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Supporting Information

Fine-Tuning Redox Properties of Heteroleptic Molybdenum Complexes through Ligand-Ligand-Cooperativity

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Experimental Procedures

Synthesis and manipulations of all complexes were carried out in a dry argon atmosphere using dry, degassed solvents unless otherwise stated. CH_3CN and CH_2Cl_2 were freshly distilled from molecular sieves, THF was distilled from sodium/benzophenone, ethanol and methanol were dried over magnesium turnings and freshly distilled prior to use. The synthesis of *p*-toluolphosphonic acid diethyl ester was prepared according to the literature.[1] Aqueous formaldehyde was purchased from BerndKraft, *t*Bu-NH_2 from AcrosOrganics. $[Mo(CO)_6]$, was purchased from Strem Chemicals, Inc. (*n*-$Bu_4N)(PF_6)$ was purchased from sigma aldrich in electrochemical quality. Na_2xdt[2], cydt[3] and $[Mo(CO)_4(NBD)]$[4] were prepared according to the literature.

X-ray structure determination

Single crystals of **2**, **3**, **4**, **5** and **6** were mounted on a glass fiber in inert paraffin oil. Data were recorded at 170 K on a STOE-IPDS 2T diffractometer with graphite-monochromated Mo-K_α-radiation (λ = 0.71073 Å). Absorption corrections were performed using X-Red32 and X-Shape by STOE & Cie GmbH. All structures were solved by direct methods (SHELXT) and refined by full-matrix least-squares techniques using the SHELXL executable and the WingX GUI.[5] All non-hydrogen-atoms were refined with anisotropic displacement parameters. All hydrogen atoms were refined isotropically at calculated positions using a riding model with their U_{iso} values constrained to 1.2 times U_{eq} of their pivot atoms for aromatic or to 1.5 times U_{eq} for all other carbon atoms.
For **2** a disorder of one tolyl substituent was modelled with SAME, SIMU and DELU constraints. Occupancies are 52% and 48%. **5** was refined with two independent molecules in the asymmetric unit. One of the two molecules has a disorder (ring pucker) in its cyclohexyl moiety. This was modelled with SAME, SIMU and DELU constraints. Occupancies are 54% and 46%. For **6** disordered solvent had to be SQUEEZED[6] from the electron density map and was refined as diffuse contribution (per formula half a molecule of acetonitrile and diethylether each; 60 electrons per unit cell; Z = 2). It also has a disorder (ring pucker) in the cyclohexyl moiety. This was refined freely without any constraints in two orientations. Occupancies are 51% and 49%. General crystallographic, crystal and refinement data for **2**, **3**, **4**, **5** and **6** are provided below (Table S9, Table S10, Table S11, Table S12 and Table S13). Crystallographic data were deposited with the Cambridge Crystallographic Data Centre, CCDC, 12 Union Road, Cambridge CB21EZ, UK. These data can be obtained free of charge on quoting the depository numbers CCDC 2238167 (**2**), 2238168 (**3**); 2238169 (**4**), 2238170 (**5**), and 2238171 (**6**) by FAX (+44-1223-336-033), email (deposit@ccdc.cam.ac.uk) or their web interface (at http://www.ccdc.cam.ac.uk).

Other physical methods

UV-vis spectra were obtained at room temperature with a Perkin Elmer Lambda 800 spectrophotometer, while IR spectra were recorded as KBr pellet using an FT-IR spectrometer Shimadzu IRAffinity-1.
Elemental analysis (C, H, N, and S) was carried out with an Elementar Vario MICRO elemental analyzer. ^{1}H, ^{13}C, ^{31}P, and 2D NMR spectra were recorded on a Bruker Avance II 300 spectrometer (300, 75, and 121.5 MHz, respectively) Chemical shifts (δ) are given in parts per million (ppm) using solvent signals as a reference relative to external tetramethylsilane (δ = 0 ppm). Electrochemical experiments were carried out in a conventional three-electrode cell using a METROHM PGStat 12 apparatus. The counter electrode and pseudo-reference electrode were made of platinum, while a glassy carbon disc (diameter: 1 mm) served as a working electrode. Cyclic voltammograms were referenced using decamethylferrocen/decamethylferrocenium but calculated for ferrocene/ferrocenium (Fc/Fc^+) = 0 V as internal standard.[7]
The SEC-UV-vis measurements were performed in a 'TSC Spectro' cell manufactured by rhd-instruments and purchased from METROHM. The cell setup is very similar to a classic three electrode setup but with adaptations: To obtain UV-vis spectra with simultaneously applied potential, the working electrode is made of a fine mesh of platinum, allowing the orthogonal light beam to pass through. Glassy carbon was used as counter electrode and a silver wire served as pseudo reference electrode. The cell length was previously spectroscopically determined to be 0.16 cm. Every experiment was started by registering a new baseline of the electrolyte (0.1 M (*n*-$Bu_4N)(PF_6$ in acetonitrile) followed by refilling the cell with the complex solution. Every refilling and cleaning step was carried out inside a glovebox filled with argon. The cell itself is airtight and thus the measurement could be performed outside the box. Vibrations potentially disturbing the diffusion layer were carefully avoided. Simultaneously to each CV-step (every 10 ms) the diode-array (manufactured by J&M, TIDAS) registered a new spectrum. The individual spectra of the species and their time/potential-dependent concentrations were extracted from the UV-vis spectra following the procedure detailed in our recently published article[8]. In short, a primary Evolving Factor Analysis (EFA) provides information about the total species count together with information about these species emerging and vanishing throughout the CV run at a certain (chosen) time frame. Once a secure frame with only three species had been found the factorization with the FacPack 1.3 program could be applied.

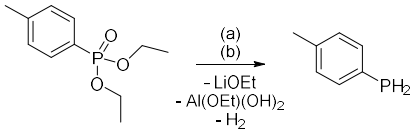
DFT-calculations

Density functional calculations, including geometry optimizations, numerical frequency, and TD-DFT calculation, were performed with the ORCA quantum chemical program package, version 5.0.3. Geometries were optimized starting with coordinates obtained from SCXRD measurements for the neutral complexes. For the case of $[Mo(CO)_2(P_2^{p\text{-tol}}N_2^{tBu})(xdt)]$ (**2**), the geometry was primarily optimized using the BP86 density functional[9] and further re-optimized by applying both the PBE0[10] and the TPSSh[11] functionals. The other three complexes and their reduced states were only optimized using the TPSSh functional. The RI-J approximation was applied jointly with the BP86 functional, while the RI-JCOSX approximation was used in the case of the (meta)-hybrid functionals PBE0 and TPSSh. Independent from the functional, the def2-TZVP[12]

valence triple-zeta basis set with polarization functions of the Karlsruhe group was applied for atoms Mo, N, S, and P, including effective core potentials[13] for Mo. Only for carbon and hydrogen atoms, def2-SVP[12] was employed. As the auxiliary basis set, def2/J was chosen[14] Environmental effects were considered with the CPCM model using acetonitrile as the solvent[15]. The atom-pairwise 2010 dispersion correction to the DFT energy with zero damping[16] was applied for the initial calculations. To yield the geometry of the 'non-stacked' complexes, a fresh optimization run with the Grimme dispersion correction switched off was performed, while the energy of the thus generated coordinates was calculated by reinstating the dispersion correction. Due to the octahedral geometry, the mono- and doubly reduced complexes might exhibit two different enantiomeric isomers (Δ and Λ). A direct comparison of the energies and bonding parameters of both isomers (of **2**$^{-1}$ and **3**$^{-1}$) revealed no significant differences. For reasons of uniformity the discussed parameters are all based on the Δ isomers. The UV-vis spectra were predicted with TD-DFT and in a similar manner, the numerical frequencies for IR-spectra were calculated with identical settings as above. Using the Tamm-Dancoff approximation, 120 roots were calculated. Line spectra were obtained with an artificial broadening described for each figure.

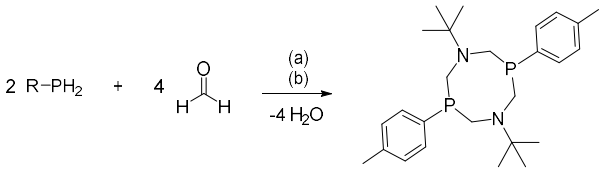
Synthetic procedures

Synthesis of p-toluene phosphane (**A**)



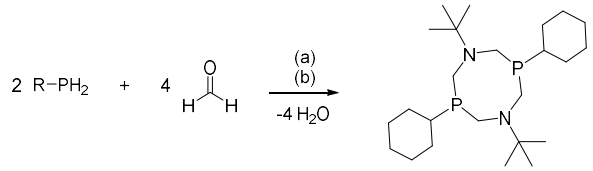
The preparation of *p*-toluene phosphane (**A**) was carried out in analogy to the literature.[17] For this purpose, $LiAlH_4$ (6.6 g, 173.91 mmol, 1.53 eq.) was placed in a pre-heated 500 ml Schlenk flask and suspended in 100 ml ice-cooled Et_2O. Under further cooling, *p*-toluene phosphonic acid diethyl ester (26 g, 113.92 mmol, 1 eq.) was added dropwise (a). The reaction takes place with a strong gas evolution and slight green-to-red coloration. After complete addition, cooling was stopped, and the solution was allowed to stir for two days to give a grayish suspension. To this solution, approximately 10 ml of an 0.2 M K_3PO_4 solution in H_2O was slowly added under ice cooling until gas evolution no longer occurred (b). The slimy suspension obtained was filtered over celite, and the remaining residue was washed several times with a total of 200 ml of Et_2O to obtain a yellowish-red solution. The excess ether was carefully removed in a fine vacuum. The product mixture was separated by fractional distillation starting at a maximum of 15 mbar and 40 °C to remove residual solvent. Distillation of the pure product was carried out at 7 mbar and 60 °C, leaving only minor amounts of the product in the sump. Finally, *p*-toluene phosphane (**A**) was obtained as a colorless, unpleasant-smelling, pyrophoric oil that solidifies in the cold. Yield: 45.6% (6.44 g, 51.92 mmol). ^{1}H NMR (300 MHz, C_6D_6): δ (ppm) = 2.01 (s, 3H, CH_3, *p*-tol-CH_3), 3.54 (s, 1H, PH), 4.20 (s, 1H, PH), 6.83 (d, J_{P-C} = 7.5 Hz, 2H, 2 · $CH_{arom.}$, *m*-CP), 7.25 (t, J_{P-C} = 7.5 Hz, 2H, 2 · $CH_{arom.}$, *o*-CP). ^{31}P NMR (121.5 MHz, C_6D_6): δ (ppm) = –125.31 (s). ^{1}H-^{31}P-COSY (300 and 121.5 MHz, C_6D_6): δ (ppm) = 3.54 (^{1}H, 1H) and -125.31 (^{31}P, PH_2), 4.20 (^{1}H, 1H) and –125.31 (^{31}P, PH_2). ^{13}C NMR (75.5 MHz, C_6D_6): δ (ppm) = 21.7 (s, $CH_{3,p\text{-tol}}$), 129.0 (s, $C_{arom.}$, CP), 130.1 (d, J_{C-P} = 6.3 Hz, $CH_{arom.}$), 135.9 (d, J_{C-P} = 15.8 Hz, $CH_{arom.}$), 160.69 (s, $C_{arom.}$, C-CH_3).

Synthesis of $P_2^{p\text{-tol}}N_2^{t\text{Bu}}$ (**1**$^{p\text{-tol}}$)



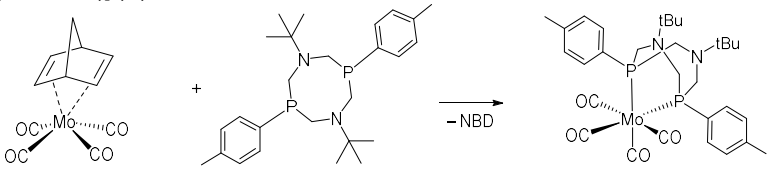
The preparation of 1,5-di-(*tert*-butyl)-3,7-di-p-tolyl-1,5,3,7-diazadiphosphocycloctane (**1**$^{p\text{-tol}}$), $P_2^{p\text{-tol}}N_2^{t\text{Bu}}$, was carried out following the procedure by Märkl et al..[18] First, *p*-toluenephosphane (**1**) (637.3 mg, 5.1 mmol, 2 eq.) was placed in a Schlenk flask, and 8 ml of ethanol was added. An aqueous 37% formaldehyde solution (0.86 ml, 10.5 mmol, 4.1 eq.) was added (a).[19] After one day, a reaction control with ^{31}P-NMR showed complete consumption of the starting material and one major new peak at -21.8 ppm representing *p*-tol-P-$(CH_2OH)_2$. This was followed (b) by the addition of the freshly distilled *t*Bu-NH_2 (380 mg, 5.2 mmol, 2.01 eq.). The mixture was refluxed at 105 °C for 6 h. After completion of the reaction (controlled via ^{31}P NMR) and further cooling to room temperature, the solid was separated aerobically over an S4 frit, washed several times (5 ml) with aerobic ethanol, and dried *in vacuo*. The product was stored anaerobically. In the NMR, two conformational isomers appear with an approximate ratio of 1 (major): 0.19 (minor). Yield: 68.1% (773.5 mg, 1.75 mmol). ^{1}H NMR (300 MHz, THF−d8): δ (ppm) = 1.04 (s, major, 18H, 6 · CH_3, *t*Bu); 1.10 (s, minor, 3.9H, 6 · CH_3, *t*Bu); 2.29 (s, minor, 1.1H, 2 · CH_3, *p*-tol); 2.31 (s, major, 6H, 2 · CH_3, *p*-tol); 3.23 (m, major+minor, 4.8H, 2 · CH_2, P_2N_2); 3.51 (m, minor, 0.8H, 2 · CH_2, P_2N_2); 3.66 (m, major, 4H, 2 · CH_2, P_2N_2); 7.14 (m, major+minor, 4.8H, 4 · CH, *p*-tol); 7.33 (m, minor, 0.8H, 4 · CH, *p*-tol); 7.42 (m, major, 4H, 4 · CH, *p*-tol). ^{31}P NMR (121.5 MHz, THF−d8): δ (ppm) = -33.08 (s, major, 1 P), -33.68 (s, minor, 0.19 P). ^{13}C NMR (75.5 MHz, THF−d8): δ (ppm) = 21.2 (s, CH_3, *p*-tol); 27.4 (s, minor, CH_3); 27.5 (s, major, CH_3); 52.1 (m, major+minor, CH_2); 55.4 (m, major+minor,, $C_{quart.}$,*t*Bu); 129.6 (m, minor, $CH_{p\text{-tol}}$); 129.7 (d, major, J_{C-P}= 7.2 Hz, $CH_{p\text{-tol}}$); 133.3 (d, minor, $CH_{p\text{-tol}}$); 133.8 (d, major, J_{C-P}= 19.8 Hz, $CH_{p\text{-tol}}$); 136.7 (d, J_{C-P}= 16.5 Hz, $C_{quart.}$, *p*-tol); 139.2 (s, $C_{quart.}$, *p*-tol). ^{135}DEPT NMR (75.5 MHz, THF−d8): δ (ppm) = 21.2 (pos., CH_3); 27.4 (pos., minor, CH_3); 27.5 (pos., major, CH_3); 52.1 (neg., major+minor, CH_2); 129.6 (pos., minor, CH); 129.7 (pos., major, CH); 133.3 (pos., minor, CH); 133.8 (pos., major, CH). IR (KBr disk, in cm^{-1}): ν = 1188; 1361; 1496; 1597; 2774 (−CH_2); 2868 (−CH_2); 2972 (−CH_2); 3013 (−CH_2). EI-MS:[M+H$^+$]= 443.7 m/z. Elemental analysis calculated for $C_{26}H_{40}N_2P_2$ (%): C: 70.56; H: 9.11; N: 6.33. Found: C: 70.64; H: 9.21; N: 6.29.

Synthesis of $P_2^{cy}N_2^{tBu}$ (**1**^{cy})



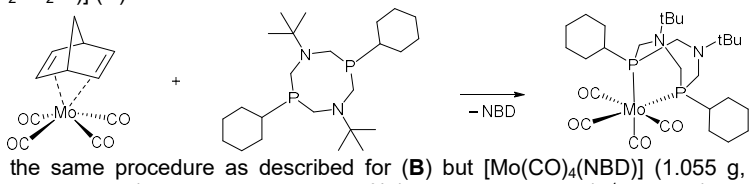
The synthesis of 1,5-di-(*tert*-butyl)-3,7-di-cyclohexyl-1,5,3,7-diazadiphosphocyclotan (**1**^{cy}), $P_2^{cy}N_2^{tBu}$, was carried out according to a procedure already published by Yang et al. and analogously to **1**$^{p\text{-tol}}$.[20] Yield: 47.2% (3.72 g, 8.7 mmol). ^{1}H NMR (300 MHz, CD_2Cl_2): δ (ppm) = 1.11 (s, minor, 10.2H, 6 · CH_3, *t*Bu); 1.15 (s, major, 18H, 6 · CH_3, *t*Bu); 1.28 (m, 13.1H, CH_2); 1.35 (m, 2.9H, CH); 1.71 (m, 16.1H, CH_2); 2.76 (s, 0.9H, CH_2); 2.80 (s, 1.3H, CH_2); 3.02 (m, 6.3H, CH_2); 3.15 (m, 2.5H, CH_2); 3.20 (m, 1.5H, CH_2). ^{31}P NMR (121.5 MHz, CD_2Cl_2): δ (ppm) = –21.9 (s, 1.75 P); –26.5 (s, 1 P). ^{13}C NMR (75.5 MHz, CD_2Cl_2): δ (ppm) = 27.0 (s, CH_2); 27.2 (s, minor, CH_3); 27.4 (m, CH_2); 27.5 (m, CH_2); 27.7 (s, major, CH_3); 30.2 (s, minor, CH_2); 30.3 (s, major, CH_2); 30.4 (s, minor, CH_2); 30.4 (s, major, CH_2); 35.9 (d, major, $J_{C\text{-}P}$= 13.2 Hz, major, CH); 37.4 (m, minor, CH); 48.1 (dd, $J_{1,C\text{-}P}$ = 12.1 Hz, $J_{2,C\text{-}P}$ = 7.7 Hz, CH_2); 49.3 (m, CH_2); 50.4 (t, major, $J_{C\text{-}P}$ = 2.8 Hz, $C_{quart.}$, *t*Bu); 56.7 (t, minor, $J_{C\text{-}P}$ = 5.5 Hz, $C_{quart.}$, *t*Bu). ^{135}DEPT NMR (75.5 MHz, CD_2Cl_2): δ (ppm) = 27.0 (neg., CH_2); 27.2 (pos., CH_3); 27.4 (neg., CH_2); 27.5 (neg., CH_2); 27.7 (pos., CH_3); 30.2 (neg., minor, CH_2); 30.3 (neg., major, CH_2); 30.4 (neg., minor, CH_2); 30.4 (neg., major, CH_2); 35.9 (pos., CH); 37.4 (pos., CH); 48.1 (neg., CH_2); 49.3 (neg., CH_2). IR (KBr disk, in cm^{-1}): ν = 1190; 1360; 1445; 1624; 2783 (−CH_2); 2849 (−CH_2); 2920 (−CH_2); 2971 (−CH_2). EI-MS:[M+H$^+$] = 426.9 m/z. Elemental analysis calculated for $C_{24}H_{48}N_2P_2$ (%): C: 67.57; H: 11.34; N: 6.57. Found: C: 67.1; H: 11.60; N: 6.48.

Synthesis of [$Mo(CO)_4(P_2^{p\text{-tol}}N_2^{tBu})$] (**B**)



[$Mo(CO)_4$(NBD)] (225 mg, 0.75 mmol, 1 eq.) was placed together with $P_2^{p\text{-tol}}N_2^{tBu}$ (**1**$^{p\text{-tol}}$) (319 mg, 0.75 mmol, 1 eq.) in a Schlenk flask connected to a reflux condenser. After the addition of 15 ml. toluene, refluxing was performed for two days. The solvent was removed, and the solid redissolved in CH_2Cl_2. Separation from polymeric residues was achieved by filtration through a 0.45 µm syringe filter. The slightly yellowish solution was poured into methanol to give a yellowish fine powder of the target product. 74.9% (389 mg, 0.56 mmol). ^{1}H NMR (300 MHz, CD_2Cl_2): δ (ppm) = 1.15 (s, 18H, 6 · CH_3, *t*Bu); 2.40 (s, 6H, 2 · CH_3, *p*-tol); 3.13 (m, 4H, 2 · CH_2, P_2N_2); 3.36 (m, 4H, 2 · CH_2, P_2N_2); 7.32 (m, 4H, 2 · 2 $CH_{arom.}$, p-tol); 7.55 (m, 4H, 2 · 2 $CH_{arom.}$, *p*-tol). ^{13}C NMR (75.5 MHz, CD_2Cl_2): δ (ppm) = 21.4 (s, 2 · CH_3, *p*-tol); 26.6 (s, 6 · CH_3, *t*Bu); 51.1 (t, $J_{C\text{-}P}$= 19.3 Hz, 4 · CH_2,P_2N_2); 57.5 (m, 2 · $C_{quart.}$, *t*Bu); 129.9 (t, $J_{C\text{-}P}$= 4.8 Hz, $CH_{arom.}$); 131.3 (t, $J_{C\text{-}P}$= 6.8 Hz, $CH_{arom.}$); 134.0 (t, $J_{C\text{-}P}$= 17.3 Hz, $C_{arom.}$); 141.7 (s, $C_{quart.}$, *p*-tol); 212.2 (t, $^2J_{P\text{-}C}$= 9.2 Hz, CO); 218.7 (t, $^2J_{P\text{-}C}$= 6.4 Hz, CO). ^{31}P NMR (121.5 MHz, CD_2Cl_2): δ (ppm) = 17.38 (s). ^{135}DEPT NMR (75.5 MHz, CD_2Cl_2): δ (ppm) = 21.4 (pos., 2 · CH_3, *p*-tol); 26.6 (pos., 6 · CH_3, *t*Bu); 51.1 (neg., 4 · CH_2,P_2N_2); 129.9 (pos., $CH_{arom.}$); 131.3 (pos., $CH_{arom.}$). HH-COSY NMR (300 MHz, CD_2Cl_2): δ (ppm) = 2.40 and 7.32 (2 · CH_3, *p*-tol with 2 · $CH_{arom.}$); 3.13 and 3.36 (CH_2, P_2N_2 with CH_2, P_2N_2); 7.32 and 7.55 (2 · $CH_{arom.}$, *p*-tol with 2 · $CH_{arom.}$, *p*-tol). HSQC NMR (300 and 75.5 MHz, CD_2Cl_2): δ (ppm) = 1.15 (1H, 6 · CH_3, *t*Bu) and 26.6 (^{13}C, 6 · CH_3); 2.40 (^{1}H, 2 · CH_3, *p*-tol) and 21.4 (^{13}C, 2 · CH_3); 3.13 (^{1}H, 2 · CH_2, P_2N_2) and 51.1 (^{13}C, 2 · CH_2); 3.34 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 51.1 (^{13}C, 2 · 0.5 · CH_2); 7.32 (^{1}H, 4 · CH, *p*-tol) and 129.9 (^{13}C, 4 · CH); 7.55 (^{1}H, 2 · CH, *p*-tol) and 131.3 (^{13}C, 4 · CH). HMBC NMR (300 and 75.5 MHz, CD_2Cl_2): δ (ppm) = 1.15 (^{1}H, 6 · CH_3, *t*Bu) and 26.6 (^{13}C, 6 · CH_3); 1.15 (^{1}H, 6 · CH_3, *t*Bu) and 57.5 (^{13}C, 2 · $C_{quart.}$); 2.40 (^{1}H, 2 · CH_3, *p*-tol) and 129.9 (^{13}C, 4 · CH); 2.40 (^{1}H, 2 · CH_3, *p*-tol) and 141.7 (^{13}C, 2 · $C_{quart.}$); 3.13 (^{1}H, 2 · CH_2, P_2N_2) and 51.1 (^{13}C, 2 · CH_2); 3.13 (^{1}H, 2 · CH_2, P_2N_2) and 57.5 (^{13}C, 2 · $C_{quart.}$, *t*Bu); 3.13 (^{1}H, 2 · CH_2, P_2N_2) and 134.0 (^{13}C, $C_{arom.}$); 3.36 (^{1}H, 2 · CH_2, P_2N_2) and 51.1 (^{13}C, 2 · CH_2); 7.32 (^{1}H, 4 · CH, *p*-tol) and 21.4 (^{13}C, 2 · CH_3, *p*-tol); 7.32 (^{1}H, 4 · CH, *p*-tol) and 129.9 (^{13}C, 4 · CH); 7.32 (^{1}H, 4 · CH, *p*-tol) and 134.0 (^{13}C, $C_{arom.}$); 7.55 (^{1}H, 2 · CH, *p*-tol) and 51.1 (^{13}C, 4 · CH_2, P_2N_2); 7.55 (^{1}H, 2 · CH, *p*-tol) and 131.3 (^{13}C, 4 · CH); 7.55 (^{1}H, 2 · CH, *p*-tol) and 141.7 (^{13}C, $C_{quart.}$,*p*-tol). ^{95}Mo NMR (19.6 MHz, CD_2Cl_2): δ (ppm) = –1831 (s, with Sat. $J_{31P\text{-}95Mo}$= 252 Hz). EI-MS:[M]= 652.3 m/z. IR (KBr disk, in cm^{-1}): ν = 1188 (s); 1364 (s); 1858 (sh, CO); 1890 (sh, CO); 1913 (s, CO); 2010 (s, CO); 2793 (sh, −CH_2); 2870 (sh, −CH_2); 2969 (s, −CH_2). Elemental analysis calculated for $C_{30}H_{40}MoN_2O_4P_2$ · 0.5 · CH_2Cl_2 (%): C: 52.86; H: 5.96; N: 4.04. Found: C: 53.08; H: 5.97; N: 4.01.

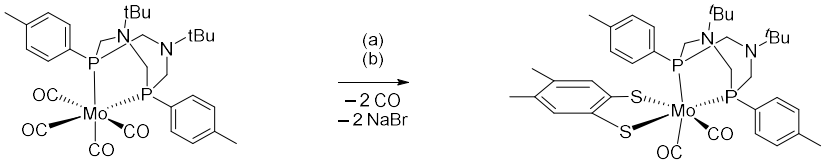
Synthesis of [$Mo(CO)_4(P_2^{cy}N_2^{tBu})$] (**C**)



The synthesis followed the same procedure as described for (**B**) but [$Mo(CO)_4$(NBD)] (1.055 g, 3.52 mmol, 1 eq.) and $P_2^{cy}N_2^{tBu}$ (**1**^{cy}) (1.5 g, 3.52 mmol, 1 eq.) were used. Yield: 76.7% (1.71 g, 2.695 mmol). ^{1}H NMR (300 MHz, CD_2Cl_2): δ (ppm) = 1.12 (s, 18H, 3 · CH_3, *t*Bu); 1.32 (m, 6H, 3 · CH_2, cy); 1.46 (m, 4H, 2 · CH_2, cy); 1.61 (m, 6H, 2 · CH_2 and 2 · CH, cy)i; 1.73 (m, 2H, 2 · 0.5 · CH_2, cy); 1.86 (m, 4H, 2 · CH_2, cy); 2.79 (m, 4H, 2 · CH_2, P_2N_2); 2.90 (m, 4H, 2 · CH_2, P_2N_2). ^{13}C NMR (75.5

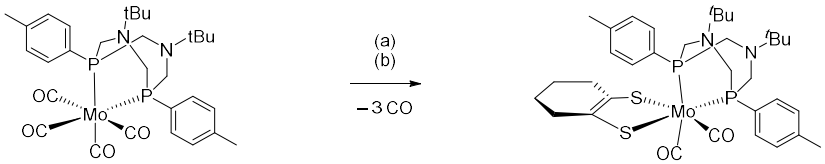
MHz, CD_2Cl_2): δ (ppm) = 26.4 (s, CH_2, cy); 26.5 (s, CH_3, *t*Bu); 26.9 (t, J_{C-P}= 6.1 Hz, CH_2, cy); 27.6 (t, J_{C-P}= 2.2 Hz, CH_2, cy); 39.4 (t, J_{C-P}= 10.4 Hz, CH, cy); 47.4 (t, J_{C-P}= 14.9 Hz, CH_2, P_2N_2); 57.3 (t, J_{C-P}= 8.8 Hz, $C_{quart.}$, *t*Bu); 212.4 (t, $^2J_{P-C}$= 9.1 Hz, CO); 219.5 (t, $^2J_{P-C}$= 6.1 Hz, CO). ^{31}P NMR (121.5 MHz, CD_2Cl_2): δ (ppm) = 24.22 (s). ^{135}DEPT NMR (75.5 MHz, CD_2Cl_2): δ (ppm) = 26.4 (neg., CH_2, cy); 26.5 (pos., 3 · CH_3, *t*Bu); 26.9 (neg., J_{C-P}= 6.1 Hz, CH_2, cy); 27.6 (neg., J_{C-P}= 2.2 Hz, CH_2, cy); 39.4 (pos., J_{C-P}= 10.4 Hz, 2 · CH, cy); 47.4 (neg., 4 · CH_2, P_2N_2). HSQC NMR (300 and 75.5 MHz, CD_2Cl_2): δ (ppm) = 1.12 (^{1}H, 3 · CH_3, *t*Bu) and 26.5 (^{13}C, 2 · CH_3); 1.32 (^{1}H, CH_2, cy) and 26.4 (^{13}C, CH_2); 1.46 (^{1}H, CH_2, cy) and 27.6 (^{13}C, CH_2); 1.61 (^{1}H, CH^2, cy) and 27.6 (^{13}C, CH_2); 1.61 (^{1}H, CH, cy) and 39.4 (^{13}C, CH); 1.73 (^{1}H, CH_2, cy) and 26.5 (^{13}C, CH_2); 1.86 (^{1}H, CH_2, cy) and 26.5 (^{13}C, CH_2); 2.79 (^{1}H, CH_2, P_2N_2) and 47.4 (^{13}C, CH_2); 2.90 (^{1}H, CH_2, P_2N_2) and 47.4 (^{13}C, CH_2). HMBC NMR[i] (300 and 75.5 MHz, CD_2Cl_2): δ (ppm) = 1.12 (^{1}H, CH_3, *t*Bu) and 26.5 (^{13}C, CH_3, *t*Bu); 1.12 (^{1}H, CH_3, *t*Bu) and 47.4 (^{13}C, CH_2, P_2N_2); 1.12 (^{1}H, CH_3, *t*Bu) and 57.3 (^{13}C, $CH_{quart.}$, *t*Bu); 2.79 (^{1}H, CH_2, P_2N_2) and 39.4 (^{13}C, CH, cy); 2.79 (^{1}H, CH_2, P_2N_2) and 47.4 (^{13}C, CH_2, P_2N_2); 2.79 (^{1}H, CH_2, P_2N_2) and 57.3 (^{13}C, $CH_{quart.}$, *t*Bu); 2.90 (^{1}H, CH_2, P_2N_2) and 47.4 (^{13}C, CH_2, P_2N_2). i: Due to the strong coupling of *t*Bu (sat.: ^{1}H-^{12}C-^{13}C; next to singulett: ^{1}H-^{13}C-^{13}C), not all signals could be assigned properly. ^{95}Mo NMR (19.6 MHz, CD_2Cl_2): δ (ppm) = –1899 (s, with Sat. $J_{31P-95Mo}$= 119 Hz). EI-MS: [M]= 636.7 m/z. IR (KBr disk; cm^{-1}): ν = 984 (s); 1194 (br); 1238 (br); 1865 (s, CO); 1883 (s, CO); 1902 (s, CO); 2002 (s, CO); 2856 (s, −CH_2); 2930 (s, −CH_2); 2968 (sh, −CH_2). Elemental analysis calculated for $C_{28}H_{48}MoN_2O_4P_2$ (%): C: 52.99; H: 7.62; N: 4.41. Found: C: 52.82; H: 7.68; N: 4.42.

Synthesis of [$Mo(CO)_2(P_2^{p\text{-}tol}N_2^{tBu})$(xdt)] (**2**)



The synthesis of [$Mo(CO)_2(P_2^{p\text{-}tol}N_2^{tBu})$(xdt)] (**2**) was carried out according to a procedure described in the literature.[21] In the first reaction step (a), [$Mo(CO)_4(P_2^{cy}N_2^{tBu})$] (**C**) (230 mg, 0. 354 mmol, 1 eq.) was oxidized using Br_2 (56.4 mg, 0.354 mmol, 1 eq.) in CH_2Cl_2. In the follow-up reaction (b), Na_2xdt (75.8 mg, 0.354 mmol, 1 eq.) in CH_3CN was added dropwise. After flash column chromatography and crystallization in CH_2Cl_2 or thf layered with methanol, red acicular crystals were obtained. Yield ((**2**) · 0.5 · CH_2Cl_2): 66.8% (200 mg, 0.236 mmol). ^{1}H NMR (300 MHz, THF-d8): δ (ppm) = 1.23 (s, 9H, 3 · CH_3, *t*Bu); 1.24 (s, 9H, 3 · CH_3, *t*Bu); 2.23 (s, 6H, 3 · CH_3, *p*-tol); 2.29 (s, 6H, 3 · CH_3, xdt); 3.45 (m, 6H, 3 · CH_2, P_2N_2); 4.04 (pdt, 2H,2 · 0.5 · CH_2, P_2N_2); 7.10 (m, 2 · 4 H, $CH_{arom.}$, *p*-tol); 7.74 (s, 2 · $CH_{arom.}$, xdt). ^{13}C NMR (75.5 MHz, THF-d8): δ (ppm) = 19.5 (s, 2 · CH_3, *p*-tol); 21.2 (s, 2 · CH_2, xdt); 26.5 (s, 3 · CH_3, *t*Bu); 26.9 (s, 3 · CH_3, *t*Bu); 46.1 (t, J_{C-P}= 21.3 Hz, 2 · CH_2, P_2N_2); 49.9 (t, J_{C-P}= 19.9 Hz, 2 · CH_2, P_2N_2); 54.9 (s, $C_{quart.}$, 2 · *t*Bu); 57.7 (s, $C_{quart.}$, 2 · *t*Bu); 130.1 (t, J_{C-P}= 4.8 Hz, $CH_{arom.}$, *p*-tol); 130.9 (s, $C_{quart.}$, xdt); 132.0 (s, $CH_{arom.}$, xdt); 133.2 (t, J_{C-P}= 4.8 Hz, $CH_{arom.}$); 141.7 (s, $C_{quart.}$, *p*-tol); 150.9 (s, $C_{quart.}$, C-S); 241.7 (m, $C_{quart.}$, CO). ^{31}P NMR (121.5 MHz, THF-d8): δ (ppm) = 40.30 (s). ^{135}DEPT NMR (75.5 MHz, THF-d8): δ (ppm) = 19.5 (pos., CH_3, *p*-tol); 21.2 (pos., CH_3, xdt); 26.5 (pos., 3 · CH_3, *t*Bu); 26.9 (pos., 3 · CH_3, *t*Bu); 46.1 (neg., 2 · CH_2, P_2N_2); 49.9 (neg., 2 · CH_2, P_2N_2); 130.1 (pos., $CH_{arom.}$, *p*-tol); 132.0 (pos., CH, xdt); 133.3 (pos., $CH_{arom.}$, *p*-tol). HH-COSY NMR (300 MHz, THF-d8): δ (ppm) = 2.23 and 7.10 (2 · CH_3, *p*-tol with CH, *p*-tol); 2.29 and 7.74 (2 · CH_3, xdt with CH, xdt); 3.45 and 4.04 (CH_2, P_2N_2 with 2 · 0.5 · CH_2, P_2N_2). HSQC NMR (300 and 75.5 MHz, THF-d8): δ (ppm) = 1.23 (^{1}H, 3 · CH_3, *t*Bu) and 26.5 (^{13}C, 3 · CH_3, *t*Bu); 1.24 (^{1}H, 3 · CH_3, *t*Bu) and 26.9 (^{13}C, 3 · CH_3, *t*Bu); 2.23 (^{1}H, 2 · CH_3, *p*-tol) and 21.2 (^{13}C, 2 · CH_3); 2.29 (^{1}H, 2 · CH_3, xdt) and 19.5 (^{13}C, 2 · CH_3); 3.45 (^{1}H, 2 · CH_2, P_2N_2) and 46.1 (^{13}C, 2 · CH_2); 3.45 (^{1}H, 2 · 0.5 · CH_2,P_2N_2) and 49.9 (^{13}C, 2 · 0.5 · CH_2); 4.04 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 49.9 (^{13}C, 2 · 0.5 · CH_2); 7.10 (^{1}H, 2 · CH, *p*-tol) and 130.1 (^{13}C, 2 · CH); 7.10 (^{1}H, 2 · CH, *p*-tol) and 133.3 (^{13}C, 2 · CH); 7.74 (^{1}H, 2 · CH, xdt) and 132.0 (^{13}C, 2 · CH). HMBC NMR (300 and 75.5 MHz, THF-d8): δ (ppm) = 1.23 (^{1}H, 3 · CH^3, *t*Bu) and 26.5 (^{13}C, 3 · CH_3, *t*Bu); 1.24 (^{1}H, 3 · CH_3, *t*Bu) and 26.9 (^{13}C, 3 · CH_3, *t*Bu); 1.23 (^{1}H, 3 · CH_3, *t*Bu) and 54.9 (^{13}C, $C_{quart.}$, *t*Bu); 1.24 (^{1}H, 3 · CH_3, *t*Bu) and 57.7 (^{13}C, $C_{quart.}$, *t*Bu); 2.23 (^{1}H, 2 · CH_3, *p*-tol) and 130.1 (^{13}C, 2 · CH); 2.23 (^{1}H, 2 · CH_3, *p*-tol) and 141.7 (^{13}C, 2 · $C_{quart.}$); 2.29 (^{1}H, 2 · CH_3, xdt) and 130.9 (^{13}C, $C_{quart.}$); 2.29 (^{1}H, 2 · CH_3, xdt) and 132.0 (^{13}C, CH); 2.29 (^{1}H, 2 · CH_3, xdt) and 150.9 (^{13}C, C−S); 3.45 (^{1}H, 2 · CH_2, P_2N_2) and 46.1 (^{13}C, 2 · CH_2, P_2N_2); 3.45 (^{1}H, 2 · CH_2, P_2N_2) and 49.9 (^{13}C, 2 · CH_2, P_2N_2); 3.45 (^{1}H, 2 · CH_2, P_2N_2) and 57.7 (^{13}C, $C_{quart.}$, *t*Bu); 4.04 (^{1}H, 2 · CH_2, P_2N_2) and 46.1 (^{13}C, 2 · CH_2, P_2N_2); 4.04 (^{1}H, 2 · CH_2, P_2N_2) and 49.9 (^{13}C, 2 · CH_2, P_2N_2); 7.10 (^{1}H, 2 · CH, *p*-tol) and 21.2 (^{13}C, 2 · CH_3, *p*-tol); 7.10 (^{1}H, 2 · CH, *p*-tol) and 130.1 (^{13}C, 2 · CH, *p*-tol); 7.10 (^{1}H, 2 · CH, *p*-tol) and 141.7 (^{13}C, 2 · CH, *p*-tol); 7.74 (^{1}H, 2 · CH, xdt) and 19.5 (^{13}C, 2 · CH_3, xdt); 7.74 (^{1}H, 2 · CH, xdt) and 132.0 (^{13}C, 2 · CH, xdt); 7.74 (^{1}H, 2 · CH, xdt) and 150.9 (^{13}C, C−S). Rf-value: 0.76 (*n*-hexane/CH_2Cl_2: 2/3). ε in CH_3CN ($M^{-1}\cdot cm^{-1}$) = 12754 (380 nm). IR (KBr disk, in cm^{-1}): ν = 1256; 1366; 1449; 1636; 1873 (CO); 1937 (CO); 2799 (−CH_2); 2861 (−CH_2); 2912 (−CH_2); 2971 (−CH_2); 3439 (br). APCI-MS:[M$^+$]= 764.3 m/z. Elemental analysis calculated for $C_{36}H_{48}MoN_2O_2P_2S_2$ · 0.5 thf (%): C: 57.13; H: 6.56; N: 3.51; S: 8.03. Found: C: 56.70; H: 6.60; N: 3.46; S: 7.77.

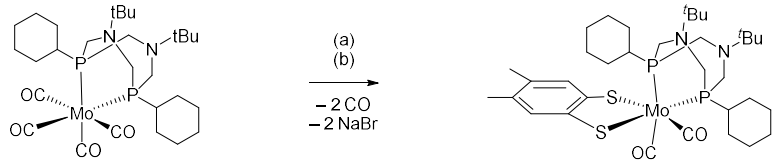
Synthesis of [$Mo(CO)_2$(cydt)($P_2^{p\text{-}tol}N_2^{tBu}$)] (**3**)



The synthesis of [$Mo(CO)_2$(cydt)($P_2^{p\text{-}tol}N_2^{tBu}$)] (**3**) is analogous to a previously reported procedure.[3] [$Mo(CO)_4(P_2^{p\text{-}tol}N_2^{tBu})$] (**B**) (1.064 g, 1.64 mmol, 1 eq.) was dissolved in 50 ml thf in a temperature-controlled jacketed vessel and irradiated at 20 °C for

about 8 h using HPM and HPA lamp to give a deep yellow solution (a). After adding protected cydt (393.4 mg, 2.28 mmol, 1.4 eq.) (b) dissolved in 15 ml, thf irradiation continued for 14 h at 10 °C. The brown-reddish reaction mixture was dried on a rotary evaporator, adsorbed on silica gel, and separated with flash column chromatography. The first orange-red fraction contained the target compound. The solvent was removed, and the compound crystallized in CH_2Cl_2 or thf layered with CH_3OH. The product crystallized as small, deep red needles suitable for X-ray diffraction. Yield: 62.3% (707 mg, 0.95 mmol). ^{1}H NMR (300 MHz, THF-d8): δ (ppm) = 1.20 (m, 9H, 3 · CH_3, *t*Bu); 1.21 (m, 9H, 3 · CH_3, *t*Bu); 1.77 (m, 4H, 2 · CH_2, cydt[i]); 2.26 (s, 6H, 2 · CH_3, *p*-tol); 2.95 (m, 4H, 2 · CH_2, cydt); 3.38 (m, 4H, 2 · CH_2, P_2N_2); 3.48 (m, 2H, 2 · 0.5 · CH_2, P_2N_2); 3.92 (pdt, 2H, 2 · 0.5 · CH_2, P_2N_2); 7.09 (m, 2 · 4 H, $CH_{arom.}$, *p*-tol). ^{13}C NMR (75.5 MHz, THF-d8): δ (ppm) = 21.2 (s, 2 · CH_3, *p*-tol); 26.4 (s, 2 · CH_2, cydt); 26.6 (s, 3 · CH_3, *t*Bu); 27.0 (s, 3 · CH_3, *t*Bu); 36.4 (s, 2 · CH_2, cydt); 46.4 (t, $J_{C\text{-}P}$= 21.7 Hz, 2 · CH_2, P_2N_2); 50.5 (t, $J_{C\text{-}P}$= 19.3 Hz, 2 · CH_2, P_2N_2); 57.6 (m, $C_{quart.}$, 2 · C_{tBu}); 130.0 (t, $J_{C\text{-}P}$= 4.8 Hz, $CH_{arom.}$); 132.5 (t, $J_{C\text{-}P}$= 24.1 Hz, $CH_{arom.}$); 133.6 (t, $J_{C\text{-}P}$= 5.2 Hz, $CH_{arom.}$); 141.4 (s, $C_{quart.}$, *p*-tol); 148.0 (s, $C_{quart.}$, C-S); 242.7 (t, $^2J_{P\text{-}C}$= 19.3 Hz, CO). ^{31}P NMR (121.5 MHz, THF-d8): δ (ppm) = 41.26 (s). ^{135}DEPT NMR (75.5 MHz, THF-d8): δ (ppm) = 21.2 (pos., 2 · CH_3, *p*-tol); 26.4 (neg., CH_2, cydt); 26.6 (pos., 3 · CH_3, *t*Bu); 27.0 (pos., 3 · CH_3, *t*Bu); 36.4 (neg., CH_2, cydt); 46.4 (neg., 2 · CH_2, P_2N_2); 50.5 (neg., 2 · CH_2, P_2N_2); 130.0 (pos., $CH_{arom.}$, *p*-tol); 132.5 (pos., $CH_{arom.}$, *p*-tol). HH-COSY NMR (300 MHz, THF-d8): δ (ppm) = 1.77 and 2.95 (2 · CH_2, cydt with CH_2, cydt); 3.48 and 3.92 (2 · 0.5 · CH_2, P_2N_2 with 2 · 0.5 · CH_2, P_2N_2). HSQC NMR (300 and 75.5 MHz, THF-d8): δ (ppm) = 1.20 (^{1}H, 3 · CH_3, *t*Bu) and 26.6 (^{13}C, 3 · CH_3); 1.21 (^{1}H, 3 · CH_3, *t*Bu) and 27.0 (^{13}C, 3 · CH_3); 1.77 (^{1}H, 2 · CH_2, cydt) and 26.4 (^{13}C, 2 · CH_2); 2.26 (^{1}H, 2 · CH_3, *p*-tol) and 21.2 (^{13}C, 2 · CH_3); 2.95 (^{1}H, 2 · CH_2, cydt) and 36.4 (^{13}C, 2 · CH_2); 3.38 (^{1}H, 2 · CH_2, P_2N_2) and 46.4 (^{13}C, 2 · CH_2); 3.48 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 50.5 (^{13}C, 2 · 0.5 · CH_2); 3.92 (1H, 2 · 0.5 · CH_2, P_2N_2) and 50.5 (^{13}C, 2 · 0.5 · CH_2); 7.10 (^{1}H, 4 · CH, *p*-tol) and 130.0 (^{13}C, 2 · CH); 7.10 (^{1}H, 4 · CH, *p*-tol) and 132.5 (^{13}C, 2 · CH). HMBC NMR[ii] (300 and 75.5 MHz, THF-d8): δ (ppm) = 1.77 (^{1}H, 2 · CH_3, cydt) and 148.0 (^{13}C, C−S); 2.26 (^{1}H, 2 · CH_3, *p*-tol) and 130.0 (^{13}C, 2 · CH); 2.26 (^{1}H, 2 · CH_3, *p*-tol) and 141.4 (^{13}C, $C_{quart.}$); 2.95 (^{1}H, 2 · CH_2, cydt) and 26.4 (^{13}C, 2 · CH_2, cydt); 2.84 (^{1}H, 2· CH_3, cydt) and 148.0 (^{13}C, C−S); 3.38 (^{1}H, 2 · CH_2, P_2N_2) and 46.4 (^{13}C, 2 · CH_2, P_2N_2); 3.92 (^{1}H, 2 · CH_2, P_2N_2) and 46.4 (^{13}C, 2 · CH_2, P_2N_2); 7.10 (^{1}H, 2 · CH, *p*-tol) and 21.2 (^{13}C, 2 · CH_3, *p*-tol); 7.10 (1H, 2 · CH, *p*-tol) and 130.0 (^{13}C, 2 · CH, *p*-tol); 7.10 (^{1}H, 2 · CH, *p*-tol) and 132.5 (^{13}C, 2 · CH, *p*-tol). i: overshadowed by thf, identified by HSQC NMR. ii: Due to the strong coupling of tBu (sat.: ^{1}H-^{12}C-^{13}C; next to singulett: ^{1}H-^{13}C-^{13}C), not all signals could be assigned properly. Rf-value: 0.366 (*n*-hexane/CH_2Cl_2: 4/1). APCI-MS:[M]= 740.15 m/z. ε in CH_3CN ($M^{-1}\cdot cm^{-1}$) = 5827 (311 nm); 6971 (405 nm). IR (KBr disk; cm^{-1}): ν = 1190; 1364; 1496; 1549; 1635; 1861 (s, CO); 1931 (s, CO); 2835 (s, −CH_2); 2924 (s, −CH_2); 2969 (sh, −CH_2). Elemental analysis calculated for $C_{34}H_{48}MoN_2O_2P_2S_2$ (%): C: 55.28; H: 6.55; N: 3.79; S: 8.68. Found: C: 55.19; H: 6.29; N: 3.85; S: 8.31.

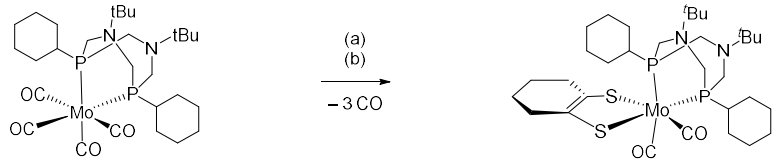
Synthesis of [$Mo(CO)_2(P_2^{cy}N_2^{tBu})$(xdt)] (**4**)



The preparation of [$Mo(CO)_2(P_2^{cy}N_2^{tBu})$(xdt)] (**4**) followed the same procedure as for (**2**) but [$Mo(CO)_4(P_2^{cy}N_2^{tBu})$] (**C**) (91.6 mg, 0.144 mmol, 1 eq.), Br_2 (22.9 mg, 0.143 mmol, 1 eq.) (a) and Na_2xdt (30.7 mg, 0.143 mmol, 1 eq.) (b) were used. Yield 80.7% (87 mg, 0.12 mmol). ^{1}H NMR (300 MHz, THF-d8): δ (ppm) = 0.83 (m. 2H, 2 · 0.5 · CH_2, cy); 1.04 (m, 4H, 2 · CH_2, cy); 1.23 (m, 9H, 3 · CH_3, *t*Bu); 1.24 (m, 9H, 3 · CH_3, *t*Bu); 1.29 (m, 4H, 2 · CH_2, cy); 1.54 (m, 4H, 2 · CH_2, cy); 1.73 (m[i], 4H, 2 · CH_2, cy); 1.83 (m, 4H, 2 · 0.5 · CH_2 and 2 · CH, cy); 2.25 (s, 6H, 2 · CH_3, xdt); 2.78 (m, 1H, 0.5 · CH_2, P_2N_2); 2.82 (m, 1H, 0.5 · CH_2, P_2N_2); 3.08 (t, 1H, J_1= 4.3 Hz, 0.5 · CH_2, P_2N_2); 3.12 (t, 1H, J_1= 4.3 Hz, 0.5 · CH_2, P_2N_2); 3.51 (m, 2H, 2 · 0.5 · CH_2, P_2N_2); 3.85 (pdt, 2H,2 · 0.5 · CH_2, P_2N_2); 7.64 (s, 2H, 2 · CH, xdt). ^{13}C NMR (75.5 MHz, THF-d8): δ (ppm) = 19.4 (s, 2 · CH_3, xdt); 26.5 (s, 3 · CH_3, *t*Bu); 26.9 (s, 3 · CH_3, *t*Bu); 26.9[ii] (CH_2, cy); 27.9 (t, J_1= 4.4 Hz, CH_2, cy); 28.2 (t, J_1= 6.4 Hz, CH_2, cy); 28.7 (m, CH_2, cy); 30.1 (s, CH_2, cy); 42.0 (t, $J_{C\text{-}P}$= 13.3 Hz, 2 · CH, P_2^{cy}); 42.4 (t, $J_{C\text{-}P}$= 17.3 Hz, 2 · CH_2, P_2N_2); 43.7 (t, $J_{C\text{-}P}$= 20.1 Hz, 2 · CH_2, P_2N_2); 57.4 (t, $J_{C\text{-}P}$= 10.4 Hz, $C_{quart.}$, *t*Bu); 58.4 (m, $J_{C\text{-}P}$= 7.6 Hz, $C_{quart.}$, *t*Bu); 130.6 (s, $C_{quart.}$, xdt); 131.9 (s, $C_{quart.}$,); 131.9 (s, CH, xdt); 150.9 (s, $C_{quart.}$, C-S); 244.5 (t, CO, $^2J_{P\text{-}C}$= 18.5 Hz). ^{31}P NMR (121.5 MHz, THF-d8): δ (ppm) = 39.45 (s). ^{135}DEPT NMR (75.5 MHz, THF-d8): δ (ppm) = 19.4 (pos., 2 · CH_3, xdt); 26.5 (pos., 3 · CH_3, *t*Bu); 26.9 (pos., 3 · CH_3, *t*Bu); 27.9 (neg., CH_2, cy); 28.2 (neg., CH_2, cy); 28.7 (neg., CH_2, cy); 30.1 (neg., CH_2, cy); 42.0 (pos., 2 · CH, P_2^{cy}); 42.4 (neg., 2 · CH_2, P_2N_2); 43.7 (neg., 2 · CH_2, P_2N_2); 131.9 (pos., 2 · CH, xdt). HH-COSY NMR (300 MHz, THF-d8): δ (ppm) = 1.04 and 1.54 (2 · 0.5 · CH_2, cy with 2 · 0.5 · CH_2, cy); 1.29 and 1.83 (2 · CH_2, cy with 2 · CH_2, cy); 2.78 and 3.12 (0.5 · CH_2, P_2N_2 with 0.5 · CH_2, P_2N_2); 2.82 and 3.08 (0.5 · CH_2, P_2N_2 with 0.5 · CH_2, P_2N_2); 2.82 and 3.51 (2 · 0.5 · CH_2, P_2N_2 with 2 · 0.5 · CH_2, P_2N_2); 2.25 and 7.64 (2 · CH_3, xdt with 2 · CH, xdt); 3.53 and 3.85 (2 · 0.5 · CH_2, P_2N_2 with 2 · 0.5 · CH_2, P_2N_2). HSQC NMR (300 and 75.5 MHz, THF-d8): δ (ppm) = 0.83 (1H, 2 · 0.5 · CH_2, cy) and 30.1 (^{13}C, 2 · CH_2); 1.04 (^{1}H, CH_2, cy) and 26.9 (^{13}C, CH_2); 1.04 (^{1}H, CH_2, cy) and 28.2 (^{13}C, CH_2); 1.23 (^{1}H, 3 · CH_3, *t*Bu) and 26.5 (^{13}C, 3 · CH_3); 1.24 (^{1}H, 3 · CH_3, *t*Bu) and 26.9 (^{13}C, 3 · CH_3); 1.29 (^{1}H, 2 · CH_2, cy) and 30.1 (^{13}C, 2 · CH_2); 1.54 (^{1}H, CH_2, cy) and 26.9 (^{13}C, CH_2); 1.54 (^{1}H, CH_2, cy) and 28.2 (^{13}C, CH_2); 1.73 (^{1}H, CH_2, cy) and 27.9 (^{13}C, CH_2); 1.83 (^{1}H, 2 · 0.5 · CH_2, cy) and 28.7 (^{13}C, CH_2); 1.83 (^{1}H, 2 · CH, cy) and 42.0 (^{13}C, CH_2); 2.25 (^{1}H, 2 · CH_3, xdt) and 19.4 (^{13}C, 2 · CH_3); 2.78 (^{1}H, 0.5 · CH_2, P_2N_2) and 43.7 (^{13}C, 2 · CH_2); 2.82 (^{1}H, 0.5 · CH_2, P_2N_2) and 43.7 (^{13}C, 2 · CH_2); 3.08 (^{1}H, 0.5 · CH_2, P_2N_2) and 43.7 (^{13}C, 2 · CH_2); 3.12 (^{1}H, 0.5 · CH_2, P_2N_2) and 43.7 (^{13}C, 2 · CH_2); 3.51 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 42.4 (^{13}C, 2 · 0.5 · CH_2); 3.85 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 42.4 (^{13}C, 2 · 0.5 · CH_2); 7.64 (^{1}H, 2 · CH, xdt) and 131.9 (^{13}C, CH). HMBC NMR (300 and 75.5 MHz, THF-d8): δ (ppm) = 0.83 (^{1}H, 2 · 0.5 · CH_2, cy) and 27.9 (^{13}C, 2 · CH_2); 1.23 (^{1}H, 3 · CH_3, *t*Bu) and 26.9 (^{13}C, 3 · CH_3); 1.23 (^{1}H, 3 · CH_3, *t*Bu) and 57.4 (^{13}C, 3 · CH_3); 1.24 (^{1}H, 3 · CH_3, *t*Bu) and 26.5 (^{13}C, 3 · CH_3); 1.24 (1H, 3 · CH_3, *t*Bu) and 58.4 (^{13}C, 3 · CH_3); 2.25 (^{1}H, 2 · CH_3, xdt) and 130.6 (^{13}C, $C_{quart.}$); 2.25 (^{1}H, 2 · CH_3, xdt) and 150.9 (^{13}C, $C_{quart.}$, C-S); 2.78 (^{1}H, 0.5 · CH_2, P_2N_2) and 43.7 (^{13}C, CH_2); 2.82 (^{1}H, 0.5 · CH_2, P_2N_2) and 43.7 (^{13}C, CH_2); 3.08 (^{1}H, 0.5 · CH_2, P_2N_2) and 43.7 (^{13}C, 2 · CH_2); 3.12 (^{1}H, 0.5 · CH_2,

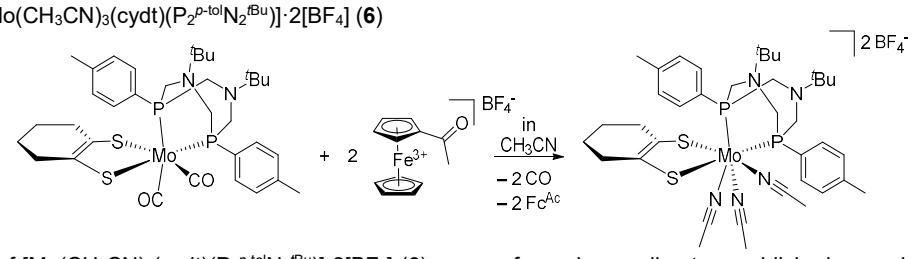
P_2N_2) and 43.7 (^{13}C, 2 · CH_2); 3.51 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 42.4 (^{13}C, 2 · 0.5 · CH_2); 3.51 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 58.4 (^{13}C, $C_{quart.}$, *t*Bu); 3.85 (^{1}H, 0.5 · CH_2, P_2N_2) and 43.7 (^{13}C, 0.5 · CH_2); 3.85 (^{1}H, 0.5 · CH_2, P_2N_2) and 43.7 (^{13}C, 0.5 · CH_2); 7.64 (^{1}H, 2 · CH, xdt) and 19.4 (^{13}C, 2 · CH_3); 7.64 (^{1}H, 2 · CH, xdt) and 130.6 (^{13}C, $C_{quart.}$, C-S); 7.64 (^{1}H, 2 · CH, xdt) and 150.9 (^{13}C, $C_{quart.}$, C-S). i: Overshadowed by thf, identified via HSQC NMR. ii: Overshadowed by $^{13}C_{tBu}$, identified via HSQC NMR. Rf-value: 0.70 (*n*-hexane/CH_2Cl_2: 2/3). IR (KBr disk, in cm^{-1}): ν = 1192 (s); 1364 (s); 1449 (s); 1853 (s, CO); 1921 (s, CO); 2856, (s, −CH_2); 2928 (s, −CH_2); 2970 (sh, −CH_2). APCI-MS:[M$^+$]= 748.4 m/z. Elemental analysis calculated for $C_{34}H_{56}MoN_2O_2P_2S_2$ (%): C: 54.68; H: 7.56; N: 3.75; S: 8.59. Found: C: 54.04; H: 7.52; N: 3.92; S: 8.32.

Synthesis of $[Mo(CO)_2(cydt)(P_2^{cy}N_2^{tBu})]$ (**5**)



The synthesis followed the same procedure as for (**3**) but $[Mo(CO)_4(P_2^{cy}N_2^{tBu})]$ (**C**) (0.965 g, 1.52 mmol, 1 eq.) (a) and protected cydt (0.366 g, 2.13 mmol, 1.4 eq.) (b) were used finally obtaining the product as deep red polyhedral crystals. Yield: 63.3% (698 mg, 0.95 mmol). ^{1}H NMR (300 MHz, THF-d8): δ (ppm) = 0.81 (m, 4H, 2 · CH_2, cy); 1.04 (m, 4H, 2 · CH_2, cy); 1.19 (m, 9H, 3 · CH_3, *t*Bu); 1.22 (m, 9H, 3 · CH_3, *t*Bu); 1.28 (m, 4H, 2 · CH_2, cy); 1.58 (m, 4H, 2 · CH_2, cy); 1.72[i] (m, 4H, 2 · CH_2, cydt); 1.74[ii] (m, 2H, 2 · CH, cy); 1.80 (m, 4H, 2 · CH_2, cy); 2.74 (m, 1H, 2 · 0.5 · CH_2, P_2N_2); 2.79 (m, 1H, 2 · 0.5 · CH_2, P_2N_2); 2.88 (m, 4H, 2 · CH_2, cydt); 3.03 (t, 1H, 2 · 0.5 · CH_2, P_2N_2); 3.07 (t, 1H, 2 · 0.5 · CH_2, P_2N_2); 3.48 (m, 2H, 2 · 0.5 · CH_2, P_2N_2); 3.71 (pdt, 2H,2 · 0.5 · CH_2, P_2N_2). ^{13}C NMR (75.5 MHz, THF-d8): δ (ppm) = 25.1[iii] (s, 2 · CH_2, cydt); 26.5 (s, 3 · CH_3, *t*Bu); 26.9 (s, 3 · CH_3, *t*Bu); 27.0[iv] (s, CH_2, cy); 27.9 (t, J_{C-P}= 4.4 Hz, CH_2, cy); 28.2 (t, J_{C-P}= 6.8 Hz, CH_2, cy); 28.6 (t, J_{C-P}= 2.8 Hz, CH_2, cy); 30.0 (s, CH_2, cy); 36.4 (s, 2 · CH_2, cydt); 42.1 (t, J_{C-P}= 13.3 Hz, 2 · CH, P_2cy); 43.1 (t, J_{C-P}= 16.9 Hz, 2 · CH_2, P_2N_2); 43.8 (t, J_{C-P}= 18.7 Hz, 2 · CH_2, P_2N_2); 57.3 (t, J_{C-P}= 10.0 Hz, $C_{quart.}$, *t*Bu); 58.2 (t, J_{C-P}= 7.6 Hz, $C_{quart.}$, *t*Bu); 147.7 (s, $C_{quart.}$, cydt); 245.5 (t, $^2J_{P-C}$= 18.1 Hz, CO). ^{31}P NMR (121.5 MHz, THF-d8): δ (ppm) = 40.24 (s). ^{135}DEPT NMR (75.5 MHz, THF-d8): δ (ppm) = 25.1 (neg., 2 · CH_2, cydt); 26.5 (pos., 3 · CH_3, *t*Bu); 26.9 (pos., 3 · CH_3, *t*Bu); 27.0 (neg., CH_2, cy); 27.9 (neg., CH_2, cy); 28.2 (neg., CH_2, cy); 28.6 (neg., CH_2, cy); 30.0 (neg., CH_2, cy); 36.4 (neg., 2 · CH_2, cydt); 42.1 (pos., 2 · CH, P_2^{cy}); 43.1 (neg., 2 · CH_2, P_2N_2); 43.8 (neg., 2 · CH_2, P_2N_2). HH-COSY NMR (300 MHz, THF-d8): δ (ppm) = 0.81 and 1.58 (2 · CH_2, cy with 2 · CH_2, cy); 1.04 and 1.58 (2 · CH_2, cy with 2 · CH_2, cy); 1.28 and 1.58 (2 · CH_2, cy with 2 · CH_2, cy); 1.72 and 2.86 (2 · CH_2, cydt with CH_2, cydt; 1.74 and 1.58 (2 · CH, cy with 2 · CH_2, cy); 3.03 and 2.74 (2 · 0.5 · CH_2, P_2N_2 with 2 · 0.5 · CH_2, P_2N_2); 3.03 and 2.79 (2 · 0.5 · CH_2, P_2N_2 with 2 · 0.5 · CH_2, P_2N_2); 3.07 and 2.74 (2 · 0.5 · CH_2, P_2N_2 with 2 · 0.5 · CH_2, P_2N_2); 3.07 and 2.79 (2 · 0.5 · CH_2, P_2N_2 with 2 · 0.5 · CH_2, P_2N_2); 3.48 and 3.71 (2 · 0.5 · CH_2, P_2N_2 with 2 · 0.5 · CH_2, P_2N_2); 3.48 and 3.71 (2 · 0.5 · CH_2, P_2N_2 with 2 · 0.5 · CH_2, P_2N_2). HSQC NMR (300 and 75.5 MHz, THF-d8): δ (ppm) = 0.81 (^{1}H, CH_2, cy) and 30.0 (^{13}C, 2 · CH_2); 1.04 (^{1}H, CH_2, cy) and 28.2 (^{13}C, CH_2); 1.19 (^{1}H, 3 · CH_3, *t*Bu) and 26.5 (^{13}C, 2 · CH_3); 1.22 (^{1}H, 3 · CH_3, *t*Bu) and 26.9 (^{13}C, 2 · CH_3); 1.28 (^{1}H, 2 · CH_2, cy) and 30.0 (^{13}C, 2 · CH_2); 1.58 (^{1}H, CH_2, cy) and 27.0 (^{13}C, CH_2); 1.72 (^{1}H, CH_2, cydt) and 25.1 (^{13}C, 2 · CH_2); 1.74 (^{1}H, CH, cy) and 42.1 (^{13}C, CH); 1.80 (^{1}H, CH_2, cy) and 28.6 (^{13}C, CH_2); 2.74 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 43.8 (^{13}C, 2 · 0.5 · CH_2); 2.79 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 43.8 (^{13}C, 2 · 0.5 · CH_2); 2.88 (^{1}H, 2 · CH_2, cydt) and 36.4 (^{13}C, 2 · CH_2); 3.03 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 43.8 (^{13}C, 2 · 0.5 · CH_2); 3.07 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 43.8 (^{13}C, 2 · 0.5 · CH_2); 3.48 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 43.1 (^{13}C, 2 · 0.5 · CH_2); 3.71 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 43.8 (^{13}C, 2 · 0.5 · CH_2). HMBC NMR[i] (300 and 75.5 MHz, THF-d8): δ (ppm) = 1.19 (^{1}H, 3 · CH_3, *t*Bu) and 26.9 (^{13}C, 2 · CH_3); 1.19 (^{1}H, 3 · CH_3, *t*Bu) and 43.8 (^{13}C, 2 · CH_2, P_2N_2); 1.22 (^{1}H, 3 · CH_3, *t*Bu) and 43.8 (^{13}C, 2 · CH_2, P_2N_2); 1.22 (^{1}H, 3 · CH_3, *t*Bu) and 57.3 (^{13}C, $C_{quart.}$, *t*Bu); 1.22 (^{1}H, 3 · CH_3, *t*Bu) and 58.2 (^{13}C, $C_{quart.}$, *t*Bu); 1.72 (^{1}H, CH_2, cydt) and 147.4 (^{13}C, C−S); 1.72 (^{1}H, CH_2, cydt) and 36.4 (^{13}C, CH_2); 2.88 (^{1}H, 2 · CH_2, cydt) and 25.1 (^{13}C, 2 · CH_2); 2.88 (^{1}H, 2 · CH_2, cydt) and 147.4 (^{13}C, C−S); 3.03 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 43.8 (^{13}C, 2 · 0.5 · CH_2); 3.07 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 43.8 (^{13}C, 2 · 0.5 · CH_2); 3.48 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 43.8 (^{13}C, 2 · 0.5 · CH_2); 3.48 (^{1}H, 2 · 0.5 · CH_2, P^2N^2) and 58.2 (^{13}C, $C_{quart.}$, *t*Bu); 3.71 (^{1}H, 2 · 0.5 · CH_2, P_2N_2) and 43.8 (^{13}C, 2 · 0.5 · CH_2). i: Due to the strong coupling of *t*Bu (sat.: ^{1}H-^{12}C-^{13}C; next to singulett: ^{1}H-^{13}C-^{13}C), not all signals could be assigned properly. ii, iii: Overshadowed by thf, identified by HSQC. iv: Overshadowed by thf, identified by ^{135}DEPT. v: signal identified in combination with ^{135}DEPT and HSQC NMR. Rf-value: 0.556 (*n*-hexane/CH_2Cl_2: 2/3). APCI-MS:[M+MeOH]= 756.35 m/z. IR (KBr disk, in cm^{-1}): ν = 1190; 1361; 1443; 1548; 1636; 1850 (CO); 1858 (CO); 1917 (CO); 1923 (CO); 2849 (−CH_2); 2930 (−CH_2); 2965 (sh, −CH_2). Elemental analysis calculated for $C_{32}H_{56}MoN_2O_2P_2S_2$ (%): C: 53.17; H: 7.81; N: 3.88; S: 8.87. Found: C: 53.27; H: 7.96; N: 4.08; S: 8.79.

Synthesis of $[Mo(CH_3CN)_3(cydt)(P_2^{p\text{-}tol}N_2^{tBu})]\cdot 2[BF_4]$ (**6**)



The synthesis of $[Mo(CH_3CN)_3(cydt)(P_2^{p\text{-}tol}N_2^{tBu})]\cdot 2[BF_4]$ (**6**) was performed according to a published procedure.[8a] In the first reaction step, $[Mo(CO)_2(cydt)(P_2^{p\text{-}tol}N_2^{tBu})]$ (**3**) (78.7 mg, 0.097 mmol, 1 eq.) was oxidized using acetyl ferrocenium tetrafluoroborate (61.4 mg, 0.195 mmol, 2. eq.) in CH_3CN. After stirring for one day, the mixture was layered with Et_2O. After

a few weeks, red crystals, which are highly sensitive towards air and moisture but suitable for X-ray single crystal structure determination were formed. Raw yield ((**6**) · Et_2O): 44% (45.6 mg, 0.043 mmol). The compound is very sensitive to air and moisture and could not be isolated purely enough for further NMR spectroscopic characterization even after several attempts of recrystallization. One (pure) single crystal could be used for IR spectroscopy before it decomposed.
IR (KBr disk, in cm^{-1}): ν = 1060 (br); 1242 (s); 1388 (br); 1500 (vbr, $C{=}C_{dithiolen}$); 1599 (sh); 1635 (br); 2316 (sw, $CN_{stretch}$); 2286 (s, $CN_{stretch}$); 2251 (sw, $CN_{stretch}$); 2859 (sh, $-CH_2$); 2932 (s, $-CH_2$); 2974 (sh, $-CH_2$); 3022 (sh, $-CH_2$).

Results and Discussion

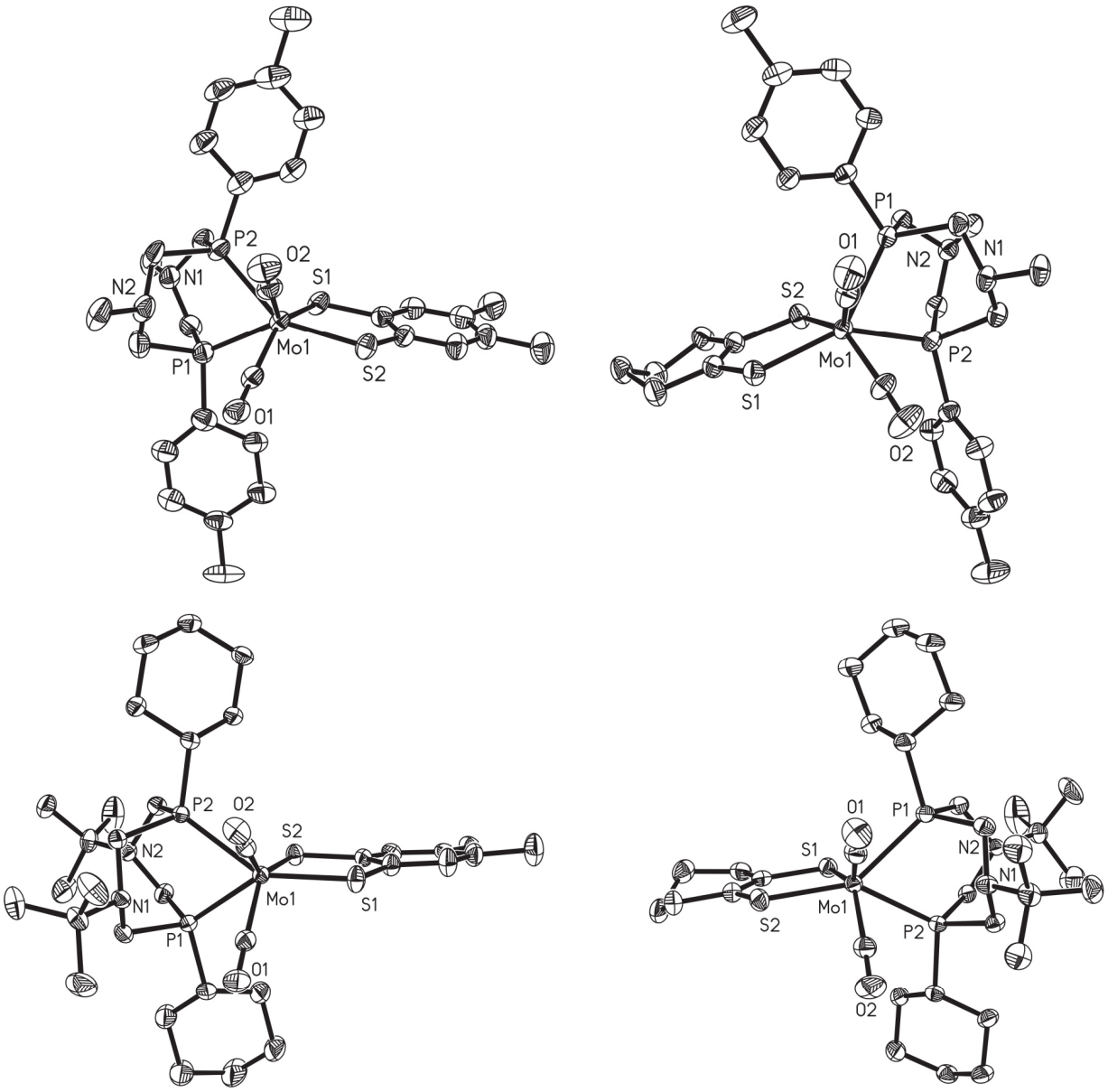


Figure S1. Molecular structures of $[Mo(CO)_2(P_2^{p\text{-}tol}N_2^{tBu})(xdt)]\cdot CH_2Cl_2$ (**2**), R= 4.30%, R_{int}= 5.88% (upper left) and $[Mo(CO)_2(cydt)(P_2^{p\text{-}tol}N_2^{tBu})]\cdot CH_2Cl_2$ (**3**), R= 4.36%, R_{int}= 7.38% (upper right) and of $[Mo(CO)_2(P_2^{cy}N_2^{tBu})(xdt)]$ (**4**), R= 3.82%, R_{int}= 6.25% (bottom right) and $[Mo(CO)_2(cydt)(P_2^{cy}N_2^{tBu})]$ (**5**), R= 4.17%, R_{int}= 10.72% (bottom right). Ellipsoids are shown at the 50% probability level. Hydrogen atoms and co-crystallized solvents were omitted for clarity reasons.

Table S1. Selected bond lengths (Å), angles (°) and torsion angles (°) in the molecular structures of $[Mo(CO)_2(dt)(P_2^{p\text{-}tol}N_2^{tBu})]$ (dt= xdt (**2**) or dt= cydt (**3**)) and $[Mo(CO)_2(dt)(P_2^{cy}N_2^{tBu})]$ (dt= xdt (**4**) or dt= cydt (**5**)). The geometrical twist resembles a Ray-Dutt type complex geometry and is therefore referred to as Ray-Dutt-Twist instead of the Bailar-Twist. The centroid for the Ray-Dutt-Twist is set between the SCC and SPP plane. CB: Chair-Boat-Conformation of the eight-membered P_2N_2 backbone.

	(**2**)	(**3**)	(**4**)	(**5**)
C=C (dithiolene)	1.382(9)	1.341(5)	1.390(3)	1.333(4)
C-S1	1.753(6)	1.754(3)	1.744(3)	1.755(3)
C-S2	1.747(6)	1.738(3)	1.756(2)	1.742(3)
CO1	1.138(7)	1.158(4)	1.148(3)	1.150(4)
CO2	1.151(7)	1.138(4)	1.150(3)	1.155(3)
Mo-P1	2.4463(19)	2.4450(10)	2.4713(8)	2.4761(11)
Mo-P2	2.4542(16)	2.4639(10)	2.4655(8)	2.4704(9)
Mo-S1	2.4217(15)	2.3536(10)	2.3482(9)	2.4167(9)
Mo-S2	2.3497(17)	2.4102(9)	2.4260(7)	2.3503(9)
Mo-CO(1)	1.965(6)	1.960(4)	1.948(3)	1.962(3)
Mo-CO(2)	1.960(6)	1.970(3)	1.962(2)	1.942(3)
S1-Mo-S2	83.30(5)	82.38(3)	83.59(3)	82.54(3)
C1-Mo-C2	72.6(2)	73.05(14)	71.83(10)	73.95(13)
P1-Mo-P2	69.61(6)	70.28(3)	70.38(3)	70.19(3)
Ray-Dutt-Twist	3.1	2.1	2.3	4.6
P_2N_2 conformation	CB	CB	CB	CB

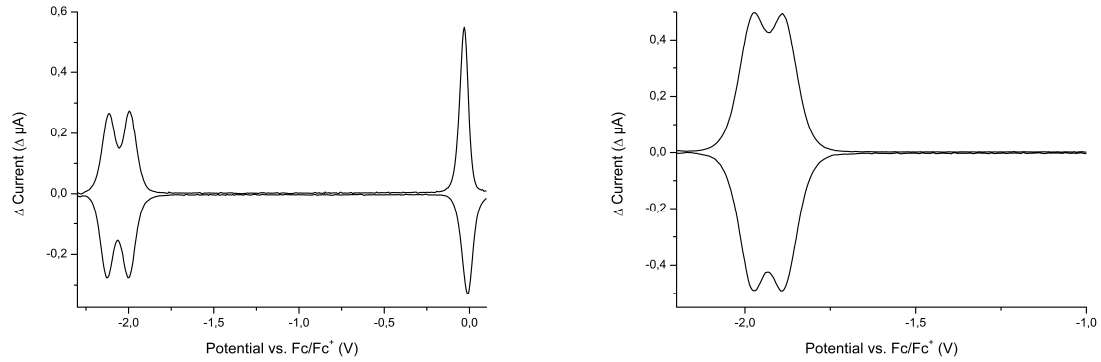


Figure S2. DPV of $[Mo(CO)_2(cydt)(P_2^{p\text{-}tol}N_2^{tBu})]$ (**3**) (left) and $[Mo(CO)_2(P_2^{p\text{-}tol}N_2^{tBu})(xdt)]$ (**2**) (right, zoomed for clarity reasons) measured in CH_3CN using $(n\text{-}Bu_4N)(PF_6)$ (0.1 M) as supporting electrolyte. Modulation amplitude: 10 mV; scan speed 5 mV/s.

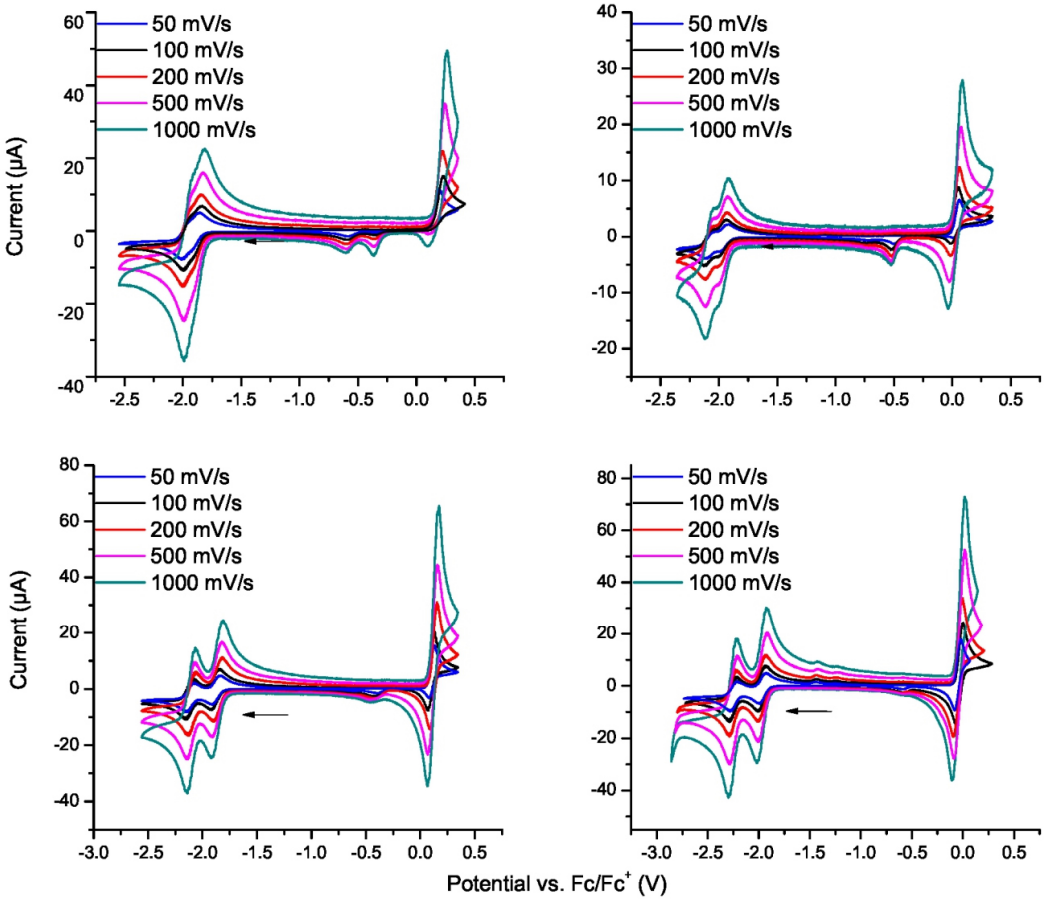


Figure S3. Scan rate dependent cyclic voltammetry of Scan rate dependent cyclic voltammetry of $[Mo(CO)_2(P_2^{p\text{-}tol}N_2^{tBu})(xdt)]$ (**2**) (top, left), $[Mo(CO)_2(cydt)(P_2^{p\text{-}tol}N_2^{tBu})]$ (**3**) (top, right), $[Mo(CO)_2(P_2^{cy}N_2^{tBu})(xdt)]$ (**4**) (bottom, left) and $[Mo(CO)_2(cydt)(P_2^{cy}N_2^{tBu})]$ (**5**) (bottom, right). The measurements were performed in CH_3CN using 0.1 M (n-Bu_4N) (PF_6) as a supporting electrolyte.

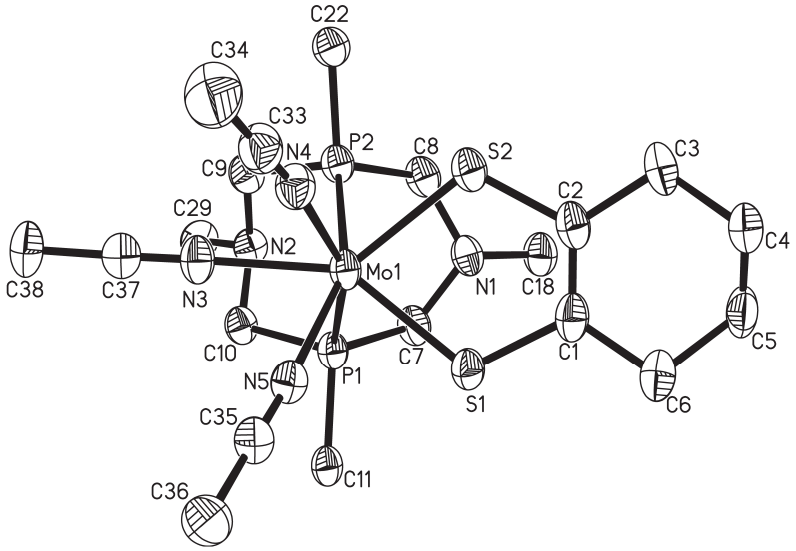


Figure S4. Molecular structure of $[Mo(CH_3CN)_3(cydt)(P_2^{p\text{-}tol}N_2^{tBu})][BF_4]_2 \cdot Et_2O$ (**6**), R= 5.41%, R_{int}= 6.80%. Ellipsoids are shown at 50% probability level. Hydrogen atoms, counterions, N- and P-substituents and the co-crystallized solvent were omitted for clarity reasons.

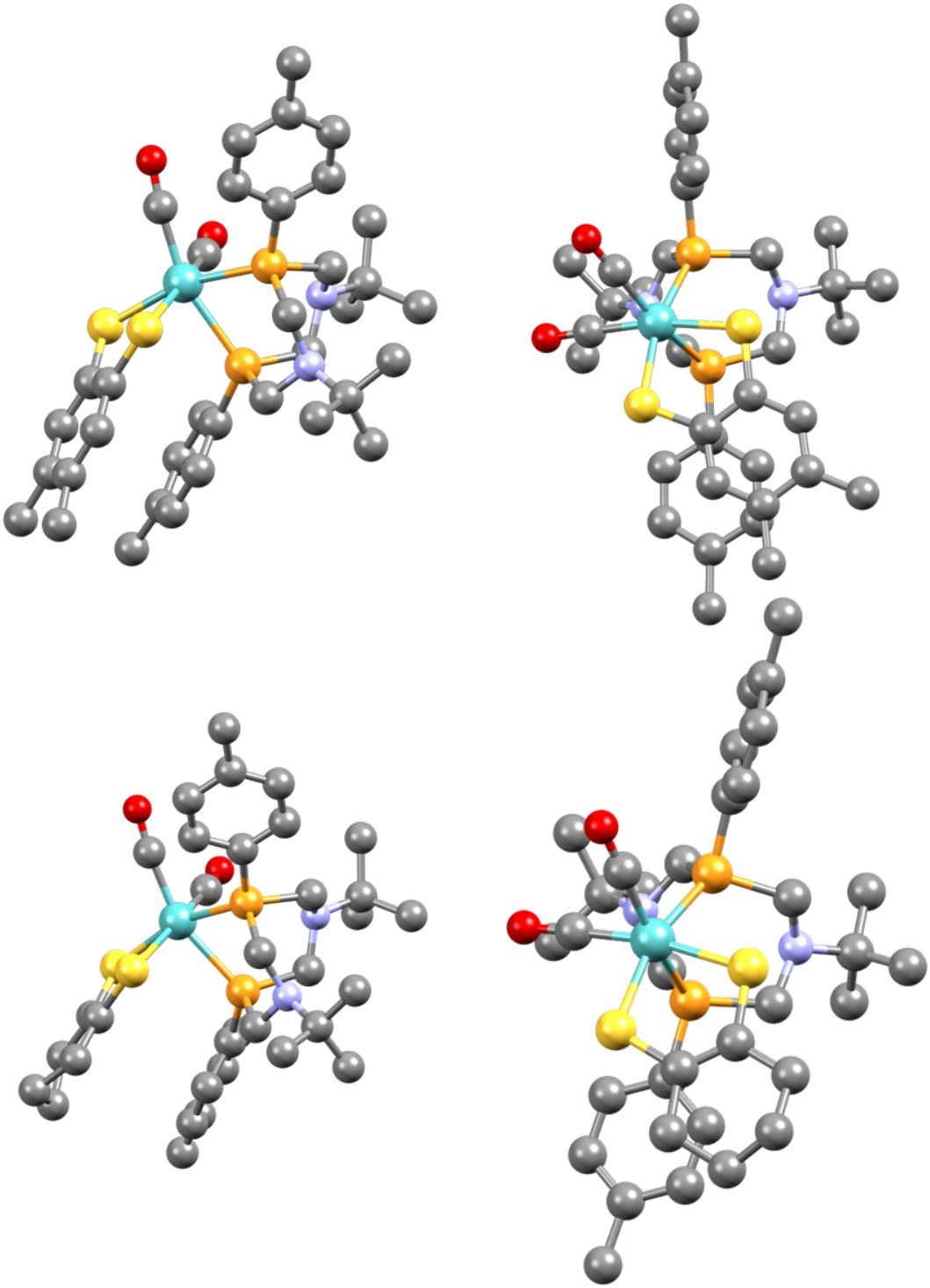


Figure S5. Ball and stick representation of $[Mo(CO)_2(P_2^{p\text{-tol}}N_2^{tBu})(xdt)]^{1-}$ (**2**$^{1-}$) (top) and $[Mo(CO)_2(cydt)(P_2^{p\text{-tol}}N_2^{tBu})]^{1-}$ (**3**$^{1-}$) (bottom) in two different perspectives. Structures calculated by DFT using the TPSSh functional. Color coding: grey: carbon, blue: nitrogen, orange: phosphane, light blue: molybdenum, red: oxygen, yellow: sulfur. Hydrogens omitted for clarity reasons. Visualized using Mercury[22]

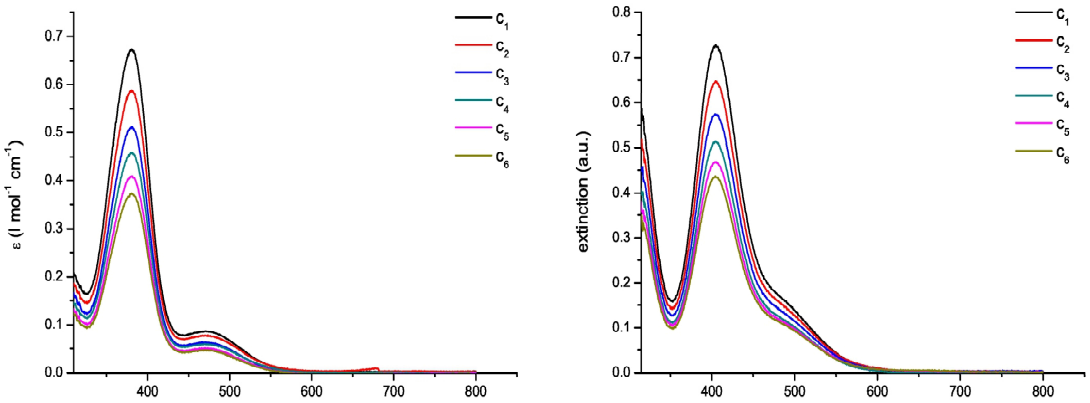


Figure S6. Concentration dependent UV-vis spectra of $[Mo(CO)_2(P_2^{p\text{-tol}}N_2^{tBu})(xdt)]$ (**2**) measured in CH_3CN at room temperature; c_1: $5.686 \cdot 10^{-5}$ mol/l, c_2: $4.975 \cdot 10^{-5}$ mol/l, c_3: $4.422 \cdot 10^{-5}$ mol/l, c_4: $3.98 \cdot 10^{-5}$ mol/l, c_5: $3.618 \cdot 10^{-5}$ mol/l, c_6: $3.317 \cdot 10^{-5}$ mol/l and dependent UVvis spectra of $[Mo(CO)_2(cydt)(P_2^{p\text{-tol}}N_2^{tBu})]$ (**3**) measured in CH_3CN at room temperature; c_1: $1.078 \cdot 10^{-4}$ mol/l, c_2: $9.539 \cdot 10^{-5}$ mol/l, c_3: $8.552 \cdot 10^{-5}$ mol/l, c_4: $7.750 \cdot 10^{-5}$ mol/l, c_5: $7.086 \cdot 10^{-5}$ mol/l, c_6: $6.526 \cdot 10^{-5}$ mol/l.

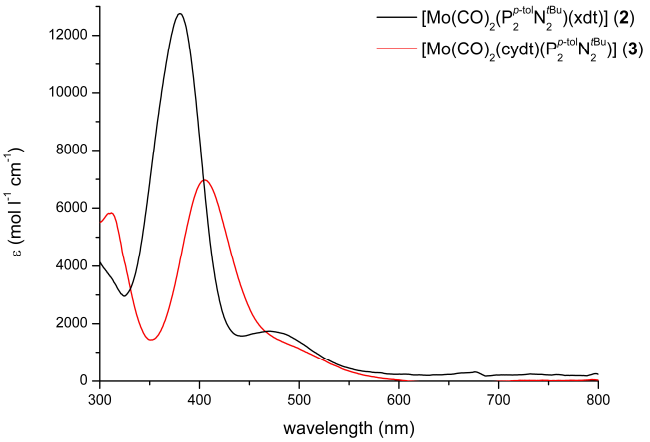


Figure S7. Pure component spectra of $[Mo(CO)_2(dt)(P_2^{p\text{-tol}}N_2^{tBu})]$ complexes (dt= xdt (**2**), black; cydt (**3**), red) measured in CH_3CN at room temperature. Maxima of the spectra: (**2**) at 380.5 nm; (**3**) at 311 nm and 405.5 nm.

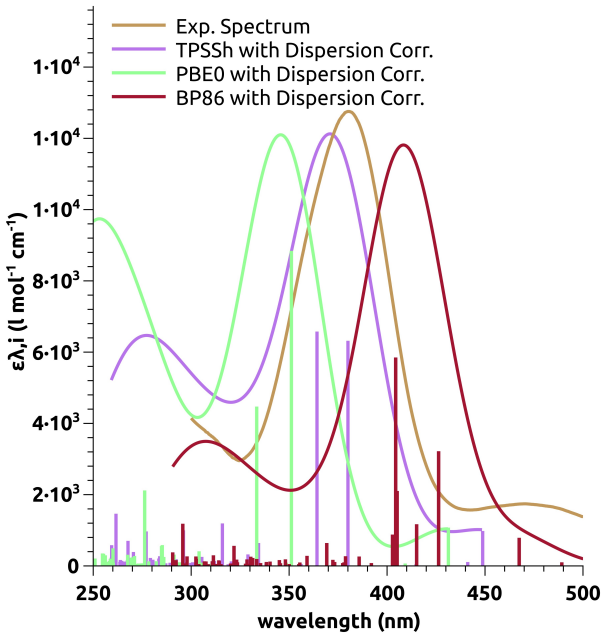


Figure S8. Experimental and calculated UV-vis spectrum of [Mo(CO)$_2$($P_2^{p\text{-tol}}N_2^{t\text{Bu}}$)(xdt)] (**2**). TD-DFT calculations performed with different functionals, namely BP86 (wine red), PBE0 (light green) and TPSSh (violet), in all cases using a structure optimized with BP86 starting with coordinates from SCXRD experiments. The best match with the experimental data (ochre) was obtained using TPSSh.

Table S2. Experimental (KBr-Pellet) and calculated vibrational frequencies for the carbonyl stretching vibration in [Mo(CO)$_2$(dt)(P_2N_2)], dt= xdt, P_2N_2= $P_2^{p\text{-tol}}N_2^{t\text{Bu}}$ (**2**), dt= cydt, P_2N_2= $P_2^{p\text{-tol}}N_2^{t\text{Bu}}$ (**3**), dt= xdt, P_2N_2= $P_2^{cy}N_2^{t\text{Bu}}$ (**4**), dt= cydt, P_2N_2= $P_2^{cy}N_2^{t\text{Bu}}$ (**5**) using the density functional specified in the table. 'Straight' (s) means a geometry optimization with the D3zero dispersion correction switched on, while 'deviant' (d) accounts for a primary optimization without any dispersion correction and a subsequent numerical frequency run with the thus achieved geometry including D3zero. {Mo} represents the whole complex.

			{Mo} (trigonal-prismatic)						{Mo}+1e$^-$ (octahedral)		{Mo}+2e$^-$ (octahedral)	
	functional	Procedure	experimental (cm^{-1})		Factor exp/dft		calc. (cm^{-1})		calc. (cm^{-1})		calc. (cm^{-1})	
2	BP86	s	1937	1873	1.031	1.026	1879	1825	1785	1712	-	-
		d			1.026	1.020	1888	1837	1788	1722	-	-
	PBE0	s			0.965	0.958	2008	1955	1914	1847	-	-
		d			0.965	0.958	2008	1955	1915	1854	-	-
	TPSSh	s			0.993	0.986	1951	1900	1855	1791	1765	1703
		d			0.993	0.986	1950	1900	1857	1798	1769	1706
3	TPSSh	s	1931	1861	0.993	0.983	1944	1893	1844	1785	1758	1698
		d			0.994	0.983	1943	1893	1847	1789	1765	1701
4	TPSSh	s	1921	1853	0.991	0.983	1938	1885	1848	1785	1755	1689
		d			0.991	0.983	1938	1885	1848	1786	1755	1689
5	TPSSh	s	1917	1850	0.993	0.986	1931	1877	1838	1777	1749	1683
		d			0.993	0.986	1930	1877	1838	1777	1751	1683

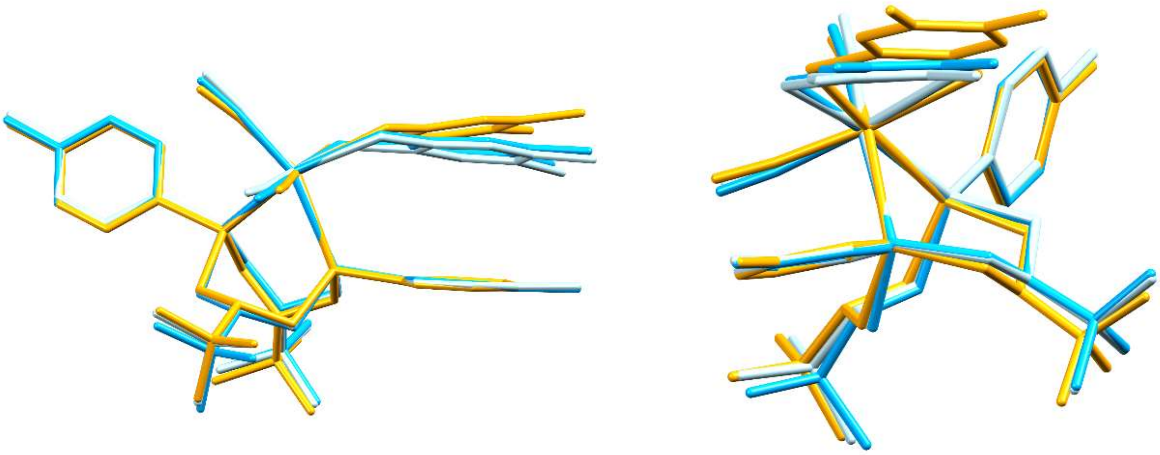


Figure S9. Additional perspectives of the superposition of the singly reduced $[Mo(CO)_2(P_2^{p\text{-tol}}N_2^{tBu})(xdt)]^{1-}$ (**2**$^{1-}$) as calculated by DFT with different density functionals (BP86: light blue; TPSSh: blue; PBE0: orange; all with D3zero dispersion corrections). Visualized with Mercury.[22]

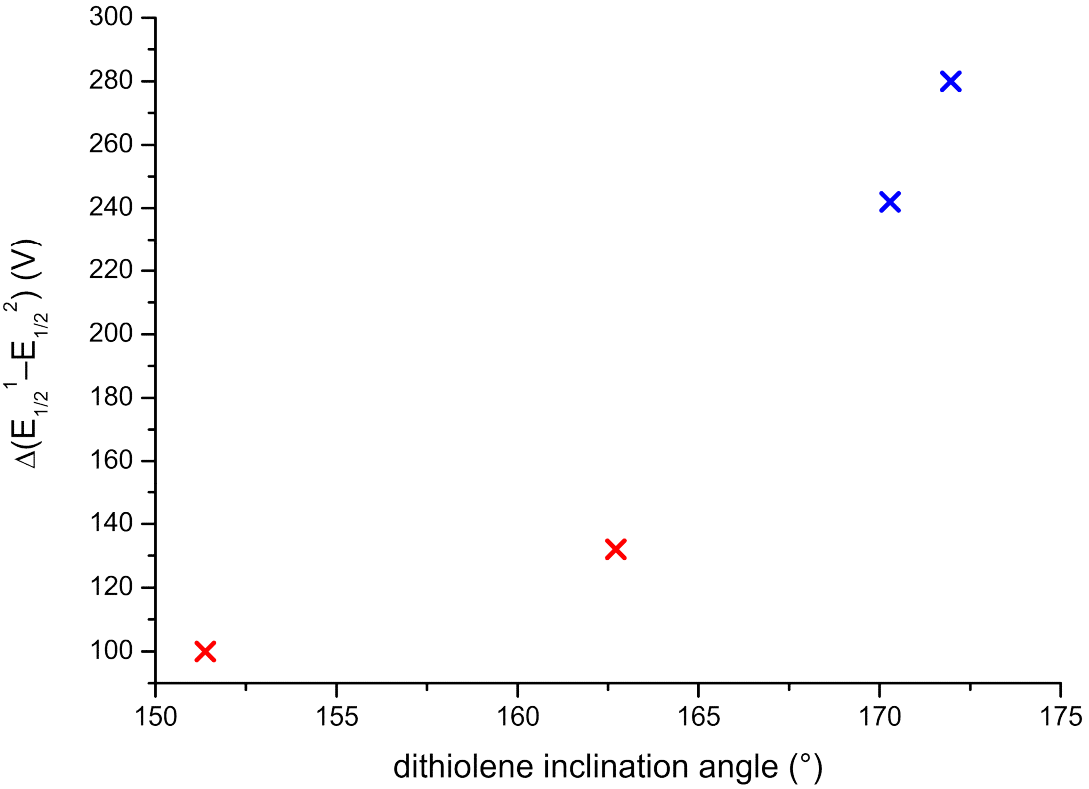


Figure S10. Inclination angle (°) of the dithiolene ligand vs. Δ ($E_{1/2}^1$–$E_{1/2}^2$) plot. The potentials were used as determined from the cyclic voltammograms (see Table 1) and the inclination angles were used as obtained from Table S6. **2**$^{1-}$: 151°, **3**$^{1-}$: 163°, **4**$^{1-}$: 170°, **5**$^{1-}$: 172°. Δ ($E_{1/2}^1$–$E_{1/2}^2$) of **2**: 100 mV, **3**: 132 mV, **4**: 242 mV, **5**: 280 mV. The larger the deviation from 180°, the smaller the potential difference between the first and second reduction. However, no finite potential difference can occur when approaching 180°, as this graph might imply. Complexes utilizing the $P_2^{p\text{-tol}}N_2^{tBu}$ ligand (**2**$^{1-}$ & **3**$^{1-}$) are marked in red, while complexes utilizing the $P_2^{cy}N_2^{tBu}$ ligand (**4**$^{1-}$ & **5**$^{1-}$) are marked in blue.

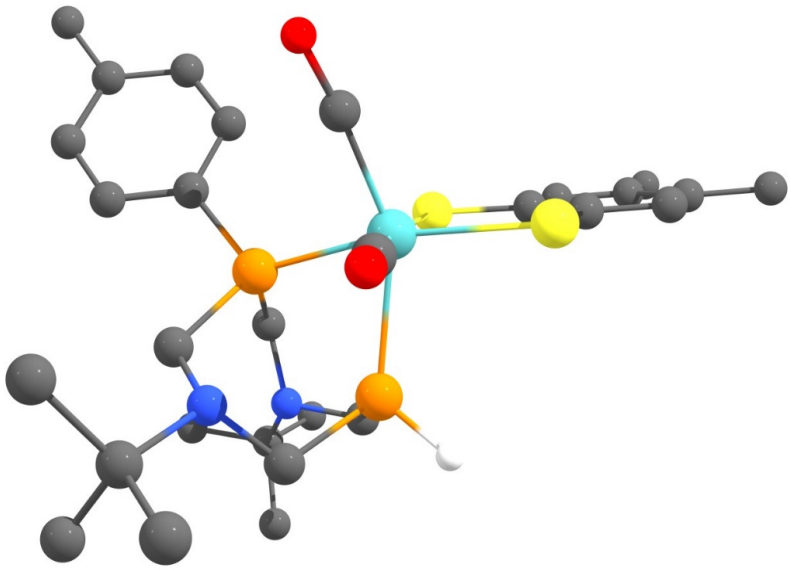


Figure S11. *In silico* exchange of the *p*-tolyl substituent on the phosphorus atom based on DFT calculations using the TPSSh density functional. All hydrogen atoms – except for the artificially added one – are omitted for clarity reasons. Color coding: grey: carbon, blue: nitrogen, orange: phosphorus, white: hydrogen, light blue: molybdenum, red: oxygen, yellow: sulfur.

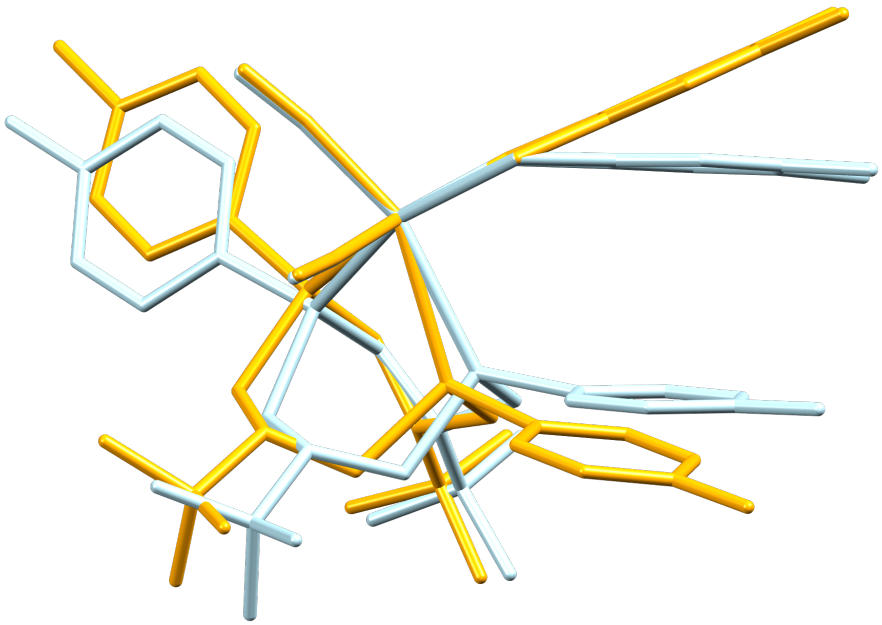


Figure S12. Superposition of the 'stacked' (blue) and 'non-stacked' (orange) structure of $[Mo(CO)_2(P_2^{p\text{-tol}}N_2^{tBu})(xdt)]^{1-}$ (**2**$^{1-}$) obtained from DFT calculations using the TPSSh functional with (light blue) or without (orange) the use of the D3zero dispersion correction. Visualized with Mercury.[22]

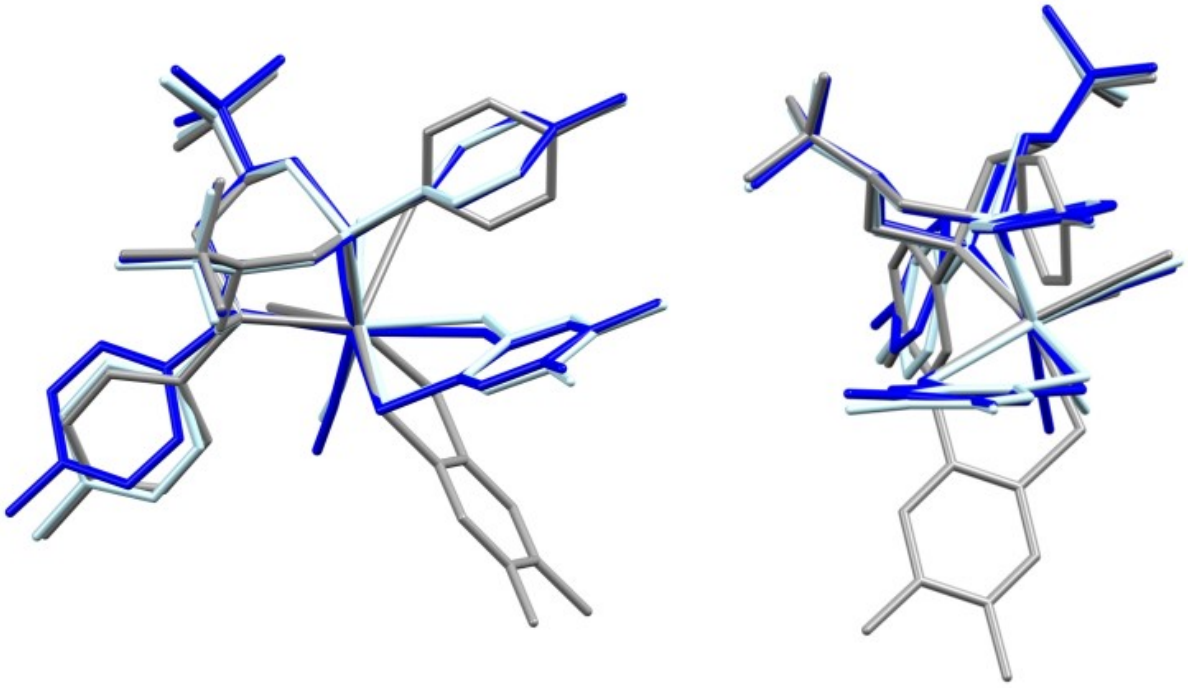


Figure S13. Structural overlays of the TPSSh calculated structures of **2** (grey, trigonal-prismatic), $\mathbf{2}^{1-}$ (light blue, distorted-octahedral) and $\mathbf{2}^{2-}$ (blue, distorted-octahedral) in two different perspectives. Visualized with Mercury.[22]

Table S3. Selected distances (Å) and angles (°) of the TPSSh calculated structures of **2**, $\mathbf{2}^{1-}$ and $\mathbf{2}^{2-}$. The elongated Mo-S distances upon reduction underline the π-antibonding character of the respective SOMO ($\mathbf{2}^{1-}$) and HOMO ($\mathbf{2}^{2-}$). The difference in C-S distances show the enhanced mobility dithiolene ligand, stabilized by the second ligand sphere interaction with the *p*-tolyl substituent of the P_2N_2 ligand upon reduction. The centroids for the calculation of the Bailar-Twist are set between the SCC and SPP plane.

	2	$\mathbf{2}^{1-}$	$\mathbf{2}^{2-}$
Mo-S1	2.439	2.544	2.624
Mo-S2	2.374	2.450	2.586
S1-$C_{dithiolene}$	1.757	1.764	1.772
S2-$C_{dithiolene}$	1.757	1.760	1.768
S1·····S2	3.192	3.254	3.287
Inclination angle	178.41	151.38	146.79
Ray-Dutt/Bailar-Twist	0.65	52.2	57.6

Table S4. Calculated Final Single Point Energies of all relevant complexes and the corresponding calculation of (non-referenced) redox potentials. {Mo} represents the whole complex $[Mo(CO)_2(dt)(P_2N_2)]$, dt= xdt, P_2N_2= $P_2^{p\text{-tol}}N_2^{tBu}$ (**2**), dt= cydt, P_2N_2= $P_2^{p\text{-tol}}N_2^{tBu}$ (**3**), dt= xdt, P_2N_2= $P_2^{cy}N_2^{tBu}$ (**4**), dt= cydt, P_2N_2= $P_2^{cy}N_2^{tBu}$ (**5**). {Mo} represents the whole complex.

compound	initial structure	Disp.-Corr.	Final Single Point Energy (Eh)			ΔFSPE (solution) (kcal/mol)		(Non-referenced) Potential (V)		Pot. Difference (V)
			{Mo}	{Mo}+1e$^-$	{Mo}+2e$^-$	{Mo} →{Mo}$^{1-}$	{Mo}$^{1-}$ →{Mo}$^{2-}$	{Mo} →{Mo}$^{1-}$	{Mo}$^{1-}$ →{Mo}$^{2-}$	
2	BP86 optimized	on	-3207.704048	-3207.807359	-3207.904814	-64.8	-61.2	2.811	2.652	0.159
	TPSSh optimized 'stacked' structure	off	-3207.585136	-3207.78485045	-3207.783791	-63.3	-61.4	2.743	2.691	0.052
	TPSSh optimized 'non-stacked' structure	on	-3207.70309	-3207.90134011	-3207.900801	-61.4	-61.1	2.732	2.663	0.069
	ΔFSPE 'non-stacked' vs. 'stacked' (kcal)			2.43	2.18					
3	SCXRD of {Mo}	on	-3131.520655	-3131.620553	-3131.713077	-62.7	-58.1	2.718	2.518	0.201
	TPSSh optimized 'stacked' structure	off	-3131.403021	-3131.500880	-3131.595301	-61.4	-59.2	2.663	2.569	0.094
	TPSSh optimized 'non-stacked' structure	on	-3131.519673	-3131.617805	-3131.710890	-61.6	-58.4	2.670	2.533	0.137
	ΔFSPE 'non-stacked' vs. 'stacked' (kcal)			1.73	1.37					
4	SCXRD of {Mo}	on	-3136.382274	-3136.48401	-3136.577418	-63.8	-58.6	2.768	2.542	0.227
	TPSSh optimized 'stacked' structure	off	-3136.251061	-3136.351149	-3136.445078	-62.8	-58.9	2.723	2.556	0.168
	TPSSh optimized 'non-stacked' structure	on	-3136.381120	-3136.482236	-3136.575502	-63.5	-58.5	2.751	2.538	0.214
	ΔFSPE 'non-stacked' vs. 'stacked' (kcal)			1.11	1.20					
5	SCXRD of {Mo}	on	-3060.198754	-3060.297838	-3060.387169	-62.2	-56.1	2.696	2.431	0.265
	TPSSh optimized 'stacked' structure	off	-3060.068772	-3060.165968	-3060.255699	-61.0	-56.3	2.645	2.442	0.203
	TPSSh optimized 'non-stacked' structure	on	-3060.197586	-3060.295918	-3060.385144	-61.7	-56.0	2.676	2.428	0.248
	ΔFSPE 'non-stacked' vs. 'stacked' (kcal)			1.21	1.27					

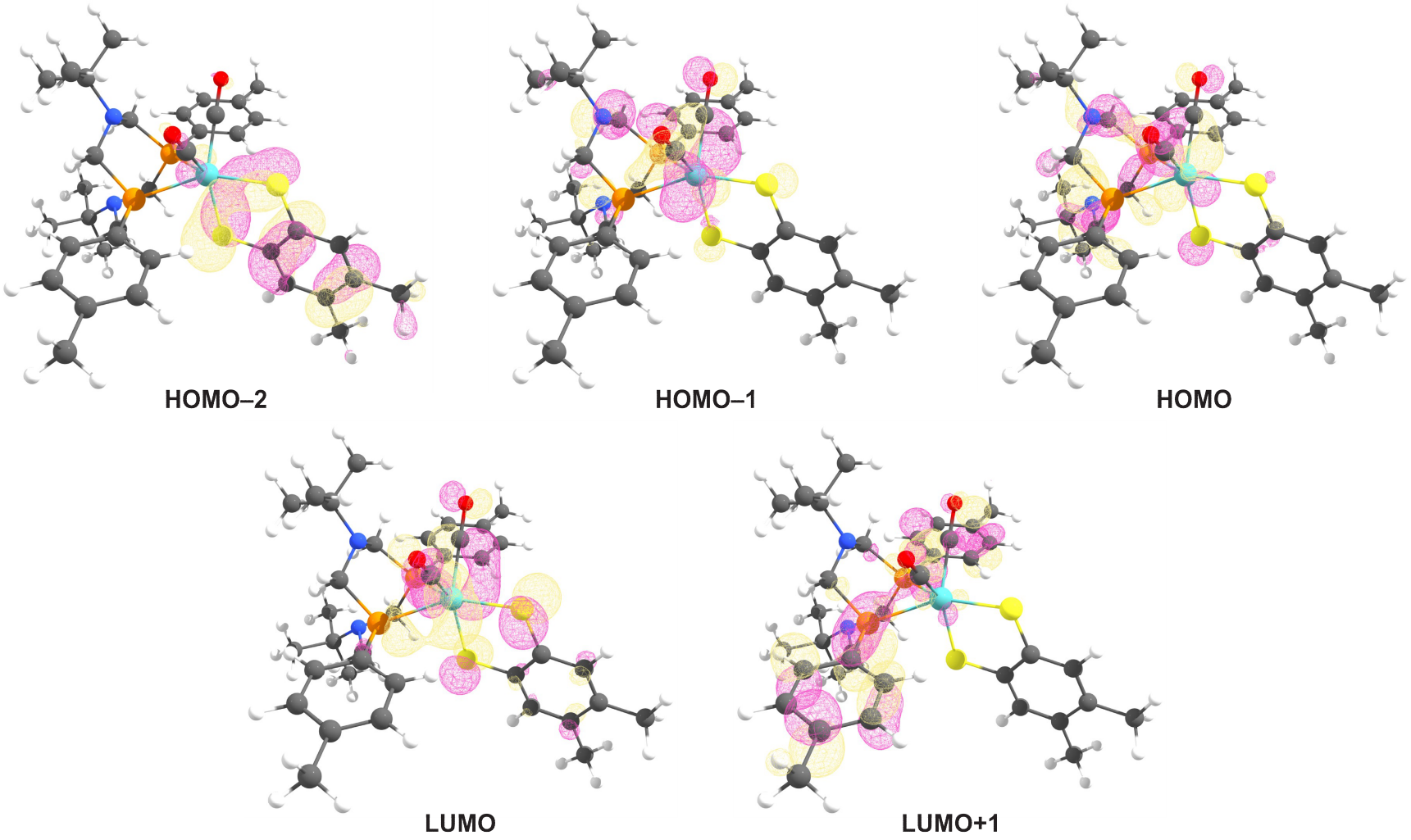


Figure S14. Contour plots of the calculated (TPSSh) molecular orbitals of **2**.

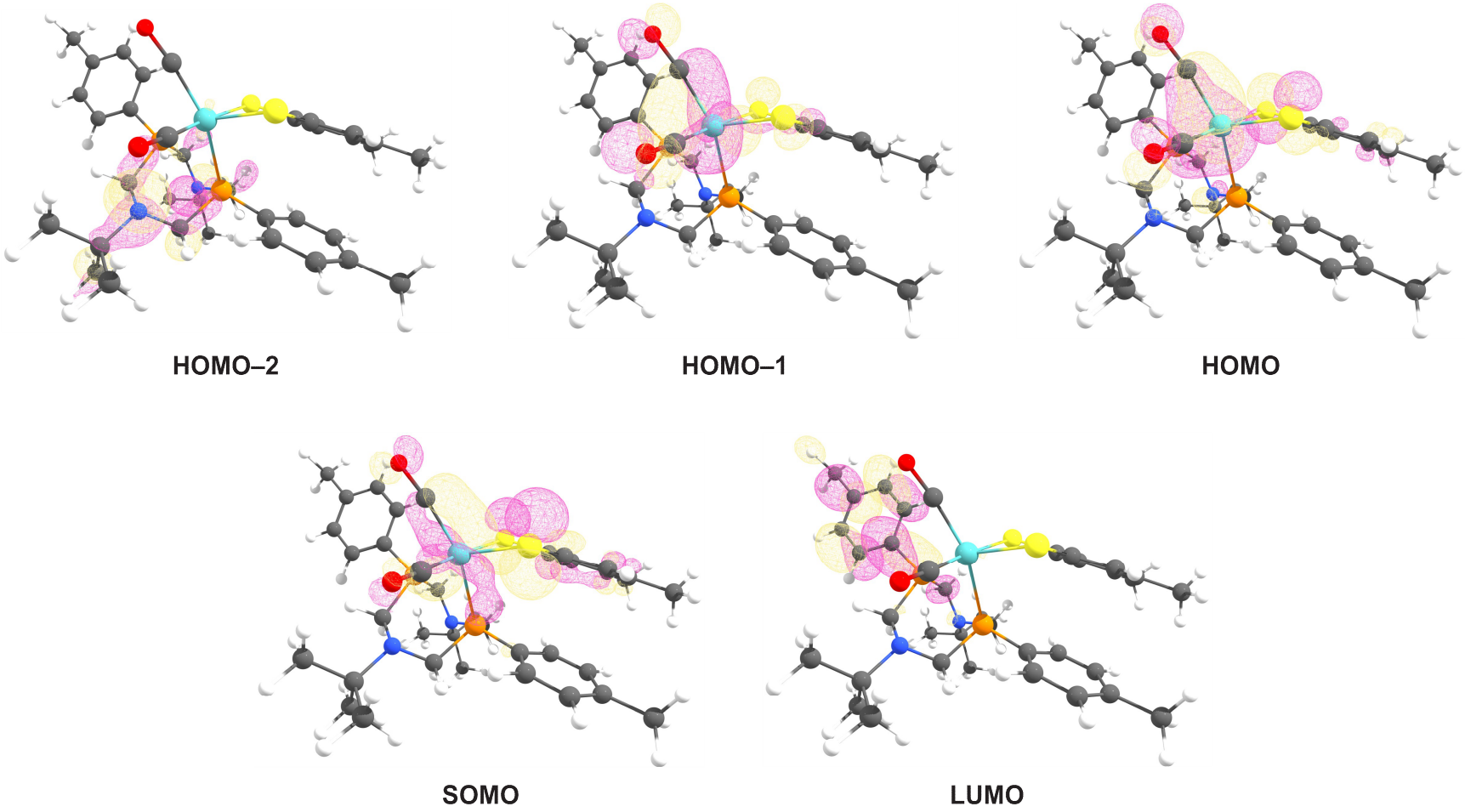


Figure S15. Contour plots of the calculated (TPSSh) molecular orbitals of $\mathbf{2}^{1-}$.

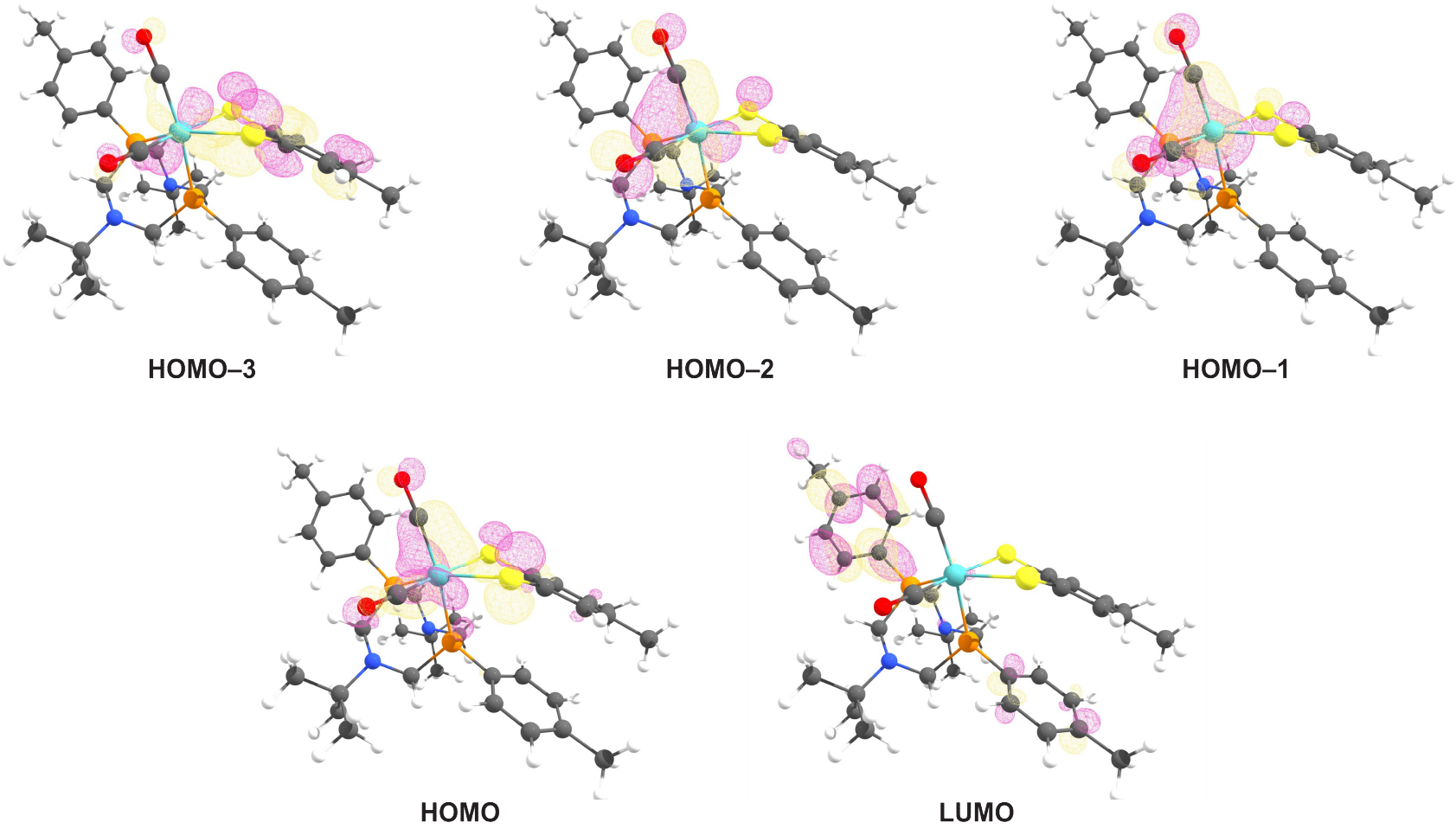


Figure S16. Contour plots of the calculated (TPSSh) molecular orbitals of $\mathbf{2}^{2-}$.

Table S5. Contributions of molybdenum's atomic orbitals to the respective molecular orbitals for $[Mo(CO)_2(P_2^{p\text{-}tol}N_2^{tBu})(xdt)]^{1-}$ **2**$^{1-}$ and $[Mo(CO)_2(P_2^{p\text{-}tol}N_2^{tBu})(xdt)]^{2-}$ **2**$^{2-}$. The trend of the contribution change of the SOMO of the mono-reduced species (non-stacked → stacked) as discussed in the main text is mirrored by the doubly reduced complexes, though with slightly distinct details, i.e. now the d_{z2} orbital (similar to the d_{xz}; both in z-direction) contributes more to the stacked HOMO (former SOMO) 0.1% → 6.6% (non-stacked → stacked) while the d_{xy} (similar to the d_{x2-y2}; both in xy-direction) loses some contribution percentage (11.9% → 7.7%; non-stacked → stacked). Both, d_{z2} and d_{xy} did not change much in the mono-reduced SOMO.

			s	pz	px	py	dz^2	dxz	dyz	dx^2y^2	dxy	Σ
		HOMO–1	0.1	0	0.4	1.0	15.1	15.4	0.4	9.7	8.6	50.7
	'non-stacked'	HOMO	0	0.3	0.2	0.2	14.2	7.4	14.2	0.6	0.5	37.6
		SOMO	0	0.1	0.3	0.1	0.3	8.2	0	12.6	6.5	28.1
2^{1-}												
		HOMO–1	0.1	0.1	1.0	0.3	11.4	9.4	1.5	24.8	1.5	50.1
	'stacked'	HOMO	0	0.5	0.4	0.1	11.2	7.8	17.8	0.4	0.3	38.5
		SOMO	0	0.2	0.3	0.1	2.6	14.3	0	6.9	6.6	31.0
		HOMO-2	0	0.3	0.1	0.2	11.1	12.5	11.6	3.2	2.0	41.0
	'non-stacked'	HOMO-1	0	0	0	0.5	22.4	16.3	2.4	9.4	3.4	54.4
		HOMO	0	0.3	0.1	0.2	0.1	11.0	0.4	9.3	11.9	33.3
2^{2-}												
		HOMO-2	0.1	0.1	0	0.2	6.1	10	0.2	30.3	0.4	47.4
	'stacked'	HOMO-1	0	0.7	0.6	0.1	14.6	6.6	22.7	0.2	0.7	46.2
		HOMO	0	0.1	0.3	0	6.6	18.7	0.1	4.4	7.7	37.9

Table S6. Mulliken Spin Population for selected atoms in the mono-reduced complexes $\mathbf{2}^{1-}$, $\mathbf{3}^{1-}$, $\mathbf{4}^{1-}$ and $\mathbf{5}^{1-}$. In all cases, a dispersion correction was applied.

	Functional	initial structure	Orientation:	Mo	S1 *trans* P	S2 *trans* CO	C1 *trans* P	O1	C2 *trans* S	O2	P1 *trans* C	P2 *trans* S	Inclination Angle (°)
$\mathbf{2}^{1-}$	BP86	SCXRD data		0.505	0.154	0.096	0.066	0.043	0.003	0.015	0.025	-0.005	152.71
		Pre-optimized one without Dispersion Corr.		0.440	0.136	0.085	0.123	0.062	0.008	0.006	0.066	-0.008	175.25
	PBE0	BP86 optimized structure		0.601	0.112	0.063	0.097	0.059	0.015	0.008	0.044	-0.021	158.66
		Pre-optimized one without Dispersion Corr.		0.537	0.109	0.053	0.138	0.077	0.029	0.001	0.068	-0.012	176.62
	TPSSh	BP86 optimized structure		0.579	0.142	0.076	0.064	0.043	-0.002	0.014	0.025	-0.011	151.38
		Pre-optimized one without Dispersion Corr.		0.509	0.129	0.071	0.123	0.066	0.018	0.004	0.056	-0.011	175.43
$\mathbf{3}^{1-}$	TPSSh	SCXRD data		0.457	0.169	0.114	0.089	0.049	-0.005	0.010	0.038	-0.011	162.72
		Pre-optimized without Dispersion Corr.		0.436	0.159	0.108	0.112	0.058	-0.011	0.006	0.051	-0.010	166.96
$\mathbf{4}^{1-}$	TPSSh	SCXRD data		0.526	0.124	0.072	0.132	0.068	0.018	0.004	0.052	-0.015	170.29
		Pre-optimized without Dispersion Corr.		0.524	0.125	0.068	0.133	0.066	0.020	0.003	0.058	-0.013	174.01
$\mathbf{5}^{1-}$	TPSSh	SCXRD data		0.458	0.149	0.102	0.130	0.064	-0.015	0.005	0.050	-0.013	171.97
		Pre-optimized without Dispersion Corr.		0.458	0.152	0.097	0.129	0.062	-0.016	0.004	0.055	-0.011	175.48

Table S7. Summarized Loewdin Orbital Composition and Energies for selected Orbitals of the mono-reduced complexes **2**$^{-}$ and **3**$^{-}$.

	initial structure	Disp. Corr.	Orientation:	Mo	S1	S2	C1	O1	C2	O2	Dithiolene C=C		P1	P2	Energy	SOMO-LUMO GAP	
				-	*trans* P	*trans* CO	*trans* P		*trans* S		*trans* P	*trans* C	*trans* C	*trans* S	Eh	Eh	kcal
	BP86 pre-optimized	on	HOMO-1	48.6	4.5	6.5	5.6	6.2	7.0	8.4	0.8	0.8	0.8	2.8	-0.16288		
			HOMO	37.5	6.7	11.8	5.9	6.1	5.0	5.3	1.0	0.1	1.6	2.3	-0.15629		
			SOMO	30.4	18.2	14.3	5.2	3.3	2.1	1.5	2.2	2.7	4.2	2.0	-0.1308	0.09896	62.1
			LUMO	0.5	0.1	0.0	0.1	0.0	0.4	0.2	0.0	0.0	0.0	9.7	-0.03184		
			LUMO+1	2.2	0.5	0.4	3.0	1.4	0.4	0.2	0.2	0.0	10.0	1.1	-0.02929		
2^{-}																	
	TPSSh without Dispersion Corr. ≈ 'non-stacked'	on	HOMO-1	49.2	3.5	8.3	3.2	3.6	8.1	9.6	1.4	0.6	0.6	3.8	-0.16216		
			HOMO	36.9	7.2	11.0	5.5	5.6	5.2	5.8	0.7	0.3	1.7	2.5	-0.15939		
			SOMO	27.8	17.0	13.2	8.7	5.4	1.2	1.0	2.0	2.5	6.8	1.4	-0.12945	0.09626	60.4
			LUMO	1.5	0.3	0.2	1.4	0.6	0.7	0.2	0.0	0.0	4.5	4.8	-0.03319		
			LUMO+1	1.1	0.0	0.2	1.5	0.5	0.2	0.1	0.0	0.0	3.8	6.1	-0.03303		
	SCXRD data from neutral species	on	HOMO-1	48.5	3.6	8.8	5.9	6.4	6.5	8.0	2.3	0.7	1.3	2.6	-0.16014		
			HOMO	48.1	4.7	4.7	5.5	5.6	7.0	7.7	1.5	0.7	1.1	3.8	-0.15498		
			SOMO	26.2	19.0	16.3	6.4	3.9	1.6	1.2	4.6	6.3	5.0	1.5	-0.12319	0.09166	57.5
			LUMO	0.8	0.0	0.0	0.0	0.0	0.4	0.2	0.0	0.0	0.0	9.7	-0.03153		
			LUMO+1	3.5	0.6	0.2	3.0	1.4	0.4	0.2	0.1	0.0	9.0	1.3	-0.02996		
3^{-}																	
	TPSSh without Dispersion Corr. ≈ 'non-stacked'	on	HOMO-1	44.9	3.3	10.9	6.3	7.0	5.2	6.5	3.6	0.3	1.8	2.3	-0.16088		
			HOMO	51.6	4.7	3.9	3.1	3.2	8.8	9.8	0.9	1.0	0.5	4.4	-0.15679		
			SOMO	24.9	18.4	15.9	7.9	4.8	1.4	1.1	4.6	6.0	6.1	1.3	-0.12374	0.09144	57.4
			LUMO	0.7	0.1	0.0	0.0	0.0	0.5	0.2	0.0	0.0	0.1	10.0	-0.0323		
			LUMO+1	3.2	0.6	0.2	2.8	1.3	0.4	0.2	0.0	0.0	8.6	1.1	-0.03135		

Table S8. Summarized Loewdin Orbital Composition and Energies for selected Orbitals of the mono-reduced complexes **4**$^{-}$ and **5**$^{-}$.

	initial structure	Disp. Corr.		Mo	S1	S2	C1	O1	C2	O2	Dithiolene C=C		P1	P2	Energy	SOMO-LUMO GAP	
			orientation:	-	*trans* P	*trans* CO	*trans* P		*trans* S		*trans* P	*trans* C	*trans* C	*trans* S	Eh	Eh	kcal
4^{-}	SCXRD data from neutral species	on	HOMO-1	49.2	3.4	7.7	4.3	4.4	7.9	9.4	1.3	0.7	0.6	3.6	-0.15962		
			HOMO	37.8	6.0	10.4	5.7	5.9	5.4	5.8	0.9	0.2	1.7	2.4	-0.15526		
			SOMO	29.3	17.0	13.2	9.0	5.5	1.4	1.0	1.8	2.2	6.6	1.2	-0.12566	0.12098	75.9
			LUMO	0.3	2.9	2.6	1.0	0.4	0.4	0.2	8.4	6.4	1.0	0.6	-0.00468		
			LUMO+1	3.1	4.7	5.3	12.8	5.7	1.8	0.7	10.0	11.0	4.9	2.8	-0.0026		
	TPSSh without Dispersion Corr. ≈ 'non-stacked'	on	HOMO-1	49.7	3.0	7.3	3.6	3.7	8.4	10.0	1.3	0.7	0.7	1.9	-0.15938		
			HOMO	36.6	6.4	11.9	5.9	6.1	4.9	5.5	0.8	0.3	1.8	2.2	-0.15735		
			SOMO	29.1	17.1	12.7	9.1	5.5	1.3	1.0	1.7	2.4	7.3	1.3	-0.12535	0.12092	75.9
			LUMO	0.3	2.8	2.5	1.1	0.3	0.4	0.4	8.0	6.5	2.2	1.7	-0.00443		
			LUMO+1	3.5	3.5	2.9	19.7	8.6	1.7	0.5	6.6	4.1	10.5	6.4	-0.00196		
5^{-}	SCXRD data from neutral species	on	HOMO-1	45.7	2.8	10.3	6.0	6.6	6.1	7.4	3.5	0.4	1.5	2.4	-0.15736		
			HOMO	48.0	4.5	4.5	4.1	4.4	7.9	8.8	1.2	0.8	1.1	3.9	-0.15399		
			SOMO	25.9	18.1	15.7	8.5	5.2	1.3	1.0	4.2	5.6	6.1	1.1	-0.11988	0.12132	76.1
			LUMO	4.1	2.5	1.8	21.8	9.8	3.5	1.3	0.7	0.7	16.8	10.9	0.00144		
			LUMO+1	4.8	2.0	4.2	19.3	8.5	6.4	2.8	0.7	0.2	14.5	7.5	0.00652		
	TPSSh without Dispersion Corr. ≈ 'non-stacked'	on	HOMO-1	42.4	3.5	11.1	6.9	7.5	5.0	6.2	3.6	0.3	1.9	2.1	-0.15857		
			HOMO	51.0	3.8	4.8	2.6	2.7	9.2	10.3	1.2	1.0	0.5	4.5	-0.15508		
			SOMO	25.7	18.6	15.1	8.8	5.3	1.2	0.9	4.1	5.8	6.8	1.3	-0.11968	0.11939	74.9
			LUMO	2.9	2.2	0.7	21.4	9.4	1.8	0.7	0.1	0.1	19.3	14.0	-0.00029		
			LUMO+1	5.9	2.0	5.1	18.3	8.1	9.5	3.8	0.7	0.3	12.4	5.4	0.00509		

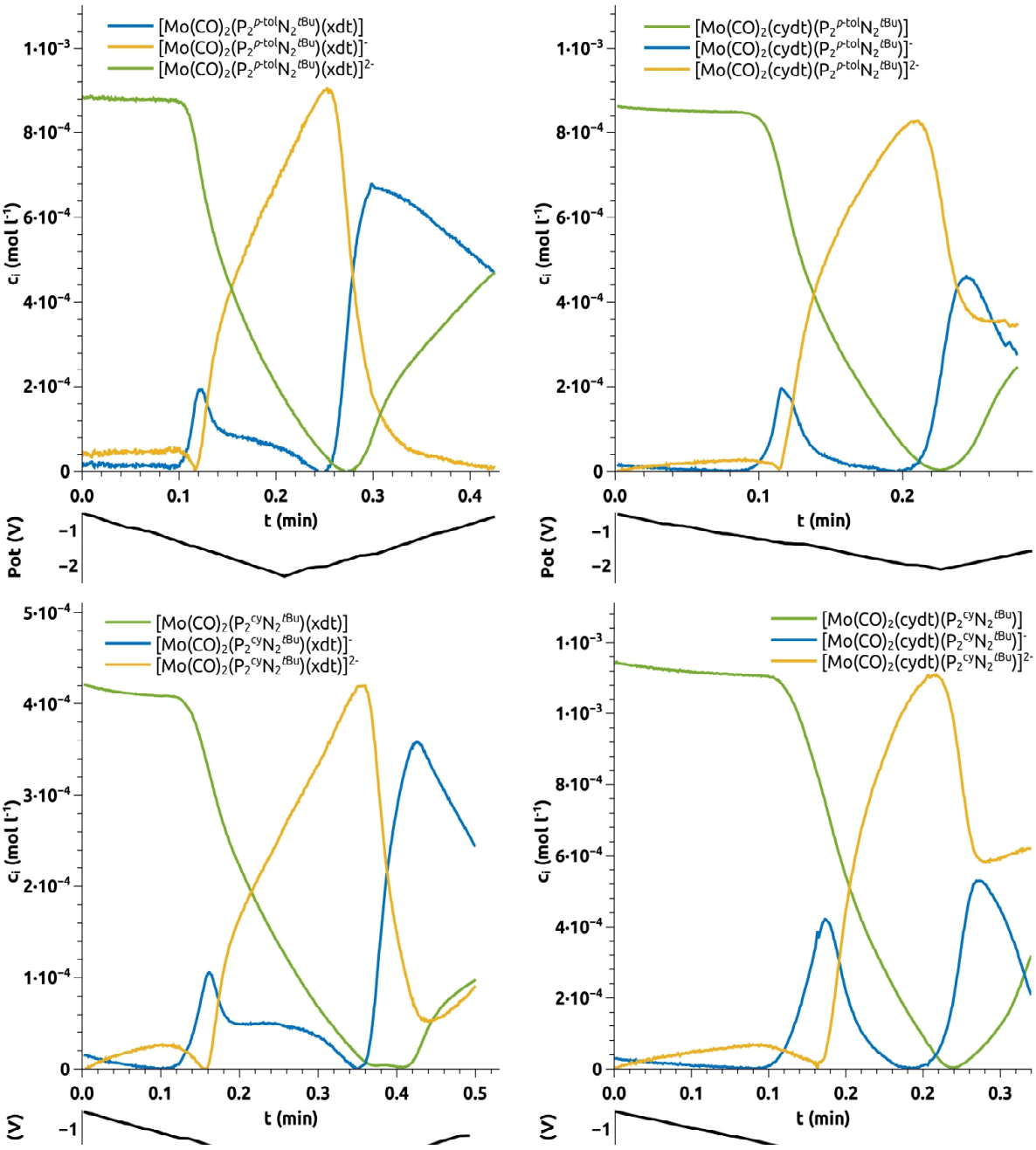


Figure S17. Concentration-time dependent data as extracted from the SEC-UV-vis data for the reductive region of the cyclic voltammetric run.[8, 23] Independent from the investigated complex, in the beginning of the cyclic voltammetric investigation the neutral complex {Mo} (green) is present. The neutral compound is reduced forming the single reduced complex $\{Mo\}^{1-}$ (blue) and subsequently the double reduced complex $\{Mo\}^{2-}$ (yellow). This concentration profile of the single reduced complex $\{Mo\}^{1-}$ is more pronounced in case of an aliphatic substituent on the P_2N_2 complex. {Mo} represents the whole complex $[Mo(CO)_2(dt)(P_2N_2)]$, with dt= xdt, P_2N_2= $P_2^{p\text{-tol}}N_2^{tBu}$ (**2**) (upper, left), dt= cydt, P_2N_2= $P_2^{p\text{-tol}}N_2^{tBu}$ (**3**) (upper, right), dt= xdt, P_2N_2= $P_2^{cy}N_2^{tBu}$ (**4**) (bottom, left), dt= cydt, P_2N_2= $P_2^{cy}N_2^{tBu}$ (**5**) (bottom, right).

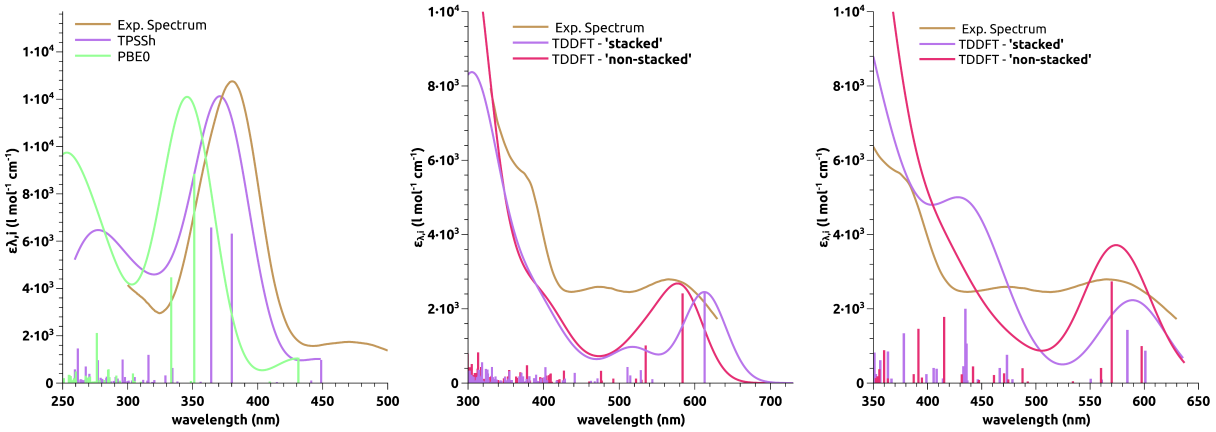


Figure S18. Experimental and TD-DFT calculated UV-vis data for [Mo(CO)$_2$(P$_2$$^{p\text{-tol}}N_2$$^{t\text{Bu}}$)(xdt)] (**2**) (left) and extracted spectra from SEC-CV-UV-vis decomposition for (**2**$^{1-}$) (middle) and (**2**$^{2-}$) (right) compared to TD-DFT spectra (TPSSh) for the structures obtained with ('stacked') and without ('non-stacked') dispersion correction using D3zero. Computed line spectra are artificially broadened by 67 nm.

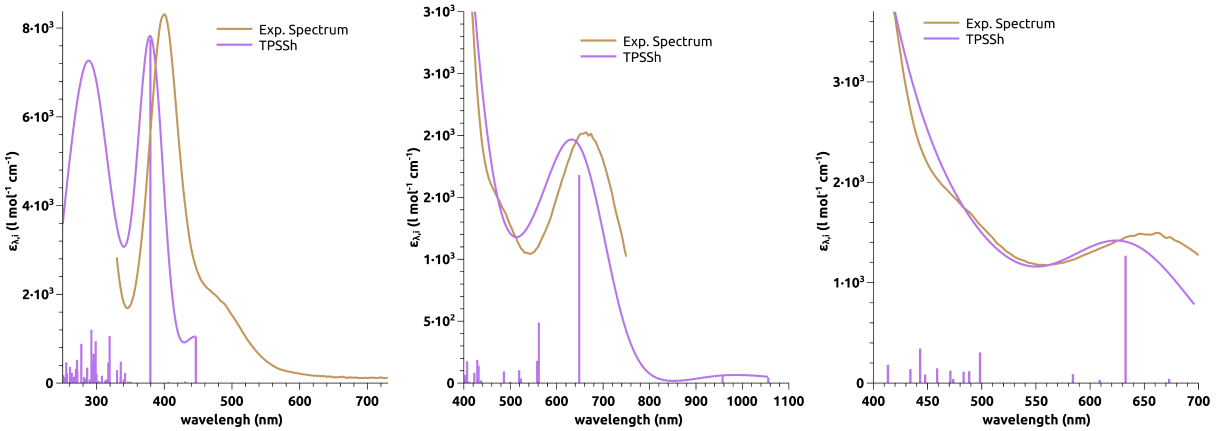


Figure S19. Experimental and TD-DFT calculated UV-vis data for [Mo(CO)$_2$(cydt)(P$_2$$^{p\text{-tol}}N_2$$^{t\text{Bu}}$)] (**3**) (left) and extracted spectra from SEC-CV-UV-vis decomposition for (**3**$^{1-}$) (middle) and (**3**$^{2-}$) (right) with dispersion correction using D3zero. Computed line spectra are artificially broadened by 143 nm.

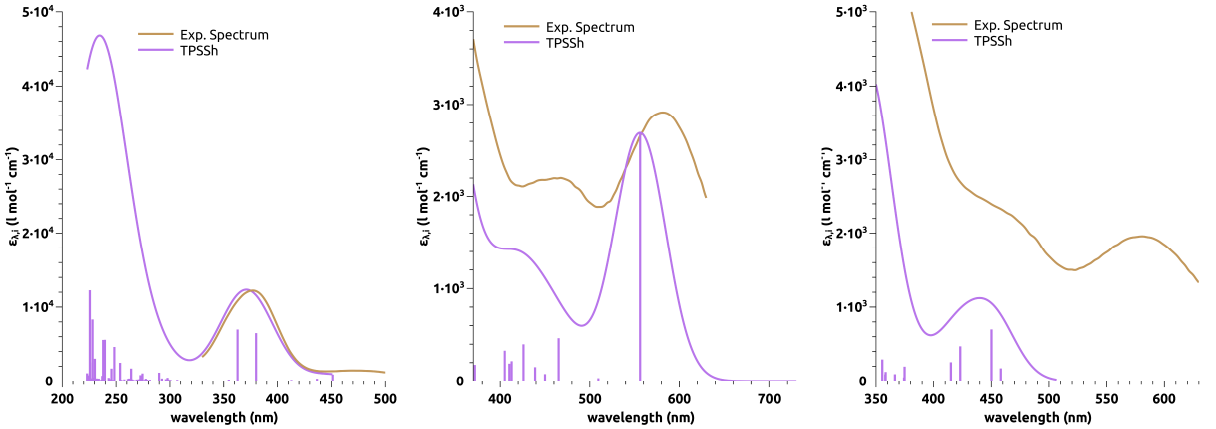


Figure S20. Experimental and TD-DFT calculated UV-vis data for [Mo(CO)$_2$(P$_2$^{cy}N$_2$$^{t\text{Bu}}$)(xdt)] (**4**) (left) and extracted spectra from SEC-CV-UV-vis decomposition for (**4**$^{1-}$) (middle) and (**4**$^{2-}$) (right) with dispersion correction using D3zero. Computed line spectra are artificially broadened by 54 nm in the case of **4** and 67 nm in the case of **4**$^{1-}$ and **4**$^{2-}$.

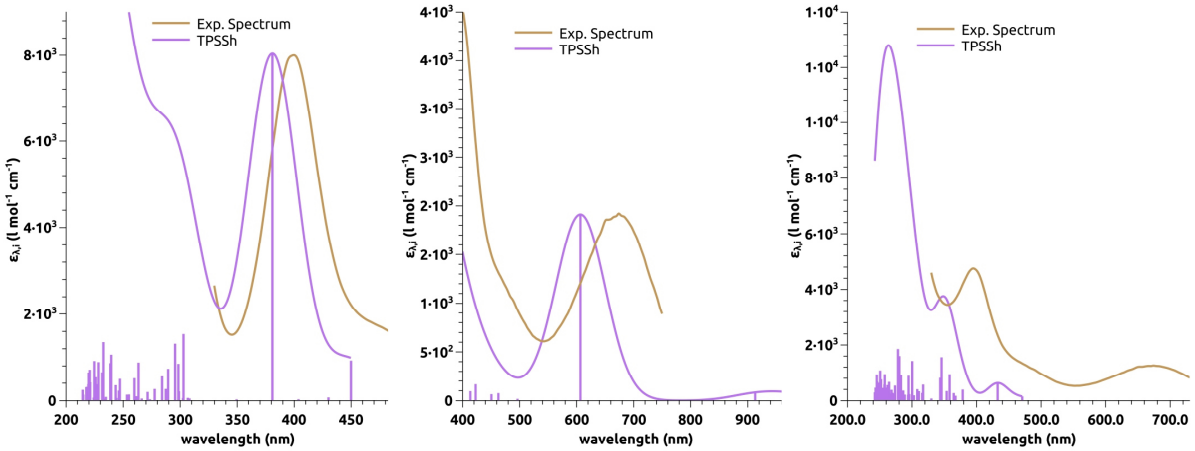


Figure S21. Experimental and TD-DFT calculated UV-vis data for $[Mo(CO)_2(cydt)(P_2^{cy}N_2^{tBu})]$ (**5**) (left) and extracted spectra from SEC-CV-UV-vis decomposition for ($\mathbf{5}^{1-}$) (middle) and ($\mathbf{5}^{2-}$) (right) with dispersion correction using D3zero. Computed line spectra are artificially broadened by 52 nm.

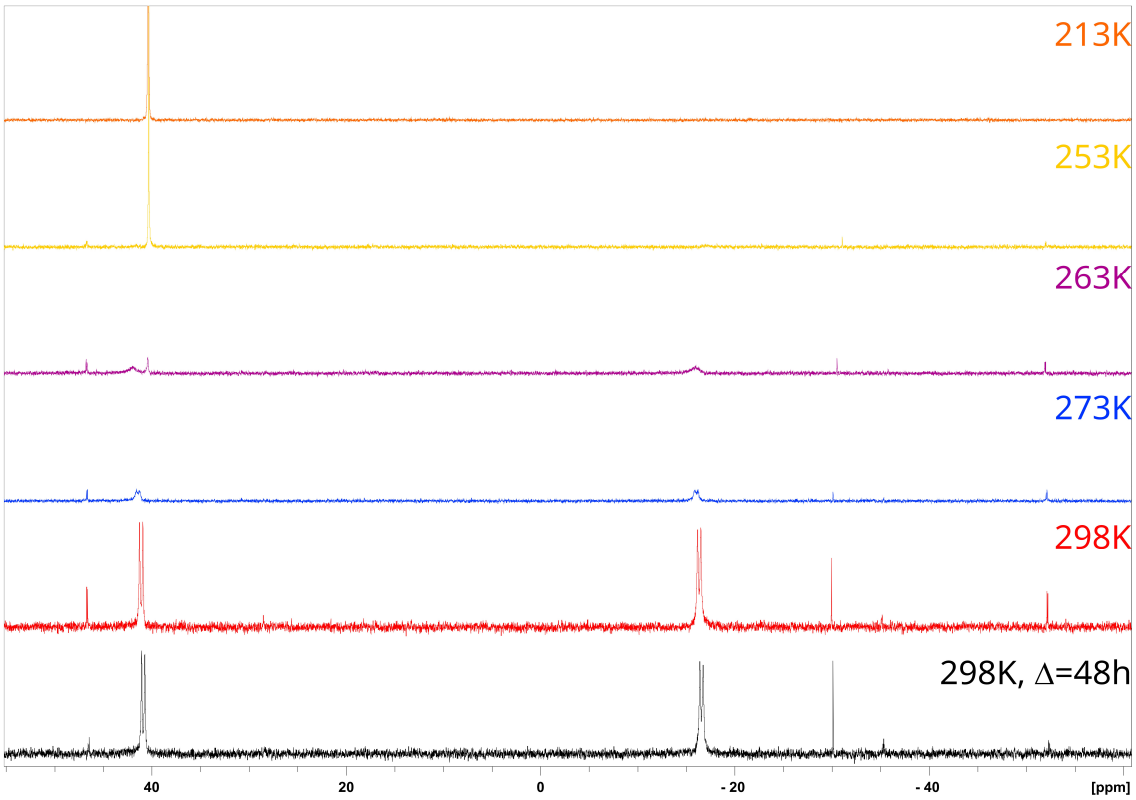


Figure S22. Reaction monitoring using ^{31}P NMR for the reaction of $[Mo(CO)_2(P_2^{p\text{-}tol}N_2^{tBu})(xdt)]$ (**2**) (crystallized in thf and MeOH to avoid side reactions[24]) with KC_8 in THF-d8. Measured at different temperatures. The initial spectrum at 213 K shows the starting compound $[Mo(CO)_2(P_2^{p\text{-}tol}N_2^{tBu})(xdt)]$ (**2**) at approximately 40.3 ppm. Following the course of the reaction, by slowly increasing the temperature, this signal decreased and finally vanished to obtain a broadened spectrum (263 K) which would be in accordance with a singly reduced, hence, paramagnetic compound. A further increase in temperature (293 K) resulted in five different sets of signals. One signal for the free ligand at approximately –30.1 ppm, two doublets at 46.5 and –52.1 ppm with a $^4J_{31P\text{-}31P}$ coupling constant of 11.7 Hz for potentially a half-detached phosphane ligand, and two more doublets at 41.8 and –16.1 ppm with a $^2J_{31P\text{-}31P}$ coupling constant of 40.2 Hz. The latter set of doublets persists even after 48 hours while the signal for the free ligand increases slowly. The coupling constant of 40.2 Hz is in accordance with two chemically inequivalent ^{31}P atoms in an octahedral complex. Repeated attempts to isolate and crystallize the resulting complex failed due to the release of the phosphane ligand during the crystallization process.

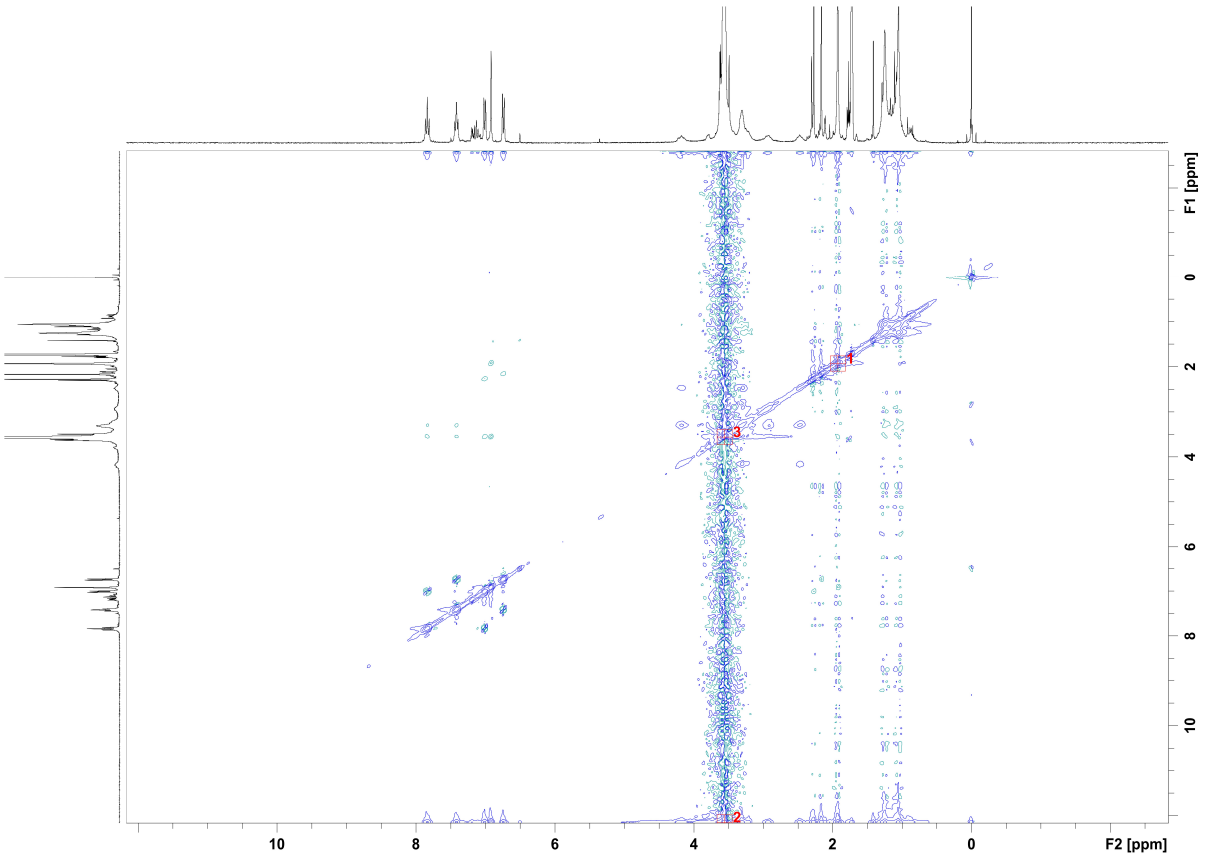


Figure S23. Full NOE spectrum 48 h after reacting [Mo(CO)$_2$($P_2^{p\text{-tol}}N_2^{tBu}$)(xdt)] (**2**) (crystallized in thf and MeOH to avoid side reactions[24]) with KC_8 in THF-d8.

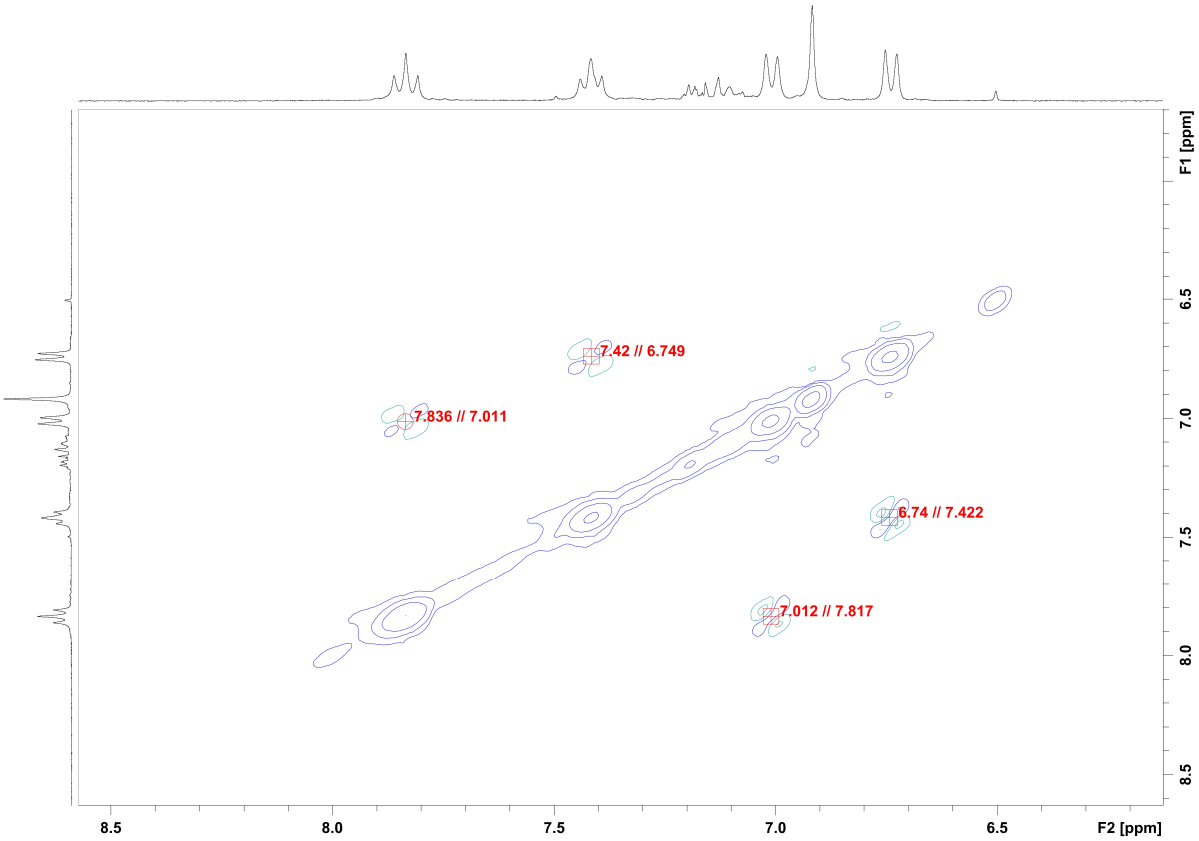


Figure S24. Zoomed in NOE spectrum 48 h after reacting [Mo(CO)$_2$($P_2^{p\text{-tol}}N_2^{t\text{Bu}}$)(xdt)] (**2**) (crystallized in thf and MeOH to avoid side reactions[24]) with KC_8 in THF-d8. Correlation signals between 7.84 and 7.01 ppm indicate proximity between the dithiolene (xdt) ligand and the *p*-tolyl substituent of the P_2N_2 ligand.

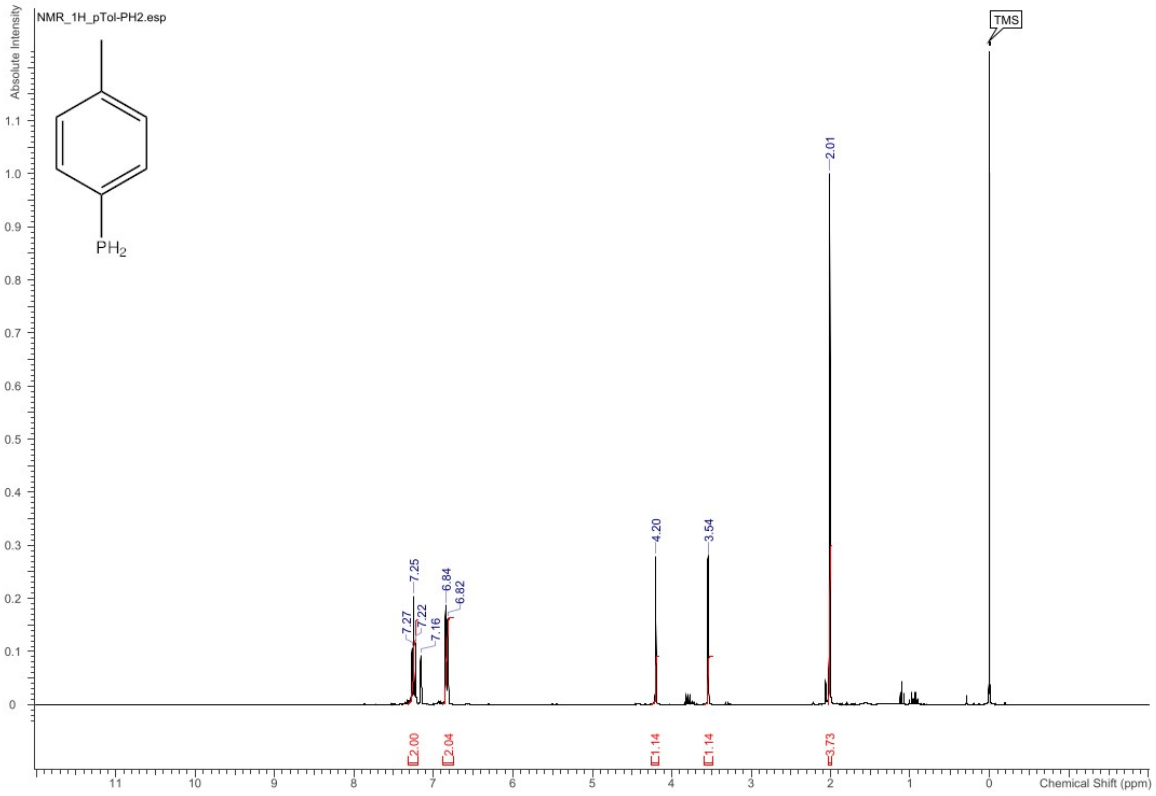


Figure S25. $^{1}H\{^{13}C\}$ NMR spectrum of *p*-toluene phosphane (**A**) measured in C_6D_6.

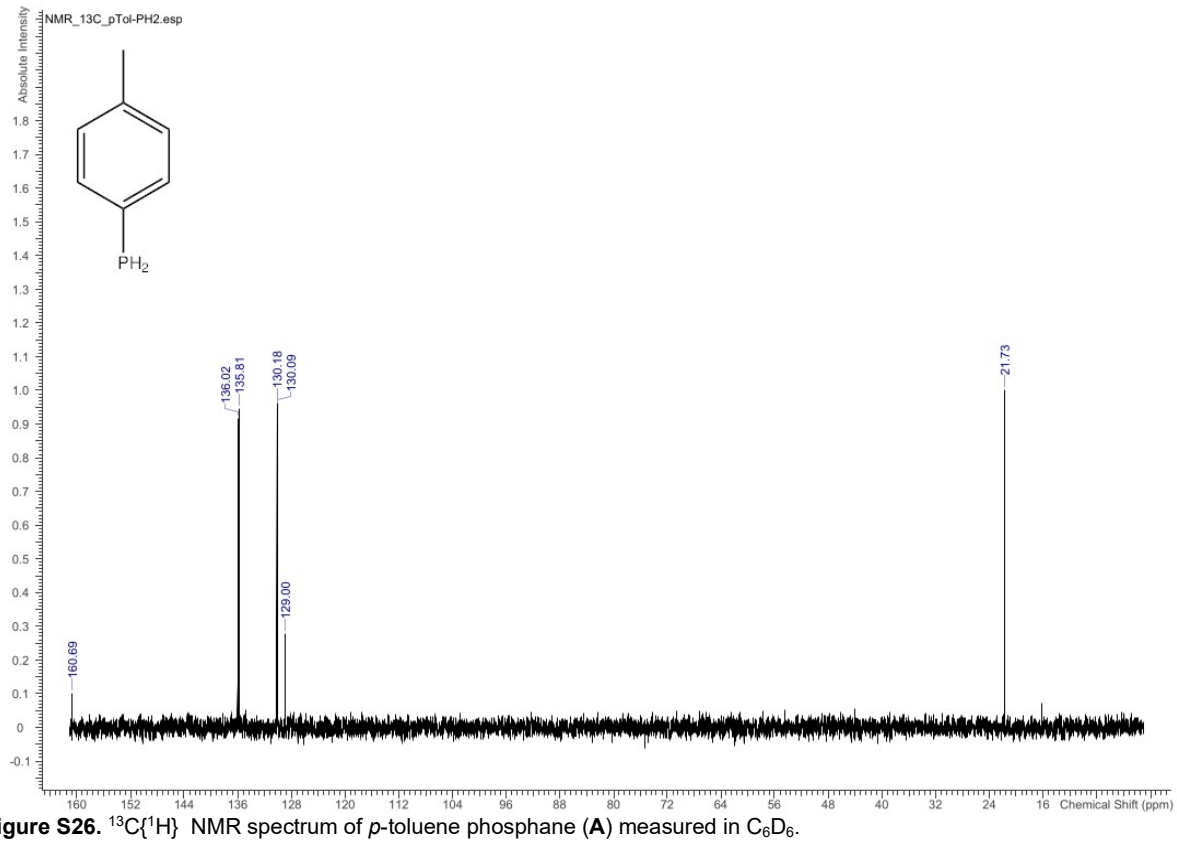


Figure S26. $^{13}C\{^{1}H\}$ NMR spectrum of *p*-toluene phosphane (**A**) measured in C_6D_6.

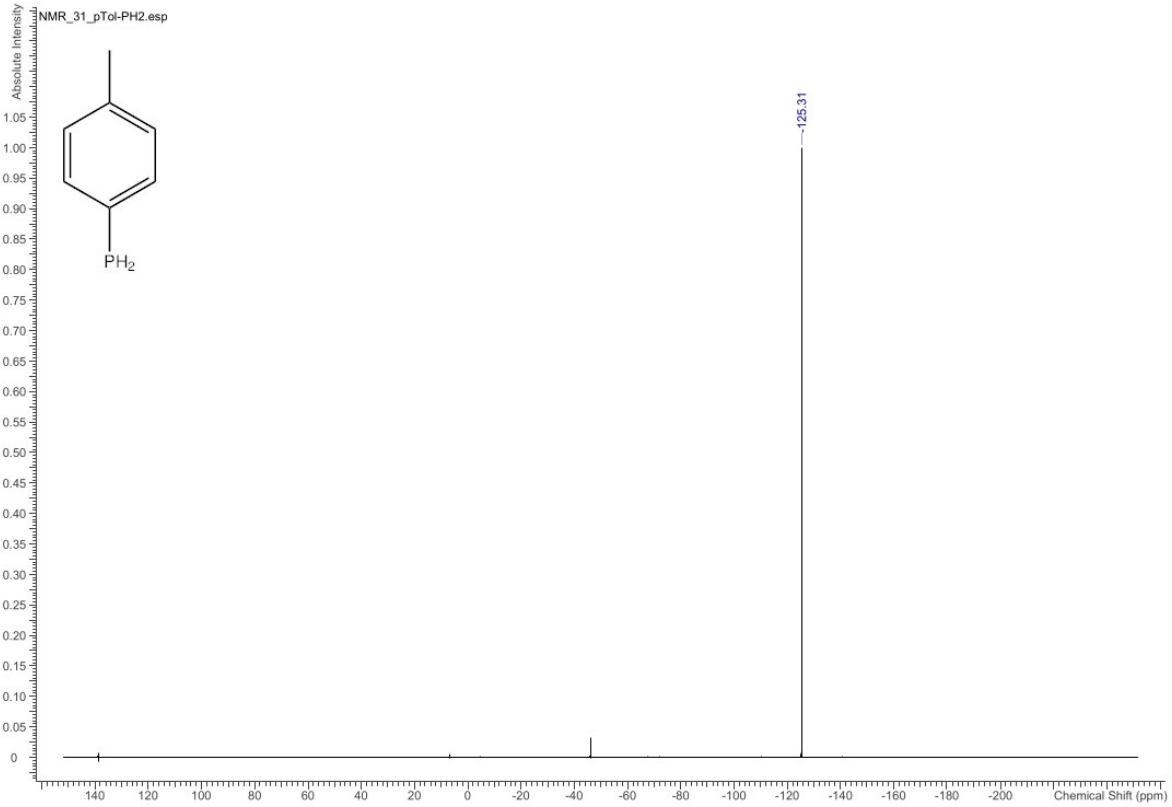


Figure S27. $^{31}P\{^{1}H\}$ NMR spectrum of *p*-toluene phosphane (**A**) measured in C_6D_6.

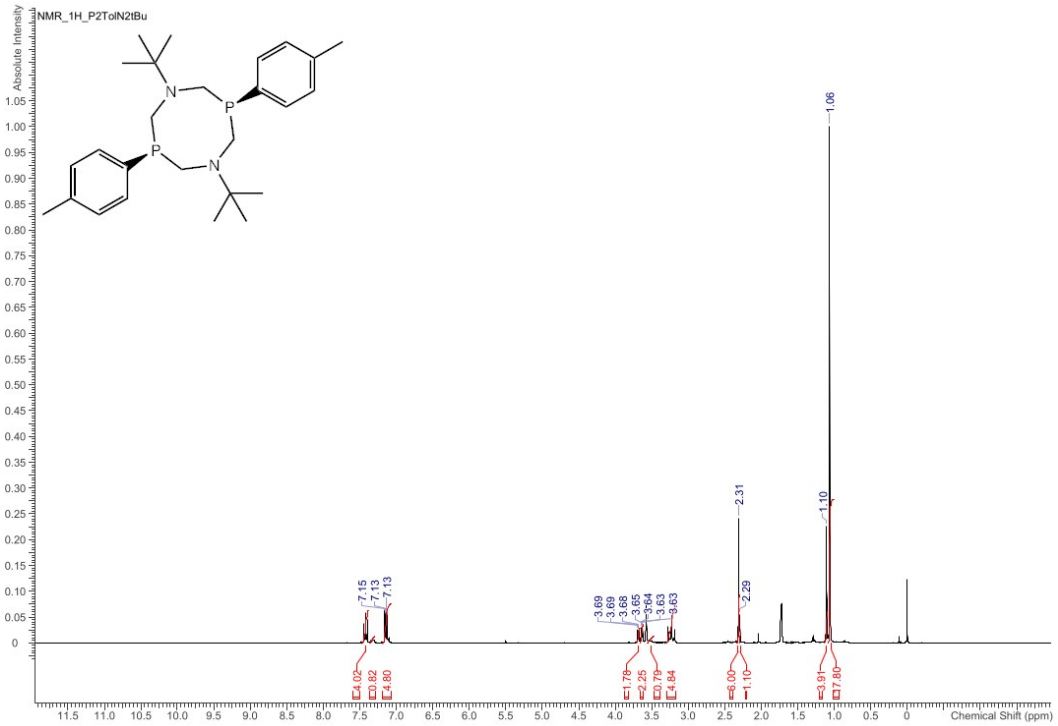


Figure S28. $^{1}H\{^{13}C\}$ NMR spectrum of 1,5-di-(*tert*-butyl)-3,7-di-*p*-tolyl-1,5,3,7-diazadiphosphocyclooctane (**1**$^{p\text{-tol}}$) measured in THF-d8.

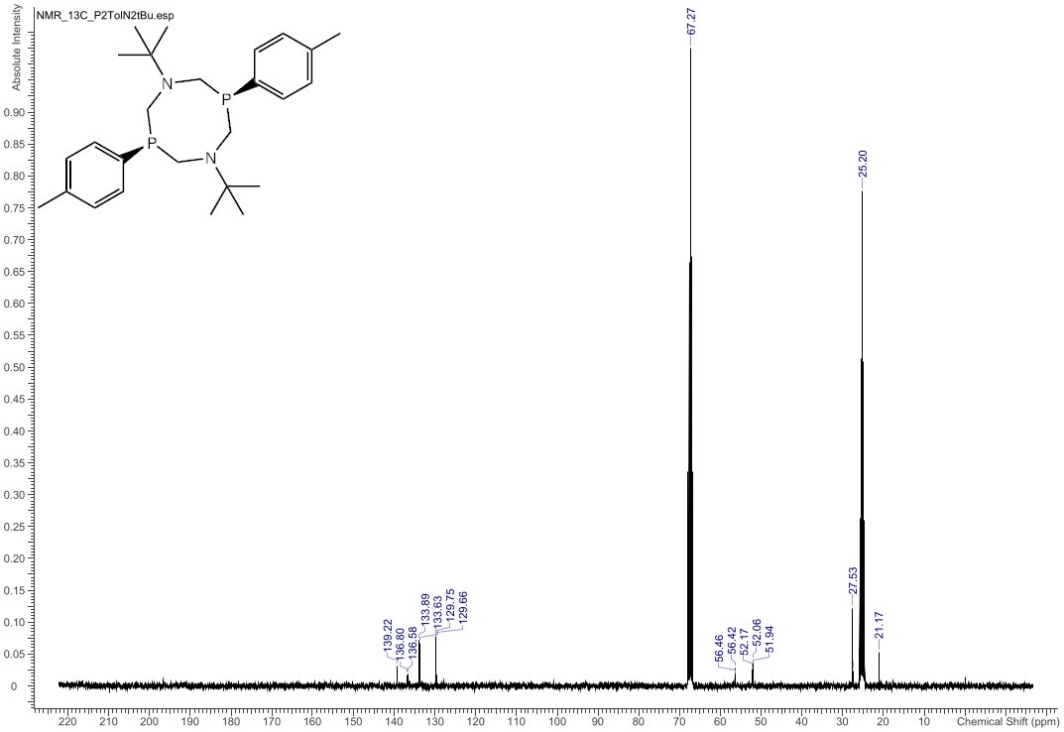


Figure S29. $^{13}C\{^{1}H\}$ NMR spectrum of 1,5-di-(*tert*-butyl)-3,7-di-*p*-tolyl-1,5,3,7-diazadiphosphocycloctane (**1**$^{p\text{-tol}}$) measured in THF-d8.

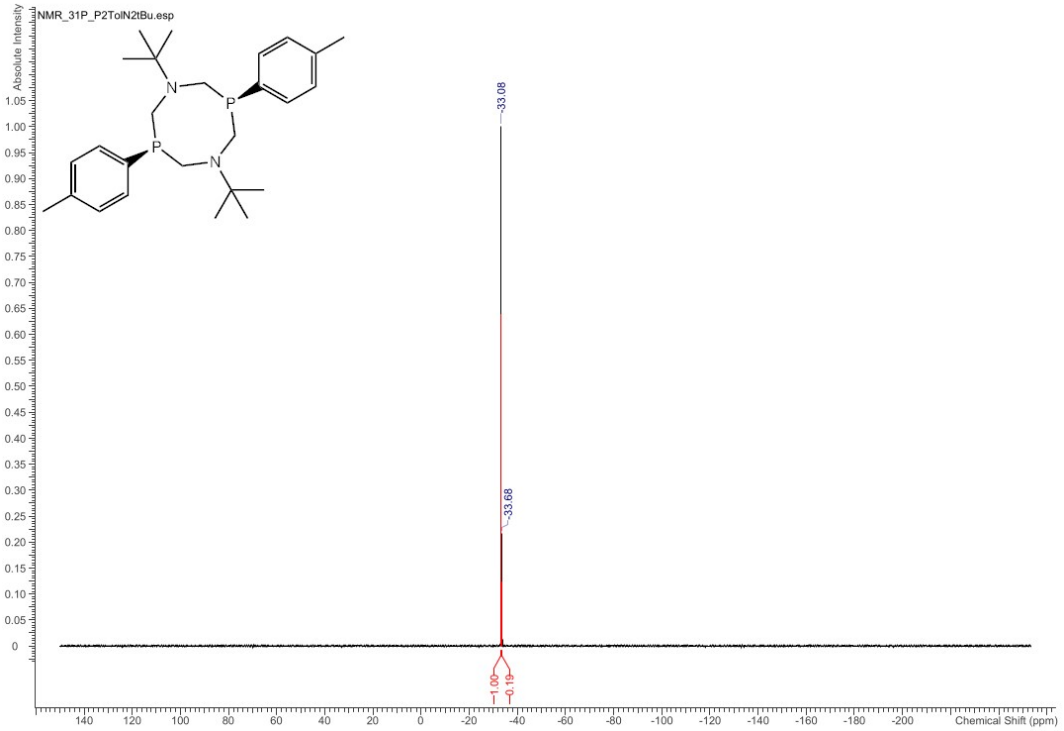


Figure S30. $^{31}P\{^{1}H\}$ NMR spectrum of 1,5-di-(*tert*-butyl)-3,7-di-*p*-tolyl-1,5,3,7-diazadiphosphocycloctane (**1**$^{p\text{-tol}}$) measured in THF-d8.

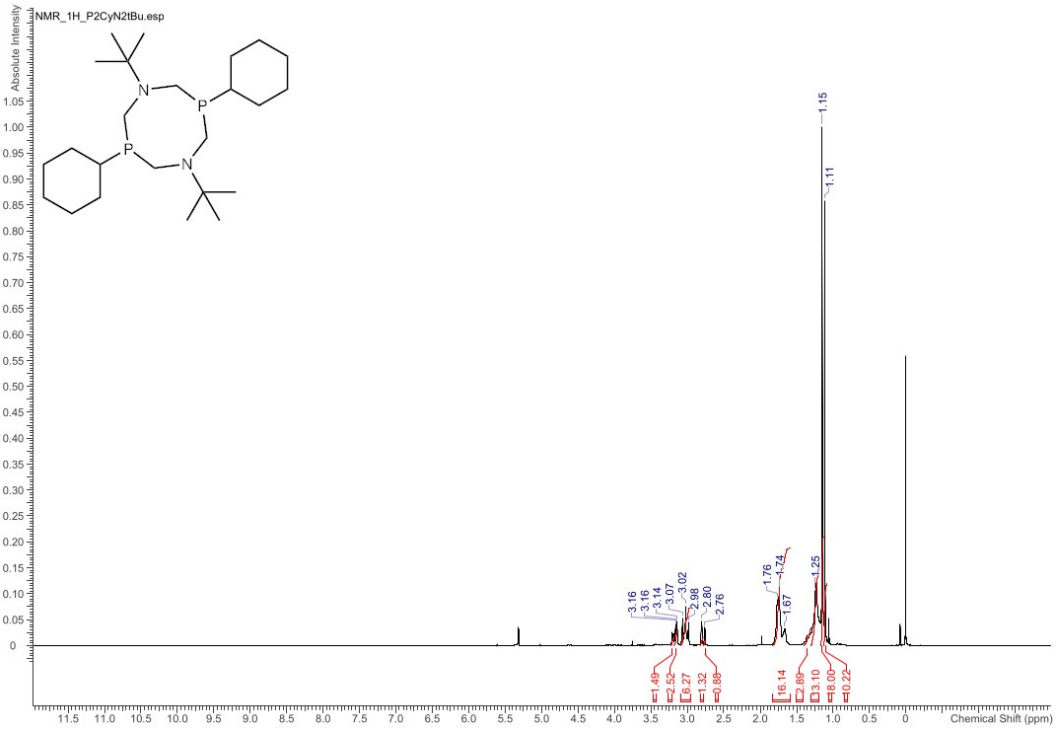


Figure S31. $^{1}H\{^{13}C\}$ NMR spectrum 1,5-di-(*tert*-butyl)-3,7-di-cyclohexyl-1,5,3,7-diazadiphosphocycloctan (**1**^{cy}) measured in CD_2Cl_2.

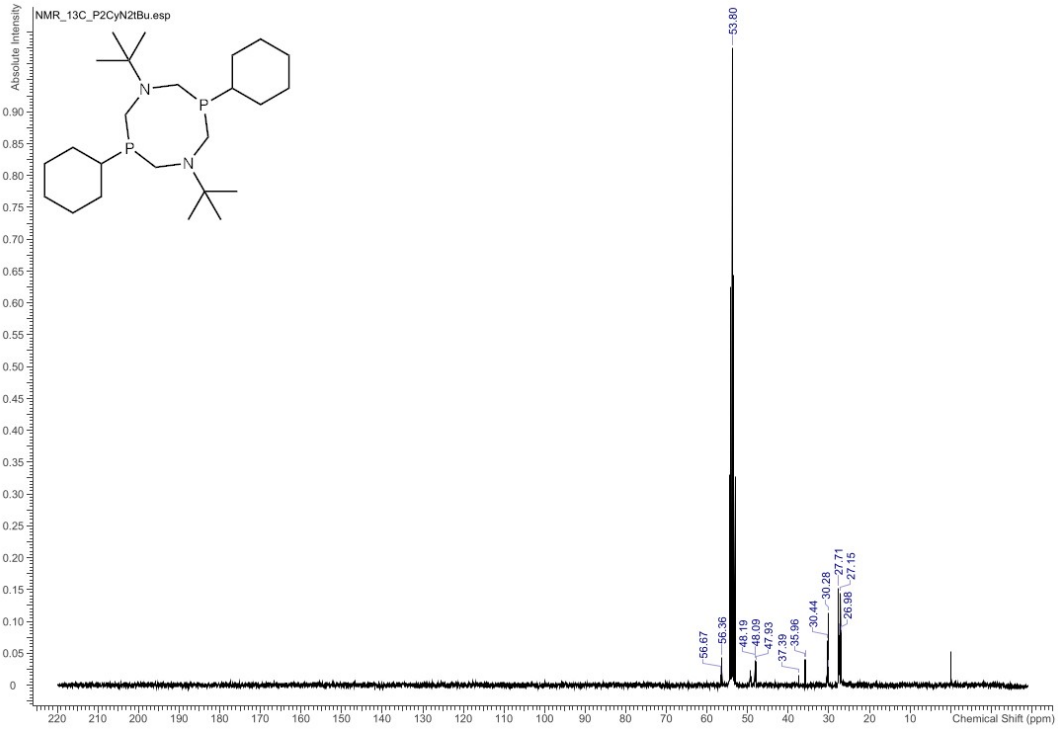


Figure S32. $^{13}C\{^{1}H\}$ NMR spectrum 1,5-di-(*tert*-butyl)-3,7-di-cyclohexyl-1,5,3,7-diazadiphosphocycloctan (**1**^{cy}) measured in CD_2Cl_2.

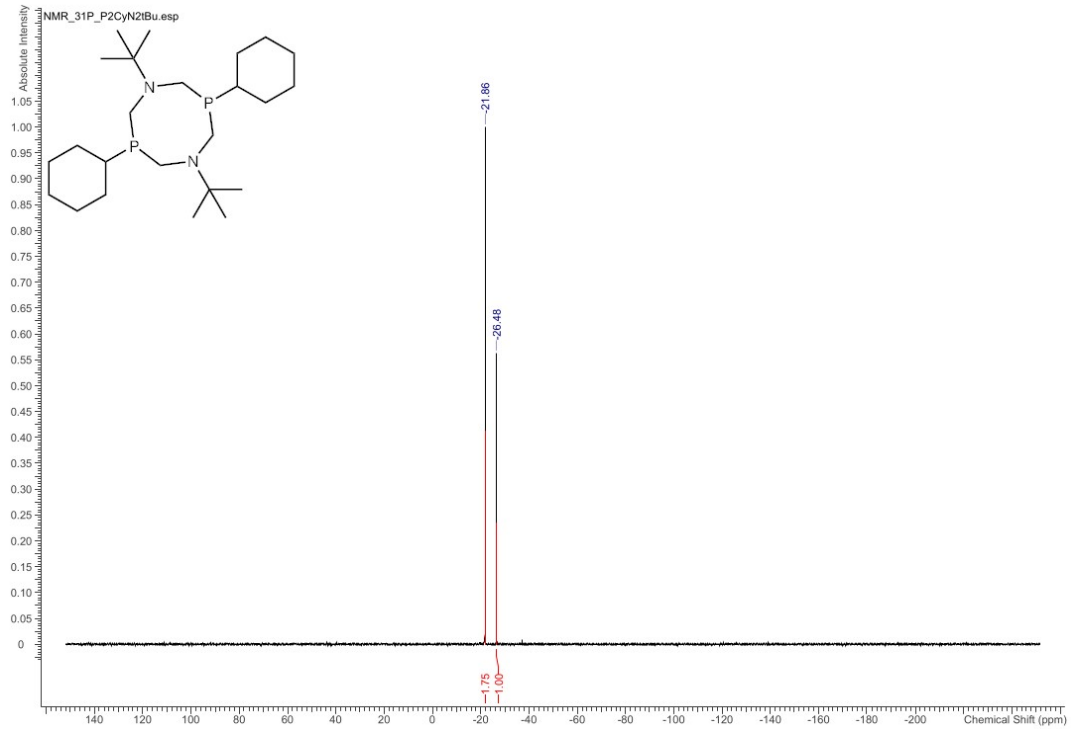


Figure S33. $^{31}P\{^{1}H\}$ NMR spectrum 1,5-di-(*tert*-butyl)-3,7-di-cyclohexyl-1,5,3,7-diazadiphosphocycloctan (**1**^{cy}) measured in CD_2Cl_2.

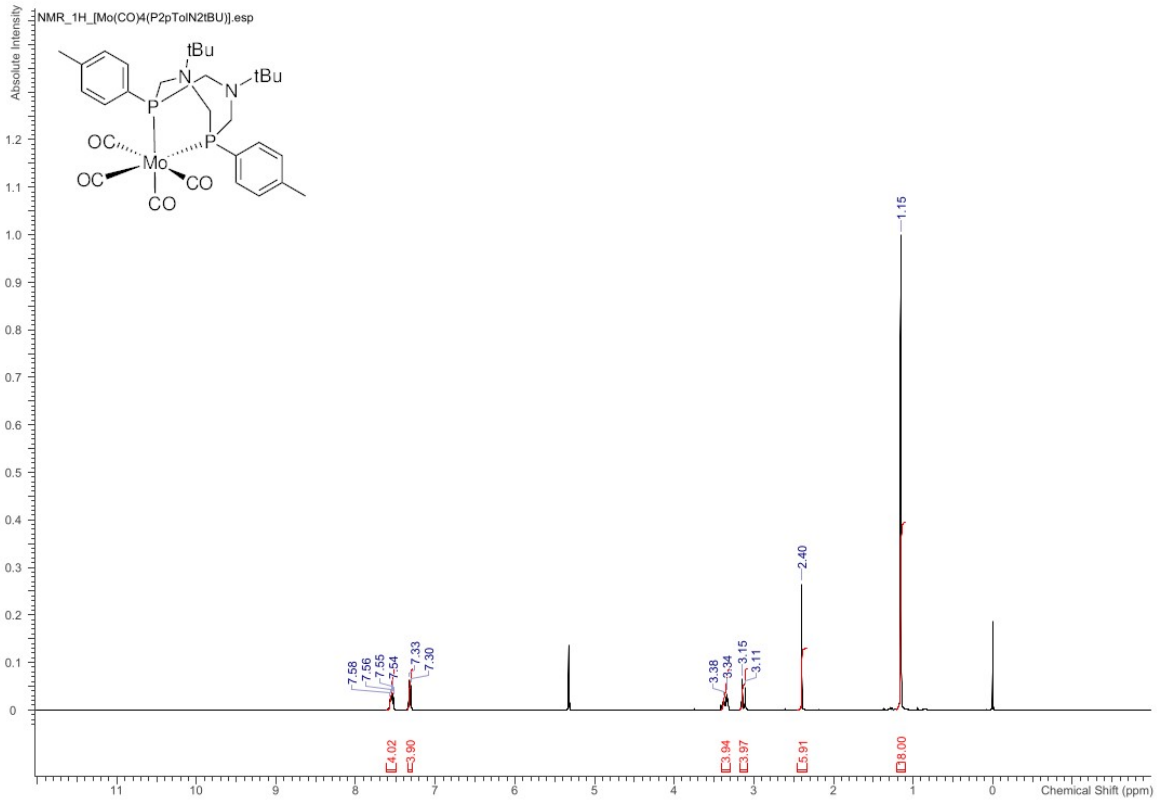


Figure S34. $^{1}H\{^{13}C\}$ NMR spectrum of $[Mo(CO)_4(P_2^{p\text{-tol}}N_2^{tBu})]$ (**B**) measured in CD_2Cl_2.

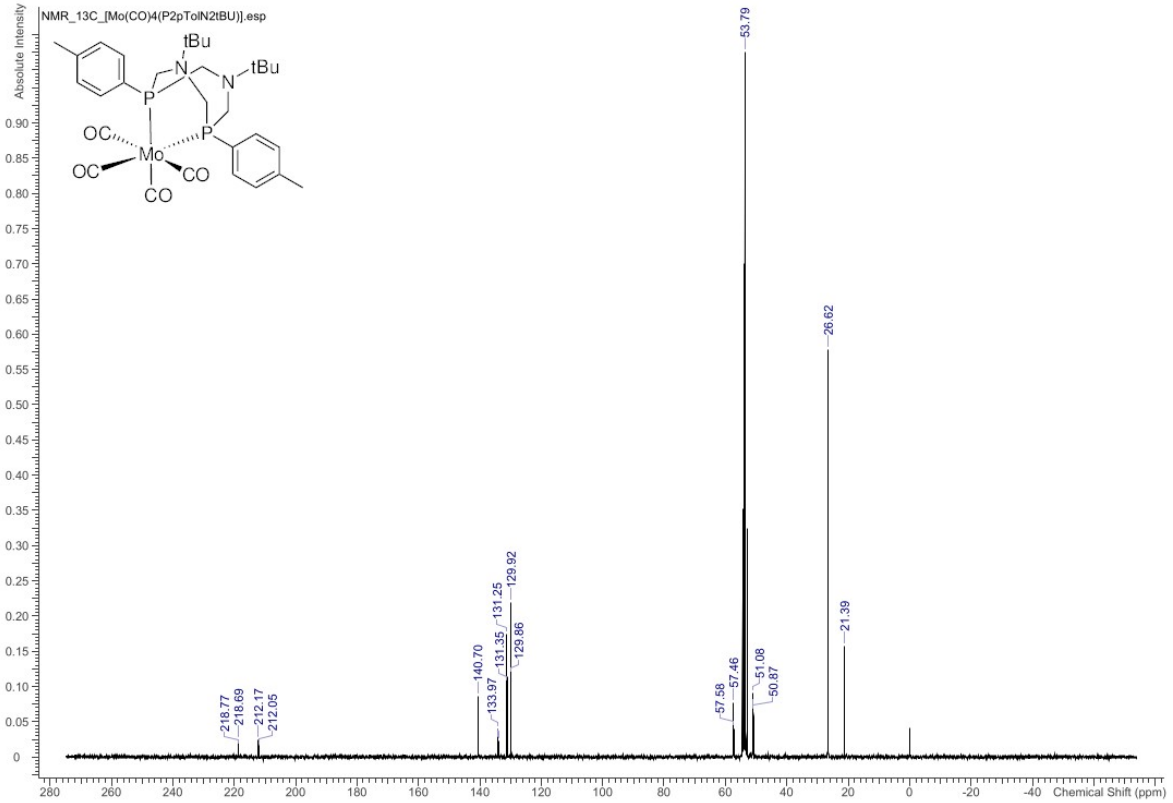


Figure S35. $^{13}C\{^{1}H\}$ NMR spectrum of $[Mo(CO)_4(P^{2p\text{-}tol}N_2^{tBu})]$ (**B**) measured in CD_2Cl_2.

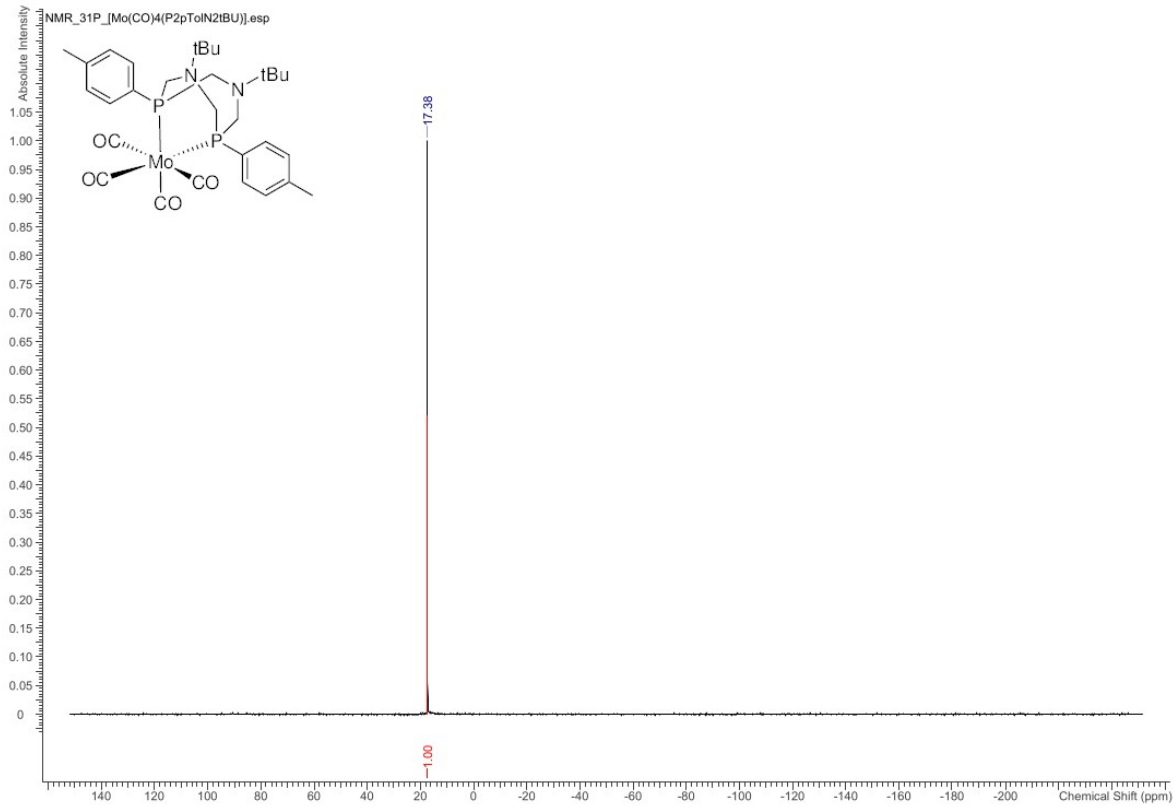


Figure S36. $^{31}P\{^{1}H\}$ NMR spectrum of $[Mo(CO)_4(P_2^{p\text{-}tol}N_2^{tBu})]$ (**B**) measured in CD_2Cl_2.

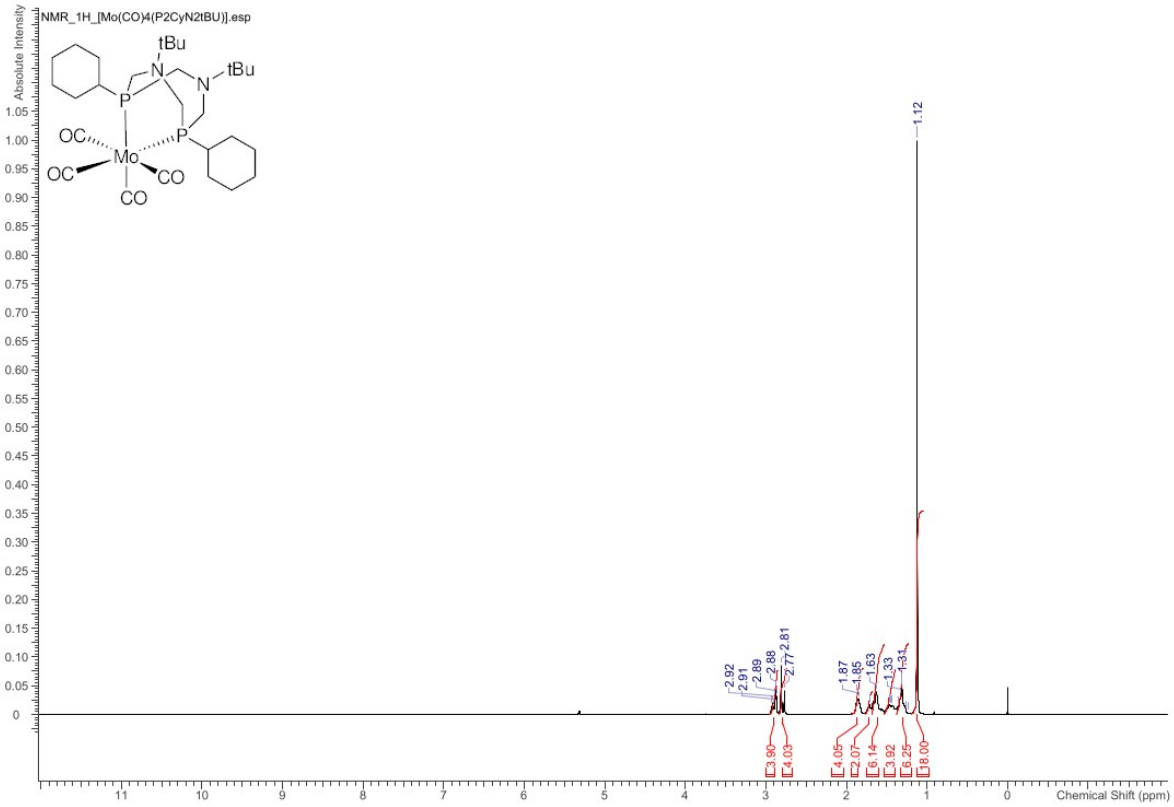


Figure S37. $^{1}H\{^{13}C\}$ NMR spectrum of $[Mo(CO)_4(P_2^{cy}N_2^{tBu})]$ (**C**) measured in CD_2Cl_2.

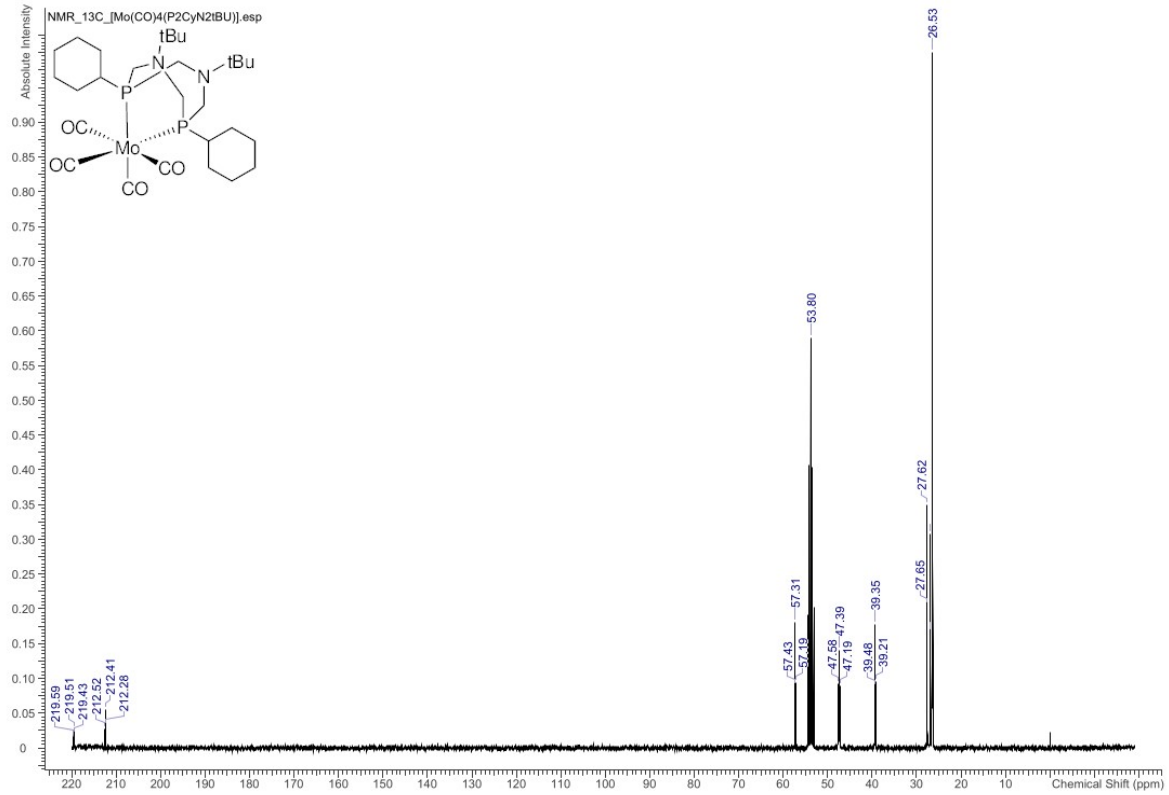


Figure S38. $^{13}C\{^{1}H\}$ NMR spectrum of $[Mo(CO)_4(P_2^{cy}N_2^{tBu})]$ (**C**) measured in CD_2Cl_2.

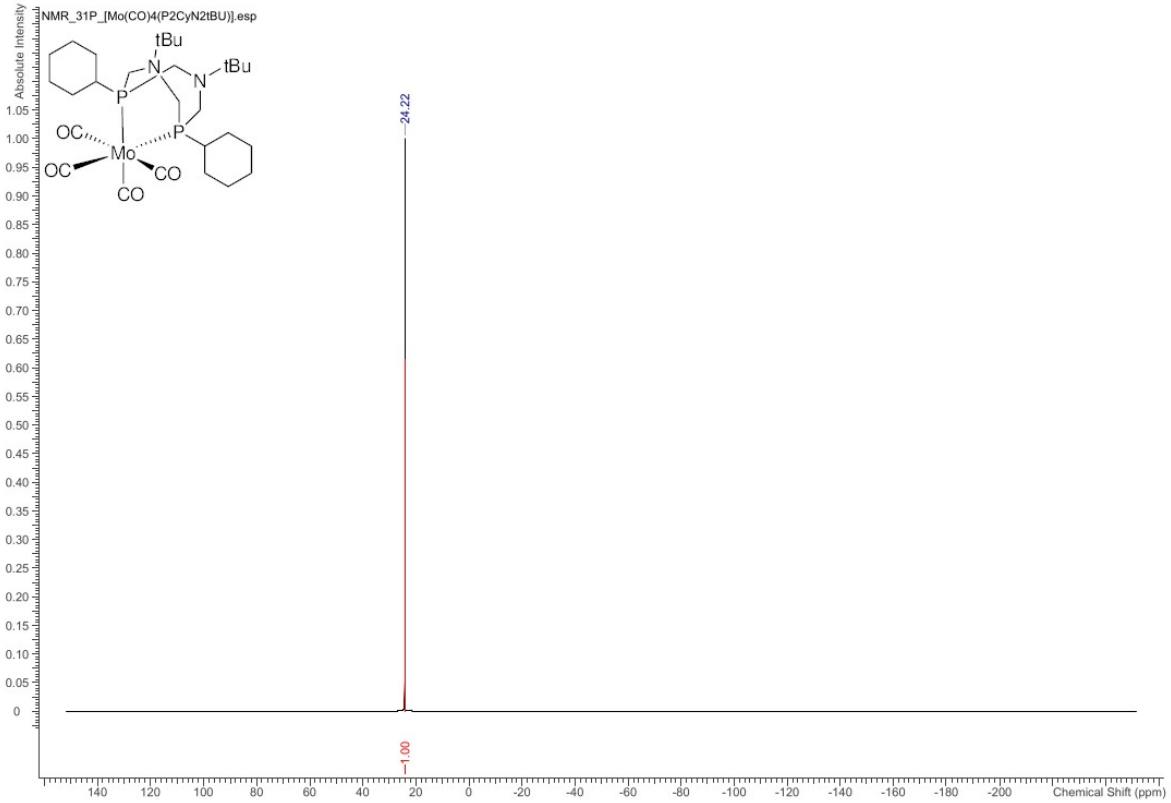


Figure S39. $^{31}P\{^{1}H\}$ NMR spectrum of $[Mo(CO)_4(P_2^{cy}N_2^{fBu})]$ (**C**).

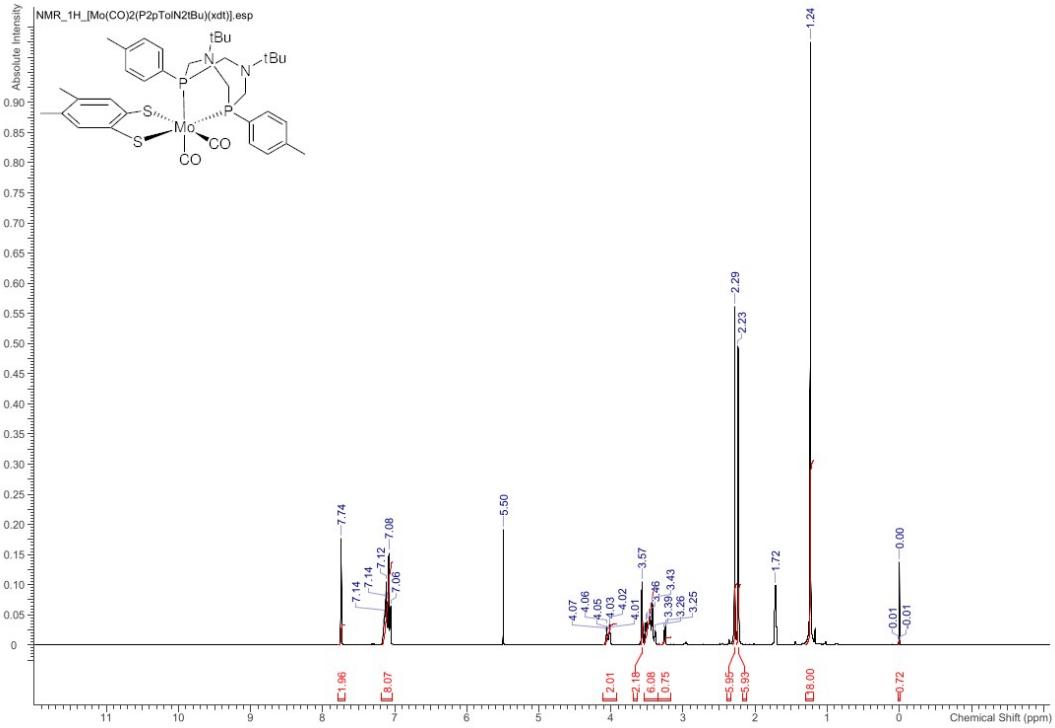


Figure S40. $^{1}H\{^{13}C\}$ NMR spectrum of $[Mo(CO)_2(P_2^{p\text{-}tol}N_2^{fBu})(xdt)]$ (**2**) measured in thf-d8. The residual solvent signal at 5.50 ppm originates from co-crystallized CH_2Cl_2 which could not be entirely removed *in vacuo*.

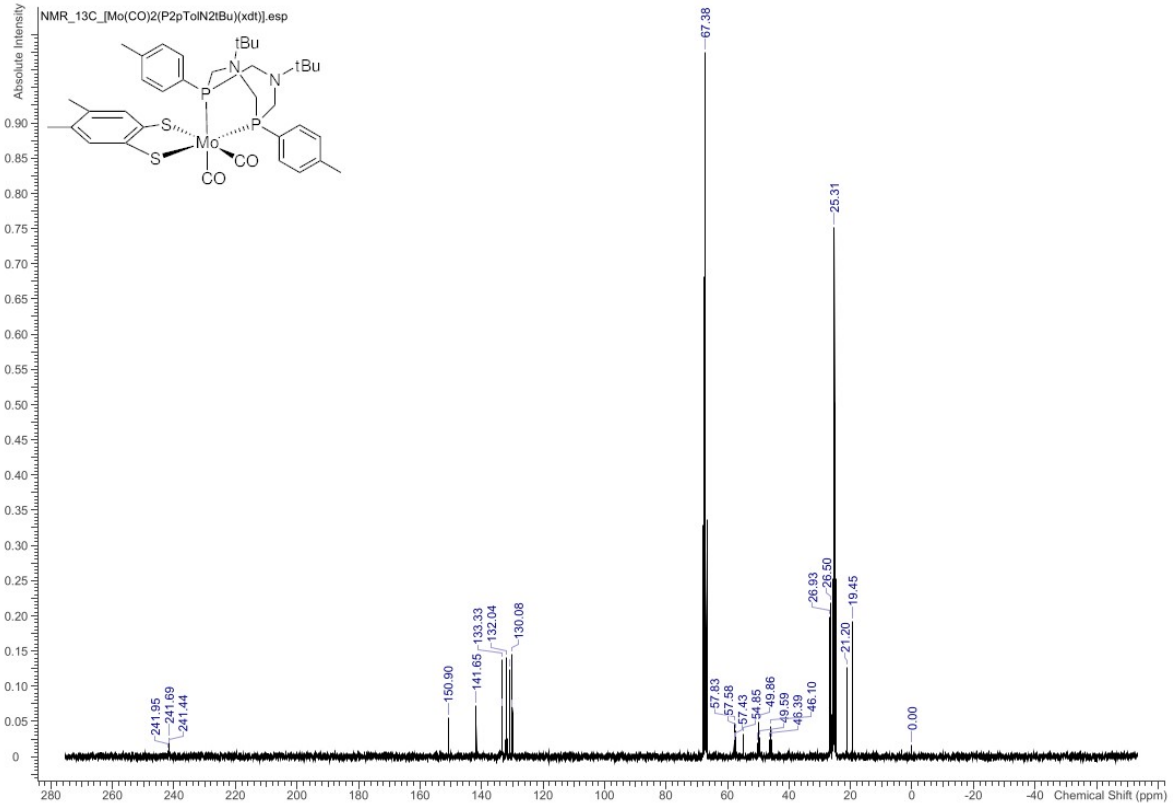


Figure S41. $^{13}C\{^{1}H\}$ NMR spectrum of $[Mo(CO)_2(P_2^{p\text{-}tol}N_2^{tBu})(xdt)]$ (**2**) measured in thf-d8.

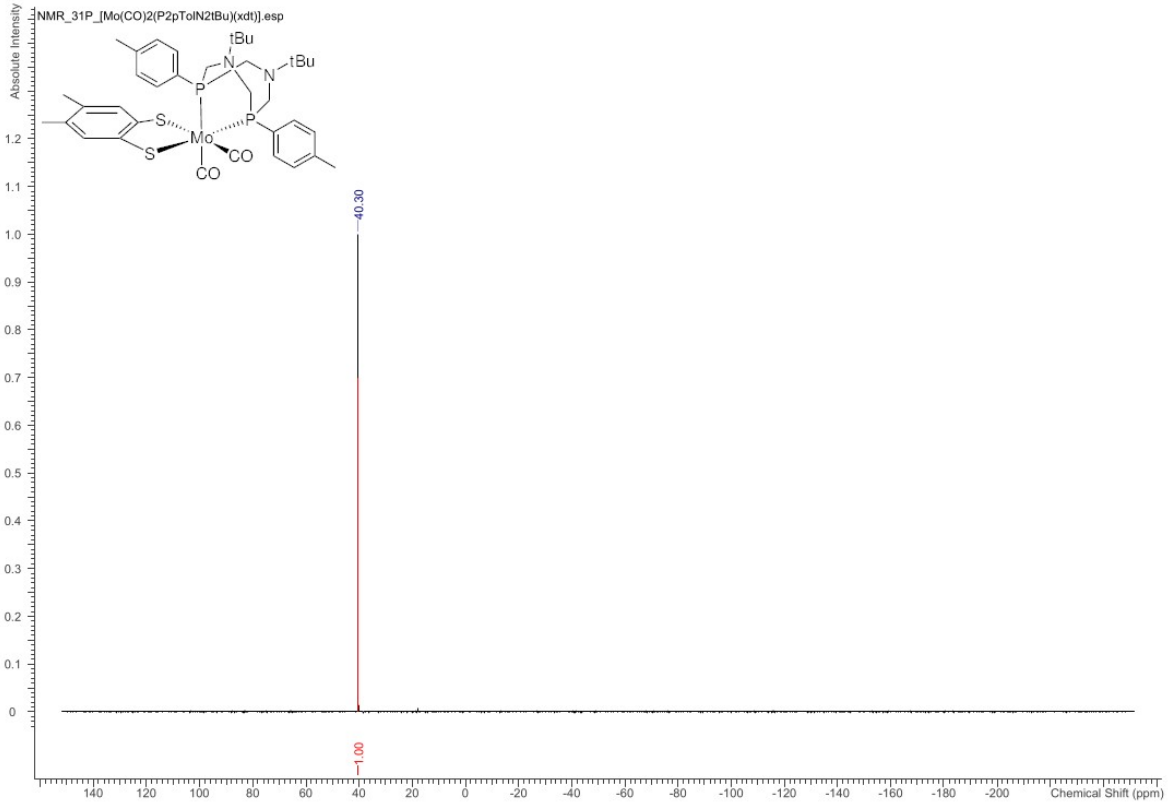


Figure S42. $^{31}P\{^{1}H\}$ NMR spectrum of $[Mo(CO)_2(P_2^{p\text{-}tol}N_2^{tBu})(xdt)]$ (**2**) measured in thf-d8.

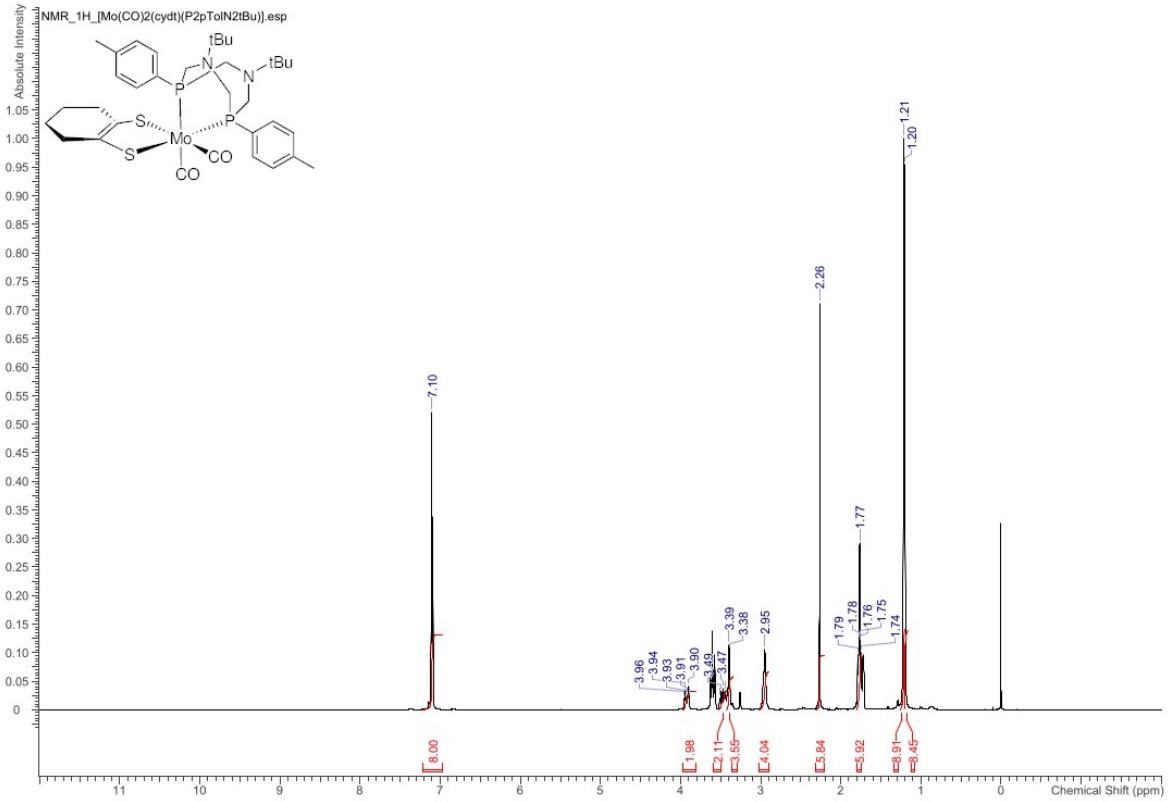


Figure S43. $^{1}H\{^{13}C\}$ NMR spectrum of $[Mo(CO)_2(cydt)(P_2^{p\text{-tol}}N_2^{tBu})]$ (**3**) measured in thf-d8.

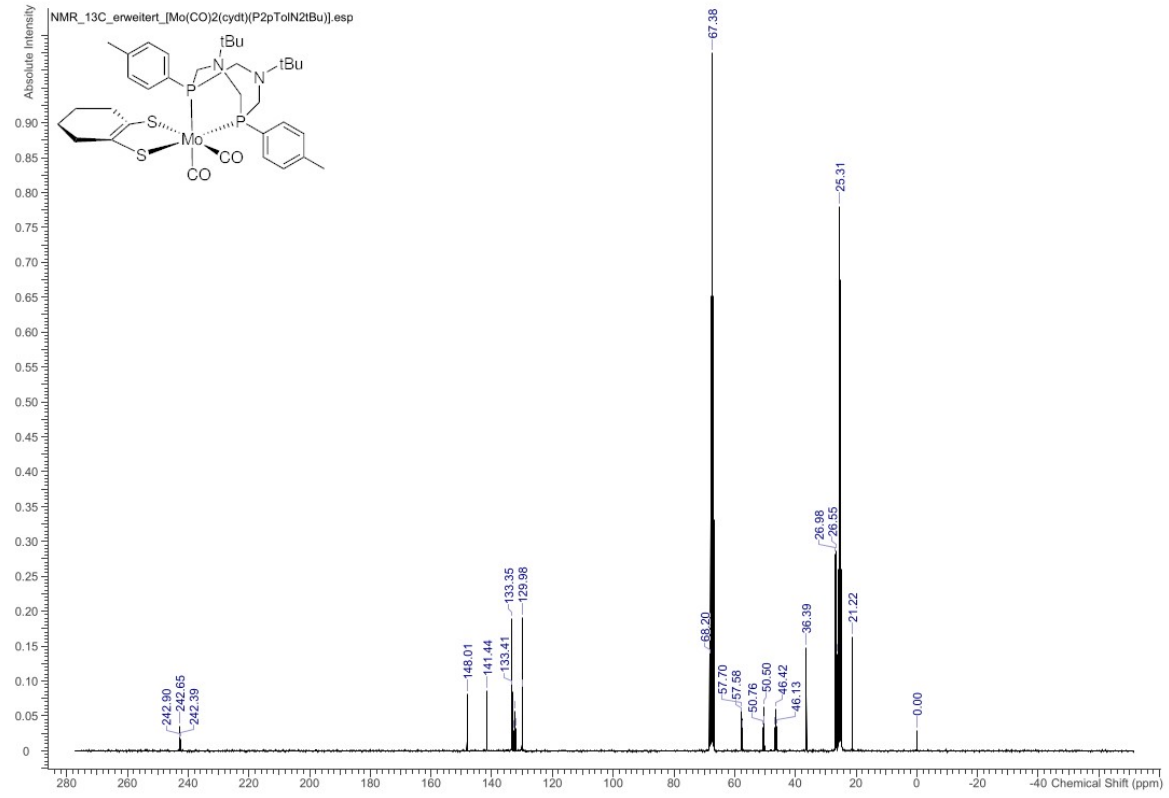


Figure S44. $^{13}C\{^{1}H\}$ NMR spectrum of $[Mo(CO)_2(cydt)(P_2^{p\text{-tol}}N_2^{tBu})]$ (**3**) measured in thf-d8.

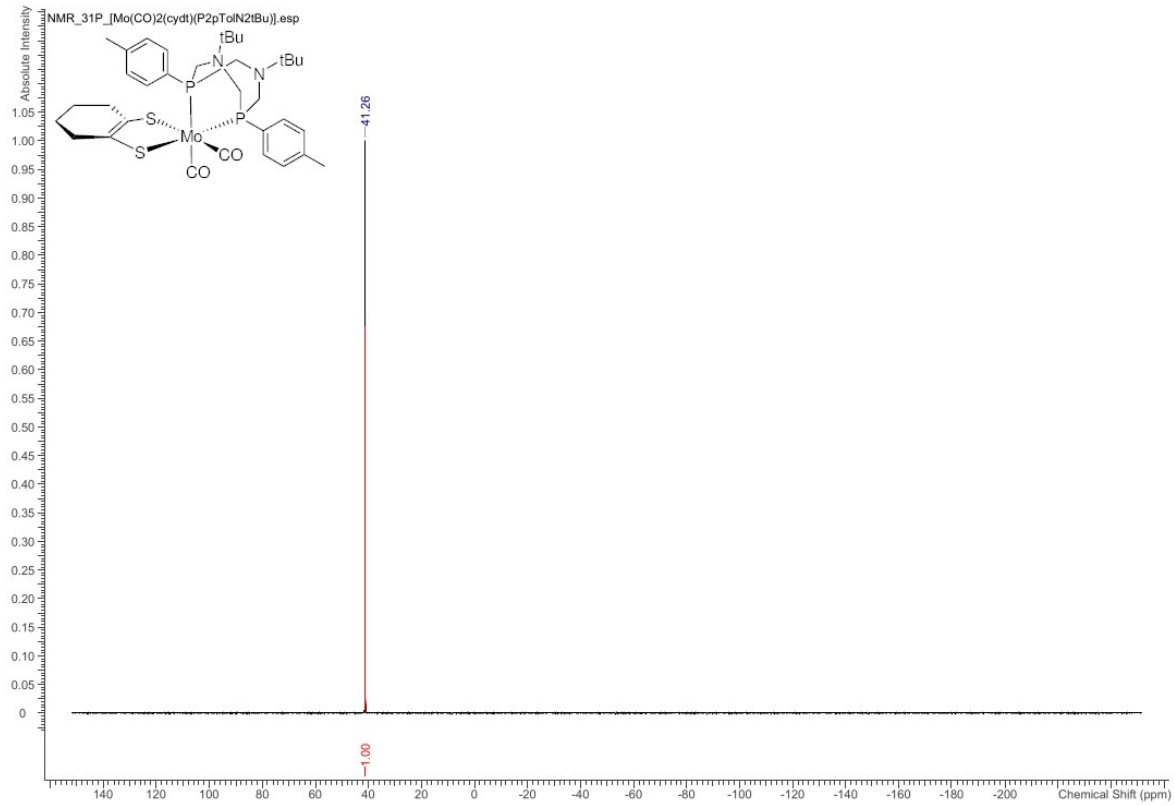


Figure S45. $^{31}P\{^{1}H\}$ NMR spectrum of $[Mo(CO)_2(cydt)(P_2^{p\text{-}tol}N_2^{tBu})]$ (**3**) measured in thf-d8.

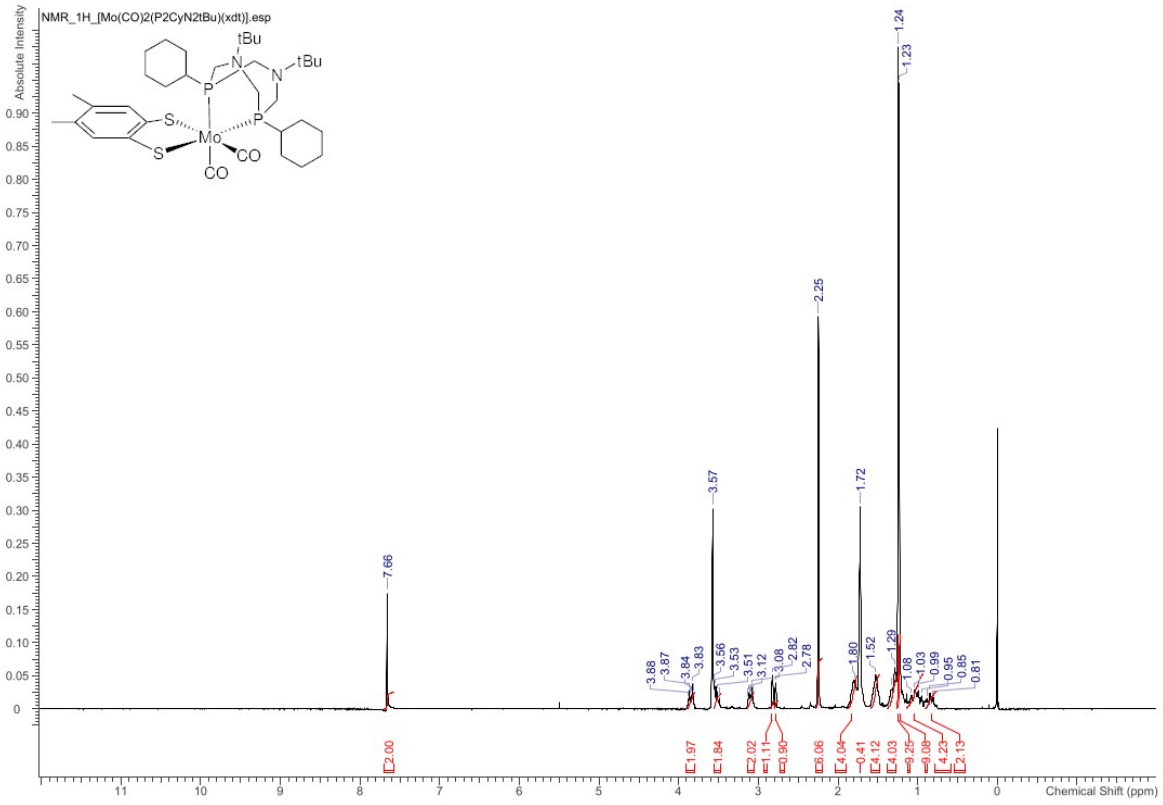


Figure S46. $^{1}H\{^{13}C\}$ NMR spectrum of $[Mo(CO)_2(P_2^{cy}N_2^{fBu})(xdt)]$ (**4**) measured in thf-d8.

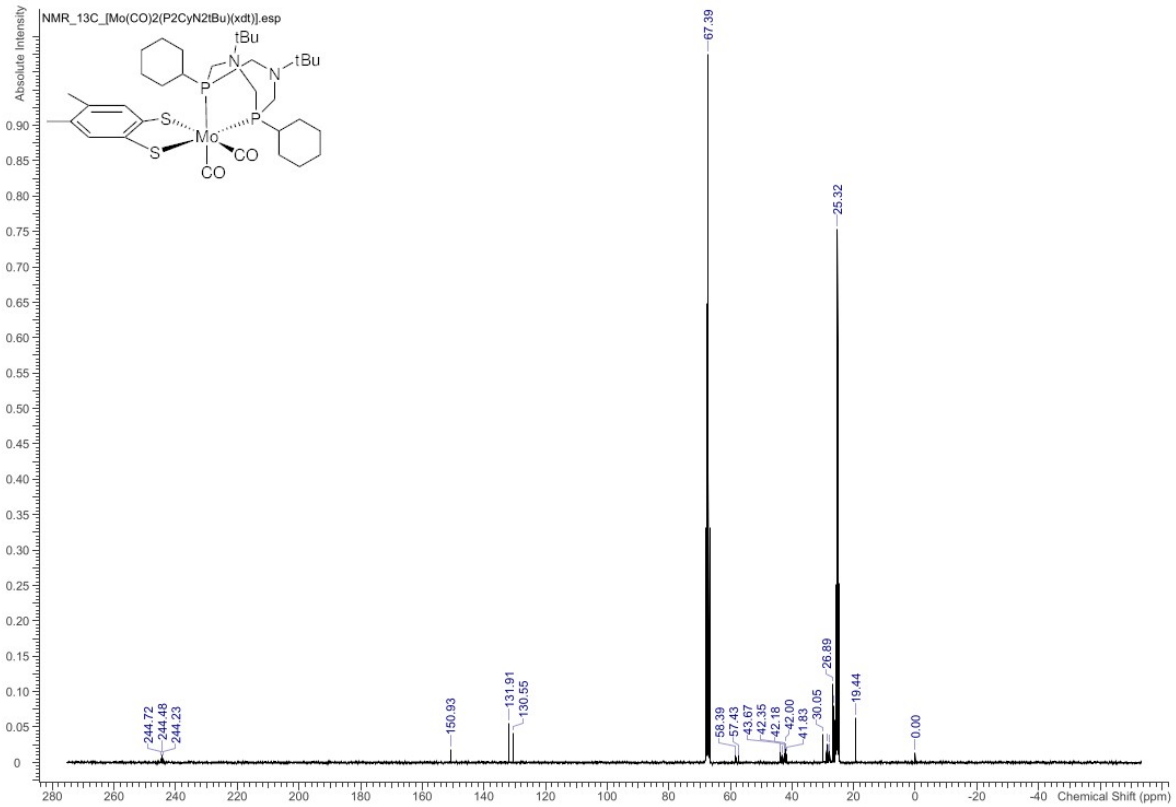


Figure S47. $^{13}C\{^{1}H\}$ NMR spectrum of $[Mo(CO)_2(P_2^{cy}N_2^{tBu})(xdt)]$ (**4**) measured in thf-d8.

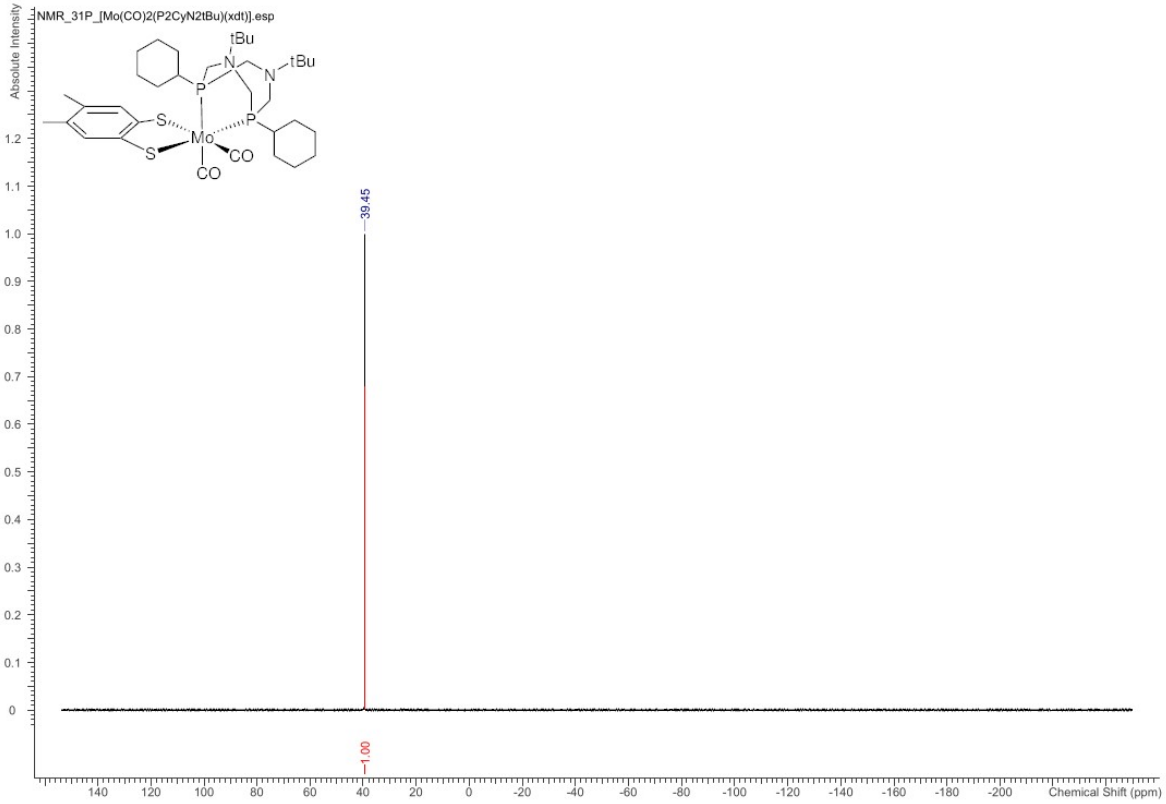


Figure S48. $^{31}P\{^{1}H\}$ NMR spectrum of $[Mo(CO)_2(P_2^{cy}N_2^{tBu})(xdt)]$ (**4**) measured in thf-d8.

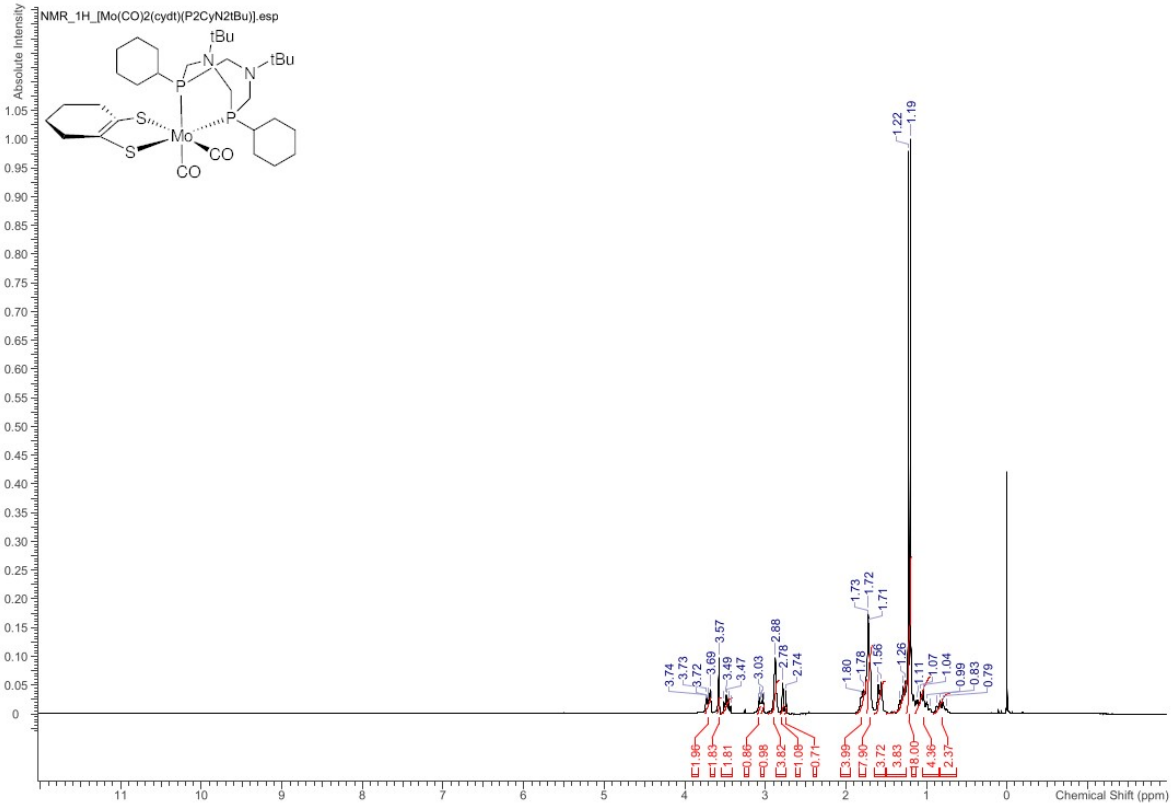


Figure S49. $^{1}H\{^{13}C\}$ NMR spectrum of $[Mo(CO)_2(cydt)(P_2^{cy}N_2^{tBu})]$ (**5**) measured in thf-d8.

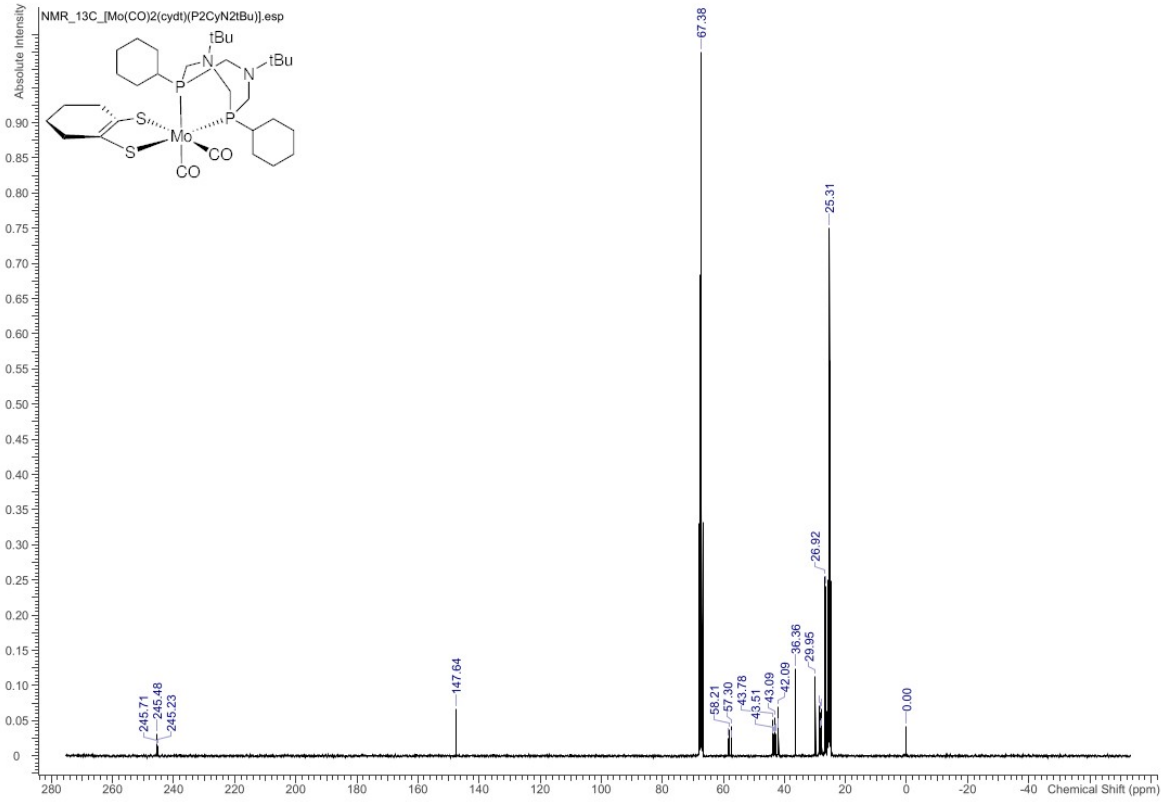


Figure S50. $^{13}C\{^{1}H\}$ NMR spectrum of $[Mo(CO)_2(cydt)(P_2^{cy}N_2^{tBu})]$ (**5**) measured in thf-d8.

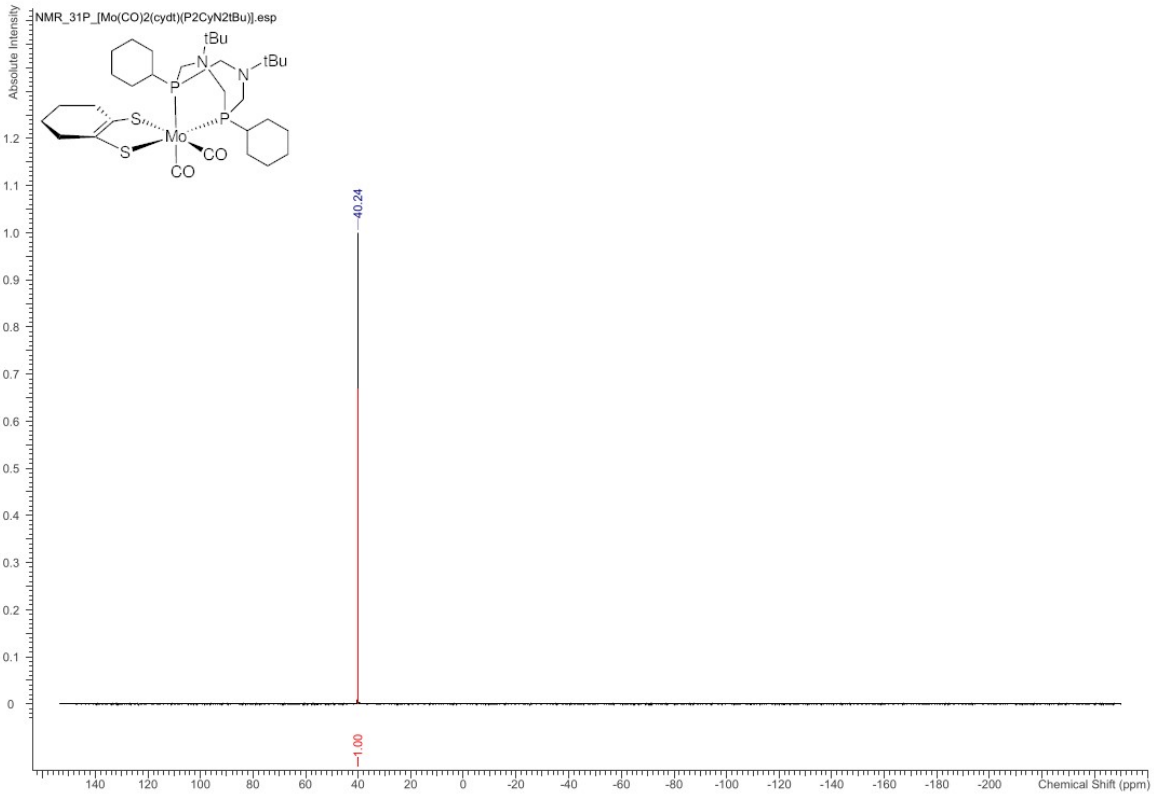


Figure S51. $^{31}P\{^{1}H\}$ NMR spectrum of $[Mo(CO)_2(cydt)(P_2{}^{cy}N_2{}^{tBu})]$ (**5**) measured in thf-d8.

Table S9. Crystal data and structure refinement for $[Mo(CO)_2(P_2^{p\text{-tol}}N_2^{tBu})(xdt)]\cdot CH_2Cl_2$ (**2**).

Table 1. Crystal data and structure refinement for be6-284-1.

Identification code	BE6-284-1
Empirical formula	C37 H50 Cl2 Mo N2 O2 P2 S2
Formula weight	847.69
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C c
Unit cell dimensions	a = 22.880(5) A alpha = 90 deg. b = 11.690(2) A beta = 103.24(3) deg. c = 15.630(3) A gamma = 90 deg.
Volume	4069.5(15) A^3
Z, Calculated density	4, 1.384 Mg/m^3
Absorption coefficient	0.668 mm^-1
F(000)	1760
Crystal size	0.182 x 0.162 x 0.153 mm
Theta range for data collection	1.967 to 29.501 deg.
Limiting indices	-31<=h<=31, -16<=k<=15, -16<=l<=21
Reflections collected / unique	22157 / 9664 [R(int) = 0.0588]
Completeness to theta = 25.242	99.9 %
Absorption correction	Numerical
Max. and min. transmission	0.9058 and 0.7941
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9664 / 379 / 499
Goodness-of-fit on F^2	0.999
Final R indices [I>2sigma(I)]	R1 = 0.0430, wR2 = 0.0950
R indices (all data)	R1 = 0.0787, wR2 = 0.1091
Absolute structure parameter	-0.04(2)
Extinction coefficient	n/a
Largest diff. peak and hole	0.593 and -1.196 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for be6-284-1.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo(1)	4935(1)	3319(1)	5325(1)	28(1)
S(1)	5228(1)	1355(1)	5162(1)	36(1)
S(2)	5354(1)	2977(1)	6821(1)	35(1)
P(1)	4009(1)	3029(1)	4201(1)	35(1)
P(2)	5107(1)	3697(1)	3857(1)	33(1)
O(1)	4017(2)	4924(4)	5905(3)	44(1)
O(2)	5480(2)	5769(4)	5520(3)	52(1)
N(1)	4321(2)	2314(4)	2678(3)	38(1)
N(2)	4180(3)	5229(4)	3698(4)	44(1)
C(1)	4349(3)	4333(5)	5685(4)	33(1)

C(2)	5276(3)	4865(5)	5440(4)	38(1)
C(3)	5587(3)	878(5)	6215(4)	34(1)
C(4)	5634(3)	1580(5)	6939(4)	34(1)
C(5)	5920(3)	1182(5)	7765(5)	41(1)
C(6)	6179(3)	107(5)	7887(5)	47(2)
C(7)	6134(3)	-604(5)	7149(5)	47(2)
C(8)	5837(3)	-212(5)	6341(5)	41(2)
C(9)	6489(4)	-289(6)	8804(5)	58(2)
C(10)	6419(4)	-1766(6)	7265(6)	65(2)
C(11)	4014(3)	1936(6)	3341(4)	40(1)
C(12)	4952(3)	2524(5)	3038(4)	36(1)
C(13)	4670(3)	4919(5)	3286(4)	45(2)
C(14)	3727(3)	4345(6)	3557(5)	48(2)
C(15)	3371(3)	2531(6)	4604(4)	42(1)
C(16)	2770(11)	2610(30)	4225(17)	54(5)
C(17)	2324(8)	2120(20)	4571(16)	54(4)
C(18)	2468(8)	1577(17)	5379(16)	43(4)
C(19)	3066(8)	1407(16)	5822(13)	43(4)
C(20)	3514(8)	1860(20)	5436(18)	39(4)
C(21)	1971(10)	1100(20)	5770(18)	69(6)
C(16')	2810(9)	2725(18)	3988(16)	33(4)
C(17')	2289(9)	2460(20)	4233(18)	57(5)
C(18')	2318(9)	1920(20)	5025(18)	51(5)
C(19')	2870(11)	1750(20)	5604(15)	51(4)
C(20')	3396(10)	2130(30)	5380(20)	46(5)
C(21')	1734(11)	1600(20)	5270(20)	81(8)
C(22)	4205(3)	1531(5)	1885(4)	45(2)
C(23)	3537(4)	1570(8)	1459(6)	70(2)
C(24)	4406(3)	309(5)	2129(5)	51(2)
C(25)	4547(4)	2006(7)	1229(5)	58(2)
C(26)	5872(3)	4010(5)	3792(4)	37(1)
C(27)	5984(3)	4582(5)	3062(5)	48(2)
C(28)	6565(3)	4780(5)	2989(5)	52(2)
C(29)	7048(4)	4397(5)	3609(6)	54(2)
C(30)	6940(3)	3824(6)	4331(5)	52(2)
C(31)	6360(3)	3651(5)	4424(5)	44(2)
C(32)	7685(4)	4605(7)	3518(7)	73(3)
C(33)	3938(4)	6423(6)	3509(5)	57(2)
C(34)	4465(5)	7265(6)	3798(7)	81(3)
C(35)	3490(4)	6634(6)	4091(6)	63(2)
C(36)	3646(6)	6608(8)	2558(6)	94(4)
Cl(1)	7597(2)	579(5)	6080(4)	208(3)
Cl(2)	7090(2)	2591(4)	6693(2)	118(1)
C(37)	7043(6)	1318(10)	6183(14)	159(8)

Table 3. Bond lengths [A] and angles [deg] for be6-284-1.

Mo(1)-C(2)	1.960(6)
Mo(1)-C(1)	1.965(6)
Mo(1)-S(2)	2.3497(17)
Mo(1)-S(1)	2.4217(15)
Mo(1)-P(1)	2.4463(19)
Mo(1)-P(2)	2.4542(16)
S(1)-C(3)	1.753(6)
S(2)-C(4)	1.747(6)
P(1)-C(15)	1.813(7)
P(1)-C(11)	1.855(6)
P(1)-C(14)	1.870(7)
P(2)-C(26)	1.816(6)
P(2)-C(13)	1.851(6)
P(2)-C(12)	1.854(6)
O(1)-C(1)	1.138(7)
O(2)-C(2)	1.151(7)
N(1)-C(12)	1.446(8)
N(1)-C(11)	1.449(8)
N(1)-C(22)	1.515(8)
N(2)-C(14)	1.444(9)
N(2)-C(13)	1.462(8)
N(2)-C(33)	1.506(8)
C(3)-C(4)	1.382(9)
C(3)-C(8)	1.392(8)
C(4)-C(5)	1.388(9)
C(5)-C(6)	1.383(9)
C(6)-C(7)	1.407(10)
C(6)-C(9)	1.519(10)
C(7)-C(8)	1.369(10)
C(7)-C(10)	1.499(9)
C(15)-C(20')	1.29(3)
C(15)-C(16)	1.37(3)

C(15)-C(16')	1.44(2)
C(15)-C(20)	1.49(2)
C(16)-C(17)	1.38(2)
C(17)-C(18)	1.38(2)
C(18)-C(19)	1.40(2)
C(18)-C(21)	1.516(16)
C(19)-C(20)	1.406(17)
C(16')-C(17')	1.369(19)
C(17')-C(18')	1.38(2)
C(18')-C(19')	1.39(2)
C(18')-C(21')	1.522(18)
C(19')-C(20')	1.397(19)
C(22)-C(23)	1.521(11)
C(22)-C(24)	1.522(9)
C(22)-C(25)	1.531(11)
C(26)-C(31)	1.376(9)
C(26)-C(27)	1.395(8)
C(27)-C(28)	1.379(10)
C(28)-C(29)	1.367(11)
C(29)-C(30)	1.383(10)
C(29)-C(32)	1.516(10)
C(30)-C(31)	1.380(10)
C(33)-C(36)	1.500(11)
C(33)-C(35)	1.538(11)
C(33)-C(34)	1.541(14)
Cl(1)-C(37)	1.573(14)
Cl(2)-C(37)	1.680(15)

C(2)-Mo(1)-C(1)	72.6(2)
C(2)-Mo(1)-S(2)	90.14(19)
C(1)-Mo(1)-S(2)	88.13(18)
C(2)-Mo(1)-S(1)	140.32(18)
C(1)-Mo(1)-S(1)	145.63(17)
S(2)-Mo(1)-S(1)	83.30(5)
C(2)-Mo(1)-P(1)	117.04(19)
C(1)-Mo(1)-P(1)	75.78(18)
S(2)-Mo(1)-P(1)	141.27(6)
S(1)-Mo(1)-P(1)	90.48(5)
C(2)-Mo(1)-P(2)	76.95(18)
C(1)-Mo(1)-P(2)	115.13(18)
S(2)-Mo(1)-P(2)	147.61(6)
S(1)-Mo(1)-P(2)	87.99(5)
P(1)-Mo(1)-P(2)	69.61(6)
C(3)-S(1)-Mo(1)	106.53(19)
C(4)-S(2)-Mo(1)	108.7(2)
C(15)-P(1)-C(11)	99.8(3)
C(15)-P(1)-C(14)	104.2(3)
C(11)-P(1)-C(14)	103.6(3)
C(15)-P(1)-Mo(1)	115.3(2)
C(11)-P(1)-Mo(1)	117.9(2)
C(14)-P(1)-Mo(1)	114.0(2)
C(26)-P(2)-C(13)	103.8(3)
C(26)-P(2)-C(12)	98.3(3)
C(13)-P(2)-C(12)	103.9(3)
C(26)-P(2)-Mo(1)	116.9(2)
C(13)-P(2)-Mo(1)	113.9(2)
C(12)-P(2)-Mo(1)	117.8(2)
C(12)-N(1)-C(11)	112.3(5)
C(12)-N(1)-C(22)	113.1(5)
C(11)-N(1)-C(22)	112.2(5)
C(14)-N(2)-C(13)	110.6(5)
C(14)-N(2)-C(33)	114.6(6)
C(13)-N(2)-C(33)	115.4(5)
O(1)-C(1)-Mo(1)	179.0(6)
O(2)-C(2)-Mo(1)	179.0(6)
C(4)-C(3)-C(8)	118.4(6)
C(4)-C(3)-S(1)	120.7(4)
C(8)-C(3)-S(1)	120.8(5)
C(3)-C(4)-C(5)	119.6(6)
C(3)-C(4)-S(2)	120.7(5)
C(5)-C(4)-S(2)	119.6(5)
C(6)-C(5)-C(4)	121.9(7)
C(5)-C(6)-C(7)	118.4(6)
C(5)-C(6)-C(9)	120.0(7)
C(7)-C(6)-C(9)	121.6(6)
C(8)-C(7)-C(6)	119.1(6)
C(8)-C(7)-C(10)	121.7(7)
C(6)-C(7)-C(10)	119.2(7)
C(7)-C(8)-C(3)	122.6(6)
N(1)-C(11)-P(1)	113.1(4)
N(1)-C(12)-P(2)	114.2(4)

N(2)-C(13)-P(2)	111.3(4)
N(2)-C(14)-P(1)	111.1(4)
C(20')-C(15)-C(16')	121.9(13)
C(16)-C(15)-C(20)	114.1(12)
C(20')-C(15)-P(1)	125.4(11)
C(16)-C(15)-P(1)	129.6(11)
C(16')-C(15)-P(1)	112.5(10)
C(20)-C(15)-P(1)	116.1(8)
C(15)-C(16)-C(17)	124.2(19)
C(18)-C(17)-C(16)	120.2(17)
C(17)-C(18)-C(19)	121.2(13)
C(17)-C(18)-C(21)	119.5(18)
C(19)-C(18)-C(21)	119.2(17)
C(18)-C(19)-C(20)	117.4(16)
C(19)-C(20)-C(15)	122.5(15)
C(17')-C(16')-C(15)	118.6(17)
C(16')-C(17')-C(18')	119.3(17)
C(17')-C(18')-C(19')	120.0(14)
C(17')-C(18')-C(21')	119(2)
C(19')-C(18')-C(21')	121(2)
C(18')-C(19')-C(20')	120.0(18)
C(15)-C(20')-C(19')	120(2)
N(1)-C(22)-C(23)	108.1(5)
N(1)-C(22)-C(24)	112.1(5)
C(23)-C(22)-C(24)	110.7(6)
N(1)-C(22)-C(25)	108.0(6)
C(23)-C(22)-C(25)	108.2(6)
C(24)-C(22)-C(25)	109.7(6)
C(31)-C(26)-C(27)	117.5(6)
C(31)-C(26)-P(2)	122.2(5)
C(27)-C(26)-P(2)	120.2(5)
C(28)-C(27)-C(26)	120.6(7)
C(29)-C(28)-C(27)	121.6(7)
C(28)-C(29)-C(30)	118.0(7)
C(28)-C(29)-C(32)	121.2(7)
C(30)-C(29)-C(32)	120.7(8)
C(31)-C(30)-C(29)	120.8(7)
C(26)-C(31)-C(30)	121.4(6)
C(36)-C(33)-N(2)	112.8(6)
C(36)-C(33)-C(35)	110.9(8)
N(2)-C(33)-C(35)	107.3(6)
C(36)-C(33)-C(34)	109.8(8)
N(2)-C(33)-C(34)	107.9(7)
C(35)-C(33)-C(34)	107.9(7)
Cl(1)-C(37)-Cl(2)	124.7(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for be6-284-1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mo(1)	35(1)	27(1)	25(1)	1(1)	10(1)	1(1)
S(1)	52(1)	31(1)	29(1)	1(1)	13(1)	4(1)
S(2)	46(1)	30(1)	28(1)	-1(1)	6(1)	0(1)
P(1)	38(1)	41(1)	28(1)	-1(1)	9(1)	7(1)
P(2)	45(1)	30(1)	28(1)	3(1)	16(1)	6(1)
O(1)	54(3)	45(2)	38(3)	-1(2)	21(2)	9(2)
O(2)	65(3)	34(2)	64(3)	-2(2)	26(3)	-7(2)
N(1)	44(3)	47(3)	24(3)	-4(2)	9(2)	11(2)
N(2)	60(4)	39(3)	37(3)	10(2)	18(3)	21(3)
C(1)	41(3)	32(3)	28(3)	2(2)	11(3)	2(2)
C(2)	41(4)	41(3)	35(4)	1(2)	17(3)	2(3)
C(3)	36(3)	30(3)	37(4)	2(2)	12(3)	0(2)
C(4)	37(3)	36(3)	29(3)	4(2)	5(3)	-4(2)
C(5)	43(4)	36(3)	39(4)	4(3)	1(3)	-4(3)
C(6)	42(4)	46(4)	47(4)	15(3)	1(3)	-4(3)
C(7)	46(4)	36(3)	62(5)	14(3)	19(3)	7(3)
C(8)	45(4)	29(3)	52(4)	4(3)	19(3)	3(2)
C(9)	63(5)	47(4)	57(5)	14(3)	1(4)	5(3)
C(10)	75(6)	52(4)	71(6)	17(4)	26(5)	19(4)
C(11)	36(4)	51(4)	32(4)	-9(3)	5(3)	3(3)
C(12)	46(4)	37(3)	26(3)	-2(2)	12(3)	5(2)
C(13)	70(5)	37(3)	32(4)	16(3)	21(3)	19(3)

C(14)	49(4)	59(4)	33(4)	2(3)	4(3)	19(3)
C(15)	39(3)	53(4)	35(4)	-14(3)	10(3)	-2(3)
C(16)	37(8)	77(11)	48(11)	2(8)	13(7)	0(7)
C(17)	40(7)	69(11)	57(12)	3(9)	15(8)	3(7)
C(18)	36(8)	54(9)	43(10)	-19(6)	17(7)	-8(7)
C(19)	36(8)	43(9)	52(9)	-9(6)	15(6)	-16(6)
C(20)	36(7)	47(11)	36(7)	-5(7)	12(6)	-7(7)
C(21)	62(11)	75(12)	88(15)	-31(10)	56(11)	-25(9)
C(16')	30(7)	25(7)	45(10)	-13(6)	12(6)	-8(5)
C(17')	36(7)	70(12)	68(12)	-4(9)	18(8)	-6(7)
C(18')	41(8)	70(12)	46(11)	-27(9)	20(8)	-18(8)
C(19')	56(10)	58(11)	45(9)	-9(7)	22(7)	1(9)
C(20')	48(9)	50(13)	39(8)	-14(7)	10(8)	-8(8)
C(21')	69(11)	83(15)	104(19)	-28(13)	48(13)	-34(11)
C(22)	53(4)	53(4)	27(3)	-9(3)	3(3)	15(3)
C(23)	63(5)	100(7)	41(5)	-17(4)	0(4)	15(5)
C(24)	64(5)	47(4)	40(4)	-9(3)	12(3)	2(3)
C(25)	82(6)	66(4)	25(4)	-3(3)	11(4)	10(4)
C(26)	52(4)	27(3)	35(3)	-3(2)	19(3)	-2(2)
C(27)	66(5)	36(3)	53(4)	12(3)	33(4)	9(3)
C(28)	69(5)	35(3)	64(5)	15(3)	40(4)	6(3)
C(29)	66(5)	32(3)	77(6)	-7(3)	46(4)	-1(3)
C(30)	52(4)	48(4)	61(5)	2(3)	25(4)	-4(3)
C(31)	59(4)	40(3)	39(4)	6(3)	22(3)	0(3)
C(32)	67(5)	50(4)	117(8)	2(4)	54(5)	-2(4)
C(33)	94(6)	47(4)	39(4)	12(3)	30(4)	37(4)
C(34)	132(9)	37(4)	93(7)	10(4)	64(6)	22(5)
C(35)	88(6)	50(4)	57(5)	11(3)	29(4)	40(4)
C(36)	158(11)	84(6)	37(5)	15(4)	16(6)	75(7)
Cl(1)	117(3)	221(5)	244(7)	-97(5)	-44(4)	58(3)
Cl(2)	75(2)	185(4)	96(3)	-26(2)	23(2)	-12(2)
C(37)	97(9)	72(7)	330(30)	15(11)	84(13)	-2(7)

Table 5. Hydrogen bonds for be6-284-1 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(11)-H(11A)...S(1)	0.99	2.94	3.558(7)	121.4
C(12)-H(12B)...S(1)	0.99	2.89	3.512(6)	121.4
C(16'^b)-H(16'^b)...Cl(2)#1	0.95	2.91	3.61(2)	131.2
C(27)-H(27)...S(2)#2	0.95	2.85	3.565(7)	132.4
C(35)-H(35A)...O(1)	0.98	2.51	3.452(9)	162.1
C(36)-H(36C)...O(1)#2	0.98	2.61	3.407(10)	138.1

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+1/2,z-1/2 #2 x,-y+1,z-1/2

Table S10. Crystal data and structure refinement for $[Mo(CO)_2(cydt)(P_2{}^{p\text{-}tol}N_2{}^{tBu})]\cdot CH_2Cl_2$ (**3**).

Table 1. Crystal data and structure refinement for be6-270-1.

Identification code	BE6-270-1
Empirical formula	C35 H50 Cl2 Mo N2 O2 P2 S2
Formula weight	823.67
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 13.009(3) A alpha = 90 deg. b = 18.560(4) A beta = 105.29(3) deg. c = 17.348(4) A gamma = 90 deg.
Volume	4040.4(15) A^3
Z, Calculated density	4, 1.354 Mg/m^3
Absorption coefficient	0.671 mm^-1
F(000)	1712
Crystal size	0.334 x 0.179 x 0.083 mm
Theta range for data collection	2.068 to 29.494 deg.
Limiting indices	-17<=h<=17, -25<=k<=25, -22<=l<=23
Reflections collected / unique	45031 / 11148 [R(int) = 0.0672]
Completeness to theta = 25.242	99.8 %
Absorption correction	Numerical
Max. and min. transmission	0.8834 and 0.8189
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11148 / 0 / 423
Goodness-of-fit on F^2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0511, wR2 = 0.1396
R indices (all data)	R1 = 0.0798, wR2 = 0.1530
Extinction coefficient	n/a
Largest diff. peak and hole	1.293 and -1.404 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for be6-270-1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo(1)	4427(1)	7422(1)	4850(1)	22(1)
S(1)	5242(1)	7735(1)	3836(1)	30(1)
S(2)	5266(1)	8520(1)	5443(1)	30(1)
P(1)	2955(1)	7744(1)	5416(1)	24(1)
P(2)	4744(1)	6914(1)	6204(1)	24(1)
O(1)	2422(2)	6866(2)	3573(2)	45(1)
O(2)	4820(3)	5814(1)	4521(2)	53(1)
N(1)	2755(2)	6290(1)	5677(2)	28(1)
N(2)	3739(2)	7771(1)	7051(2)	26(1)
C(1)	3163(3)	7074(2)	4050(2)	32(1)
C(2)	4677(3)	6399(2)	4659(2)	33(1)
C(3)	5913(3)	8556(2)	4095(2)	30(1)
C(4)	5930(3)	8885(2)	4786(2)	29(1)
C(5)	6512(3)	9584(2)	5038(2)	37(1)

C(6)	7296(3)	9752(2)	4554(2)	41(1)
C(7)	6759(3)	9643(2)	3665(2)	41(1)
C(8)	6477(3)	8846(2)	3501(2)	43(1)
C(9)	2168(3)	6968(2)	5623(2)	29(1)
C(10)	3703(3)	6284(2)	6347(2)	28(1)
C(11)	4810(3)	7548(2)	7036(2)	28(1)
C(12)	3272(3)	8239(2)	6375(2)	27(1)
C(13)	1960(3)	8343(2)	4811(2)	26(1)
C(14)	1020(3)	8507(2)	5032(2)	33(1)
C(15)	301(3)	8996(2)	4597(2)	38(1)
C(16)	473(3)	9325(2)	3921(2)	38(1)
C(17)	1381(3)	9157(2)	3700(2)	37(1)
C(18)	2127(3)	8678(2)	4144(2)	32(1)
C(19)	-313(4)	9863(3)	3442(3)	57(1)
C(20)	2055(3)	5641(2)	5633(2)	35(1)
C(21)	2736(4)	4963(2)	5640(3)	55(1)
C(22)	1197(3)	5663(2)	4842(2)	49(1)
C(23)	1548(4)	5610(2)	6326(3)	54(1)
C(24)	5984(3)	6415(2)	6570(2)	28(1)
C(25)	6053(3)	5687(2)	6402(2)	33(1)
C(26)	6991(3)	5318(2)	6689(2)	40(1)
C(27)	7900(3)	5651(2)	7147(2)	42(1)
C(28)	7838(3)	6393(2)	7292(2)	39(1)
C(29)	6897(3)	6769(2)	7010(2)	32(1)
C(30)	8916(4)	5245(3)	7483(3)	66(1)
C(31)	3656(3)	8054(2)	7841(2)	36(1)
C(32)	4106(4)	7493(2)	8481(2)	49(1)
C(33)	4276(4)	8759(2)	8053(3)	56(1)
C(34)	2486(4)	8163(3)	7797(2)	58(1)
Cl(1)	8796(3)	6794(2)	5513(2)	159(1)
Cl(2)	8691(3)	8219(2)	6166(3)	196(1)
C(35)	7946(5)	7595(3)	5416(5)	91(2)

Table 3. Bond lengths [A] and angles [deg] for be6-270-1.

Mo(1)-C(1)	1.960(4)
Mo(1)-C(2)	1.970(3)
Mo(1)-S(1)	2.3536(10)
Mo(1)-S(2)	2.4102(9)
Mo(1)-P(1)	2.4450(10)
Mo(1)-P(2)	2.4639(10)
S(1)-C(3)	1.754(3)
S(2)-C(4)	1.738(3)
P(1)-C(13)	1.816(3)
P(1)-C(12)	1.851(3)
P(1)-C(9)	1.856(3)
P(2)-C(24)	1.822(3)
P(2)-C(11)	1.846(3)
P(2)-C(10)	1.855(3)
O(1)-C(1)	1.158(4)
O(2)-C(2)	1.138(4)
N(1)-C(10)	1.454(4)
N(1)-C(9)	1.461(4)
N(1)-C(20)	1.499(4)
N(2)-C(12)	1.457(4)
N(2)-C(11)	1.459(4)
N(2)-C(31)	1.498(4)
C(3)-C(4)	1.341(5)
C(3)-C(8)	1.513(5)
C(4)-C(5)	1.507(5)
C(5)-C(6)	1.514(5)
C(6)-C(7)	1.530(5)
C(7)-C(8)	1.534(5)
C(13)-C(18)	1.379(5)
C(13)-C(14)	1.407(5)
C(14)-C(15)	1.377(5)
C(15)-C(16)	1.391(5)
C(16)-C(17)	1.372(5)
C(16)-C(19)	1.511(5)
C(17)-C(18)	1.390(5)
C(20)-C(23)	1.517(5)
C(20)-C(22)	1.524(5)
C(20)-C(21)	1.538(5)
C(24)-C(25)	1.389(4)
C(24)-C(29)	1.396(5)
C(25)-C(26)	1.373(5)
C(26)-C(27)	1.384(6)
C(27)-C(28)	1.406(6)
C(27)-C(30)	1.500(5)

C(28)-C(29)	1.382(5)
C(31)-C(34)	1.518(6)
C(31)-C(32)	1.522(5)
C(31)-C(33)	1.530(6)
Cl(1)-C(35)	1.834(6)
Cl(2)-C(35)	1.820(8)

C(1)-Mo(1)-C(2)	73.05(14)
C(1)-Mo(1)-S(1)	90.69(10)
C(2)-Mo(1)-S(1)	89.16(11)
C(1)-Mo(1)-S(2)	141.43(10)
C(2)-Mo(1)-S(2)	144.12(11)
S(1)-Mo(1)-S(2)	82.38(3)
C(1)-Mo(1)-P(1)	76.41(10)
C(2)-Mo(1)-P(1)	119.01(11)
S(1)-Mo(1)-P(1)	142.63(3)
S(2)-Mo(1)-P(1)	86.37(3)
C(1)-Mo(1)-P(2)	116.57(10)
C(2)-Mo(1)-P(2)	78.34(10)
S(1)-Mo(1)-P(2)	144.28(3)
S(2)-Mo(1)-P(2)	88.45(3)
P(1)-Mo(1)-P(2)	70.28(3)
C(3)-S(1)-Mo(1)	108.35(11)
C(4)-S(2)-Mo(1)	107.32(12)
C(13)-P(1)-C(12)	99.87(15)
C(13)-P(1)-C(9)	104.00(15)
C(12)-P(1)-C(9)	102.42(15)
C(13)-P(1)-Mo(1)	115.58(11)
C(12)-P(1)-Mo(1)	118.04(11)
C(9)-P(1)-Mo(1)	114.73(11)
C(24)-P(2)-C(11)	101.43(15)
C(24)-P(2)-C(10)	104.09(15)
C(11)-P(2)-C(10)	100.54(15)
C(24)-P(2)-Mo(1)	115.90(11)
C(11)-P(2)-Mo(1)	117.56(11)
C(10)-P(2)-Mo(1)	115.06(11)
C(10)-N(1)-C(9)	112.2(3)
C(10)-N(1)-C(20)	114.2(3)
C(9)-N(1)-C(20)	112.8(3)
C(12)-N(2)-C(11)	110.6(2)
C(12)-N(2)-C(31)	114.3(3)
C(11)-N(2)-C(31)	114.5(3)
O(1)-C(1)-Mo(1)	179.3(3)
O(2)-C(2)-Mo(1)	177.5(3)
C(4)-C(3)-C(8)	123.4(3)
C(4)-C(3)-S(1)	121.0(3)
C(8)-C(3)-S(1)	115.6(3)
C(3)-C(4)-C(5)	122.7(3)
C(3)-C(4)-S(2)	120.9(3)
C(5)-C(4)-S(2)	116.4(2)
C(4)-C(5)-C(6)	112.1(3)
C(5)-C(6)-C(7)	109.7(3)
C(6)-C(7)-C(8)	109.7(3)
C(3)-C(8)-C(7)	110.6(3)
N(1)-C(9)-P(1)	112.0(2)
N(1)-C(10)-P(2)	112.6(2)
N(2)-C(11)-P(2)	110.3(2)
N(2)-C(12)-P(1)	111.9(2)
C(18)-C(13)-C(14)	118.2(3)
C(18)-C(13)-P(1)	120.9(3)
C(14)-C(13)-P(1)	120.8(3)
C(15)-C(14)-C(13)	120.4(3)
C(14)-C(15)-C(16)	120.9(3)
C(17)-C(16)-C(15)	118.5(3)
C(17)-C(16)-C(19)	120.2(4)
C(15)-C(16)-C(19)	121.2(4)
C(16)-C(17)-C(18)	121.2(3)
C(13)-C(18)-C(17)	120.7(3)
N(1)-C(20)-C(23)	112.1(3)
N(1)-C(20)-C(22)	108.4(3)
C(23)-C(20)-C(22)	110.3(4)
N(1)-C(20)-C(21)	108.4(3)
C(23)-C(20)-C(21)	109.4(3)
C(22)-C(20)-C(21)	108.2(3)
C(25)-C(24)-C(29)	118.6(3)
C(25)-C(24)-P(2)	121.5(3)
C(29)-C(24)-P(2)	119.9(3)
C(26)-C(25)-C(24)	120.7(3)
C(25)-C(26)-C(27)	121.9(4)
C(26)-C(27)-C(28)	117.3(3)
C(26)-C(27)-C(30)	122.1(4)

C(28)-C(27)-C(30)	120.6(4)
C(29)-C(28)-C(27)	121.2(4)
C(28)-C(29)-C(24)	120.2(3)
N(2)-C(31)-C(34)	108.3(3)
N(2)-C(31)-C(32)	108.7(3)
C(34)-C(31)-C(32)	108.3(3)
N(2)-C(31)-C(33)	111.1(3)
C(34)-C(31)-C(33)	110.9(4)
C(32)-C(31)-C(33)	109.4(4)
Cl(2)-C(35)-Cl(1)	104.9(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for be6-270-1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mo(1)	26(1)	18(1)	22(1)	-1(1)	5(1)	-1(1)
S(1)	40(1)	27(1)	27(1)	-4(1)	13(1)	-2(1)
S(2)	38(1)	25(1)	31(1)	-7(1)	15(1)	-9(1)
P(1)	27(1)	21(1)	23(1)	1(1)	5(1)	-1(1)
P(2)	27(1)	19(1)	23(1)	-1(1)	3(1)	-1(1)
O(1)	43(2)	48(2)	36(1)	-3(1)	-6(1)	-9(1)
O(2)	76(2)	28(1)	45(2)	-11(1)	-2(2)	9(1)
N(1)	31(2)	22(1)	29(1)	1(1)	3(1)	-8(1)
N(2)	31(2)	25(1)	23(1)	0(1)	6(1)	2(1)
C(1)	40(2)	28(2)	26(2)	0(1)	6(1)	-2(1)
C(2)	43(2)	22(2)	29(2)	-2(1)	2(2)	3(1)
C(3)	32(2)	25(2)	35(2)	1(1)	12(1)	-1(1)
C(4)	30(2)	21(1)	37(2)	-1(1)	14(1)	-2(1)
C(5)	40(2)	27(2)	49(2)	-6(2)	20(2)	-9(2)
C(6)	36(2)	38(2)	50(2)	2(2)	14(2)	-8(2)
C(7)	37(2)	41(2)	48(2)	7(2)	16(2)	-10(2)
C(8)	53(2)	38(2)	44(2)	2(2)	25(2)	-5(2)
C(9)	29(2)	25(2)	31(2)	2(1)	7(1)	-4(1)
C(10)	33(2)	23(2)	26(2)	1(1)	4(1)	-3(1)
C(11)	34(2)	24(2)	24(1)	-4(1)	5(1)	-1(1)
C(12)	31(2)	27(2)	23(1)	-1(1)	7(1)	1(1)
C(13)	25(2)	24(2)	26(2)	-1(1)	2(1)	2(1)
C(14)	25(2)	37(2)	35(2)	-2(1)	6(1)	1(1)
C(15)	28(2)	41(2)	42(2)	-8(2)	6(2)	4(2)
C(16)	35(2)	35(2)	39(2)	-4(2)	0(2)	8(2)
C(17)	46(2)	34(2)	29(2)	4(1)	7(2)	12(2)
C(18)	36(2)	31(2)	29(2)	4(1)	7(1)	7(1)
C(19)	55(3)	58(3)	52(3)	6(2)	2(2)	26(2)
C(20)	41(2)	27(2)	35(2)	2(1)	5(2)	-14(2)
C(21)	60(3)	27(2)	69(3)	-5(2)	1(2)	-11(2)
C(22)	47(2)	44(2)	47(2)	1(2)	-3(2)	-20(2)
C(23)	64(3)	50(2)	50(2)	6(2)	21(2)	-26(2)
C(24)	31(2)	27(2)	23(1)	1(1)	6(1)	5(1)
C(25)	32(2)	29(2)	33(2)	-7(1)	-1(1)	2(1)
C(26)	46(2)	34(2)	37(2)	-6(2)	7(2)	11(2)
C(27)	40(2)	49(2)	35(2)	0(2)	8(2)	13(2)
C(28)	30(2)	53(2)	32(2)	-4(2)	4(2)	-1(2)
C(29)	31(2)	31(2)	31(2)	-4(1)	7(1)	0(1)
C(30)	44(3)	75(3)	69(3)	-2(3)	0(2)	28(2)
C(31)	50(2)	33(2)	25(2)	1(1)	13(2)	10(2)
C(32)	73(3)	50(2)	28(2)	10(2)	22(2)	19(2)
C(33)	87(4)	40(2)	37(2)	-15(2)	11(2)	-2(2)
C(34)	55(3)	91(4)	34(2)	0(2)	20(2)	20(3)
Cl(1)	252(3)	140(2)	113(2)	28(2)	95(2)	38(2)
Cl(2)	208(3)	143(3)	235(4)	3(3)	58(3)	-14(2)
C(35)	68(4)	95(5)	115(6)	-10(4)	32(4)	15(3)

Table S11. Crystal data and structure refinement for [Mo(CO)$_2$($P_2^{cy}N_2^{tBu}$)(xdt)] (**4**).

Table 1. Crystal data and structure refinement for be6-273-1.

Identification code	BE6-273-1
Empirical formula	C34 H56 Mo N2 O2 P2 S2
Formula weight	746.80
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 9.857(2) A alpha = 90 deg. b = 20.079(4) A beta = 97.29(3) deg. c = 18.626(4) A gamma = 90 deg.
Volume	3656.9(13) A^3
Z, Calculated density	4, 1.356 Mg/m^3
Absorption coefficient	0.592 mm^-1
F(000)	1576
Crystal size	0.324 x 0.226 x 0.111 mm
Theta range for data collection	2.028 to 29.495 deg.
Limiting indices	-13<=h<=12, -27<=k<=27, -25<=l<=25
Reflections collected / unique	40649 / 10113 [R(int) = 0.0625]
Completeness to theta = 25.242	100.0 %
Absorption correction	Numerical
Max. and min. transmission	0.9596 and 0.7960
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10113 / 0 / 397
Goodness-of-fit on F^2	1.086
Final R indices [I>2sigma(I)]	R1 = 0.0382, wR2 = 0.0866
R indices (all data)	R1 = 0.0673, wR2 = 0.0998
Extinction coefficient	0.0030(2)
Largest diff. peak and hole	0.968 and -1.155 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for be6-273-1.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo(1)	7352(1)	6803(1)	5743(1)	19(1)
S(1)	8592(1)	6583(1)	6879(1)	29(1)
S(2)	5708(1)	6038(1)	6154(1)	25(1)
P(1)	5354(1)	7409(1)	5125(1)	21(1)
P(2)	6894(1)	6431(1)	4474(1)	19(1)
O(1)	8205(2)	8286(1)	5893(1)	41(1)
O(2)	10154(2)	6986(1)	5164(1)	35(1)
N(1)	7131(2)	7775(1)	4170(1)	22(1)
N(2)	4207(2)	6666(1)	4003(1)	23(1)
C(1)	7876(3)	7738(1)	5833(1)	27(1)
C(2)	9115(2)	6910(1)	5371(1)	23(1)

C(3)	7663(2)	6020(1)	7338(1)	26(1)
C(4)	6368(2)	5812(1)	7040(1)	23(1)
C(5)	5617(2)	5415(1)	7460(1)	26(1)
C(6)	6140(3)	5194(1)	8139(1)	27(1)
C(7)	7478(3)	5365(1)	8418(1)	32(1)
C(8)	8202(3)	5781(1)	8021(1)	35(1)
C(9)	5286(3)	4769(1)	8574(2)	35(1)
C(10)	8123(3)	5089(2)	9140(2)	50(1)
C(11)	5785(2)	7936(1)	4366(1)	25(1)
C(12)	7159(2)	7117(1)	3839(1)	23(1)
C(13)	5165(2)	6117(1)	4137(1)	24(1)
C(14)	3879(2)	6929(1)	4684(1)	26(1)
C(15)	4579(3)	8006(1)	5711(1)	29(1)
C(16)	3281(3)	8343(2)	5353(2)	48(1)
C(17)	2798(4)	8871(2)	5854(2)	62(1)
C(18)	2563(4)	8564(2)	6571(2)	61(1)
C(19)	3839(4)	8229(2)	6927(2)	51(1)
C(20)	4347(3)	7699(2)	6433(2)	40(1)
C(21)	7777(3)	8310(1)	3768(1)	28(1)
C(22)	7616(3)	8983(1)	4124(2)	46(1)
C(23)	7176(3)	8352(2)	2971(2)	43(1)
C(24)	9306(3)	8164(1)	3823(2)	43(1)
C(25)	7985(2)	5736(1)	4224(1)	21(1)
C(26)	7896(3)	5614(1)	3411(1)	27(1)
C(27)	8716(3)	5002(1)	3233(1)	32(1)
C(28)	8318(3)	4391(1)	3633(1)	28(1)
C(29)	8489(3)	4515(1)	4439(1)	29(1)
C(30)	7643(3)	5109(1)	4630(1)	25(1)
C(31)	3031(2)	6540(1)	3425(1)	29(1)
C(32)	2221(3)	5919(2)	3580(2)	58(1)
C(33)	3593(3)	6454(2)	2709(1)	38(1)
C(34)	2115(3)	7145(2)	3353(2)	54(1)

Table 3. Bond lengths [A] and angles [deg] for be6-273-1.

Mo(1)-C(1)	1.948(3)
Mo(1)-C(2)	1.962(2)
Mo(1)-S(1)	2.3482(9)
Mo(1)-S(2)	2.4260(7)
Mo(1)-P(2)	2.4655(8)
Mo(1)-P(1)	2.4713(8)
S(1)-C(3)	1.744(3)
S(2)-C(4)	1.756(2)
P(1)-C(14)	1.847(2)
P(1)-C(15)	1.852(2)
P(1)-C(11)	1.857(2)
P(2)-C(13)	1.850(2)
P(2)-C(12)	1.856(2)
P(2)-C(25)	1.857(2)
O(1)-C(1)	1.148(3)
O(2)-C(2)	1.150(3)
N(1)-C(11)	1.456(3)
N(1)-C(12)	1.460(3)
N(1)-C(21)	1.497(3)
N(2)-C(14)	1.448(3)
N(2)-C(13)	1.452(3)
N(2)-C(31)	1.500(3)
C(3)-C(4)	1.390(3)
C(3)-C(8)	1.400(3)
C(4)-C(5)	1.394(3)
C(5)-C(6)	1.378(3)
C(6)-C(7)	1.397(4)
C(6)-C(9)	1.506(3)
C(7)-C(8)	1.374(4)
C(7)-C(10)	1.517(3)
C(15)-C(20)	1.522(4)
C(15)-C(16)	1.525(4)
C(16)-C(17)	1.529(4)
C(17)-C(18)	1.516(5)
C(18)-C(19)	1.504(4)
C(19)-C(20)	1.532(4)
C(21)-C(22)	1.522(4)
C(21)-C(24)	1.526(4)
C(21)-C(23)	1.530(4)
C(25)-C(26)	1.526(3)
C(25)-C(30)	1.529(3)
C(26)-C(27)	1.529(3)
C(27)-C(28)	1.514(4)
C(28)-C(29)	1.510(3)

C(29)-C(30)	1.522(3)
C(31)-C(34)	1.509(4)
C(31)-C(33)	1.518(4)
C(31)-C(32)	1.529(4)
C(1)-Mo(1)-C(2)	71.83(10)
C(1)-Mo(1)-S(1)	90.12(7)
C(2)-Mo(1)-S(1)	87.43(7)
C(1)-Mo(1)-S(2)	139.76(8)
C(2)-Mo(1)-S(2)	146.84(7)
S(1)-Mo(1)-S(2)	83.59(3)
C(1)-Mo(1)-P(2)	112.90(7)
C(2)-Mo(1)-P(2)	75.98(7)
S(1)-Mo(1)-P(2)	144.88(3)
S(2)-Mo(1)-P(2)	93.55(3)
C(1)-Mo(1)-P(1)	75.69(7)
C(2)-Mo(1)-P(1)	118.10(7)
S(1)-Mo(1)-P(1)	143.70(3)
S(2)-Mo(1)-P(1)	86.23(3)
P(2)-Mo(1)-P(1)	70.38(3)
C(3)-S(1)-Mo(1)	108.52(8)
C(4)-S(2)-Mo(1)	106.13(8)
C(14)-P(1)-C(15)	103.86(12)
C(14)-P(1)-C(11)	101.68(11)
C(15)-P(1)-C(11)	103.40(11)
C(14)-P(1)-Mo(1)	119.06(9)
C(15)-P(1)-Mo(1)	114.07(8)
C(11)-P(1)-Mo(1)	112.91(8)
C(13)-P(2)-C(12)	103.53(11)
C(13)-P(2)-C(25)	101.37(10)
C(12)-P(2)-C(25)	105.35(11)
C(13)-P(2)-Mo(1)	118.53(8)
C(12)-P(2)-Mo(1)	111.24(8)
C(25)-P(2)-Mo(1)	115.29(7)
C(11)-N(1)-C(12)	111.87(19)
C(11)-N(1)-C(21)	115.13(18)
C(12)-N(1)-C(21)	113.95(19)
C(14)-N(2)-C(13)	109.78(19)
C(14)-N(2)-C(31)	116.89(19)
C(13)-N(2)-C(31)	114.96(19)
O(1)-C(1)-Mo(1)	178.8(2)
O(2)-C(2)-Mo(1)	178.3(2)
C(4)-C(3)-C(8)	118.9(2)
C(4)-C(3)-S(1)	120.81(18)
C(8)-C(3)-S(1)	120.31(18)
C(3)-C(4)-C(5)	118.3(2)
C(3)-C(4)-S(2)	120.62(19)
C(5)-C(4)-S(2)	121.05(18)
C(6)-C(5)-C(4)	122.4(2)
C(5)-C(6)-C(7)	119.2(2)
C(5)-C(6)-C(9)	120.4(2)
C(7)-C(6)-C(9)	120.4(2)
C(8)-C(7)-C(6)	118.6(2)
C(8)-C(7)-C(10)	120.8(2)
C(6)-C(7)-C(10)	120.6(2)
C(7)-C(8)-C(3)	122.3(2)
N(1)-C(11)-P(1)	111.58(15)
N(1)-C(12)-P(2)	112.99(16)
N(2)-C(13)-P(2)	110.55(16)
N(2)-C(14)-P(1)	109.18(16)
C(20)-C(15)-C(16)	110.8(2)
C(20)-C(15)-P(1)	112.25(18)
C(16)-C(15)-P(1)	114.55(18)
C(15)-C(16)-C(17)	110.5(2)
C(18)-C(17)-C(16)	110.5(3)
C(19)-C(18)-C(17)	111.0(3)
C(18)-C(19)-C(20)	111.4(3)
C(15)-C(20)-C(19)	110.3(2)
N(1)-C(21)-C(22)	110.2(2)
N(1)-C(21)-C(24)	107.89(19)
C(22)-C(21)-C(24)	107.3(2)
N(1)-C(21)-C(23)	112.9(2)
C(22)-C(21)-C(23)	109.0(2)
C(24)-C(21)-C(23)	109.4(2)
C(26)-C(25)-C(30)	111.75(19)
C(26)-C(25)-P(2)	114.09(16)
C(30)-C(25)-P(2)	108.86(16)
C(25)-C(26)-C(27)	112.2(2)
C(28)-C(27)-C(26)	111.6(2)
C(29)-C(28)-C(27)	110.6(2)
C(28)-C(29)-C(30)	111.5(2)
C(29)-C(30)-C(25)	111.5(2)

N(2)-C(31)-C(34)	109.1(2)
N(2)-C(31)-C(33)	108.4(2)
C(34)-C(31)-C(33)	107.1(2)
N(2)-C(31)-C(32)	112.1(2)
C(34)-C(31)-C(32)	110.6(3)
C(33)-C(31)-C(32)	109.3(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for be6-273-1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mo(1)	21(1)	18(1)	18(1)	0(1)	1(1)	-1(1)
S(1)	26(1)	36(1)	23(1)	6(1)	-3(1)	-9(1)
S(2)	24(1)	26(1)	24(1)	3(1)	-2(1)	-5(1)
P(1)	24(1)	21(1)	19(1)	-1(1)	4(1)	2(1)
P(2)	19(1)	18(1)	19(1)	0(1)	2(1)	1(1)
O(1)	57(1)	24(1)	41(1)	-6(1)	1(1)	-8(1)
O(2)	27(1)	34(1)	45(1)	5(1)	8(1)	-1(1)
N(1)	24(1)	18(1)	23(1)	2(1)	6(1)	1(1)
N(2)	19(1)	28(1)	20(1)	-1(1)	-1(1)	3(1)
C(1)	29(1)	26(1)	24(1)	-2(1)	1(1)	-2(1)
C(2)	23(1)	21(1)	25(1)	2(1)	3(1)	0(1)
C(3)	26(1)	28(1)	24(1)	2(1)	0(1)	-3(1)
C(4)	26(1)	20(1)	22(1)	0(1)	0(1)	0(1)
C(5)	27(1)	22(1)	31(1)	1(1)	4(1)	-1(1)
C(6)	36(1)	19(1)	26(1)	2(1)	9(1)	3(1)
C(7)	40(2)	32(1)	24(1)	5(1)	1(1)	-2(1)
C(8)	34(1)	41(2)	28(1)	9(1)	-6(1)	-8(1)
C(9)	43(2)	28(1)	37(2)	9(1)	13(1)	3(1)
C(10)	58(2)	55(2)	33(2)	16(1)	-7(1)	-10(2)
C(11)	28(1)	21(1)	26(1)	5(1)	5(1)	5(1)
C(12)	28(1)	21(1)	21(1)	2(1)	5(1)	2(1)
C(13)	22(1)	22(1)	26(1)	-1(1)	1(1)	-1(1)
C(14)	22(1)	33(1)	23(1)	-2(1)	3(1)	2(1)
C(15)	35(1)	27(1)	26(1)	-1(1)	8(1)	10(1)
C(16)	56(2)	58(2)	30(2)	0(1)	8(1)	33(2)
C(17)	79(2)	68(2)	38(2)	-3(2)	9(2)	50(2)
C(18)	65(2)	84(3)	38(2)	-7(2)	15(2)	39(2)
C(19)	66(2)	63(2)	26(1)	0(1)	12(1)	30(2)
C(20)	53(2)	43(2)	27(1)	3(1)	12(1)	16(1)
C(21)	28(1)	23(1)	32(1)	9(1)	5(1)	2(1)
C(22)	59(2)	24(1)	58(2)	2(1)	19(2)	-6(1)
C(23)	46(2)	47(2)	35(2)	19(1)	3(1)	-1(1)
C(24)	27(1)	36(2)	66(2)	18(1)	6(1)	-4(1)
C(25)	20(1)	19(1)	23(1)	-1(1)	2(1)	1(1)
C(26)	34(1)	25(1)	23(1)	0(1)	8(1)	1(1)
C(27)	34(1)	30(1)	33(1)	-7(1)	13(1)	1(1)
C(28)	27(1)	23(1)	34(1)	-7(1)	2(1)	1(1)
C(29)	32(1)	21(1)	32(1)	-1(1)	-1(1)	3(1)
C(30)	31(1)	21(1)	24(1)	1(1)	5(1)	2(1)
C(31)	24(1)	39(1)	23(1)	1(1)	-3(1)	-3(1)
C(32)	43(2)	84(3)	42(2)	13(2)	-12(1)	-31(2)
C(33)	44(2)	45(2)	23(1)	-3(1)	-2(1)	5(1)
C(34)	40(2)	82(3)	37(2)	-9(2)	-13(1)	31(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for be6-273-1.

	x	y	z	U(eq)
H(5)	4712	5291	7271	32
H(8)	9100	5911	8216	42
H(9A)	4350	4742	8325	53
H(9B)	5272	4967	9054	53
H(9C)	5679	4321	8627	53
H(10A)	7621	5252	9526	75
H(10B)	9078	5234	9233	75
H(10C)	8087	4601	9126	75

H(11A)	5089	7869	3940	30
H(11B)	5764	8410	4507	30
H(12A)	8051	7054	3657	28
H(12B)	6436	7095	3418	28
H(13A)	5199	5865	3683	28
H(13B)	4850	5812	4498	28
H(14A)	3668	6558	5003	31
H(14B)	3065	7220	4598	31
H(15)	5267	8369	5826	35
H(16A)	2554	8005	5238	57
H(16B)	3462	8554	4894	57
H(17A)	3494	9228	5939	74
H(17B)	1937	9074	5622	74
H(18A)	2282	8915	6895	74
H(18B)	1815	8233	6490	74
H(19A)	3648	8017	7384	61
H(19B)	4562	8567	7048	61
H(20A)	5213	7505	6670	48
H(20B)	3663	7337	6350	48
H(22A)	6660	9126	4029	69
H(22B)	8202	9311	3925	69
H(22C)	7882	8944	4647	69
H(23A)	7411	7948	2719	65
H(23B)	7554	8742	2748	65
H(23C)	6180	8394	2934	65
H(24A)	9691	8138	4334	65
H(24B)	9761	8521	3586	65
H(24C)	9448	7739	3585	65
H(25)	8955	5856	4400	25
H(26A)	8245	6010	3177	32
H(26B)	6926	5552	3209	32
H(27A)	8555	4917	2705	38
H(27B)	9704	5091	3366	38
H(28A)	7354	4274	3465	34
H(28B)	8898	4010	3526	34
H(29A)	9466	4599	4610	35
H(29B)	8204	4113	4689	35
H(30A)	7820	5191	5158	30
H(30B)	6659	5005	4508	30
H(32A)	2836	5534	3637	87
H(32B)	1501	5839	3176	87
H(32C)	1806	5985	4026	87
H(33A)	4130	6848	2613	56
H(33B)	2834	6401	2319	56
H(33C)	4178	6058	2731	56
H(34A)	1607	7171	3771	81
H(34B)	1471	7110	2908	81
H(34C)	2673	7547	3332	81

Table 6. Hydrogen bonds for be6-273-1 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(14)-H(14A)...S(2)	0.99	2.94	3.562(3)	121.9
C(23)-H(23C)...S(1)#1	0.98	3.02	3.849(3)	143.5
C(22)-H(22C)...O(1)	0.98	2.65	3.559(4)	153.7

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+3/2,z-1/2

Table S12. Crystal data and structure refinement for [$Mo(CO)_2$(cydt)($P_2^{cy}N_2^{tBu}$)] (**5**).

Table 1. Crystal data and structure refinement for be6-272-1.

Identification code	BE6-272-1
Empirical formula	C32 H56 Mo N2 O2 P2 S2
Formula weight	722.78
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 18.521(4) A alpha = 90 deg. b = 18.654(4) A beta = 112.90(3) deg. c = 22.552(5) A gamma = 90 deg.
Volume	7177(3) A^3
Z, Calculated density	8, 1.338 Mg/m^3
Absorption coefficient	0.601 mm^-1
F(000)	3056
Crystal size	0.313 x 0.235 x 0.133 mm
Theta range for data collection	1.857 to 29.526 deg.
Limiting indices	-25<=h<=25, -25<=k<=25, -31<=l<=25
Reflections collected / unique	81662 / 19855 [R(int) = 0.1072]
Completeness to theta = 25.242	99.9 %
Absorption correction	Numerical
Max. and min. transmission	0.8672 and 0.7625
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	19855 / 126 / 779
Goodness-of-fit on F^2	0.917
Final R indices [I>2sigma(I)]	R1 = 0.0417, wR2 = 0.0769
R indices (all data)	R1 = 0.1095, wR2 = 0.0932
Extinction coefficient	n/a
Largest diff. peak and hole	1.197 and -2.525 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for be6-272-1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo(1)	6055(1)	6943(1)	3237(1)	21(1)
S(1)	5775(1)	7293(1)	4158(1)	26(1)
S(2)	6779(1)	8015(1)	3473(1)	29(1)
P(1)	4742(1)	6402(1)	2682(1)	22(1)
P(2)	6086(1)	5670(1)	3548(1)	20(1)
O(1)	5665(1)	7213(1)	1784(1)	44(1)
O(2)	7440(1)	6311(1)	2963(1)	44(1)
N(1)	5533(1)	5416(1)	2233(1)	23(1)
N(2)	4611(1)	5255(1)	3378(1)	22(1)
C(1)	5806(2)	7114(2)	2320(2)	30(1)
C(2)	6917(2)	6537(2)	3062(2)	29(1)
C(3)	6289(2)	8094(2)	4448(2)	26(1)
C(4)	6721(2)	8393(2)	4160(2)	29(1)

C(5)	7181(2)	9082(2)	4393(2)	38(1)
C(6)	7295(2)	9260(2)	5078(2)	41(1)
C(7)	6539(2)	9177(2)	5174(2)	40(1)
C(8)	6209(2)	8415(2)	5030(2)	32(1)
C(9)	4749(2)	5691(2)	2112(1)	26(1)
C(10)	5883(2)	5060(1)	2854(1)	22(1)
C(11)	5380(2)	5357(1)	3890(1)	22(1)
C(12)	4260(2)	5954(1)	3159(2)	24(1)
C(13)	3950(2)	7020(2)	2194(2)	30(1)
C(14)	3712(2)	7498(2)	2642(2)	37(1)
C(15)	3095(2)	8046(2)	2258(2)	53(1)
C(16)	2388(2)	7688(2)	1765(2)	57(1)
C(17)	2613(2)	7215(2)	1319(2)	52(1)
C(18)	3227(2)	6658(2)	1700(2)	38(1)
C(19)	5573(2)	4976(2)	1687(1)	28(1)
C(20)	5196(2)	5394(2)	1062(2)	38(1)
C(21)	5166(2)	4247(2)	1624(2)	38(1)
C(22)	6432(2)	4869(2)	1805(2)	35(1)
C(23)	7020(2)	5325(1)	4156(1)	22(1)
C(24)	7064(2)	4509(2)	4228(2)	30(1)
C(25)	7836(2)	4263(2)	4738(2)	31(1)
C(26)	7984(2)	4612(2)	5380(2)	30(1)
C(27)	7958(2)	5424(2)	5313(2)	33(1)
C(28)	7189(2)	5681(2)	4806(1)	26(1)
C(29)	4077(2)	4722(2)	3500(2)	29(1)
C(30)	4518(2)	4022(2)	3729(2)	64(1)
C(31)	3406(2)	4576(2)	2861(2)	50(1)
C(32)	3769(3)	4992(2)	3989(2)	68(1)
Mo(1B)	9105(1)	2733(1)	1848(1)	18(1)
S(1B)	8290(1)	3529(1)	1014(1)	28(1)
S(2B)	7946(1)	2047(1)	1516(1)	29(1)
P(1B)	9842(1)	3768(1)	2470(1)	18(1)
P(2B)	10206(1)	3020(1)	1538(1)	19(1)
O(3)	9508(1)	2283(1)	3266(1)	34(1)
O(4)	10060(1)	1319(1)	2102(1)	38(1)
N(1B)	10521(1)	4461(1)	1739(1)	20(1)
N(2B)	11127(1)	2868(1)	2824(1)	19(1)
C(1B)	9356(2)	2458(1)	2742(2)	23(1)
C(2B)	9706(2)	1850(1)	2005(2)	25(1)
C(3B)	7374(2)	3120(2)	667(2)	28(1)
C(4B)	7227(2)	2487(2)	878(2)	28(1)
C(5B)	6447(2)	2107(2)	581(2)	40(1)
C(6B)	5953(9)	2434(6)	-43(9)	60(4)
C(7B)	5938(5)	3240(4)	13(6)	64(3)
C(8B)	6743(9)	3558(11)	171(10)	43(4)
C(6B')	5812(10)	2566(8)	86(9)	51(3)
C(7B')	6108(5)	2978(6)	-335(5)	51(3)
C(8B')	6791(11)	3454(12)	48(12)	41(4)
C(9B)	10871(2)	3549(1)	2994(1)	20(1)
C(10B)	11180(2)	2912(1)	2197(1)	21(1)
C(11B)	10242(2)	3927(1)	1223(1)	23(1)
C(12B)	9937(2)	4563(1)	2020(1)	20(1)
C(13B)	9474(2)	4158(1)	3052(1)	19(1)
C(14B)	8659(2)	4478(2)	2726(2)	29(1)
C(15B)	8360(2)	4733(2)	3231(2)	34(1)
C(16B)	8913(2)	5268(2)	3691(2)	31(1)
C(17B)	9728(2)	4959(2)	4014(2)	26(1)
C(18B)	10035(2)	4695(1)	3515(1)	21(1)
C(19B)	11840(2)	2548(1)	3339(1)	23(1)
C(20B)	11743(2)	2562(2)	3979(1)	29(1)
C(21B)	12587(2)	2940(2)	3408(2)	41(1)
C(22B)	11882(2)	1758(2)	3171(2)	36(1)
C(23B)	10292(2)	2437(1)	903(1)	21(1)
C(24B)	9563(2)	2443(2)	289(2)	30(1)
C(25B)	9646(2)	1893(2)	-183(2)	36(1)
C(26B)	10379(2)	2016(2)	-315(2)	31(1)
C(27B)	11108(2)	2029(2)	303(2)	29(1)
C(28B)	11027(2)	2589(2)	765(2)	27(1)
C(29B)	10807(2)	5149(2)	1558(2)	28(1)
C(30B)	11233(2)	5569(2)	2176(2)	38(1)
C(31B)	10144(2)	5588(2)	1083(2)	45(1)
C(32B)	11411(2)	4967(2)	1273(2)	44(1)

Table 3. Bond lengths [A] and angles [deg] for be6-272-1.

Mo(1)-C(2)	1.942(3)
Mo(1)-C(1)	1.962(3)
Mo(1)-S(2)	2.3503(9)
Mo(1)-S(1)	2.4167(9)

Mo(1)-P(2)	2.4704(9)
Mo(1)-P(1)	2.4761(11)
S(1)-C(3)	1.755(3)
S(2)-C(4)	1.742(3)
P(1)-C(12)	1.843(3)
P(1)-C(9)	1.851(3)
P(1)-C(13)	1.854(3)
P(2)-C(11)	1.853(3)
P(2)-C(10)	1.853(3)
P(2)-C(23)	1.854(3)
O(1)-C(1)	1.150(4)
O(2)-C(2)	1.155(3)
N(1)-C(10)	1.455(3)
N(1)-C(9)	1.463(4)
N(1)-C(19)	1.505(4)
N(2)-C(11)	1.455(4)
N(2)-C(12)	1.455(3)
N(2)-C(29)	1.503(3)
C(3)-C(4)	1.333(4)
C(3)-C(8)	1.501(4)
C(4)-C(5)	1.518(4)
C(5)-C(6)	1.512(5)
C(6)-C(7)	1.506(5)
C(7)-C(8)	1.531(4)
C(13)-C(18)	1.526(4)
C(13)-C(14)	1.537(4)
C(14)-C(15)	1.526(4)
C(15)-C(16)	1.505(5)
C(16)-C(17)	1.514(5)
C(17)-C(18)	1.532(4)
C(19)-C(22)	1.521(4)
C(19)-C(20)	1.522(4)
C(19)-C(21)	1.533(4)
C(23)-C(28)	1.528(4)
C(23)-C(24)	1.529(4)
C(24)-C(25)	1.517(4)
C(25)-C(26)	1.511(4)
C(26)-C(27)	1.522(4)
C(27)-C(28)	1.515(4)
C(29)-C(32)	1.511(5)
C(29)-C(31)	1.517(5)
C(29)-C(30)	1.520(4)
Mo(1B)-C(2B)	1.943(3)
Mo(1B)-C(1B)	1.953(3)
Mo(1B)-S(2B)	2.3564(9)
Mo(1B)-S(1B)	2.4111(10)
Mo(1B)-P(2B)	2.4597(9)
Mo(1B)-P(1B)	2.4644(9)
S(1B)-C(3B)	1.745(3)
S(2B)-C(4B)	1.741(3)
P(1B)-C(12B)	1.844(3)
P(1B)-C(13B)	1.847(3)
P(1B)-C(9B)	1.856(3)
P(2B)-C(11B)	1.845(3)
P(2B)-C(10B)	1.850(3)
P(2B)-C(23B)	1.854(3)
O(3)-C(1B)	1.150(3)
O(4)-C(2B)	1.160(3)
N(1B)-C(12B)	1.462(3)
N(1B)-C(11B)	1.465(3)
N(1B)-C(29B)	1.504(3)
N(2B)-C(10B)	1.456(3)
N(2B)-C(9B)	1.459(3)
N(2B)-C(19B)	1.502(4)
C(3B)-C(4B)	1.339(4)
C(3B)-C(8B)	1.51(2)
C(3B)-C(8B')	1.53(3)
C(4B)-C(5B)	1.512(4)
C(5B)-C(6B)	1.479(16)
C(5B)-C(6B')	1.530(19)
C(6B)-C(7B)	1.508(13)
C(7B)-C(8B)	1.514(11)
C(6B')-C(7B')	1.484(13)
C(7B')-C(8B')	1.511(12)
C(13B)-C(14B)	1.522(4)
C(13B)-C(18B)	1.526(4)
C(14B)-C(15B)	1.524(4)
C(15B)-C(16B)	1.515(4)
C(16B)-C(17B)	1.512(4)
C(17B)-C(18B)	1.527(4)
C(19B)-C(21B)	1.520(4)

C(19B)-C(20B)	1.522(4)
C(19B)-C(22B)	1.531(4)
C(23B)-C(24B)	1.510(4)
C(23B)-C(28B)	1.536(4)
C(24B)-C(25B)	1.529(4)
C(25B)-C(26B)	1.517(4)
C(26B)-C(27B)	1.518(4)
C(27B)-C(28B)	1.524(4)
C(29B)-C(31B)	1.518(4)
C(29B)-C(30B)	1.524(4)
C(29B)-C(32B)	1.530(4)

C(2)-Mo(1)-C(1)	73.95(13)
C(2)-Mo(1)-S(2)	86.36(9)
C(1)-Mo(1)-S(2)	88.87(9)
C(2)-Mo(1)-S(1)	138.46(10)
C(1)-Mo(1)-S(1)	145.13(9)
S(2)-Mo(1)-S(1)	82.54(3)
C(2)-Mo(1)-P(2)	75.68(9)
C(1)-Mo(1)-P(2)	115.16(9)
S(2)-Mo(1)-P(2)	143.65(3)
S(1)-Mo(1)-P(2)	90.25(3)
C(2)-Mo(1)-P(1)	117.45(10)
C(1)-Mo(1)-P(1)	75.57(9)
S(2)-Mo(1)-P(1)	145.39(3)
S(1)-Mo(1)-P(1)	92.74(3)
P(2)-Mo(1)-P(1)	70.19(3)
C(3)-S(1)-Mo(1)	106.43(11)
C(4)-S(2)-Mo(1)	108.58(10)
C(12)-P(1)-C(9)	102.50(13)
C(12)-P(1)-C(13)	100.18(14)
C(9)-P(1)-C(13)	104.49(14)
C(12)-P(1)-Mo(1)	119.55(11)
C(9)-P(1)-Mo(1)	111.92(10)
C(13)-P(1)-Mo(1)	116.19(10)
C(11)-P(2)-C(10)	102.33(13)
C(11)-P(2)-C(23)	100.87(13)
C(10)-P(2)-C(23)	103.59(13)
C(11)-P(2)-Mo(1)	118.67(9)
C(10)-P(2)-Mo(1)	112.11(9)
C(23)-P(2)-Mo(1)	117.13(9)
C(10)-N(1)-C(9)	112.2(2)
C(10)-N(1)-C(19)	113.0(2)
C(9)-N(1)-C(19)	113.6(2)
C(11)-N(2)-C(12)	108.9(2)
C(11)-N(2)-C(29)	116.8(2)
C(12)-N(2)-C(29)	114.6(2)
O(1)-C(1)-Mo(1)	179.4(3)
O(2)-C(2)-Mo(1)	178.3(3)
C(4)-C(3)-C(8)	122.7(3)
C(4)-C(3)-S(1)	121.1(2)
C(8)-C(3)-S(1)	116.2(2)
C(3)-C(4)-C(5)	123.2(3)
C(3)-C(4)-S(2)	121.3(2)
C(5)-C(4)-S(2)	115.5(2)
C(6)-C(5)-C(4)	112.1(3)
C(7)-C(6)-C(5)	110.9(3)
C(6)-C(7)-C(8)	112.4(3)
C(3)-C(8)-C(7)	113.0(3)
N(1)-C(9)-P(1)	113.3(2)
N(1)-C(10)-P(2)	113.58(18)
N(2)-C(11)-P(2)	110.0(2)
N(2)-C(12)-P(1)	110.46(19)
C(18)-C(13)-C(14)	110.0(3)
C(18)-C(13)-P(1)	115.2(2)
C(14)-C(13)-P(1)	109.5(2)
C(15)-C(14)-C(13)	111.0(3)
C(16)-C(15)-C(14)	111.4(3)
C(15)-C(16)-C(17)	111.4(3)
C(16)-C(17)-C(18)	111.0(3)
C(13)-C(18)-C(17)	111.0(3)
N(1)-C(19)-C(22)	108.0(2)
N(1)-C(19)-C(20)	109.0(2)
C(22)-C(19)-C(20)	107.5(3)
N(1)-C(19)-C(21)	112.4(2)
C(22)-C(19)-C(21)	110.1(3)
C(20)-C(19)-C(21)	109.6(3)
C(28)-C(23)-C(24)	110.4(2)
C(28)-C(23)-P(2)	110.03(19)
C(24)-C(23)-P(2)	114.9(2)
C(25)-C(24)-C(23)	112.2(3)

C(26)-C(25)-C(24)	111.2(2)
C(25)-C(26)-C(27)	110.3(3)
C(28)-C(27)-C(26)	111.9(3)
C(27)-C(28)-C(23)	111.6(2)
N(2)-C(29)-C(32)	112.1(3)
N(2)-C(29)-C(31)	107.4(3)
C(32)-C(29)-C(31)	110.5(3)
N(2)-C(29)-C(30)	108.9(3)
C(32)-C(29)-C(30)	110.1(3)
C(31)-C(29)-C(30)	107.6(3)
C(2B)-Mo(1B)-C(1B)	72.51(12)
C(2B)-Mo(1B)-S(2B)	89.06(9)
C(1B)-Mo(1B)-S(2B)	90.40(9)
C(2B)-Mo(1B)-S(1B)	143.60(9)
C(1B)-Mo(1B)-S(1B)	142.47(9)
S(2B)-Mo(1B)-S(1B)	82.60(4)
C(2B)-Mo(1B)-P(2B)	75.91(8)
C(1B)-Mo(1B)-P(2B)	117.37(9)
S(2B)-Mo(1B)-P(2B)	141.41(3)
S(1B)-Mo(1B)-P(2B)	88.85(3)
C(2B)-Mo(1B)-P(1B)	114.18(9)
C(1B)-Mo(1B)-P(1B)	76.18(8)
S(2B)-Mo(1B)-P(1B)	147.24(3)
S(1B)-Mo(1B)-P(1B)	90.08(4)
P(2B)-Mo(1B)-P(1B)	69.76(3)
C(3B)-S(1B)-Mo(1B)	106.51(10)
C(4B)-S(2B)-Mo(1B)	108.37(10)
C(12B)-P(1B)-C(13B)	102.47(12)
C(12B)-P(1B)-C(9B)	103.50(13)
C(13B)-P(1B)-C(9B)	101.87(13)
C(12B)-P(1B)-Mo(1B)	117.83(10)
C(13B)-P(1B)-Mo(1B)	115.91(9)
C(9B)-P(1B)-Mo(1B)	113.22(9)
C(11B)-P(2B)-C(10B)	103.86(13)
C(11B)-P(2B)-C(23B)	102.38(13)
C(10B)-P(2B)-C(23B)	101.98(13)
C(11B)-P(2B)-Mo(1B)	117.86(10)
C(10B)-P(2B)-Mo(1B)	113.88(9)
C(23B)-P(2B)-Mo(1B)	114.92(9)
C(12B)-N(1B)-C(11B)	110.0(2)
C(12B)-N(1B)-C(29B)	113.8(2)
C(11B)-N(1B)-C(29B)	114.6(2)
C(10B)-N(2B)-C(9B)	111.0(2)
C(10B)-N(2B)-C(19B)	113.8(2)
C(9B)-N(2B)-C(19B)	114.8(2)
O(3)-C(1B)-Mo(1B)	178.6(3)
O(4)-C(2B)-Mo(1B)	179.3(3)
C(4B)-C(3B)-C(8B)	122.4(5)
C(4B)-C(3B)-C(8B')	121.1(6)
C(4B)-C(3B)-S(1B)	121.5(2)
C(8B)-C(3B)-S(1B)	115.7(5)
C(8B')-C(3B)-S(1B)	116.7(6)
C(3B)-C(4B)-C(5B)	123.2(3)
C(3B)-C(4B)-S(2B)	121.0(2)
C(5B)-C(4B)-S(2B)	115.9(2)
C(6B)-C(5B)-C(4B)	111.0(5)
C(4B)-C(5B)-C(6B')	113.0(6)
C(5B)-C(6B)-C(7B)	110.9(12)
C(6B)-C(7B)-C(8B)	111.2(11)
C(3B)-C(8B)-C(7B)	111.8(13)
C(7B')-C(6B')-C(5B)	112.7(11)
C(6B')-C(7B')-C(8B')	112.0(13)
C(7B')-C(8B')-C(3B)	114.8(15)
N(2B)-C(9B)-P(1B)	112.51(19)
N(2B)-C(10B)-P(2B)	111.94(18)
N(1B)-C(11B)-P(2B)	111.82(19)
N(1B)-C(12B)-P(1B)	112.22(17)
C(14B)-C(13B)-C(18B)	110.9(2)
C(14B)-C(13B)-P(1B)	112.4(2)
C(18B)-C(13B)-P(1B)	113.77(19)
C(13B)-C(14B)-C(15B)	109.9(3)
C(16B)-C(15B)-C(14B)	111.8(2)
C(17B)-C(16B)-C(15B)	111.2(2)
C(16B)-C(17B)-C(18B)	110.8(3)
C(13B)-C(18B)-C(17B)	111.5(2)
N(2B)-C(19B)-C(21B)	112.2(2)
N(2B)-C(19B)-C(20B)	109.6(2)
C(21B)-C(19B)-C(20B)	109.5(3)
N(2B)-C(19B)-C(22B)	107.7(2)
C(21B)-C(19B)-C(22B)	110.8(3)
C(20B)-C(19B)-C(22B)	106.8(2)

C(24B)-C(23B)-C(28B)	111.1(2)
C(24B)-C(23B)-P(2B)	112.90(19)
C(28B)-C(23B)-P(2B)	113.34(19)
C(23B)-C(24B)-C(25B)	109.7(2)
C(26B)-C(25B)-C(24B)	112.1(3)
C(25B)-C(26B)-C(27B)	111.5(3)
C(26B)-C(27B)-C(28B)	110.5(2)
C(27B)-C(28B)-C(23B)	110.1(2)
N(1B)-C(29B)-C(31B)	112.2(3)
N(1B)-C(29B)-C(30B)	107.7(2)
C(31B)-C(29B)-C(30B)	110.9(3)
N(1B)-C(29B)-C(32B)	108.5(2)
C(31B)-C(29B)-C(32B)	110.2(3)
C(30B)-C(29B)-C(32B)	107.1(3)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for be6-272-1.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mo(1)	18(1)	21(1)	24(1)	3(1)	9(1)	-1(1)
S(1)	24(1)	26(1)	31(1)	-1(1)	13(1)	-2(1)
S(2)	28(1)	27(1)	35(1)	1(1)	15(1)	-5(1)
P(1)	18(1)	23(1)	24(1)	4(1)	7(1)	1(1)
P(2)	17(1)	22(1)	19(1)	1(1)	7(1)	0(1)
O(1)	50(2)	52(2)	29(2)	12(1)	13(1)	-8(1)
O(2)	36(2)	49(2)	59(2)	10(1)	32(1)	9(1)
N(1)	22(1)	28(1)	18(1)	1(1)	6(1)	2(1)
N(2)	17(1)	20(1)	27(2)	4(1)	8(1)	-2(1)
C(1)	26(2)	31(2)	33(2)	7(1)	11(2)	-3(1)
C(2)	26(2)	31(2)	30(2)	5(1)	13(2)	0(1)
C(3)	20(2)	26(2)	31(2)	3(1)	8(1)	5(1)
C(4)	25(2)	24(2)	36(2)	-1(1)	11(2)	-1(1)
C(5)	37(2)	26(2)	48(2)	0(2)	14(2)	-7(1)
C(6)	44(2)	26(2)	44(2)	-7(2)	8(2)	-3(2)
C(7)	47(2)	33(2)	35(2)	-7(2)	12(2)	4(2)
C(8)	25(2)	36(2)	35(2)	2(2)	10(2)	3(1)
C(9)	24(2)	30(2)	20(2)	3(1)	6(1)	1(1)
C(10)	25(2)	23(2)	20(2)	-1(1)	9(1)	3(1)
C(11)	22(2)	20(1)	27(2)	5(1)	12(1)	0(1)
C(12)	23(2)	24(2)	28(2)	5(1)	12(1)	2(1)
C(13)	24(2)	29(2)	32(2)	9(1)	4(2)	1(1)
C(14)	28(2)	26(2)	47(2)	-3(2)	5(2)	5(1)
C(15)	38(2)	37(2)	61(3)	-5(2)	-5(2)	10(2)
C(16)	34(2)	42(2)	73(3)	-1(2)	-5(2)	15(2)
C(17)	37(2)	49(2)	46(3)	4(2)	-9(2)	12(2)
C(18)	29(2)	38(2)	34(2)	-2(2)	-1(2)	9(2)
C(19)	30(2)	34(2)	17(2)	-4(1)	7(2)	-1(1)
C(20)	41(2)	48(2)	24(2)	-4(2)	11(2)	0(2)
C(21)	43(2)	34(2)	32(2)	-11(2)	10(2)	-6(2)
C(22)	38(2)	43(2)	26(2)	-9(2)	16(2)	1(2)
C(23)	18(2)	25(2)	22(2)	3(1)	8(1)	0(1)
C(24)	28(2)	27(2)	29(2)	-1(1)	5(2)	8(1)
C(25)	28(2)	30(2)	31(2)	5(1)	8(2)	8(1)
C(26)	25(2)	34(2)	27(2)	7(1)	4(2)	2(1)
C(27)	30(2)	31(2)	29(2)	-3(1)	3(2)	-1(1)
C(28)	26(2)	24(2)	25(2)	-3(1)	5(1)	2(1)
C(29)	27(2)	25(2)	38(2)	6(1)	14(2)	-6(1)
C(30)	43(2)	27(2)	115(4)	26(2)	24(3)	-5(2)
C(31)	36(2)	51(2)	54(3)	8(2)	7(2)	-23(2)
C(32)	93(4)	66(3)	73(3)	-14(2)	64(3)	-36(2)
Mo(1B)	19(1)	17(1)	19(1)	-2(1)	8(1)	-1(1)
S(1B)	24(1)	25(1)	32(1)	6(1)	6(1)	-2(1)
S(2B)	26(1)	28(1)	29(1)	4(1)	6(1)	-7(1)
P(1B)	19(1)	17(1)	19(1)	-1(1)	9(1)	1(1)
P(2B)	22(1)	18(1)	18(1)	-2(1)	9(1)	-1(1)
O(3)	48(2)	26(1)	25(1)	0(1)	13(1)	-7(1)
O(4)	43(2)	19(1)	58(2)	0(1)	28(1)	4(1)
N(1B)	25(1)	15(1)	23(1)	-4(1)	14(1)	-5(1)
N(2B)	20(1)	18(1)	19(1)	-1(1)	8(1)	5(1)
C(1B)	28(2)	17(1)	23(2)	0(1)	10(1)	-4(1)
C(2B)	31(2)	16(1)	35(2)	-2(1)	19(2)	-4(1)
C(3B)	22(2)	30(2)	28(2)	4(1)	5(1)	1(1)
C(4B)	21(2)	34(2)	29(2)	0(1)	9(1)	-5(1)

C(5B)	25(2)	42(2)	45(2)	6(2)	4(2)	-9(1)
C(6B)	28(6)	69(5)	57(7)	15(5)	-11(4)	-23(5)
C(7B)	29(4)	71(5)	67(6)	29(4)	-9(4)	-5(4)
C(8B)	29(4)	45(6)	40(8)	12(4)	-3(4)	-5(4)
C(6B')	22(5)	69(7)	52(7)	12(5)	4(4)	-5(4)
C(7B')	34(4)	58(5)	43(5)	12(4)	-4(4)	-11(4)
C(8B')	35(5)	40(6)	41(7)	13(5)	5(4)	3(4)
C(9B)	21(2)	20(1)	19(2)	-2(1)	6(1)	3(1)
C(10B)	20(2)	24(2)	21(2)	-2(1)	9(1)	2(1)
C(11B)	29(2)	19(1)	24(2)	1(1)	13(1)	-2(1)
C(12B)	24(2)	16(1)	24(2)	0(1)	12(1)	1(1)
C(13B)	23(2)	17(1)	21(2)	-1(1)	13(1)	1(1)
C(14B)	20(2)	30(2)	37(2)	-13(1)	12(2)	-1(1)
C(15B)	22(2)	38(2)	48(2)	-16(2)	19(2)	-2(1)
C(16B)	32(2)	25(2)	42(2)	-12(1)	22(2)	-3(1)
C(17B)	32(2)	25(2)	26(2)	-6(1)	15(2)	-2(1)
C(18B)	20(2)	20(1)	22(2)	-2(1)	7(1)	2(1)
C(19B)	24(2)	22(1)	22(2)	4(1)	11(1)	5(1)
C(20B)	36(2)	28(2)	24(2)	5(1)	12(2)	13(1)
C(21B)	20(2)	59(2)	42(2)	21(2)	10(2)	4(2)
C(22B)	49(2)	30(2)	27(2)	3(1)	14(2)	18(2)
C(23B)	26(2)	17(1)	21(2)	-6(1)	12(1)	-2(1)
C(24B)	25(2)	40(2)	25(2)	-7(1)	10(2)	-2(1)
C(25B)	35(2)	47(2)	26(2)	-14(2)	12(2)	-10(2)
C(26B)	35(2)	36(2)	24(2)	-8(1)	15(2)	-2(1)
C(27B)	33(2)	32(2)	27(2)	-2(1)	17(2)	4(1)
C(28B)	26(2)	35(2)	23(2)	-5(1)	13(1)	1(1)
C(29B)	34(2)	20(2)	36(2)	-2(1)	19(2)	-6(1)
C(30B)	42(2)	28(2)	51(2)	-12(2)	26(2)	-11(2)
C(31B)	58(3)	28(2)	47(2)	14(2)	18(2)	-3(2)
C(32B)	56(2)	35(2)	59(3)	-13(2)	43(2)	-22(2)

Table 5. Hydrogen bonds for be6-272-1 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(11B)-H(11B)...S(1B)	0.99	2.90	3.537(3)	122.7
C(12B)-H(12A)...S(1B)	0.99	2.95	3.576(3)	122.1
C(18B)-H(18A)...O(4)#1	0.99	2.38	3.309(3)	155.3
C(22B)-H(22B)...O(2)#2	0.98	2.45	3.363(4)	155.4

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,y+1/2,-z+1/2 #2 -x+2,y-1/2,-z+1/2

Table S13. Crystal data and structure refinement for $[Mo(CH_3CN)_3(cydt)(P_2^{p\text{-tol}}N_2^{tBu})][BF_4]_2 \cdot Et_2O$ (6).

Table 1. Crystal data and structure refinement for be6-295-1_sq.

Identification code	BE6-295-1
Empirical formula	C40 H60 B2 F8 Mo N6 P2 S2
Formula weight	1020.56
Temperature	170(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 10.899(2) A alpha = 90.63(3) deg. b = 12.999(3) A beta = 96.26(3) deg. c = 20.262(4) A gamma = 112.68(3) deg.
Volume	2628.5(11) A^3
Z, Calculated density	2, 1.289 Mg/m^3
Absorption coefficient	0.451 mm^-1
F(000)	1056
Crystal size	0.393 x 0.183 x 0.140 mm
Theta range for data collection	2.087 to 29.491 deg.
Limiting indices	-15<=h<=14, -18<=k<=17, -27<=l<=27
Reflections collected / unique	29110 / 14404 [R(int) = 0.0680]
Completeness to theta = 25.242	99.5 %
Absorption correction	Numerical
Max. and min. transmission	0.9211 and 0.7779
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14404 / 0 / 581
Goodness-of-fit on F^2	0.967
Final R indices [I>2sigma(I)]	R1 = 0.0541, wR2 = 0.1268
R indices (all data)	R1 = 0.1090, wR2 = 0.1421
Extinction coefficient	n/a
Largest diff. peak and hole	0.967 and -1.168 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for be6-295-1_sq. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo(1)	8032(1)	6680(1)	7173(1)	28(1)
S(1)	9756(1)	8435(1)	7195(1)	33(1)
S(2)	9180(1)	6829(1)	8239(1)	35(1)
P(1)	6872(1)	7937(1)	6868(1)	29(1)
P(2)	6340(1)	6378(1)	7936(1)	31(1)
N(1)	7458(3)	8689(2)	8202(1)	34(1)
N(2)	4341(3)	6893(2)	7230(1)	32(1)
N(3)	6249(3)	5456(2)	6561(1)	37(1)
N(4)	8336(3)	5114(2)	7191(1)	37(1)
N(5)	8693(3)	6631(2)	6200(1)	34(1)
C(1)	10766(3)	8825(3)	7936(2)	37(1)
C(2)	10502(3)	8086(3)	8415(2)	36(1)
C(3)	11365(4)	8277(3)	9076(2)	44(1)

C(4)	12717(18)	9200(15)	9065(10)	55(4)
C(5)	12527(10)	10203(8)	8758(5)	48(3)
C(4')	12460(20)	9529(19)	9137(11)	66(5)
C(5')	13054(11)	9933(10)	8520(6)	62(4)
C(6)	11951(4)	9932(3)	8004(2)	46(1)
C(7)	6929(3)	8909(3)	7551(2)	34(1)
C(8)	6585(4)	7641(3)	8449(2)	36(1)
C(9)	4586(3)	5982(3)	7554(2)	36(1)
C(10)	5044(3)	7250(3)	6645(2)	32(1)
C(11)	7386(3)	8762(3)	6159(2)	31(1)
C(12)	8306(4)	9874(3)	6213(2)	41(1)
C(13)	8689(4)	10436(3)	5657(2)	47(1)
C(14)	8224(4)	9938(3)	5022(2)	41(1)
C(15)	7340(4)	8830(3)	4971(2)	43(1)
C(16)	6917(4)	8249(3)	5526(2)	40(1)
C(17)	8647(5)	10566(3)	4416(2)	54(1)
C(18)	7826(4)	9660(3)	8698(2)	42(1)
C(19)	8557(5)	9442(4)	9325(2)	70(2)
C(20)	6616(4)	9884(4)	8865(2)	53(1)
C(21)	8792(5)	10696(3)	8411(2)	66(1)
C(22)	6104(3)	5256(3)	8507(2)	36(1)
C(23)	6268(6)	5400(4)	9171(2)	73(2)
C(24)	6113(7)	4510(4)	9574(2)	91(2)
C(25)	5829(5)	3462(4)	9315(2)	60(1)
C(26)	5722(6)	3331(4)	8630(3)	81(2)
C(27)	5864(6)	4213(4)	8233(2)	72(1)
C(28)	5680(6)	2512(4)	9761(3)	88(2)
C(29)	2883(3)	6708(3)	7107(2)	39(1)
C(30)	2289(4)	6452(4)	7757(2)	60(1)
C(31)	2085(4)	5763(4)	6584(2)	54(1)
C(32)	2786(4)	7796(3)	6886(2)	55(1)
C(33)	8483(4)	4308(3)	7126(2)	44(1)
C(34)	8692(6)	3269(4)	7046(3)	71(1)
C(35)	8992(4)	6539(3)	5696(2)	37(1)
C(36)	9391(5)	6426(3)	5046(2)	56(1)
C(37)	5365(4)	4815(3)	6232(2)	38(1)
C(38)	4182(4)	4024(3)	5838(2)	49(1)
F(2)	6403(3)	4045(2)	4955(1)	64(1)
F(1)	6863(3)	2499(2)	4865(1)	82(1)
F(3)	8255(3)	3975(2)	5528(1)	71(1)
F(4)	6243(3)	2946(2)	5825(1)	67(1)
B(1)	6938(5)	3347(4)	5292(2)	48(1)
F(5)	744(3)	1856(2)	7279(1)	79(1)
F(6)	2664(5)	3335(3)	7232(2)	153(2)
F(7)	2308(5)	1765(4)	6714(3)	164(2)
F(8)	1220(3)	2786(3)	6352(2)	96(1)
B(2)	1724(6)	2457(4)	6914(3)	59(1)
N(6)	5623(9)	946(8)	7194(5)	156(4)
C(39)	5186(6)	323(5)	5917(5)	127(3)
C(40)	5413(7)	647(7)	6630(6)	115(3)

Table 3. Bond lengths [A] and angles [deg] for be6-295-1_sq.

Mo(1)-N(5)	2.180(3)
Mo(1)-N(4)	2.185(3)
Mo(1)-N(3)	2.212(3)
Mo(1)-S(1)	2.3254(13)
Mo(1)-S(2)	2.3420(11)
Mo(1)-P(2)	2.4544(12)
Mo(1)-P(1)	2.4681(11)
S(1)-C(1)	1.708(4)
S(2)-C(2)	1.712(4)
P(1)-C(11)	1.810(4)
P(1)-C(10)	1.842(3)
P(1)-C(7)	1.843(3)
P(2)-C(22)	1.828(4)
P(2)-C(8)	1.847(3)
P(2)-C(9)	1.851(3)
N(1)-C(7)	1.456(4)
N(1)-C(8)	1.460(5)
N(1)-C(18)	1.502(4)
N(2)-C(9)	1.458(4)
N(2)-C(10)	1.464(4)
N(2)-C(29)	1.503(4)
N(3)-C(37)	1.138(4)
N(4)-C(33)	1.128(4)
N(5)-C(35)	1.123(4)
C(1)-C(2)	1.347(5)
C(1)-C(6)	1.511(5)

C(2)-C(3)	1.510(5)
C(3)-C(4)	1.50(2)
C(3)-C(4')	1.60(2)
C(4)-C(5)	1.53(2)
C(5)-C(6)	1.569(10)
C(4')-C(5')	1.48(3)
C(5')-C(6)	1.506(10)
C(11)-C(16)	1.388(4)
C(11)-C(12)	1.401(5)
C(12)-C(13)	1.365(5)
C(13)-C(14)	1.385(5)
C(14)-C(15)	1.385(5)
C(14)-C(17)	1.496(5)
C(15)-C(16)	1.382(5)
C(18)-C(19)	1.513(6)
C(18)-C(21)	1.522(6)
C(18)-C(20)	1.526(5)
C(22)-C(23)	1.341(5)
C(22)-C(27)	1.376(5)
C(23)-C(24)	1.391(6)
C(24)-C(25)	1.360(6)
C(25)-C(26)	1.383(7)
C(25)-C(28)	1.507(6)
C(26)-C(27)	1.377(6)
C(29)-C(30)	1.514(5)
C(29)-C(31)	1.528(5)
C(29)-C(32)	1.528(5)
C(33)-C(34)	1.463(5)
C(35)-C(36)	1.453(5)
F(2)-B(1)	1.401(5)
F(1)-B(1)	1.364(5)
F(3)-B(1)	1.377(5)
F(4)-B(1)	1.378(5)
F(5)-B(2)	1.357(6)
F(6)-B(2)	1.306(6)
F(7)-B(2)	1.367(6)
F(8)-B(2)	1.355(6)
N(6)-C(40)	1.174(12)
C(39)-C(40)	1.466(11)
N(5)-Mo(1)-N(4)	79.17(11)
N(5)-Mo(1)-N(3)	75.76(11)
N(4)-Mo(1)-N(3)	74.98(11)
N(5)-Mo(1)-S(1)	78.84(8)
N(4)-Mo(1)-S(1)	124.05(8)
N(3)-Mo(1)-S(1)	144.30(9)
N(5)-Mo(1)-S(2)	130.09(8)
N(4)-Mo(1)-S(2)	78.48(8)
N(3)-Mo(1)-S(2)	137.83(9)
S(1)-Mo(1)-S(2)	77.86(5)
N(5)-Mo(1)-P(2)	154.12(8)
N(4)-Mo(1)-P(2)	102.55(8)
N(3)-Mo(1)-P(2)	79.76(8)
S(1)-Mo(1)-P(2)	118.60(4)
S(2)-Mo(1)-P(2)	74.74(4)
N(5)-Mo(1)-P(1)	95.04(8)
N(4)-Mo(1)-P(1)	156.74(8)
N(3)-Mo(1)-P(1)	81.76(8)
S(1)-Mo(1)-P(1)	75.90(4)
S(2)-Mo(1)-P(1)	120.67(4)
P(2)-Mo(1)-P(1)	73.07(4)
C(1)-S(1)-Mo(1)	113.84(14)
C(2)-S(2)-Mo(1)	112.98(13)
C(11)-P(1)-C(10)	102.10(16)
C(11)-P(1)-C(7)	106.82(16)
C(10)-P(1)-C(7)	99.57(15)
C(11)-P(1)-Mo(1)	116.26(10)
C(10)-P(1)-Mo(1)	115.60(12)
C(7)-P(1)-Mo(1)	114.50(11)
C(22)-P(2)-C(8)	106.48(16)
C(22)-P(2)-C(9)	99.60(17)
C(8)-P(2)-C(9)	100.73(16)
C(22)-P(2)-Mo(1)	117.40(11)
C(8)-P(2)-Mo(1)	113.63(12)
C(9)-P(2)-Mo(1)	116.81(12)
C(7)-N(1)-C(8)	112.9(3)
C(7)-N(1)-C(18)	112.1(3)
C(8)-N(1)-C(18)	112.3(3)
C(9)-N(2)-C(10)	113.8(3)
C(9)-N(2)-C(29)	113.7(3)
C(10)-N(2)-C(29)	113.2(3)
C(37)-N(3)-Mo(1)	177.3(3)

C(33)-N(4)-Mo(1)	172.3(3)
C(35)-N(5)-Mo(1)	175.9(3)
C(2)-C(1)-C(6)	123.7(3)
C(2)-C(1)-S(1)	117.4(3)
C(6)-C(1)-S(1)	118.7(3)
C(1)-C(2)-C(3)	123.5(3)
C(1)-C(2)-S(2)	117.9(3)
C(3)-C(2)-S(2)	118.5(3)
C(4)-C(3)-C(2)	111.9(9)
C(2)-C(3)-C(4')	108.7(9)
C(3)-C(4)-C(5)	108.7(12)
C(4)-C(5)-C(6)	110.9(10)
C(5')-C(4')-C(3)	115.1(14)
C(4')-C(5')-C(6)	108.0(13)
C(5')-C(6)-C(1)	111.9(5)
C(1)-C(6)-C(5)	108.5(5)
N(1)-C(7)-P(1)	114.5(2)
N(1)-C(8)-P(2)	114.7(2)
N(2)-C(9)-P(2)	113.5(2)
H(9A)-C(9)-H(9B)	107.7
N(2)-C(10)-P(1)	112.1(2)
H(10A)-C(10)-H(10B)	107.9
C(16)-C(11)-C(12)	117.7(3)
C(16)-C(11)-P(1)	118.5(3)
C(12)-C(11)-P(1)	123.6(3)
C(13)-C(12)-C(11)	120.5(3)
C(12)-C(13)-C(14)	122.4(3)
C(15)-C(14)-C(13)	116.9(3)
C(15)-C(14)-C(17)	121.3(3)
C(13)-C(14)-C(17)	121.8(3)
C(16)-C(15)-C(14)	121.8(3)
C(15)-C(16)-C(11)	120.6(3)
N(1)-C(18)-C(19)	109.0(3)
N(1)-C(18)-C(21)	108.4(3)
C(19)-C(18)-C(21)	107.6(4)
N(1)-C(18)-C(20)	113.0(3)
C(19)-C(18)-C(20)	109.9(3)
C(21)-C(18)-C(20)	108.8(3)
C(23)-C(22)-C(27)	117.9(4)
C(23)-C(22)-P(2)	124.6(3)
C(27)-C(22)-P(2)	117.2(3)
C(22)-C(23)-C(24)	121.3(4)
C(25)-C(24)-C(23)	121.8(5)
C(24)-C(25)-C(26)	116.6(4)
C(24)-C(25)-C(28)	120.9(5)
C(26)-C(25)-C(28)	122.5(5)
C(27)-C(26)-C(25)	121.4(5)
C(22)-C(27)-C(26)	121.0(4)
N(2)-C(29)-C(30)	108.8(3)
N(2)-C(29)-C(31)	112.9(3)
C(30)-C(29)-C(31)	109.7(3)
N(2)-C(29)-C(32)	108.2(3)
C(30)-C(29)-C(32)	107.4(3)
C(31)-C(29)-C(32)	109.8(3)
N(4)-C(33)-C(34)	179.2(5)
N(5)-C(35)-C(36)	179.5(5)
N(3)-C(37)-C(38)	176.1(4)
F(1)-B(1)-F(3)	110.0(4)
F(1)-B(1)-F(4)	111.5(4)
F(3)-B(1)-F(4)	108.6(4)
F(1)-B(1)-F(2)	109.6(4)
F(3)-B(1)-F(2)	108.2(4)
F(4)-B(1)-F(2)	108.9(3)
F(6)-B(2)-F(8)	108.5(4)
F(6)-B(2)-F(5)	114.8(5)
F(8)-B(2)-F(5)	111.7(4)
F(6)-B(2)-F(7)	107.9(5)
F(8)-B(2)-F(7)	106.4(5)
F(5)-B(2)-F(7)	107.3(4)
N(6)-C(40)-C(39)	177.5(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for be6-295-1_sq.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mo(1)	22(1)	32(1)	30(1)	-5(1)	-1(1)	11(1)
S(1)	24(1)	37(1)	34(1)	-4(1)	-1(1)	9(1)
S(2)	28(1)	41(1)	34(1)	-3(1)	-2(1)	14(1)
P(1)	24(1)	32(1)	30(1)	-4(1)	0(1)	11(1)
P(2)	28(1)	35(1)	31(1)	-2(1)	1(1)	13(1)
N(1)	35(2)	37(2)	31(2)	-8(1)	-1(1)	17(1)
N(2)	25(1)	38(2)	35(2)	0(1)	5(1)	14(1)
N(3)	27(2)	40(2)	41(2)	-11(1)	-1(1)	13(1)
N(4)	37(2)	35(2)	39(2)	-3(1)	0(1)	16(1)
N(5)	31(2)	32(2)	36(2)	-4(1)	2(1)	11(1)
C(1)	23(2)	42(2)	42(2)	-11(2)	-1(2)	11(2)
C(2)	27(2)	46(2)	34(2)	-9(2)	-3(1)	16(2)
C(3)	35(2)	52(2)	40(2)	-11(2)	-12(2)	16(2)
C(4)	40(8)	55(9)	50(9)	2(7)	-15(6)	1(5)
C(5)	36(5)	46(5)	45(5)	-13(4)	-7(4)	1(4)
C(4')	47(9)	83(15)	45(7)	-19(9)	-15(6)	7(7)
C(5')	36(6)	70(7)	60(7)	-15(5)	-12(5)	4(5)
C(6)	33(2)	43(2)	53(2)	-8(2)	-7(2)	9(2)
C(7)	35(2)	36(2)	34(2)	-7(1)	2(2)	18(2)
C(8)	36(2)	43(2)	32(2)	-6(2)	3(2)	19(2)
C(9)	26(2)	44(2)	37(2)	0(2)	2(1)	15(2)
C(10)	24(2)	39(2)	34(2)	-2(1)	0(1)	14(1)
C(11)	22(2)	37(2)	34(2)	-5(1)	-1(1)	11(1)
C(12)	35(2)	36(2)	42(2)	-5(2)	-1(2)	4(2)
C(13)	41(2)	36(2)	50(2)	3(2)	-1(2)	2(2)
C(14)	37(2)	40(2)	41(2)	6(2)	6(2)	11(2)
C(15)	50(2)	40(2)	37(2)	-1(2)	3(2)	14(2)
C(16)	48(2)	32(2)	37(2)	-4(2)	1(2)	13(2)
C(17)	58(3)	51(2)	47(2)	13(2)	8(2)	14(2)
C(18)	42(2)	41(2)	40(2)	-11(2)	1(2)	14(2)
C(19)	84(4)	78(3)	53(3)	-36(2)	-29(2)	48(3)
C(20)	58(3)	55(2)	52(2)	-15(2)	9(2)	28(2)
C(21)	59(3)	51(3)	66(3)	-25(2)	12(2)	-2(2)
C(22)	31(2)	40(2)	38(2)	2(2)	1(2)	14(2)
C(23)	123(5)	45(2)	43(2)	1(2)	3(3)	26(3)
C(24)	157(6)	58(3)	44(3)	10(2)	-9(3)	33(4)
C(25)	53(3)	50(3)	68(3)	13(2)	-7(2)	13(2)
C(26)	125(5)	44(3)	74(4)	12(2)	16(3)	31(3)
C(27)	110(4)	50(3)	50(3)	3(2)	13(3)	25(3)
C(28)	101(5)	61(3)	88(4)	30(3)	-2(3)	21(3)
C(29)	25(2)	45(2)	50(2)	2(2)	6(2)	17(2)
C(30)	45(2)	87(3)	63(3)	10(2)	19(2)	40(2)
C(31)	24(2)	63(3)	69(3)	-8(2)	-5(2)	13(2)
C(32)	43(2)	59(3)	75(3)	9(2)	10(2)	32(2)
C(33)	41(2)	44(2)	45(2)	-1(2)	-3(2)	16(2)
C(34)	92(4)	47(3)	79(3)	-5(2)	-17(3)	39(3)
C(35)	33(2)	38(2)	38(2)	-4(2)	2(2)	13(2)
C(36)	68(3)	51(2)	43(2)	-8(2)	20(2)	14(2)
C(37)	34(2)	41(2)	41(2)	-4(2)	3(2)	16(2)
C(38)	35(2)	46(2)	55(2)	-19(2)	-4(2)	8(2)
F(2)	70(2)	68(2)	64(2)	14(1)	13(1)	36(1)
F(1)	113(3)	68(2)	71(2)	-12(1)	18(2)	42(2)
F(3)	51(2)	75(2)	82(2)	6(2)	9(1)	20(1)
F(4)	71(2)	72(2)	69(2)	22(1)	29(1)	36(2)
B(1)	40(3)	46(3)	56(3)	-1(2)	9(2)	15(2)
F(5)	71(2)	83(2)	73(2)	15(2)	11(2)	17(2)
F(6)	156(4)	99(3)	94(3)	7(2)	-43(3)	-54(3)
F(7)	187(5)	154(4)	219(5)	71(4)	118(4)	116(4)
F(8)	83(2)	95(2)	78(2)	30(2)	-18(2)	7(2)
B(2)	53(3)	48(3)	68(3)	9(3)	-2(3)	13(3)
N(6)	127(7)	169(8)	183(8)	83(7)	18(6)	66(6)
C(39)	61(4)	70(4)	232(10)	66(5)	-24(5)	15(3)
C(40)	50(4)	86(5)	198(10)	72(7)	3(6)	17(3)

Table 5. Hydrogen bonds for be6-295-1_sq [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(6)-H(6A^a)...F(5)#1	0.99	2.53	3.512(5)	172.4
C(9)-H(9A)...N(3)	0.99	2.54	3.087(4)	114.5
C(9)-H(9A)...F(6)	0.99	2.56	3.279(5)	129.4
C(10)-H(10B)...N(3)	0.99	2.52	3.096(4)	116.9
C(12)-H(12)...F(5)#1	0.95	2.62	3.422(5)	142.8
C(30)-H(30B)...S(2)#2	0.98	2.94	3.830(4)	151.9
C(32)-H(32B)...S(1)#2	0.98	2.88	3.813(4)	159.9
C(34)-H(34B)...F(3)	0.98	2.50	3.256(6)	133.9

C(34)-H(34C)...N(6)	0.98	2.67	3.585(11)	156.3
C(36)-H(36A)...F(3)#3	0.98	2.40	3.143(5)	132.2
C(36)-H(36B)...F(8)#4	0.98	2.28	3.115(5)	142.8
C(36)-H(36C)...F(3)	0.98	2.47	3.151(5)	126.0
C(38)-H(38A)...F(4)	0.98	2.55	3.074(5)	113.7
C(38)-H(38C)...F(8)	0.98	2.55	3.296(5)	132.5

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y+1,z #2 x-1,y,z #3 -x+2,-y+1,-z+1
#4 -x+1,-y+1,-z+1

Table S14. Coordinates for geometry optimized structures from DFT calculations of **2** using different functionals.

	2																	
	PBE0; Disp. ON			PBE0; Disp. OFF			TPSSh; Disp. ON			TPSSh; Disp. OFF			BP86; Disp. ON			BP86; Disp. OFF		
Mo	9.509205	3.838239	8.13897	9.447472	3.824356	8.166389	9.483275	3.857363	8.15322	9.456099	3.852252	8.190213	9.465088	3.869419	8.145987	8.861083	3.756909	8.458061
S	10.132625	1.495076	7.934605	10.136178	1.500553	7.934763	10.133851	1.516479	7.944154	10.128618	1.51745	7.950713	10.130858	1.52155	7.949519	9.588179	1.236742	8.339066
S	10.096856	3.505546	10.402324	10.060285	3.476951	10.420884	10.068579	3.518655	10.429294	10.062038	3.482359	10.45525	10.052481	3.550336	10.431492	10.90324	3.796645	10.003767
P	7.744543	3.440617	6.479999	7.690471	3.465387	6.47481	7.719669	3.43466	6.477852	7.68514	3.470382	6.486365	7.700334	3.429593	6.464111	7.284525	3.618882	6.640588
P	10.367721	4.230689	5.867751	10.329865	4.245999	5.89679	10.364979	4.220639	5.870749	10.344477	4.25427	5.898146	10.362219	4.219822	5.860503	10.135165	4.134348	6.236286
O	7.241332	5.750537	9.052193	7.11163	5.60508	9.173511	7.136302	5.721769	9.053755	7.114266	5.659636	9.217709	7.085842	5.724338	8.992163	6.74264	3.31824	10.732905
O	10.684824	6.705257	8.249415	10.55762	6.71414	8.381899	10.675055	6.748271	8.244551	10.663433	6.729918	8.426456	10.634396	6.775226	8.197282	8.317744	6.778131	9.07381
N	8.92689	2.693671	4.136571	8.906044	2.693877	4.134047	8.912881	2.692499	4.131585	8.90417	2.696649	4.134938	8.911764	2.671866	4.120634	8.697397	2.584117	4.395792
N	8.260216	5.995021	5.573114	8.238855	6.035365	5.586115	8.256757	5.992345	5.561508	8.23645	6.044611	5.575761	8.247919	5.990073	5.543391	8.205011	6.076355	5.546204
C	8.080962	5.035643	8.691192	7.975849	4.94229	8.773839	8.010889	5.032027	8.703604	7.980953	4.992828	8.808544	7.983949	5.034191	8.664252	7.577425	3.443642	9.870596
C	10.242119	5.633671	8.195318	10.133989	5.638806	8.276204	10.222867	5.672517	8.20101	10.202943	5.662849	8.312681	10.183562	5.686047	8.171688	8.52274	5.625928	8.759972
C	10.613137	0.957902	9.5281	10.666099	0.964186	9.513096	10.628341	0.973486	9.540338	10.653943	0.961003	9.532635	10.634051	0.99271	9.553352	10.866943	1.02341	9.553131
C	10.597546	1.844286	10.616563	10.628189	1.835433	10.612264	10.598285	1.856621	10.638114	10.621693	1.828899	10.641205	10.599055	1.888107	10.651839	11.444049	2.125651	10.258605
C	10.98527	1.38112	11.885957	11.055638	1.375532	11.870195	10.998924	1.391713	11.9082	11.048386	1.357493	11.900515	11.01001	1.432537	11.928574	12.482669	1.852771	11.187081
H	10.967976	2.07905	12.7288	11.020586	2.062406	12.721493	10.971512	2.083504	12.755386	11.018994	2.038977	12.755947	10.979913	2.134604	12.778311	12.929063	2.704542	11.730363
C	11.38442	0.065179	12.098656	11.52018	0.077551	12.060575	11.426285	0.077734	12.109908	11.506431	0.050523	12.080957	11.452455	0.117712	12.13855	12.96623	0.557796	11.455226
C	11.403836	-0.831635	10.999257	11.564089	-0.804257	10.949188	11.459625	-0.814807	11.001172	11.542694	-0.82791	10.960201	11.489223	-0.786648	11.030202	12.385974	-0.54145	10.757436
C	11.019398	-0.371313	9.742692	11.137736	-0.347056	9.704772	11.061339	-0.353695	9.744031	11.116773	-0.359522	9.714356	11.080701	-0.334691	9.765876	11.35865	-0.278513	9.830585
H	11.03197	-1.061354	8.893562	11.169782	-1.025781	8.847111	11.084875	-1.037272	8.890319	11.143068	-1.032444	8.852307	11.10738	-1.02933	8.910163	10.909499	-1.128556	9.287026
C	11.786543	-0.399428	13.468105	11.966383	-0.38045	13.41884	11.846544	-0.388961	13.481892	11.95597	-0.419032	13.443011	11.885033	-0.340104	13.511392	14.071173	0.340959	12.4661
H	12.821379	-0.779955	13.476755	13.016958	-0.715184	13.408144	12.889868	-0.747768	13.480252	13.006758	-0.755062	13.425976	12.937255	-0.697722	13.507046	14.961257	-0.14871	12.012549
H	11.147642	-1.228571	13.815008	11.370357	-1.238731	13.771272	11.224066	-1.232824	13.825204	11.356389	-1.277813	13.790121	11.27018	-1.195077	13.866721	13.749848	-0.322467	13.299457
H	11.716291	0.414639	14.2031	11.873343	0.425005	14.160729	11.763208	0.421428	14.220399	11.865415	0.384912	14.187659	11.802974	0.473984	14.257649	14.405631	1.299627	12.910808
C	11.832252	-2.257118	11.191891	12.063912	-2.210279	11.113255	11.91964	-2.240222	11.182884	12.035775	-2.245963	11.113154	11.962864	-2.20791	11.222295	12.857171	-1.95776	11.005539
H	12.86029	-2.317047	11.585996	13.101133	-2.227577	11.487116	12.952516	-2.279617	11.568765	13.075793	-2.270857	11.480796	13.005326	-2.238886	11.606286	13.941512	-2.081478	10.78933
H	11.795233	-2.817999	10.247683	12.035729	-2.757465	10.160764	11.885847	-2.793771	10.233524	11.997633	-2.783677	10.15493	11.929019	-2.780945	10.275318	12.30472	-2.683	10.374937
H	11.188911	-2.774378	11.922927	11.460318	-2.769893	11.847009	11.289679	-2.772946	11.915436	11.429624	-2.805086	11.846166	11.3422	-2.744831	11.971653	12.721312	-2.263873	12.066679
C	8.039052	2.187861	5.155955	7.995639	2.214051	5.148196	8.016964	2.170668	5.151504	7.994541	2.202637	5.159609	8.007537	2.157596	5.135882	7.5991	2.29049	5.314697
H	8.383983	1.256544	5.64547	8.32073	1.281846	5.650821	8.367827	1.239981	5.636637	8.336109	1.27705	5.662021	8.352704	1.221483	5.636457	7.7308	1.332841	5.880033

H	7.048913	1.992596	4.730779	7.01034	2.025582	4.706958	7.030242	1.976701	4.718252	7.011984	2.004612	4.716747	7.014972	1.959542	4.697357	6.659786	2.213818	4.740577
C	10.270497	2.86081	4.635177	10.240641	2.878674	4.654814	10.268049	2.836568	4.638872	10.25215	2.870303	4.657109	10.264434	2.822245	4.630203	9.991722	2.659214	5.077243
H	10.93976	3.165943	3.823704	10.916237	3.189781	3.850379	10.942662	3.127877	3.826983	10.926175	3.171041	3.847577	10.950167	3.109135	3.815354	10.791841	2.76212	4.323939
H	10.705195	1.957242	5.105891	10.679932	1.979237	5.130469	10.67909	1.926161	5.115495	10.677159	1.967895	5.138498	10.682658	1.911529	5.12204	10.206366	1.759139	5.703892
C	9.524666	5.619907	4.97778	9.50909	5.651607	5.007014	9.525978	5.607258	4.954664	9.514125	5.654839	4.986213	9.517201	5.608942	4.936756	9.478397	5.499791	5.117902
H	10.223432	6.460187	5.049885	10.214428	6.485319	5.094287	10.222436	6.449766	5.015613	10.212156	6.495513	5.060578	10.220271	6.456909	4.992783	10.250769	6.287565	5.130537
H	9.450849	5.321125	3.914467	9.448428	5.363314	3.939343	9.44069	5.293139	3.897567	9.442191	5.350556	3.924436	9.435093	5.285288	3.872509	9.450563	5.072145	4.086027
C	7.273911	4.938974	5.500038	7.24793	4.982351	5.501075	7.255935	4.934616	5.477491	7.238096	4.982361	5.486793	7.242733	4.938203	5.457331	7.092235	5.126837	5.512389
H	7.05776	4.59456	4.4706	7.039837	4.645358	4.466985	7.054714	4.588308	4.446499	7.045517	4.636739	4.453248	7.038127	4.585703	4.418899	6.854441	4.756545	4.482548
H	6.336606	5.284075	5.949759	6.307385	5.334134	5.939953	6.318865	5.29217	5.91672	6.29612	5.342216	5.914887	6.298025	5.29777	5.898346	6.194218	5.641012	5.897079
C	6.182415	2.831903	7.182125	6.10586	2.863085	7.141817	6.149104	2.830915	7.178427	6.095401	2.868693	7.15939	6.126968	2.81772	7.164744	5.495113	3.158842	6.902358
C	5.01024	2.839286	6.408963	4.933209	2.932869	6.372373	4.968974	2.848838	6.408766	4.916228	2.922872	6.389069	4.94308	2.840051	6.390324	4.3998	3.703729	6.192122
H	5.021924	3.226896	5.386248	4.952118	3.361314	5.36652	4.977983	3.244532	5.389594	4.929516	3.347032	5.381804	4.951962	3.246499	5.366496	4.554713	4.471486	5.419657
C	3.818863	2.35003	6.932516	3.728205	2.45618	6.87717	3.775018	2.357886	6.937585	3.713837	2.432406	6.900052	3.744599	2.339967	6.916715	3.085636	3.271919	6.445349
H	2.915396	2.365418	6.316104	2.825807	2.525186	6.262838	2.868135	2.382592	6.326967	2.810341	2.488249	6.286344	2.830713	2.368702	6.30158	2.252667	3.723662	5.880978
C	3.756967	1.831936	8.235874	3.650618	1.886487	8.157756	3.719368	1.826684	8.240912	3.645235	1.863821	8.186763	3.68783	1.794234	8.221125	2.810983	2.265373	7.397059
C	4.933198	1.817966	8.994773	4.827619	1.804187	8.910797	4.903759	1.801416	8.995918	4.827663	1.800484	8.942186	4.877846	1.765745	8.979705	3.909395	1.70327	8.086119
H	4.914139	1.412215	10.010152	4.798671	1.355951	9.907942	4.889339	1.386823	10.007555	4.805929	1.356302	9.941131	4.863166	1.339434	9.995605	3.732608	0.906925	8.828342
C	6.130515	2.313241	8.479409	6.037954	2.287705	8.414601	6.103341	2.298871	8.476208	6.035365	2.297753	8.440314	6.082042	2.272415	8.463827	5.220329	2.148093	7.850936
H	7.034109	2.294141	9.095951	6.93969	2.216573	9.029716	7.012029	2.272949	9.085172	6.94025	2.24054	9.05223	6.996215	2.243656	9.078995	6.058159	1.71585	8.420823
C	2.460452	1.329746	8.798283	2.340199	1.403241	8.704591	2.417619	1.320823	8.809696	2.335878	1.358147	8.738302	2.384542	1.279811	8.782951	1.394628	1.824595	7.687891
H	2.621976	0.691684	9.678496	2.484727	0.724775	9.557035	2.585011	0.67702	9.685368	2.494351	0.693855	9.600092	2.544802	0.638317	9.671522	1.350246	0.752578	7.967622
H	1.894198	0.758327	8.047598	1.752786	0.881822	7.934137	1.848565	0.754158	8.056532	1.764807	0.813065	7.970925	1.818758	0.700309	8.025203	0.729244	1.988062	6.816591
H	1.822177	2.173491	9.110089	1.729883	2.252704	9.05479	1.783354	2.165739	9.129078	1.706661	2.200497	9.074154	1.732659	2.125331	9.09293	0.965263	2.398496	8.538535
C	8.805342	2.054944	2.793783	8.813695	1.992891	2.815696	8.788387	2.067398	2.7679	8.806231	1.992608	2.801461	8.78052	2.06827	2.744697	8.719124	1.73427	3.137526
C	7.350604	2.161606	2.326966	7.386928	2.143228	2.277493	7.324346	2.181361	2.308799	7.369414	2.149448	2.271258	7.31532	2.208471	2.283235	7.324845	1.755969	2.473457
H	7.280586	1.849651	1.274954	7.344209	1.762969	1.246543	7.251515	1.885123	1.251758	7.320574	1.767831	1.240238	7.232903	1.914026	1.218519	7.395755	1.307508	1.462403
H	6.996525	3.201225	2.405288	7.085744	3.202148	2.268661	6.9727	3.220408	2.406839	7.074089	3.21033	2.265136	6.97691	3.259867	2.383767	6.952709	2.795203	2.360799
H	6.668312	1.514409	2.896495	6.646095	1.573687	2.856956	6.647972	1.524621	2.875725	6.632653	1.582775	2.859956	6.619671	1.558708	2.849874	6.569812	1.171161	3.034264
C	9.243011	0.587913	2.828811	9.175954	0.508259	2.933448	9.232513	0.594345	2.782314	9.171483	0.500361	2.912835	9.205926	0.585161	2.745389	9.121287	0.269967	3.432803
H	9.15044	0.131477	1.831322	9.115916	0.020188	1.948477	9.134922	0.15109	1.778613	9.10349	0.0169	1.925243	9.111433	0.146286	1.731047	9.087347	-0.339339	2.506009
H	8.620618	0.003936	3.524369	8.48844	-0.022459	3.609849	8.613596	0.003752	3.47618	8.487416	-0.029932	3.593978	8.57112	-0.010155	3.433153	8.430469	-0.19552	4.165727

H	10.293752	0.494925	3.144418	10.202296	0.375116	3.309591	10.285568	0.503855	3.092554	10.201184	0.369016	3.281787	10.262277	0.475487	3.065814	10.151215	0.203263	3.838525
C	9.662839	2.836392	1.793691	9.751832	2.675598	1.815802	9.645514	2.875553	1.777879	9.744747	2.687862	1.79921	9.654267	2.877555	1.763993	9.709491	2.356849	2.127985
H	10.742032	2.696595	1.951516	10.813786	2.473257	2.016902	10.725268	2.746019	1.94455	10.807588	2.487111	2.000958	10.739836	2.729305	1.928379	10.764329	2.298313	2.461007
H	9.435888	3.912557	1.847942	9.59441	3.765515	1.812635	9.403815	3.947871	1.847155	9.581913	3.777249	1.80466	9.429646	3.960759	1.845795	9.461783	3.421934	1.941887
H	9.442269	2.487023	0.774831	9.540377	2.295346	0.806046	9.433201	2.534515	0.753712	9.530579	2.310704	0.788045	9.440145	2.553841	0.72655	9.64715	1.813359	1.163735
C	12.137993	4.63674	5.792839	12.108614	4.6357	5.840889	12.141823	4.622122	5.807423	12.128118	4.650568	5.831329	12.146873	4.610982	5.802293	11.955199	4.451497	6.168265
C	12.691741	5.202218	4.632532	12.686427	5.181604	4.682215	12.716487	5.169388	4.642572	12.706733	5.20133	4.669259	12.728538	5.142701	4.626606	12.454564	5.721498	6.555391
H	12.064929	5.408334	3.760007	12.07405	5.395569	3.801542	12.101252	5.368822	3.760792	12.093214	5.41537	3.790048	12.110884	5.340816	3.73588	11.7532	6.54057	6.784533
C	14.046319	5.508963	4.577662	14.048232	5.457201	4.635535	14.079182	5.463544	4.600896	14.07278	5.480549	4.623297	14.10063	5.421634	4.581513	13.832158	5.964801	6.650724
H	14.458747	5.956297	3.668682	14.476622	5.886397	3.725145	14.506618	5.894841	3.691394	14.499133	5.91319	3.713847	14.536714	5.84223	3.660995	14.182636	6.970221	6.938236
C	14.893987	5.254445	5.668172	14.88251	5.191702	5.733635	14.91356	5.213544	5.708557	14.91051	5.212958	5.724147	14.937712	5.170832	5.695198	14.779568	4.946501	6.38927
C	14.336598	4.67474	6.813168	14.300927	4.638962	6.879719	14.33505	4.653472	6.858887	14.328872	4.653079	6.872803	14.349406	4.627914	6.857093	14.282423	3.675554	6.031268
H	14.976017	4.46058	7.674097	14.928006	4.418488	7.748155	14.961591	4.444313	7.730179	14.956197	4.430661	7.740337	14.978993	4.418292	7.73666	14.992066	2.857187	5.824054
C	12.976675	4.371791	6.879082	12.933631	4.366657	6.936805	12.967352	4.363438	6.911946	12.957724	4.377834	6.929731	12.972739	4.353376	6.914756	12.901531	3.427806	5.925377
H	12.563532	3.929448	7.790392	12.504858	3.940842	7.848471	12.536221	3.936327	7.82227	12.527722	3.948734	7.839241	12.534494	3.937751	7.836692	12.571838	2.416187	5.644541
C	16.350076	5.607806	5.598387	16.349098	5.500987	5.670797	16.382013	5.552114	5.652089	16.383892	5.529456	5.66397	16.412079	5.488613	5.630307	16.262362	5.212048	6.513079
H	16.895568	5.252793	6.483639	16.873574	5.153267	6.57143	16.911544	5.19566	6.547161	16.907582	5.16914	6.560815	16.947199	5.146785	6.537429	16.861681	4.369524	6.115185
H	16.482296	6.69997	5.531121	16.516694	6.586125	5.575484	16.525122	6.643374	5.579744	16.545778	6.617622	5.585441	16.574063	6.582973	5.528158	16.557437	5.361434	7.574574
H	16.819641	5.173587	4.701999	16.815808	5.028146	4.792505	16.855067	5.105221	4.762948	16.850281	5.06997	4.777665	16.884306	5.013574	4.745193	16.557129	6.134181	5.969792
C	7.755882	7.339491	5.157363	7.742669	7.382335	5.157909	7.757772	7.352089	5.140073	7.735655	7.400048	5.126492	7.760822	7.372112	5.176284	7.902119	7.421738	4.920355
C	8.827117	8.389893	5.467351	8.830513	8.428385	5.424109	8.840033	8.397358	5.464624	8.820549	8.454378	5.413648	8.844839	8.39749	5.569599	9.01918	8.418469	5.306238
H	9.70045	8.318682	4.80331	9.683153	8.344947	4.734966	9.720593	8.312678	4.810707	9.692089	8.360138	4.748991	9.750977	8.331107	4.935591	9.992816	8.18199	4.833694
H	9.16899	8.298618	6.50938	9.202389	8.353758	6.457207	9.166316	8.301882	6.51127	9.162014	8.389412	6.458114	9.144836	8.257138	6.626955	9.160459	8.441988	6.405922
H	8.402498	9.394384	5.328056	8.405992	9.432973	5.284432	8.424193	9.40512	5.316854	8.39703	9.456628	5.249765	8.444854	9.423227	5.447531	8.740372	9.437472	4.970553
C	6.51932	7.68749	5.992141	6.528806	7.761502	6.012566	6.512805	7.70225	5.974341	6.49853	7.774764	5.962696	6.498579	7.691494	6.004648	6.580398	7.97686	5.497389
H	6.723891	7.548875	7.064304	6.761455	7.667568	7.084028	6.714631	7.558167	7.046461	6.712201	7.679227	7.038216	6.673158	7.479952	7.078518	6.584597	7.943711	6.60607
H	5.638478	7.087762	5.721475	5.639986	7.153548	5.790992	5.633503	7.102747	5.695569	5.618018	7.161305	5.720505	5.609835	7.1206	5.670431	5.688231	7.431169	5.13222
H	6.250606	8.739927	5.822125	6.255665	8.807203	5.809786	6.250166	8.757051	5.804845	6.228523	8.820971	5.754256	6.248086	8.76464	5.89352	6.461511	9.034133	5.186862
C	7.402072	7.383352	3.665816	7.357522	7.411983	3.672999	7.41439	7.399629	3.638726	7.376937	7.421792	3.62695	7.444264	7.481108	3.668563	7.787617	7.344195	3.377936
H	7.026367	8.381086	3.391851	7.004686	8.416213	3.392063	7.04144	8.399345	3.365376	7.011989	8.420989	3.340595	7.06652	8.494488	3.422209	7.533097	8.337994	2.954652
H	6.618232	6.65115	3.417908	6.547374	6.700854	3.450122	6.632492	6.666102	3.386455	6.583254	6.695049	3.392572	6.667489	6.747603	3.370246	6.992559	6.634891	3.068407
H	8.281758	7.172832	3.038376	8.216984	7.169123	3.029159	8.301338	7.188557	3.020898	8.254182	7.192809	3.001531	8.348568	7.297838	3.053244	8.740642	7.017517	2.914354

Table S15. Coordinates for geometry optimized structures from DFT calculations of **3**, **4** and **5**.

	3							**4**							**5**						
	TPSSh; Disp ON			TPSSh; Disp OFF				TPSSh; Disp ON			TPSSh; Disp OFF				TPSSh; Disp ON			TPSSh; Disp OFF		
Mo	3.48299	13.86865	8.117185	3.506699	13.865685	8.100557	Mo	5.880729	13.763983	10.649209	5.887765	13.747234	10.684524	Mo	8.410091	12.835766	6.742804	8.409801	12.876746	6.758468
S	5.032082	14.445455	6.418126	5.058527	14.483209	6.418293	S	6.737853	13.221615	12.803536	6.718077	13.172139	12.839628	S	6.896473	13.376478	8.57846	6.882468	13.391993	8.593007
S	4.462121	15.827742	9.182797	4.456786	15.833728	9.182644	S	4.197896	12.094087	11.235066	4.192506	12.078354	11.24283	S	9.388498	14.895431	7.405527	9.367944	14.932209	7.45992
P	1.302588	14.446577	9.125453	1.296546	14.412106	9.103467	P	4.100229	15.018123	9.459507	4.12062	15.035541	9.469515	P	6.460752	11.850973	5.564718	6.469831	11.865673	5.54434
P	3.297761	12.880756	10.372453	3.29358	12.836458	10.353127	P	5.698511	12.979786	8.298358	5.724665	12.989295	8.303271	P	8.171611	10.436718	7.333431	8.189292	10.45021	7.326299
O	1.392782	12.951081	5.970774	1.500831	12.979693	5.862417	O	6.708583	16.75133	11.065082	6.75701	16.697674	11.260286	O	9.005101	13.522059	3.751042	9.057034	13.698325	3.809645
O	4.042535	10.82872	7.638821	4.176917	10.866027	7.50968	O	8.799675	14.087319	9.573432	8.85649	14.038632	9.739884	O	11.246866	11.687462	6.089104	11.306072	11.854362	6.151593
N	0.96255	11.715214	9.448466	0.947433	11.665691	9.416493	N	6.046929	15.633327	7.588367	6.075317	15.656784	7.582183	N	8.236168	9.952856	4.604829	8.259326	9.955891	4.582312
N	1.576779	14.417666	11.851678	1.576735	14.407971	11.854218	N	3.125971	13.405843	7.479463	3.120784	13.39631	7.487316	N	5.52675	9.772462	7.085237	5.52045	9.780423	7.090326
C	2.169143	13.290891	6.775361	2.235628	13.306313	6.710557	C	6.388663	15.638288	10.897869	6.412978	15.605512	11.020505	C	8.770547	13.255723	4.86736	8.79438	13.370017	4.902815
C	3.822982	11.962397	7.821645	3.911085	11.979348	7.747048	C	7.701987	13.964067	9.958831	7.736746	13.928799	10.060215	C	10.180893	12.103743	6.338335	10.213369	12.208009	6.380211
C	5.927588	15.867356	6.900998	5.931898	15.91435	6.90967	C	5.722421	11.981295	13.52559	5.689979	11.935853	13.547449	C	7.402285	14.910247	9.248117	7.377429	14.916426	9.292297
C	5.688956	16.458464	8.106557	5.677149	16.495173	8.117003	C	4.601896	11.483985	12.830224	4.573156	11.452878	12.838202	C	8.490559	15.563917	8.749878	8.464826	15.582315	8.808682
C	6.443423	17.687055	8.577149	6.40772	17.735389	8.596469	C	3.810358	10.485019	13.435314	3.766672	10.4575	13.429645	C	8.970355	16.895898	9.294736	8.938272	16.907748	9.375933
H	6.677725	17.586928	9.650078	6.640907	17.633074	9.669408	H	2.942185	10.100767	12.891794	2.90039	10.084073	12.875707	H	10.072319	16.902255	9.339496	10.040002	16.915821	9.425767
H	5.777686	18.566531	8.4928	5.726492	18.603488	8.517102	C	4.105766	9.975721	14.701994	4.044131	9.938391	14.696835	H	8.690803	17.695474	8.583	8.6617	17.718253	8.67542
C	7.723014	17.924996	7.766134	7.685677	18.003604	7.791364	C	5.236839	10.479657	15.404523	5.173285	10.428238	15.413743	C	8.374056	17.201526	10.674193	8.335555	17.192251	10.757624
H	8.486955	17.18275	8.059695	8.467096	17.282179	8.090626	C	6.020193	11.46912	14.805965	5.971271	11.413989	14.827824	H	8.859704	16.563574	11.434484	8.826652	16.552636	11.512934
H	8.132013	18.920347	8.002907	8.06849	19.008843	8.030681	H	6.891339	11.859362	15.340562	6.840386	11.793939	15.373015	H	8.586044	18.247877	10.947194	8.537793	18.237649	11.041837
C	7.443018	17.791879	6.267784	7.421315	17.865767	6.290524	C	3.238386	8.905041	15.317205	3.157281	8.87305	15.294205	C	6.868107	16.930919	10.67855	6.831603	16.910211	10.759437
H	8.339456	18.039658	5.676823	8.320977	18.125152	5.709344	H	2.412899	8.625973	14.646526	2.338066	8.610161	14.609531	H	6.386766	17.54581	9.896879	6.342525	17.540213	9.994862
H	6.656672	18.512573	5.979778	6.630447	18.577583	5.993157	H	2.805145	9.242306	16.274262	2.714249	9.207482	16.247793	H	6.418466	17.223894	11.640973	6.383893	17.179415	11.729794
C	6.980656	16.369098	5.9316	6.981099	16.43736	5.946658	H	3.822839	7.996071	15.539838	3.726827	7.954674	15.517019	C	6.585773	15.447915	10.407992	6.554731	15.431527	10.458548
H	6.587656	16.322754	4.902105	6.591942	16.390166	4.915758	C	5.584109	9.950953	16.774488	5.505417	9.892059	16.784952	H	6.817005	14.852268	11.311132	6.781265	14.819814	11.352176
H	7.84567	15.679891	5.957239	7.856776	15.761596	5.970063	H	4.755013	10.106687	17.485595	4.673632	10.052795	17.491829	H	5.513086	15.288143	10.207498	5.483314	15.273149	10.250378
C	0.219635	12.970912	9.470203	0.213187	12.928044	9.43858	H	6.47936	10.446183	17.177417	6.401778	10.380017	17.194225	C	6.899243	10.490006	4.380037	6.92488	10.503665	4.35817
H	-0.300616	13.164003	10.426917	-0.309616	13.120773	10.394823	H	5.775032	8.864484	16.747282	5.689198	8.804349	16.757486	H	6.094498	9.732526	4.436968	6.117175	9.74799	4.40694
H	-0.520766	12.962668	8.663665	-0.528206	12.922906	8.632383	C	4.709901	16.022595	8.022135	4.740413	16.042235	8.030445	H	6.865931	10.956892	3.389831	6.897922	10.971584	3.367689
C	1.930771	11.626005	10.535173	1.923694	11.575381	10.497873	H	3.942398	15.956226	7.227886	3.968368	15.981653	7.239205	C	8.349463	9.278334	5.892937	8.371445	9.293315	5.878362

H	2.433638	10.654846	10.490173	2.426846	10.604177	10.444268	H	4.740059	17.054019	8.38984	4.77408	17.07387	8.398752	H	9.357556	8.860211	5.986331	9.378826	8.87237	5.972265
H	1.488578	11.749797	11.541832	1.484291	11.687421	11.507896	C	6.067356	14.285469	7.031053	6.094131	14.30299	7.036385	H	7.617402	8.461321	6.037111	7.639693	8.47598	6.025276
C	2.966808	13.989114	11.823829	2.958576	13.947849	11.808233	H	7.079317	14.061587	6.676462	7.105222	14.078994	6.678019	C	6.573606	9.892537	8.093189	6.584076	9.903078	8.083566
H	3.181535	13.371367	12.701881	3.166125	13.32914	12.68822	H	5.360614	14.136051	6.19328	5.386474	14.149674	6.199323	H	6.770923	8.909076	8.529657	6.77966	8.919536	8.522857
H	3.70276	14.815414	11.796982	3.710636	14.760152	11.77592	C	4.0645	12.319665	7.731744	4.08401	12.328065	7.738742	H	6.327474	10.588727	8.916694	6.347645	10.603543	8.906959
C	1.275709	15.328578	10.757545	1.26451	15.294609	10.741011	H	4.268362	11.79372	6.794746	4.283685	11.79887	6.801555	C	5.122339	11.081085	6.585538	5.129517	11.086577	6.566937
H	1.958735	16.196233	10.682041	1.937505	16.169428	10.650458	H	3.710733	11.576046	8.470466	3.745414	11.583864	8.484621	H	4.835615	11.795983	7.379323	4.84102	11.812602	7.350749
H	0.254474	15.710318	10.862273	0.239384	15.66699	10.846607	C	2.709828	14.048048	8.720262	2.726475	14.063857	8.724602	H	4.268341	10.965135	5.911529	4.27654	10.963285	5.891573
C	0.269081	15.559679	8.116665	0.253109	15.53013	8.100507	H	2.328336	13.345829	9.484666	2.342843	13.375914	9.501787	C	5.543764	13.073958	4.513419	5.542139	13.072325	4.468905
C	-1.105676	15.71305	8.384214	-1.126253	15.668343	8.355442	H	1.920532	14.775319	8.507145	1.940833	14.793883	8.503906	H	6.32026	13.416888	3.806387	6.326239	13.414934	3.76956
H	-1.578919	15.15597	9.197338	-1.604747	15.095383	9.153944	C	3.237317	16.25259	10.53877	3.252675	16.291842	10.534663	C	5.076845	14.289839	5.33563	5.0483	14.296975	5.262916
C	-1.880796	16.580355	7.613534	-1.902904	16.541233	7.591924	H	4.059491	16.914072	10.864371	4.082413	16.947392	10.854692	H	4.332897	13.960895	6.082699	4.293799	13.974339	6.001977
H	-2.947429	16.682965	7.831966	-2.972195	16.629169	7.80392	C	2.189973	17.12269	9.817305	2.218005	17.168726	9.800556	H	5.925238	14.712744	5.897504	5.883138	14.737453	5.831265
C	-1.313358	17.327284	6.562599	-1.33464	17.311356	6.558545	H	1.361016	16.490061	9.456215	1.381397	16.543665	9.44387	C	4.451661	15.355784	4.42543	4.428808	15.346029	4.327541
C	0.061282	17.180218	6.314259	0.043433	17.179736	6.321468	H	2.627046	17.61552	8.934588	2.663249	17.647152	8.914067	H	4.092357	16.200292	5.036627	4.04931	16.192807	4.923413
H	0.528579	17.755271	5.510161	0.513529	17.772062	5.531564	C	1.621215	18.177685	10.779234	1.658797	18.245921	10.744841	H	5.234056	15.75601	3.755167	5.218857	15.749786	3.668542
C	0.843472	16.306781	7.076973	0.826759	16.300519	7.077071	H	2.431111	18.868157	11.07657	2.474072	18.935189	11.03001	C	3.30801	14.778301	3.582695	3.306709	14.750511	3.468795
H	1.910917	16.200905	6.861462	1.896585	16.20961	6.868289	H	0.861615	18.781782	10.255992	0.906357	18.847873	10.208629	H	2.900292	15.550523	2.909266	2.91312	15.510566	2.773298
C	-2.168352	18.239892	5.719809	-2.18849	18.232012	5.72301	C	1.020676	17.526542	12.030721	1.048936	17.626975	12.007725	H	2.484132	14.471043	4.252726	2.466701	14.4534	4.123137
H	-2.764271	17.65255	5.000034	-2.768119	17.655206	4.981671	H	0.643186	18.299986	12.72015	0.688874	18.419245	12.685218	C	3.775553	13.561548	2.775453	3.795966	13.522841	2.691891
H	-1.554544	18.950453	5.147446	-1.573462	18.960403	5.175047	H	0.151544	16.910501	11.73538	0.165649	17.024681	11.726405	H	4.534674	13.87946	2.038194	4.561054	13.833207	1.957603
H	-2.878345	18.806341	6.342266	-2.91304	18.778154	6.346651	C	2.049117	16.637464	12.740147	2.061771	16.730627	12.730014	H	2.936071	13.130211	2.205436	2.967884	13.073996	2.11847
C	0.095471	10.492159	9.282918	0.065171	10.445287	9.269086	H	1.593017	16.136991	13.610298	1.594597	16.247246	13.604107	C	4.382858	12.484607	3.688422	4.399252	12.464235	3.630258
C	0.999052	9.250382	9.184597	0.953267	9.192326	9.16329	H	2.871145	17.266785	13.126877	2.89053	17.352227	13.114769	H	3.594845	12.109231	4.363818	3.603206	12.088401	4.29597
H	1.799113	9.411456	8.445887	1.73402	9.327534	8.398775	C	2.63628	15.584931	11.789597	2.637391	15.655449	11.79585	H	4.72268	11.628946	3.083919	4.756607	11.605875	3.040109
H	0.394048	8.3896	8.863254	0.327695	8.33596	8.869976	H	3.40633	14.98745	12.304528	3.397262	15.057203	12.324612	C	8.7966	9.169587	3.44608	8.799586	9.141752	3.428288
H	1.455885	8.982763	10.149084	1.433125	8.929992	10.117974	H	1.842103	14.881763	11.482009	1.832942	14.958913	11.500252	C	8.74447	10.048055	2.182744	8.735244	9.987701	2.142888
C	-0.673256	10.611295	7.954733	-0.725336	10.560809	7.952583	C	6.751811	16.663998	6.744218	6.756698	16.685337	6.707797	H	7.720467	10.185294	1.804318	7.707753	10.122415	1.773109
H	0.021581	10.801065	7.123003	-0.046866	10.735786	7.10381	C	6.795569	17.992101	7.521284	6.804516	18.027336	7.461478	H	9.322678	9.563883	1.381678	9.299211	9.475269	1.349012
H	-1.427582	11.411835	7.972729	-1.476088	11.364598	7.97623	H	5.809076	18.47465	7.588886	5.81601	18.50334	7.544143	H	9.183158	11.037445	2.38324	9.187052	10.978898	2.303281
H	-1.207404	9.669358	7.759639	-1.267104	9.61942	7.775639	H	7.462726	18.694531	6.999899	7.452694	18.725158	6.910361	C	8.024824	7.858646	3.2023	8.019605	7.828292	3.218674
C	-0.896062	10.324806	10.450904	-0.913727	10.285643	10.450143	H	7.181211	17.831195	8.539459	7.21925	17.89436	8.47252	H	8.07753	7.194549	4.0794	8.085226	7.173709	4.102034

H	-1.59161	11.176513	10.508242	-1.602689	11.141905	10.519004	C	6.05571	16.875793	5.386424	6.037369	16.87778	5.357665	H	8.45453	7.318908	2.34357	8.435275	7.275896	2.360919
H	-0.365964	10.243266	11.413033	-0.376019	10.193549	11.407084	H	6.033824	15.94379	4.799962	6.013502	15.942128	4.777071	H	6.96443	8.058001	2.980823	6.956036	8.023538	3.008779
H	-1.492681	9.409055	10.314158	-1.520294	9.375834	10.316544	H	6.594234	17.634313	4.796424	6.563572	17.634152	4.753727	C	10.278	8.862959	3.732005	10.283793	8.828894	3.694697
C	4.792777	12.008222	10.946739	4.781478	11.956052	10.950788	H	5.019948	17.225496	5.521269	5.00169	17.224554	5.500691	H	10.814603	9.784067	4.005765	10.842393	9.751581	3.91509
C	4.738526	11.150421	12.061284	4.711802	11.087196	12.056504	C	8.205295	16.208049	6.523462	8.210985	16.243372	6.461547	H	10.742345	8.441307	2.82803	10.720396	8.365649	2.796979
H	3.796706	10.987405	12.592423	3.762288	10.913607	12.569707	H	8.676186	15.946995	7.483303	8.714904	16.013071	7.412821	H	10.411598	8.125004	4.537125	10.429384	8.121576	4.524715
C	5.890042	10.495749	12.505004	5.857454	10.43343	12.51755	H	8.776997	17.027436	6.062822	8.757208	17.062136	5.969407	C	9.445375	9.846495	8.54425	9.469148	9.838891	8.534075
H	5.827899	9.829438	13.369818	5.77983	9.759533	13.375277	H	8.279336	15.342941	5.847706	8.28311	15.365549	5.802223	H	10.395359	10.047607	8.017746	10.415729	10.05041	8.004532
C	7.126939	10.680834	11.860961	7.106814	10.62889	11.901643	C	6.88932	11.619274	7.891512	6.92425	11.632387	7.872545	C	9.39382	8.340303	8.863921	9.424648	8.326225	8.829626
C	7.174185	11.550647	10.756851	7.170588	11.508401	10.806153	H	7.869365	12.104244	8.048864	7.899834	12.122707	8.04407	H	8.442635	8.095254	9.366813	8.477314	8.069244	9.333905
H	8.124577	11.718547	10.242598	8.129581	11.685919	10.311341	C	6.836735	11.127754	6.432455	6.885754	11.168317	6.402601	H	9.434593	7.740825	7.940736	9.461859	7.742229	7.896664
C	6.025545	12.203111	10.302019	6.027591	12.159474	10.334244	H	6.930137	11.971029	5.73012	6.981812	12.025134	5.717377	C	10.555879	7.951495	9.791537	10.593869	7.919357	9.741876
H	6.083365	12.869366	9.436164	6.101644	12.833102	9.475758	H	5.862646	10.648605	6.234928	5.915606	10.688997	6.186637	H	10.495559	6.876106	10.02725	10.530057	6.840295	9.959864
C	8.364742	9.953649	12.323245	8.338751	9.906561	12.387156	C	7.95134	10.101407	6.176499	8.00853	10.15385	6.128818	H	11.510813	8.109949	9.258552	11.545261	8.079838	9.203219
H	8.233212	9.536287	13.332089	8.17084	9.445066	13.370886	H	7.893436	9.745596	5.134526	7.951364	9.817916	5.080083	C	10.546787	8.784791	11.078563	10.602087	8.729657	11.043218
H	9.239621	10.622226	12.328159	9.197827	10.591609	12.46089	H	8.931936	10.597238	6.292739	8.985818	10.654836	6.250646	H	11.402615	8.510395	11.717574	11.469108	8.446958	11.663457
H	8.597891	9.118754	11.640241	8.622193	9.10662	11.681899	C	7.856984	8.922859	7.152964	7.92782	8.955292	7.081268	H	9.631374	8.552048	11.653076	9.698076	8.483073	11.6298
C	1.050506	14.839626	13.198187	1.111431	14.902862	13.205245	H	6.914992	8.374955	6.966753	6.997069	8.394048	6.87921	C	10.575545	10.285866	10.76659	10.622415	10.235932	10.757794
C	1.348994	13.727995	14.219295	1.37818	13.810799	14.25667	H	8.680151	8.211234	6.974046	8.763721	8.261087	6.892487	H	10.522009	10.875009	11.697102	10.572663	10.807332	11.699675
H	1.023914	12.749484	13.831848	0.967521	12.843037	13.928069	C	7.877696	9.405108	8.608533	7.934999	9.408945	8.545909	H	11.53547	10.539905	10.281215	11.579227	10.503277	10.273503
H	0.798197	13.935344	15.148709	0.8846	14.093499	15.198646	H	8.859614	9.862445	8.827966	8.912692	9.867058	8.781869	C	9.426082	10.689575	9.83323	9.46439	10.656245	9.840436
H	2.415794	13.668113	14.481792	2.448409	13.684618	14.478583	H	7.760451	8.553388	9.298858	7.819711	8.542271	9.2179	H	9.490574	11.760883	9.581935	9.52923	11.731975	9.609864
C	1.681418	16.165403	13.660469	1.821482	16.207655	13.613752	C	6.777979	10.441995	8.877472	6.824332	10.431294	8.831761	H	8.461821	10.541825	10.351389	8.506101	10.500337	10.367063
H	2.777686	16.076881	13.722148	2.912234	16.066133	13.67379	H	6.842897	10.810885	9.914138	6.884451	10.77743	9.876389	C	4.392776	8.85235	7.454477	4.367802	8.896796	7.510715
H	1.305663	16.44279	14.658007	1.470197	16.539063	14.603929	H	5.786826	9.966512	8.769942	5.839447	9.945934	8.712327	C	4.972774	7.460996	7.765777	4.912927	7.495543	7.842792
H	1.436974	16.985065	12.966677	1.614955	17.017344	12.89621	C	2.006205	13.081351	6.526632	1.968426	13.010281	6.587588	H	5.633535	7.129048	6.949659	5.530854	7.112756	7.015423
C	-0.478771	14.977823	13.100663	-0.410995	15.125488	13.149987	C	1.019907	12.065257	7.130563	1.04248	11.970761	7.247857	H	4.148925	6.738643	7.865141	4.066982	6.807348	7.990177
H	-0.790057	15.821067	12.466489	-0.694445	15.98539	12.524907	H	1.531292	11.124047	7.387529	1.59134	11.049782	7.500637	H	5.538752	7.436991	8.708861	5.508776	7.475521	8.76741
H	-0.892105	15.158605	14.104251	-0.782712	15.328427	14.165671	H	0.220281	11.832275	6.409839	0.225646	11.697746	6.560886	C	3.465773	8.703661	6.235319	3.402316	8.741132	6.321903
H	-0.922301	14.052989	12.699344	-0.919703	14.227234	12.766256	H	0.548875	12.465558	8.04206	0.587791	12.368636	8.168744	H	2.890467	9.617764	6.02646	2.840156	9.661851	6.106175
							C	2.609832	12.52416	5.225011	2.532691	12.447804	5.269928	H	2.738384	7.901072	6.428189	2.664173	7.960328	6.559107
							H	3.416769	13.180351	4.862169	3.288557	13.129058	4.848434	H	4.048916	8.440374	5.338668	3.948412	8.438307	5.414538

			H	1.826025	12.476333	4.454653	1.713017	12.347837	4.542758	C	3.600092	9.380896	8.663378	3.613939	9.468698	8.726635
			H	3.009627	11.505888	5.342652	2.982249	11.450549	5.387798	H	4.246767	9.470226	9.550521	4.276138	9.555845	9.602468
			C	1.274465	14.388369	6.17266	1.167521	14.277777	6.236978	H	2.775559	8.694371	8.912504	2.777493	8.807025	9.002968
			H	0.708888	14.802419	7.020549	0.61427	14.6859	7.095889	H	3.165512	10.369775	8.447927	3.196319	10.463616	8.505383
			H	0.551153	14.193232	5.366869	0.424468	14.029404	5.464259							
			H	1.991801	15.14789	5.824467	1.83176	15.061652	5.840482							

Table S 16. Coordinates for geometry optimized structures from DFT calculations of the mono reduced complexes $\mathbf{2}^{1-}$ & $\mathbf{3}^{1-}$.

	$\mathbf{2}^{1-}$							$\mathbf{3}^{1-}$						
	TPSSh; Disp ON			TPSSh; Disp OFF				TPSSh; Disp ON			TPSSh; Disp OFF			
Mo	4.270525	12.983218	8.231853	3.911875	13.382175	8.194212	Mo	4.149301	13.137374	8.191915	4.044095	13.306582	8.189404
S	4.532222	14.300295	6.182037	4.312645	14.804713	6.237924	S	4.381273	14.601708	6.24158	4.4664	14.743219	6.247398
S	5.628943	14.912279	9.183593	5.293015	15.191119	9.313502	S	5.537702	14.982567	9.226794	5.480187	15.085254	9.279026
P	2.220115	14.296593	8.983715	1.700248	14.30685	9.047113	P	2.047197	14.309059	8.983449	1.863375	14.342097	8.99439
P	3.64221	12.230425	10.486545	3.443957	12.430843	10.430282	P	3.582435	12.309538	10.431037	3.504446	12.404164	10.421388
O	2.622939	10.93081	6.535914	2.293814	11.549	6.247629	O	2.473689	11.197997	6.393337	2.401203	11.476585	6.257512
O	6.25877	10.568001	7.929931	5.847331	10.948243	7.734619	O	6.15928	10.749851	7.796541	5.97525	10.86329	7.760857
N	1.055911	11.814519	9.504608	0.919119	11.646581	9.519103	N	1.000598	11.776734	9.508799	0.956223	11.725581	9.48654
N	2.351307	14.366038	11.717997	1.907507	14.34917	11.790334	N	2.217448	14.389653	11.705569	2.032054	14.399167	11.742768
C	3.191414	11.702091	7.230213	2.853001	12.226756	7.04207	C	3.062084	11.921482	7.125763	2.969927	12.156486	7.045709
C	5.237945	20.061173	8.082626	7.406881	19.807012	7.905817	C	5.478509	11.708309	7.93828	5.327681	11.838971	7.927485
C	4.794925	15.948581	6.740787	5.187354	16.244775	6.748146	C	4.927545	16.159291	6.829705	5.334385	16.173781	6.77346
C	5.246407	16.217755	8.06041	5.61806	16.409121	8.08762	C	5.435678	16.314917	8.092273	5.777027	16.310694	8.060913
C	5.398338	17.565793	8.449944	6.33538	17.580021	8.422436	C	5.945443	17.652595	8.597866	6.551503	17.533821	8.523927
H	0.126564	15.991504	13.754408	-0.317444	15.763656	13.985771	H	-0.015662	15.934742	13.793013	-0.176962	15.89718	13.898057
H	-0.168413	14.933964	12.343887	-0.614353	14.825174	12.497636	H	-0.300985	14.934856	12.339851	-0.483215	14.936211	12.425894
C	5.111577	18.637596	7.596413	6.634336	18.577853	7.489443	C	6.203488	18.6586	7.471651	7.111774	18.362772	7.362258
H	0.571493	16.547824	12.134343	0.068885	16.476877	12.412609	H	0.428039	16.561667	12.198558	0.23371	16.571586	12.314148
H	5.734988	17.777096	9.470093	6.670427	17.705471	9.457244	H	4.101501	18.934263	7.059279	5.171452	19.079262	6.735586
C	4.679565	18.363647	6.272593	6.199252	18.412377	6.145634	C	5.021188	18.678677	6.502343	6.043089	18.567688	6.287821
C	0.530268	15.662035	12.785194	0.073495	15.535923	12.982639	C	0.392179	15.64914	12.811713	0.215751	15.641959	12.902197
H	2.581517	16.535721	14.421582	2.108629	16.426543	14.577483	H	2.436375	16.506734	14.451179	2.262272	16.508389	14.503796
C	4.545012	17.0311	5.874374	5.489493	17.255666	5.809016	C	4.848372	17.307941	5.838946	5.603974	17.219514	5.704458
H	3.037804	16.875958	12.732667	2.557359	16.825921	12.900952	H	2.899948	16.871218	12.768851	2.722134	16.88252	12.824528
H	4.191327	16.814005	4.861388	5.153927	17.121992	4.775262	H	3.770892	15.608379	13.68439	3.603782	15.624675	13.737096
C	0.744159	13.236936	9.394391	0.412451	13.014092	9.460606	C	0.629031	13.185397	9.430234	0.511307	13.112708	9.401032
H	0.287062	13.663753	10.307185	-0.070051	13.352804	10.397714	H	0.195229	13.581731	10.367576	0.025427	13.483922	10.324221
H	0.046916	13.381218	8.563391	-0.326875	13.080918	8.656768	H	-0.109873	13.312573	8.633931	-0.209301	13.200343	8.582261
C	1.936405	11.490643	10.624215	1.873701	11.433386	10.603843	C	1.917582	11.484949	10.606109	1.884021	11.486807	10.589354
H	2.105999	10.408773	10.619817	2.197618	10.387101	10.574142	H	2.137006	10.412064	10.593941	2.156076	10.425421	10.583844
H	1.523761	11.774169	11.612317	1.45486	11.637971	11.608712	H	1.51255	11.745916	11.603896	1.460498	11.730685	11.583361
C	3.546122	13.539691	11.822921	3.2066	13.683006	11.812559	C	3.445169	13.607093	11.780922	3.304113	13.683607	11.787164
H	3.51936	12.984023	12.765449	3.299767	13.111187	12.742381	H	3.456614	13.044065	12.719759	3.366953	13.121852	12.725505
H	4.492741	14.112045	11.78502	4.063897	14.381537	11.752361	H	4.366693	14.218128	11.733775	4.187418	14.348767	11.725418
C	2.398337	15.25829	10.564825	1.77327	15.2548	10.65232	C	2.206835	15.290111	10.55712	1.947852	15.298999	10.595251
H	3.33025	15.848623	10.500094	2.598515	15.987928	10.574567	H	3.114565	15.916214	10.481144	2.800523	16.00093	10.525771
H	1.546165	15.944541	10.60431	0.826759	15.799934	10.732529	H	1.329136	15.942879	10.608388	1.020893	15.879199	10.658234
C	1.561419	15.546573	7.83179	0.790493	15.45767	7.951199	C	1.307017	15.507239	7.827413	1.010144	15.524162	7.884342
C	0.986565	15.120032	6.618718	0.121487	14.961251	6.816072	C	0.582363	15.045762	6.711519	0.335538	15.048375	6.74101
H	0.863537	14.051648	6.418703	0.084144	13.885527	6.625238	H	0.379311	13.977861	6.59214	0.260753	13.973574	6.555109
C	0.581206	16.046878	5.657137	-0.50465	15.828263	5.915943	C	0.125756	15.936734	5.738255	-0.244429	15.93236	5.829832

H	0.133811	15.690777	4.7244	-1.027954	15.412559	5.049947	H	-0.44299	15.553794	4.885819	-0.771312	15.531315	4.958901
C	0.751445	17.429991	5.860493	-0.472708	17.221513	6.100572	C	0.391557	17.315866	5.829864	-0.160593	17.326644	6.008862
C	1.326109	17.847957	7.070448	0.211425	17.714423	7.226016	C	1.121883	17.769292	6.940959	0.528794	17.797154	7.137672
H	1.478881	18.915004	7.254455	0.256597	18.793611	7.399663	H	1.344888	18.835582	7.039752	0.614628	18.874874	7.304555
C	1.73103	16.925553	8.040215	0.834672	16.853882	8.134512	C	1.576797	16.883858	7.923862	1.10723	16.916431	8.060189
H	2.202675	17.299324	8.949903	1.357923	17.286553	8.989588	H	2.156846	17.27918	8.760112	1.637288	17.333873	8.91866
C	0.374213	18.423452	4.789642	-1.128468	18.1597	5.117103	C	-0.061945	18.267535	4.750182	-0.779467	18.274671	5.011136
H	1.161186	18.473806	4.016805	-0.370298	18.683883	4.510109	H	0.668079	18.289196	3.922019	-0.270173	18.206338	4.034893
H	0.253306	19.434885	5.205323	-1.71743	18.932841	5.635598	H	-0.156982	19.294385	5.133896	-0.714022	19.316673	5.356431
H	-0.560719	18.135253	4.284184	-1.793212	17.616833	4.429348	H	-1.029122	17.959029	4.32448	-1.840444	18.031817	4.837823
C	-0.150349	10.918286	9.401303	-0.150274	10.583468	9.432173	C	-0.166077	10.830425	9.415499	-0.155341	10.707936	9.396173
C	0.316654	9.450953	9.355754	0.526511	9.210304	9.254515	C	0.36715	9.387292	9.342729	0.464717	9.307779	9.222304
H	1.103193	9.31847	8.596576	1.25166	9.239752	8.426313	H	1.148831	9.302865	8.571655	1.183244	9.303082	8.387981
H	-0.536055	8.807985	9.090383	-0.240033	8.456918	9.01741	H	-0.457479	8.707995	9.079113	-0.332949	8.583614	8.996701
H	0.697701	9.095941	10.324868	1.043559	8.868417	10.163431	H	0.778422	9.038632	10.301708	0.975641	8.951079	10.128944
C	-0.874273	11.208252	8.072421	-1.013602	10.829751	8.17997	C	-0.926127	11.103702	8.103199	-1.002665	10.988449	8.140047
H	-0.162202	11.18309	7.233471	-0.381609	10.963464	7.288737	H	-0.228594	11.11701	7.25189	-0.360889	11.10839	7.253678
H	-1.385798	12.182137	8.070928	-1.671526	11.705634	8.282074	H	-1.476648	12.055994	8.121492	-1.632765	11.884255	8.24461
H	-1.643683	10.440014	7.902498	-1.662948	9.95654	8.015472	H	-1.666947	10.306695	7.938592	-1.678163	10.137347	7.965203
C	-1.125455	11.115679	10.579275	-1.056719	10.557005	10.680322	C	-1.127875	10.96949	10.612618	-1.068629	10.719851	10.639699
H	-1.498616	12.151222	10.616301	-1.569417	11.521771	10.821729	H	-1.548556	11.985909	10.66732	-1.53089	11.709226	10.785248
H	-0.638112	10.888695	11.540673	-0.479568	10.334189	11.591448	H	-0.612773	10.756632	11.562683	-0.509298	10.460668	11.552336
H	-1.99396	10.446118	10.473064	-1.829017	9.778169	10.573857	H	-1.96582	10.260793	10.515045	-1.879904	9.983225	10.523074
C	4.704518	11.049793	11.403677	4.700207	11.38664	11.275737	C	4.706193	11.17454	11.33635	4.691038	11.310328	11.307432
C	4.215261	10.085225	12.304073	4.378083	10.351447	12.173925	C	4.265639	10.218896	12.271264	4.301733	10.314587	12.223355
H	3.141766	9.963885	12.464585	3.337091	10.092582	12.378586	H	3.200317	10.078452	12.466977	3.245625	10.117412	12.419305
C	5.096478	9.26853	13.019925	5.385061	9.636204	12.829705	C	5.185183	9.43669	12.97689	5.259691	9.560526	12.908909
H	4.691968	8.520947	13.708592	5.106899	8.831951	13.517191	H	4.818223	8.69548	13.692999	4.929461	8.788021	13.609707
C	6.48987	9.396783	12.880062	6.744492	9.935892	12.629985	C	6.570665	9.591737	12.791889	6.635769	9.781752	12.722442
C	6.973187	10.378499	11.99712	7.060453	10.984792	11.748995	C	7.005627	10.564483	11.874643	7.019859	10.792277	11.823579
H	8.052323	10.509341	11.874755	8.108365	11.249481	11.580223	H	8.077598	10.715796	11.717648	8.082776	10.996235	11.664202
C	6.097264	11.186751	11.267529	6.058239	11.693121	11.078868	C	6.09051	11.338499	11.155369	6.066348	11.538506	11.124253
H	6.495058	11.935277	10.576763	6.328239	12.49704	10.388714	H	6.448757	12.082438	10.438467	6.387898	12.311536	10.420885
C	7.435653	8.49318	13.632212	7.827017	9.142019	13.319238	C	7.557511	8.724545	13.534201	7.665075	8.94646	13.443715
H	6.987481	8.135628	14.571503	7.476887	8.739186	14.281503	H	7.143471	8.375197	14.49207	7.265494	8.544908	14.386957
H	8.380458	9.007643	13.864813	8.722104	9.756765	13.497622	H	8.496256	9.264465	13.730961	8.571467	9.530561	13.664268
H	7.686085	7.604865	13.026175	8.13652	8.284315	12.696535	H	7.811844	7.830431	12.938375	7.972933	8.086741	12.822985
C	1.910951	15.016108	13.002325	1.480958	14.926799	13.120321	C	1.777387	15.005944	13.005758	1.609332	15.005959	13.060271
C	1.73808	13.92811	14.077979	1.378958	13.782064	14.146025	C	1.615447	13.889214	14.053336	1.475502	13.881462	14.104391
H	1.11483	13.105153	13.693669	0.732661	12.977367	13.761958	H	0.985969	13.07877	13.653119	0.820411	13.080509	13.727301
H	1.240023	14.363107	14.957403	0.938292	14.168333	15.077774	H	1.130008	14.300056	14.951346	1.029539	14.292226	15.023038
H	2.696919	13.512267	14.420597	2.357397	13.351715	14.405542	H	2.577314	13.461297	14.371419	2.443314	13.440272	14.384362
C	2.921529	16.075278	13.480231	2.463884	16.000926	13.625253	C	2.782548	16.060324	13.505278	2.611281	16.066664	13.556587
H	3.909512	15.622762	13.660555	3.46505	15.576518	13.799573	H	5.202503	18.071656	9.304526	5.887077	18.168556	9.142169

H	4.271214	20.590956	8.021804	6.82649	20.729828	7.731844	H	3.880674	17.264278	5.309838	4.702236	17.348611	5.081261
H	5.949988	20.638261	7.467549	8.342076	19.912723	7.32903	H	5.624054	17.171392	5.060371	6.387942	16.843284	5.018391
C	4.331145	19.484977	5.324576	6.496614	19.460271	5.099575	H	7.118871	18.372044	6.922339	7.97736	17.83903	6.917017
C	5.585341	11.534775	8.037819	5.200928	11.920116	7.914952	H	6.383696	19.660032	7.896731	7.482826	19.330541	7.738877
H	5.581417	20.097144	9.127085	7.668717	19.766821	8.973505	H	5.154413	19.454166	5.729849	6.41625	19.220159	5.480898
H	4.035955	19.093655	4.339646	6.085754	19.169227	4.121464	H	6.861862	17.492237	9.191959	7.365983	17.215248	9.197257
H	5.178869	20.176547	5.179763	7.582642	19.617635	4.979226							
H	3.49282	20.090087	5.712144	6.0668	20.440072	5.371485							

Table S17. Coordinates for geometry optimized structures from DFT calculations of the mono reduced complexes $\mathbf{4}^{1-}$ and $\mathbf{5}^{1-}$.

	$\mathbf{4}^{1-}$							$\mathbf{5}^{1-}$						
	TPSSh; Disp ON			TPSSh; Disp OFF				TPSSh; Disp ON			TPSSh; Disp OFF			
Mo	6.535103	13.339057	10.473644	6.420517	13.372575	10.533261	Mo	8.949124	12.687149	7.042195	8.847576	12.74927	7.036237	
S	6.444843	13.741981	12.894785	6.365925	13.659817	12.97342	S	7.635249	13.284086	9.128494	7.494469	13.284568	9.120564	
S	5.111675	11.341706	11.132646	4.962981	11.37361	11.132483	S	8.860573	15.127273	6.781005	8.835689	15.201664	6.913347	
P	4.501505	14.648748	9.73245	4.43977	14.745272	9.696617	P	6.820358	12.052164	5.829083	6.757289	12.031026	5.750639	
P	6.081457	12.835551	8.102512	6.034039	12.870177	8.129819	P	8.497867	10.298775	7.426744	8.453813	10.326953	7.401995	
O	8.209081	15.972492	10.277624	8.10781	16.000447	10.520501	O	10.472712	12.61498	4.313764	10.406951	12.875415	4.33441	
O	9.426218	12.268549	9.859199	9.348458	12.348332	10.031606	O	11.889793	12.010694	7.924516	11.815422	12.178588	7.894876	
N	6.08419	15.585541	7.609326	6.122737	15.622575	7.605133	N	8.295801	9.968857	4.655315	8.325317	9.970131	4.616804	
N	3.371886	13.200443	7.688536	3.310609	13.248681	7.647017	N	5.760381	9.933193	7.231217	5.701811	9.900216	7.192131	
C	7.54392	14.991342	10.289059	7.438529	15.023656	10.453071	C	9.861582	12.57925	5.33091	9.782005	12.75517	5.337493	
C	8.33019	12.593737	10.168969	8.230374	12.648293	10.280105	C	10.778367	12.342329	7.675651	10.685295	12.449126	7.660523	
C	5.290633	12.612368	13.599471	5.275598	12.463677	13.668021	C	7.287642	15.00013	9.01419	7.282735	15.026988	9.15297	
C	4.712258	11.56996	12.830517	4.669637	11.466454	12.864462	C	7.816311	15.78692	8.027874	7.856872	15.844863	8.219777	
C	3.786527	10.708344	13.460946	3.817951	10.528065	13.490476	C	7.495014	17.265632	7.902827	7.680321	17.354014	8.238475	
H	3.339835	9.903974	12.867357	3.351432	9.755956	12.869821	H	8.410656	17.821471	7.635468	8.636256	17.838572	7.974113	
C	3.411098	10.848469	14.800587	3.546155	10.547158	14.862483	H	6.802071	17.405824	7.050093	6.969167	17.646366	7.441109	
C	3.986183	11.897739	15.567284	4.151618	11.551159	15.666563	C	6.866856	17.851628	9.171922	7.173328	17.877086	9.587454	
C	4.910231	12.748325	14.952696	4.998646	12.479989	15.053281	H	7.644484	17.974079	9.947911	7.991727	17.842483	10.329598	
H	5.353254	13.561223	15.537397	5.468702	13.254742	15.668073	H	6.463081	18.855923	8.961146	6.873871	18.934112	9.490808	
C	2.406342	9.906169	15.4191	2.623138	9.519461	15.473333	C	5.774348	16.922098	9.701123	6.00714	17.022927	10.08683	
H	2.063089	9.155792	14.691581	2.248485	8.821276	14.710265	H	5.009441	16.777564	8.915843	5.19376	17.047873	9.338663	
H	1.520947	10.449249	15.793015	1.752011	9.993128	15.958742	H	5.262597	17.368507	10.569952	5.592049	17.431537	11.023282	
H	2.834063	9.372308	16.285414	3.133084	8.92945	16.254683	C	6.371713	15.564673	10.087369	6.457197	15.573666	10.306496	
C	3.601692	12.093967	17.014132	3.88706	11.617788	17.152074	H	6.938895	15.66688	11.033164	7.053238	15.509414	11.237883	
H	2.518733	12.279054	17.122596	2.813326	11.757423	17.367755	H	5.56772	14.839028	10.298107	5.581769	14.922033	10.471009	
H	4.138453	12.946297	17.456463	4.437032	12.450754	17.614612	C	7.058526	10.73234	4.54074	7.069718	10.701942	4.477045	
H	3.827144	11.197709	17.617917	4.189078	10.685949	17.661179	H	6.143668	10.106641	4.53542	6.174183	10.048513	4.463866	
C	4.854608	15.841368	8.351061	4.870978	15.907347	8.29989	H	7.09065	11.28659	3.596168	7.098864	11.246601	3.526095	
H	3.946549	15.887835	7.716711	3.988179	15.947681	7.630079	C	8.431244	9.228824	5.904841	8.444233	9.244802	5.878722	
H	4.958071	16.806071	8.859864	4.965085	16.884147	8.787984	H	9.398175	8.712127	5.890709	9.417345	8.739143	5.889815	
C	6.118422	14.289111	6.941495	6.138445	14.316307	6.953191	H	7.641229	8.469403	6.062528	7.66063	8.475513	6.023009	
H	7.075084	14.20279	6.413817	7.101706	14.199667	6.44286	C	6.851809	9.883838	8.202928	6.801125	9.881531	8.158992	
H	5.305872	14.146356	6.203923	5.336521	14.18865	6.200391	H	6.937658	8.866515	8.596074	6.903477	8.868151	8.560151	
C	4.386787	12.148412	7.731608	4.334834	12.204125	7.717266	H	6.700611	10.568978	9.05803	6.637629	10.569755	9.01037	
H	4.448131	11.663982	6.752209	4.418393	11.721637	6.738078	C	5.459367	11.311574	6.855813	5.392862	11.265054	6.76584	
H	4.165974	11.36824	8.483342	4.100416	11.421464	8.463588	H	5.304533	11.974024	7.727581	5.201176	11.950963	7.613172	
C	3.072668	13.690542	9.02988	3.012367	13.788478	8.973436	H	4.555833	11.335248	6.238224	4.502283	11.248846	6.128912	
H	2.823262	12.884001	9.745128	2.743756	13.00696	9.71019	C	5.903618	13.383828	4.906715	5.81586	13.298594	4.741908	
H	2.229956	14.388374	8.987356	2.174755	14.490331	8.897537	H	6.709641	13.909716	4.362379	6.61129	13.741872	4.113263	
C	3.656419	15.708155	11.006672	3.575076	15.894718	10.893794	C	5.294066	14.371061	5.920757	5.265534	14.409467	5.658612	
H	4.504754	16.205393	11.512331	4.419345	16.459709	11.332109	H	4.491884	13.86243	6.484585	4.493085	13.984185	6.324537	

C	2.689395	16.792932	10.500463	2.58194	16.906872	10.288752	H	6.058726	14.677751	6.650268	6.072939	14.7947	6.302262
H	1.843726	16.321129	9.968922	1.744443	16.366216	9.813624	C	4.694958	15.590429	5.209462	4.638637	15.54817	4.840621
H	3.185223	17.464313	9.782088	3.061747	17.509327	9.502107	H	4.249829	16.27454	5.951919	4.229635	16.314597	5.52068
C	2.149628	17.617232	11.682245	2.022036	17.840533	11.375517	H	5.506211	16.149267	4.707934	5.427925	16.040759	4.243739
H	2.989967	18.167617	12.143226	2.846791	18.457228	11.776758	C	3.647215	15.163619	4.173729	3.543931	15.026977	3.901838
H	1.437575	18.374635	11.313385	1.29543	18.537631	10.924993	H	3.252549	16.042808	3.636862	3.136915	15.850121	3.290395
C	1.484921	16.732224	12.744885	1.371743	17.056122	12.521206	H	2.791251	14.700875	4.698977	2.704351	14.636527	4.506205
H	1.149115	17.347884	13.596403	1.020467	17.747122	13.306094	C	4.230021	14.152987	3.17777	4.076406	13.908582	2.998405
H	0.580124	16.266655	12.312292	0.47776	16.530378	12.138086	H	5.016771	14.647529	2.579297	4.837237	14.324531	2.313002
C	2.43343	15.625331	13.22138	2.344815	16.028178	13.110579	H	3.45296	13.820514	2.468916	3.26658	13.507215	2.365852
H	1.924712	14.963437	13.942566	1.847282	15.432581	13.894524	C	4.842365	12.933425	3.887719	4.707775	12.765706	3.812397
H	3.292691	16.074399	13.752528	3.184929	16.555745	13.598199	H	4.041328	12.375487	4.404606	3.919521	12.281562	4.415394
C	2.955254	14.802787	12.037288	2.902857	15.093658	12.026615	H	5.273426	12.253031	3.136875	5.099671	12.000682	3.124176
H	3.646283	14.021064	12.384509	3.624462	14.385856	12.464752	C	8.626029	9.14852	3.437117	8.689865	9.137258	3.411158
H	2.102296	14.294107	11.554097	2.073152	14.497393	11.606824	C	8.523385	10.032714	2.180094	8.581692	9.996987	2.137292
C	6.519488	16.723261	6.724551	6.611383	16.741928	6.717251	H	7.482652	10.272593	1.915923	7.539476	10.208903	1.855533
C	6.479006	18.040021	7.521973	6.583755	18.070487	7.495915	H	8.959651	9.49477	1.324891	9.039914	9.451092	1.298557
H	5.452243	18.386753	7.711397	5.562161	18.445685	7.65707	H	9.080192	10.972413	2.320129	9.116822	10.951691	2.259072
H	6.986451	18.826169	6.942767	7.122723	18.834696	6.915528	C	7.692235	7.930691	3.281103	7.78905	7.893458	3.256803
H	6.999871	17.928566	8.485855	7.081543	17.966781	8.472611	H	7.794908	7.234809	4.128441	7.898341	7.205437	4.109712
C	5.630423	16.86044	5.471607	5.763987	16.892316	5.436322	H	7.933447	7.377168	2.359356	8.057167	7.338931	2.342997
H	5.704537	15.971399	4.826048	5.824414	15.993961	4.802295	H	6.638508	8.246653	3.220265	6.72787	8.178893	3.177023
H	5.93766	17.735275	4.876319	6.122094	17.74722	4.840296	C	10.088733	8.675676	3.543343	10.162255	8.700149	3.538233
H	4.573878	16.996162	5.753185	4.705082	17.073359	5.681114	H	10.753683	9.531951	3.735507	10.810529	9.574584	3.704404
C	7.984164	16.488508	6.307402	8.080811	16.467707	6.341575	H	10.391134	8.202712	2.596519	10.47738	8.206235	2.606174
H	8.612967	16.333911	7.197794	8.688138	16.315608	7.247334	H	10.237946	7.930186	4.338431	10.325966	7.98208	4.355399
H	8.357392	17.369112	5.762557	8.4849	17.332694	5.793432	C	9.663996	9.343582	8.518528	9.633136	9.38982	8.511661
H	8.102311	15.621398	5.640896	8.197784	15.58891	5.690266	H	10.649318	9.541451	8.058156	10.614157	9.599032	8.046068
C	7.177218	11.60654	7.238113	7.140452	11.614897	7.29575	C	9.463005	7.81824	8.581671	9.457526	7.860115	8.579333
H	8.190819	12.010786	7.4134	8.150771	12.021664	7.48642	H	8.474557	7.589381	9.017526	8.475175	7.615475	9.020335
C	6.978058	11.454382	5.71871	6.975389	11.450379	5.772195	H	9.478185	7.372751	7.574676	9.475626	7.412431	7.573434
H	7.06811	12.426142	5.209012	7.074822	12.418279	5.257073	C	10.551099	7.16432	9.44902	10.559414	7.219877	9.440988
H	5.961169	11.077415	5.510995	5.964638	11.068751	5.544317	H	10.38032	6.075872	9.502198	10.399726	6.12968	9.495067
C	8.001755	10.467662	5.133873	8.013269	10.463019	5.211455	H	11.53233	7.309761	8.961372	11.536043	7.372944	8.946463
H	7.830581	10.353125	4.05025	7.859365	10.342347	4.125805	C	10.591024	7.769016	10.857444	10.603743	7.823741	10.849316
H	9.015861	10.890556	5.253818	9.024048	10.890356	5.342987	H	11.402061	7.310414	11.447965	11.430252	7.379839	11.429735
C	7.935964	9.104713	5.8334	7.942477	9.103169	5.915924	H	9.644742	7.53264	11.378368	9.669405	7.568305	11.38253
H	6.953865	8.640155	5.627394	6.970909	8.626921	5.688099	C	10.764125	9.291963	10.801981	10.749588	9.349239	10.793384
H	8.701572	8.425672	5.421719	8.723975	8.429239	5.525982	H	10.743201	9.719613	11.81848	10.722475	9.775818	11.810327
C	8.11049	9.251955	7.349979	8.081191	9.259202	7.435056	H	11.754135	9.532627	10.373211	11.736239	9.606361	10.366523
H	9.12873	9.623234	7.56711	9.095747	9.627469	7.673353	C	9.677402	9.944224	9.936908	9.650965	9.988819	9.931468
H	8.014839	8.271512	7.846152	7.972901	8.281171	7.933694	H	9.826486	11.033972	9.878622	9.791328	11.079575	9.874257
C	7.087779	10.235226	7.934847	7.0461	10.245238	7.996521	H	8.692346	9.781626	10.410637	8.670897	9.818355	10.412667
H	7.237371	10.355738	9.019637	7.179708	10.370405	9.082649	C	4.561935	9.096403	7.584489	4.49805	9.084654	7.60049

H	6.07192	9.822634	7.797224	6.034458	9.826851	7.846652	C	5.012104	7.63221	7.738242	4.937064	7.625323	7.824995
C	2.175307	12.882414	6.835294	2.093802	12.873565	6.834271	H	5.575174	7.310072	6.84808	5.497794	7.251428	6.953782
C	1.438641	11.622472	7.326568	1.331868	11.679327	7.441779	H	4.127041	6.986936	7.845535	4.04425	6.995657	7.958909
H	2.089408	10.735802	7.270102	1.967694	10.780983	7.485393	H	5.640289	7.471271	8.626645	5.559108	7.499428	8.723384
H	0.547323	11.428468	6.708603	0.44799	11.435882	6.830258	C	3.562067	9.142868	6.414825	3.481888	9.076377	6.443199
H	1.108856	11.745094	8.370659	0.982301	11.907205	8.461278	H	3.06277	10.118531	6.320534	2.983217	10.047254	6.305919
C	2.650841	12.692656	5.383256	2.538694	12.533726	5.399537	H	2.775434	8.390495	6.576849	2.695504	8.336686	6.65764
H	3.213249	13.578213	5.047795	3.156018	13.345379	4.983356	H	4.072557	8.916211	5.465177	3.972467	8.795629	5.497657
H	1.77814	12.56104	4.725519	1.648072	12.414716	4.763783	C	3.882432	9.581819	8.878496	3.827203	9.630573	8.876648
H	3.290267	11.806695	5.257035	3.106811	11.593766	5.339291	H	4.574908	9.522784	9.733036	4.521016	9.611654	9.731915
C	1.217147	14.086899	6.844456	1.157846	14.092939	6.739184	H	3.002027	8.961667	9.111722	2.95028	9.01812	9.142052
H	0.683601	14.198185	7.800092	0.652564	14.318222	7.690009	H	3.545105	10.625628	8.777125	3.481687	10.666677	8.733083
H	0.4561	13.951378	6.061249	0.372051	13.8882	5.996182							
H	1.767651	15.018675	6.63732	1.715354	14.98633	6.415684							

Table S18. Coordinates for geometry optimized structures from DFT calculations of the double reduced complexes $\mathbf{2}^{2-}$ and $\mathbf{3}^{2-}$.

	$\mathbf{2}^{2-}$							$\mathbf{3}^{2-}$						
	TPSSh; Disp ON			TPSSh; Disp OFF				TPSSh; Disp ON			TPSSh; Disp OFF			
Mo	4.441391	12.906138	8.248968	4.02016	13.402176	8.245687	Mo	4.330519	13.197357	8.245752	4.10912	13.34399	8.220216
S	4.802786	14.300671	6.101224	4.22812	14.963127	6.22513	S	4.481317	14.691306	6.167538	4.385451	14.886615	6.190748
S	5.777605	14.968608	9.16848	5.183502	15.464421	9.363368	S	5.538785	15.291811	9.253938	5.34587	15.376989	9.322925
P	2.365891	14.25765	8.867022	1.731899	14.29331	8.9992	P	2.137658	14.318079	8.941591	1.855883	14.328816	8.961453
P	3.724575	12.163496	10.390425	3.500357	12.406018	10.371612	P	3.738326	12.348369	10.414097	3.546064	12.389158	10.3557
O	2.973717	10.568932	6.784875	2.828208	11.097074	6.509258	O	2.976751	10.861689	6.672525	2.829829	11.074066	6.498512
O	6.905379	10.967742	8.187644	6.689057	11.859068	7.677209	O	6.96048	11.597284	7.638386	6.72984	11.717442	7.659319
N	1.091039	11.818816	9.439204	0.945119	11.624967	9.4573	N	1.12699	11.769628	9.491665	0.959104	11.699417	9.448908
N	2.458352	14.333217	11.626694	1.909113	14.288499	11.764845	N	2.276383	14.381953	11.680013	2.0274	14.3461	11.728125
C	3.490962	11.480525	7.375995	3.229469	11.979774	7.220692	C	3.44825	11.762383	7.31678	3.266477	11.94745	7.202583
C	4.940703	20.080602	8.128831	7.492276	19.925859	7.765841	C	5.976058	12.232567	7.895827	5.756727	12.3749	7.893049
C	4.906971	15.960058	6.70288	5.177863	16.373888	6.711731	C	4.966847	16.297792	6.735703	5.365449	16.273008	6.702185
C	5.301841	16.24931	8.0397	5.596897	16.582824	8.054676	C	5.426361	16.539833	7.996919	5.783252	16.461124	7.98628
C	5.320298	17.598574	8.449487	6.346688	17.745219	8.343951	C	5.852788	17.926459	8.449805	6.625019	17.661472	8.392874
H	0.276873	16.065765	13.629063	-0.33115	15.692346	13.954484	H	-0.003444	15.850649	13.773532	-0.169274	15.839514	13.901739
H	-0.069511	14.857784	12.357025	-0.617972	14.752539	12.464806	H	-0.253519	14.893891	12.285639	-0.483765	14.876843	12.431992
C	4.960941	18.662824	7.608896	6.691231	18.703509	7.381118	C	6.056097	18.913942	7.295754	7.255533	18.396529	7.204558
H	0.628229	16.446537	11.935441	0.05425	16.407661	12.38164	H	0.452803	16.534497	12.205124	0.223843	16.514714	12.313349
H	5.611054	17.819589	9.482518	6.669387	17.903692	9.379172	H	3.948835	19.013297	6.834006	5.370317	19.181239	6.50346
C	4.590561	18.37462	6.274241	6.268533	18.497895	6.043195	C	4.89791	18.808966	6.304789	6.220181	18.600728	6.099123
C	0.637367	15.637965	12.68089	0.064281	15.467191	12.952253	C	0.422691	15.603022	12.78944	0.216223	15.58567	12.902446
H	2.734739	16.607818	14.241309	2.087885	16.370591	14.553758	H	2.42661	16.477846	14.449599	2.270812	16.463666	14.485359
C	4.585867	17.038002	5.8547	5.529226	17.345081	5.74705	C	4.847888	17.403127	5.697977	5.718874	17.245795	5.587641
H	3.091809	16.924375	12.5245	2.536482	16.775245	12.878302	H	2.924064	16.850636	12.778145	2.713018	16.839892	12.801627
H	4.27749	16.812817	4.827846	5.203379	17.184231	4.713073	H	3.786698	15.594746	13.709985	3.610896	15.588335	13.705719
C	0.853031	13.253678	9.311758	0.443305	12.996238	9.416057	C	0.729671	13.168401	9.37754	0.514073	13.089799	9.387401
H	0.427304	13.712275	10.224865	-0.02965	13.320778	10.363418	H	0.261285	13.568779	10.297809	0.050254	13.44426	10.328573
H	0.144333	13.415638	8.493696	-0.310275	13.067094	8.625288	H	0.003989	13.262524	8.564152	-0.233333	13.180549	8.592654
C	1.996866	11.452306	10.52611	1.923463	11.390531	10.518106	C	2.051301	11.520043	10.592326	1.926896	11.443046	10.514815
H	2.151394	10.369124	10.473384	2.261304	10.350528	10.442972	H	2.282676	10.449921	10.614825	2.220358	10.388509	10.458657
H	1.599518	11.690619	11.534632	1.507437	11.540076	11.535647	H	1.636582	11.801619	11.580998	1.517043	11.628634	11.528913
C	3.614443	13.454741	11.758687	3.207225	13.616682	11.79741	C	3.54976	13.666687	11.75289	3.300659	13.628093	11.768124
H	3.52628	12.889125	12.691292	3.276983	13.026726	12.717912	H	3.614603	13.155812	12.717718	3.350284	13.048237	12.696306
H	4.583543	13.992416	11.767821	4.063365	14.320925	11.77786	H	4.424878	14.337388	11.659611	4.181445	14.300659	11.737105
C	2.551934	15.210975	10.461521	1.790027	15.206656	10.632376	C	2.222722	15.286943	10.533908	1.942052	15.255908	10.585546
H	3.508245	15.762114	10.406601	2.629381	15.926578	10.570636	H	3.098702	15.959307	10.47356	2.807322	15.943732	10.519358
H	1.727376	15.930262	10.495102	0.851135	15.76306	10.719518	H	1.309409	15.888594	10.584748	1.022931	15.845872	10.664833
C	1.622664	15.540195	7.781129	0.732088	15.462633	7.984661	C	1.304873	15.521152	7.837169	0.910745	15.527345	7.930463
C	0.962077	15.143306	6.600668	0.057446	14.989787	6.839023	C	0.595301	15.063455	6.709229	0.213102	15.073307	6.790659
H	0.827167	14.079207	6.382762	0.054392	13.920344	6.608666	H	0.452048	13.990336	6.551838	0.148876	14.00179	6.579799
C	0.478926	16.089119	5.691945	-0.619491	15.862251	5.983925	C	0.068013	15.95945	5.774219	-0.408163	15.967358	5.915975

H	-0.033377	15.749996	4.786235	-1.146208	15.456975	5.114437
C	0.64297	17.467995	5.91919	-0.635215	17.250227	6.218038
C	1.303721	17.86011	7.094989	0.057403	17.724569	7.343744
H	1.45414	18.924279	7.298494	0.067855	18.798245	7.555152
C	1.793163	16.918077	8.003839	0.731058	16.852922	8.2088
H	2.334416	17.275825	8.880755	1.255206	17.276022	9.068586
C	0.169496	18.487575	4.911836	-1.34519	18.191356	5.275044
H	0.946696	18.669733	4.148615	-0.737133	18.376293	4.372128
H	-0.049885	19.453622	5.391739	-1.537734	19.164664	5.75044
H	-0.733673	18.144199	4.384033	-2.305348	17.770638	4.937249
C	-0.175502	11.005491	9.403124	-0.141326	10.581727	9.380021
C	0.172995	9.506247	9.466534	0.498608	9.181511	9.306722
H	0.945186	9.254931	8.722558	1.275819	9.14788	8.527171
H	-0.728701	8.915904	9.242823	-0.277092	8.443228	9.051767
H	0.52645	9.195908	10.460925	0.944255	8.867613	10.262184
C	-0.884642	11.249093	8.056157	-0.940042	10.779749	8.075879
H	-0.186188	11.084084	7.22084	-0.262249	10.829794	7.209531
H	-1.296869	12.265288	7.970595	-1.560425	11.688281	8.087862
H	-1.727397	10.548474	7.951952	-1.621196	9.926539	7.933963
C	-1.129676	11.353783	10.564652	-1.104996	10.637381	10.58467
H	-1.460124	12.40286	10.509602	-1.6278	11.605541	10.635657
H	-0.636814	11.198347	11.537656	-0.56629	10.48502	11.533411
H	-2.026948	10.714801	10.532304	-1.868861	9.847216	10.501007
C	4.683899	10.945071	11.401177	4.680593	11.318746	11.308379
C	4.139305	9.891783	12.159558	4.291216	10.329933	12.23336
H	3.062347	9.711663	12.174456	3.234231	10.13285	12.42602
C	4.962844	9.053826	12.921317	5.24596	9.584665	12.934195
H	4.511236	8.238034	13.49437	4.912914	8.818179	13.640842
C	6.353972	9.245398	12.973964	6.623168	9.807973	12.757006
C	6.894011	10.313023	12.234326	7.009513	10.810123	11.850177
H	7.972858	10.494701	12.26091	8.073292	11.016277	11.696619
C	6.076725	11.138319	11.457478	6.05686	11.543859	11.135287
H	6.51967	11.945935	10.868032	6.374878	12.305315	10.4183
C	7.241663	8.321251	13.771892	7.650414	8.983732	13.494795
H	6.69911	7.876877	14.620187	7.251663	8.605477	14.448214
H	8.126264	8.850572	14.158103	8.559864	9.56865	13.700918
H	7.606208	7.490542	13.142187	7.95424	8.108091	12.894425
C	2.038929	15.034409	12.889903	1.476112	14.866117	13.091253
C	1.917465	14.004865	14.028797	1.376266	13.72537	14.122553
H	1.331343	13.13207	13.698606	0.744642	12.910674	13.734475
H	1.399905	14.468249	14.882436	0.919563	14.109526	15.047669
H	2.895445	13.655065	14.390952	2.356947	13.307925	14.393943
C	3.037889	16.136659	13.292435	2.448152	15.948649	13.601457
H	4.046861	15.715459	13.42795	3.452685	15.532504	13.776381
H	-0.487778	15.572066	4.914851	-0.953927	15.576796	5.051459
C	0.245601	17.347243	5.913202	-0.342726	17.358372	6.123177
C	0.967392	17.802425	7.030772	0.372863	17.812561	7.242663
H	1.124903	18.876519	7.168224	0.446804	18.887763	7.432643
C	1.490085	16.910441	7.972784	0.990794	16.919484	8.127512
H	2.058928	17.312482	8.814019	1.537206	17.327451	8.980817
C	-0.283581	18.312388	4.880147	-0.994794	18.320393	5.15965
H	0.490943	18.539482	4.126357	-0.41961	18.387379	4.219763
H	-0.58181	19.267715	5.339036	-1.057247	19.332542	5.58601
H	-1.150161	17.893814	4.346178	-2.011529	17.991122	4.892041
C	-0.021197	10.803495	9.413523	-0.17084	10.702381	9.390212
C	0.526299	9.363252	9.402679	0.408825	9.275089	9.348169
H	1.325243	9.258391	8.652026	1.187259	9.191628	8.57339
H	-0.286508	8.666953	9.145577	-0.396816	8.565548	9.104611
H	0.920993	9.053956	10.38171	0.836852	8.962214	10.311971
C	-0.763674	11.01659	8.07931	-0.956864	10.907426	8.079536
H	-0.051929	11.007932	7.239142	-0.275768	10.904197	7.214374
H	-1.324823	11.962472	8.051268	-1.532077	11.845181	8.068183
H	-1.491982	10.204766	7.929944	-1.678612	10.085283	7.955606
C	-1.007814	10.968232	10.588196	-1.134715	10.823964	10.590108
H	-1.452083	11.976046	10.595078	-1.616936	11.813798	10.618546
H	-0.501065	10.807743	11.553115	-0.605429	10.669804	11.543871
H	-1.828205	10.236659	10.508928	-1.930273	10.064448	10.519875
C	4.718277	11.130557	11.41567	4.674903	11.263246	11.311444
C	4.243471	10.587026	12.628203	4.240513	10.302638	12.246125
H	3.264354	10.878173	13.018382	3.175332	10.151133	12.434732
C	5.011549	9.676011	13.356473	5.159594	9.528128	12.962845
H	4.619098	9.270843	14.294392	4.790939	8.785214	13.676985
C	6.285078	9.273956	12.90859	6.545719	9.693038	12.792519
C	6.75776	9.820924	11.705189	6.977981	10.666904	11.875348
H	7.745998	9.531385	11.334811	8.050229	10.827761	11.726318
C	5.985682	10.730806	10.970654	6.060524	11.429559	11.144929
H	6.364225	11.144017	10.033346	6.41393	12.169094	10.42132
C	7.099343	8.273698	13.69277	7.533894	8.838302	13.548715
H	7.076954	8.498434	14.770965	7.103375	8.465503	14.49036
H	8.147742	8.260381	13.359771	8.453071	9.398344	13.779864
H	6.693249	7.255126	13.566178	7.829751	7.958716	12.950166
C	1.815355	14.974402	12.981871	1.614842	14.9553	13.046288
C	1.656178	13.840726	14.012713	1.493598	13.835646	14.097992
H	1.022561	13.039168	13.601324	0.845773	13.026332	13.725533
H	1.17772	14.235481	14.92206	1.045002	14.245966	15.015802
H	2.61814	13.402401	14.315751	2.466183	13.404575	14.376869
C	2.798003	16.03703	13.510297	2.613721	16.023566	13.534881
H	5.089507	18.32816	9.147301	5.99744	18.370291	8.970887

H	3.926058	20.514991	8.077153	6.942637	20.859842	7.552186	H	3.904483	17.269843	5.138074	4.83557	17.38912	4.939373
H	5.593897	20.745032	7.536268	8.440733	19.988384	7.203501	H	5.655339	17.295901	4.945478	6.489961	16.792148	4.932318
C	4.163223	19.475128	5.333023	6.604368	19.493975	4.957584	H	7.00144	18.682072	6.771102	8.097498	17.801616	6.804749
C	5.998719	11.750474	8.185098	5.699286	12.489488	7.91212	H	6.151589	19.94086	7.688443	7.676323	19.361001	7.537042
H	5.272912	20.125373	9.177166	7.736443	19.917047	8.838933	H	4.988511	19.564554	5.505663	6.640595	19.188755	5.265236
H	3.924908	19.074545	4.335992	6.191384	19.17623	3.988194	H	6.778219	17.845686	9.048651	7.412165	17.332937	9.095359
H	4.946356	20.244305	5.214029	7.695252	19.616988	4.83634							
H	3.265136	19.996459	5.708668	6.201851	20.497164	5.184296							

Table S19. Coordinates for geometry optimized structures from DFT calculations of the double reduced complexes $\mathbf{4}^{2-}$ and $\mathbf{5}^{2-}$.

	$\mathbf{4}^{2-}$							$\mathbf{5}^{2-}$						
	TPSSh; Disp ON			TPSSh; Disp OFF				TPSSh; Disp ON			TPSSh; Disp OFF			
Mo	6.610883	13.17577	10.45713	6.481886	13.221302	10.514172	Mo	9.032688	12.679783	7.190114	8.918571	12.715785	7.153041
S	6.466405	13.747422	12.958614	6.325253	13.728728	13.028338	S	7.487391	13.427796	9.179503	7.358849	13.421631	9.146642
S	4.946744	11.314971	11.257722	4.766098	11.381405	11.266306	S	8.912381	15.211276	6.755029	8.822827	15.268208	6.808596
P	4.574739	14.5859	9.809875	4.48554	14.695073	9.753972	P	6.8996	12.133755	5.883304	6.798623	12.081351	5.784723
P	6.181476	12.802547	8.137848	6.125514	12.844425	8.163368	P	8.597084	10.348336	7.460214	8.53497	10.357919	7.416608
O	8.747232	15.375897	9.875117	8.680528	15.40107	10.127292	O	11.006713	12.193823	4.820647	10.978426	12.36962	4.835533
O	9.190252	11.40152	10.336139	9.026265	11.402787	10.609754	O	11.68617	12.417994	8.836039	11.583515	12.58507	8.785615
N	6.120324	15.591234	7.671157	6.143418	15.632682	7.654205	N	8.331717	10.025546	4.656758	8.34154	10.019333	4.606993
N	3.464651	13.190078	7.685218	3.388927	13.229304	7.636354	N	5.855771	9.942802	7.233656	5.768213	9.89823	7.211453
C	7.876173	14.565327	10.060904	7.789859	14.595214	10.220432	C	10.198113	12.34524	5.701965	10.130175	12.454742	5.688349
C	8.179634	12.041963	10.461767	8.020978	12.062133	10.622462	C	10.653159	12.595167	8.244004	10.534399	12.688997	8.205672
C	5.288875	12.657681	13.701316	5.241534	12.547179	13.77347	C	7.224899	15.169052	8.952437	7.246303	15.19259	9.082916
C	4.641847	11.61581	12.976024	4.581483	11.535597	13.020393	C	7.819297	15.901684	7.966251	7.852764	15.951242	8.124826
C	3.700546	10.816389	13.663088	3.73894	10.635736	13.711657	C	7.528913	17.381339	7.772838	7.712397	17.465965	8.089073
H	3.201078	10.016999	13.104125	3.233554	9.856355	13.130166	H	8.468188	17.9108	7.530911	8.684677	17.915334	7.81821
C	3.361965	11.001698	15.010058	3.513079	10.690619	15.093865	H	6.885748	17.502653	6.877389	7.02197	17.749882	7.268819
C	4.00052	12.043103	15.728972	4.164534	11.702934	15.843185	C	6.848774	18.038018	8.977931	7.205582	18.065125	9.405559
C	4.942331	12.835133	15.060155	5.005317	12.596941	15.166792	H	7.586447	18.179576	9.789524	8.01417	18.040762	10.159411
H	5.434234	13.643132	15.61351	5.510621	13.378472	15.745604	H	6.478682	19.040945	8.703961	6.937269	19.125727	9.260056
C	2.333382	10.118289	15.676151	2.594092	9.693974	15.761534	C	5.712613	17.15186	9.485783	6.013059	17.264336	9.927342
H	1.93993	9.365964	14.97573	2.179183	8.985795	15.028247	H	4.98738	16.990244	8.666405	5.207965	17.280977	9.16935
H	1.47895	10.704749	16.058192	1.74703	10.19075	16.26729	H	5.163876	17.641344	10.308625	5.598589	17.721228	10.842448
H	2.756324	9.58409	16.545376	3.118093	9.10822	16.537707	C	6.264944	15.8003	9.949996	6.426215	15.814253	10.203754
C	3.668543	12.298888	17.180355	3.96097	11.81952	17.33603	H	6.774378	15.926952	10.927029	7.003808	15.770625	11.149672
H	2.599521	12.540846	17.317045	2.900269	11.989935	17.59277	H	5.433016	15.099464	10.141988	5.529935	15.19345	10.383497
H	4.258468	13.136756	17.581909	4.546302	12.653943	17.751218	C	7.105398	10.815989	4.585474	7.067546	10.729794	4.520555
H	3.868232	11.411811	17.807183	4.263674	10.89803	17.864327	H	6.181776	10.203788	4.586885	6.187441	10.057504	4.564133
C	4.890585	15.796286	8.431062	4.87697	15.8632	8.344772	H	7.127536	11.373093	3.640549	7.038	11.24907	3.55479
H	3.979084	15.828733	7.801414	4.000844	15.864979	7.665386	C	8.547623	9.303767	5.908244	8.54422	9.299418	5.863079
H	4.97243	16.76402	8.940902	4.927794	16.851277	8.818397	H	9.551822	8.864532	5.863803	9.553598	8.870606	5.840903
C	6.240093	14.29453	7.010053	6.250788	14.324009	7.013025	H	7.828836	8.475608	6.07349	7.830663	8.46249	6.011345
H	7.24129	14.243277	6.565658	7.25836	14.244623	6.587157	C	6.949649	9.84273	8.199486	6.88987	9.813889	8.149466
H	5.505192	14.140133	6.194094	5.527759	14.177391	6.184455	H	7.048057	8.802291	8.524558	7.011017	8.771125	8.461701
C	4.489809	12.147183	7.661019	4.431763	12.200141	7.655309	H	6.782845	10.468016	9.098862	6.728453	10.425596	9.060229
H	4.576177	11.752519	6.643975	4.536761	11.787111	6.646335	C	5.566198	11.343468	6.923746	5.480499	11.291914	6.856453
H	4.255899	11.30194	8.337751	4.190263	11.36354	8.340908	H	5.461112	11.965641	7.832339	5.385015	11.942714	7.747436
C	3.176162	13.604146	9.058424	3.089188	13.708137	8.988721	H	4.634283	11.404795	6.35307	4.537614	11.330684	6.300821
H	2.987442	12.745426	9.730223	2.865166	12.882878	9.692801	C	5.872042	13.387495	4.942731	5.747294	13.265818	4.76057
H	2.291867	14.249287	9.065598	2.217854	14.369773	8.946427	H	6.626079	13.925209	4.336455	6.49565	13.713823	4.077652
C	3.610255	15.659156	11.00666	3.513058	15.863459	10.868614	C	5.275178	14.395218	5.943252	5.206256	14.397445	5.656739
H	4.404849	16.226229	11.528547	4.314838	16.493194	11.301715	H	4.526009	13.878441	6.570672	4.482875	13.977685	6.379946

C	2.603811	16.670013	10.426719	2.480369	16.799874	10.210761	H	6.064045	14.76042	6.619128	6.034824	14.830506	6.241691
H	1.816847	16.132086	9.867506	1.680677	16.19828	9.742782	C	4.583998	15.558754	5.221686	4.504563	15.486063	4.831182
H	3.09263	17.349699	9.710939	2.942341	17.394369	9.407053	H	4.150953	16.255877	5.959945	4.100357	16.264728	5.50082
C	1.949105	17.495244	11.547857	1.845846	17.74623	11.244347	H	5.339624	16.12971	4.650831	5.250396	15.981826	4.182665
H	2.726132	18.113371	12.034136	2.62527	18.425963	11.635252	C	3.500168	15.046921	4.264551	3.38736	14.900012	3.959285
H	1.211232	18.193845	11.117437	1.090499	18.382746	10.752059	H	3.032926	15.885695	3.720664	2.927442	15.688827	3.339568
C	1.286259	16.602891	12.605282	1.215583	16.975261	12.410411	H	2.6989	14.564756	4.855066	2.587236	14.505538	4.613033
H	0.861129	17.221125	13.414419	0.808242	17.676921	13.158356	C	4.075181	14.026234	3.274209	3.915269	13.766886	3.071337
H	0.440832	16.060414	12.142497	0.3606	16.384412	12.032398	H	4.805745	14.533484	2.617449	4.631816	14.182739	2.339176
C	2.282084	15.583032	13.170478	2.232116	16.028698	13.060194	H	3.277436	13.635176	2.619543	3.091345	13.321432	2.487498
H	1.783172	14.914688	13.893279	1.752927	15.442594	13.863093	C	4.780382	12.862877	3.992675	4.617673	12.673905	3.895801
H	3.077994	16.113146	13.725768	3.031244	16.625317	13.537693	H	4.031391	12.288933	4.567841	3.868192	12.185853	4.544397
C	2.92198	14.756628	12.048318	2.86436	15.082202	12.028714	H	5.200354	12.174214	3.242684	5.003299	11.896798	3.216979
H	3.649482	14.042661	12.460707	3.620395	14.440628	12.509574	C	8.544755	9.173969	3.433265	8.649251	9.199212	3.379025
H	2.131881	14.165642	11.550601	2.079015	14.416069	11.626736	C	8.583914	10.083485	2.18906	8.676349	10.125381	2.14622
C	6.46162	16.754051	6.779535	6.560403	16.78052	6.769733	H	7.5988	10.506987	1.943445	7.678677	10.497913	1.870219
C	6.568181	18.030891	7.636809	6.646368	18.067054	7.61545	H	8.912877	9.498988	1.316054	9.064619	9.568094	1.279632
H	5.59048	18.376959	8.003543	5.659169	18.438606	7.927932	H	9.293292	10.911991	2.343351	9.335537	10.989071	2.326797
H	6.994775	18.845527	7.031627	7.118232	18.863432	7.019407	C	7.443326	8.106386	3.255153	7.626032	8.066075	3.146355
H	7.226569	17.856757	8.502481	7.259572	17.897821	8.514602	H	7.391101	7.442482	4.132631	7.585624	7.384748	4.011114
C	5.416513	16.970094	5.663958	5.590241	17.008487	5.590002	H	7.652876	7.484237	2.370066	7.905754	7.471247	2.261514
H	5.324946	16.074089	5.02972	5.525704	16.114636	4.949317	H	6.454832	8.570984	3.114465	6.614718	8.46717	2.97462
H	5.711103	17.813757	5.018942	5.936945	17.846691	4.963712	C	9.914071	8.473354	3.528091	10.057429	8.585822	3.510787
H	4.424911	17.197968	6.085527	4.576512	17.252627	5.944967	H	10.705354	9.199214	3.773693	10.794341	9.354287	3.792757
C	7.844156	16.519568	6.139952	7.973437	16.512902	6.214132	H	10.154744	8.012888	2.557628	10.357809	8.159857	2.541063
H	8.583604	16.242497	6.907805	8.667417	16.239022	7.02442	H	9.925423	7.672241	4.281628	10.098467	7.772001	4.249829
H	8.180893	17.446349	5.65069	8.351206	17.427286	5.731184	C	9.73778	9.293447	8.513846	9.692149	9.33226	8.499309
H	7.824319	15.73356	5.370811	7.986395	15.716076	5.455939	H	10.73893	9.584459	8.143836	10.688161	9.643599	8.131077
C	7.254726	11.613219	7.161471	7.209206	11.621684	7.219858	C	9.615433	7.761842	8.405634	9.6129	7.796014	8.403162
H	8.277712	11.939717	7.427626	8.228746	11.945977	7.503146	H	8.612937	7.441833	8.74308	8.619333	7.449247	8.740627
C	7.13335	11.623917	5.626181	7.125366	11.61503	5.680766	H	9.719829	7.428397	7.36182	9.729999	7.457266	7.362354
H	7.308568	12.633048	5.222235	7.31593	12.618384	5.269538	C	10.679533	7.061784	9.267731	10.693513	7.128575	9.272444
H	6.108381	11.336596	5.32975	6.106638	11.329611	5.361681	H	10.55991	5.967091	9.196173	10.599806	6.030883	9.207001
C	8.130295	10.642446	4.987223	8.132113	10.62324	5.071606	H	11.679852	7.299521	8.86133	11.688851	7.385511	8.865497
H	8.010694	10.647568	3.89024	8.032381	10.618922	3.972523	C	10.613187	7.511875	10.731869	10.615862	7.583973	10.734276
H	9.158159	10.991474	5.196896	9.157433	10.971578	5.294507	H	11.412208	7.027423	11.318763	11.431376	7.128022	11.321496
C	7.961697	9.220862	5.536599	7.950369	9.206852	5.629273	H	9.652445	7.180577	11.168053	9.668299	7.223742	11.176209
H	6.96854	8.834673	5.240496	6.967501	8.814153	5.308633	C	10.711724	9.038187	10.845158	10.667801	9.112768	10.840057
H	8.711256	8.545444	5.08999	8.713282	8.528888	5.209709	H	10.614815	9.352529	11.898509	10.552279	9.428766	11.891186
C	8.066586	9.205587	7.066433	8.014789	9.205253	7.161247	H	11.710291	9.368385	10.504294	11.660309	9.470237	10.509142
H	9.090594	9.494171	7.367189	9.034362	9.484054	7.485441	C	9.640347	9.726074	9.988829	9.583446	9.769356	9.973353
H	7.896287	8.186324	7.453478	7.82514	8.190716	7.552073	H	9.726415	10.82151	10.061394	9.645295	10.866751	10.042518
C	7.065709	10.181827	7.698601	7.006602	10.194359	7.764405	H	8.643243	9.453273	10.380015	8.592258	9.477584	10.36573
H	7.162496	10.18311	8.795401	7.084377	10.203287	8.862818	C	4.642827	9.11708	7.559303	4.545863	9.111685	7.619213

H	6.04112	9.839337	7.464872	5.985204	9.852234	7.51675	C	5.073534	7.654222	7.773688	4.953023	7.662062	7.943819
C	2.245716	12.904714	6.853334	2.168195	12.864879	6.82632	H	5.706648	7.315142	6.937932	5.57683	7.243036	7.138008
C	1.412277	11.74143	7.424553	1.395645	11.674267	7.429328	H	4.180144	7.012647	7.817578	4.046284	7.044288	8.034019
H	2.015764	10.821693	7.48479	2.030994	10.776074	7.484993	H	5.626246	7.507331	8.713305	5.501149	7.576844	8.893649
H	0.540031	11.535013	6.783405	0.518461	11.428076	6.808895	C	3.695029	9.132018	6.345293	3.576961	9.046533	6.422788
H	1.04236	11.979151	8.434368	1.035154	11.906542	8.443905	H	3.246217	10.120431	6.168303	3.144356	10.025973	6.170401
C	2.685021	12.574456	5.414823	2.599469	12.524203	5.386984	H	2.868436	8.424727	6.514228	2.739011	8.374174	6.664456
H	3.391425	13.335506	5.046222	3.236822	13.322599	4.974468	H	4.23657	8.827929	5.435356	4.092405	8.653915	5.532039
H	1.803513	12.56723	4.755634	1.704313	12.434094	4.752464	C	3.907105	9.634585	8.810295	3.828629	9.726462	8.838665
H	3.161291	11.586292	5.332817	3.143275	11.570626	5.31859	H	4.575482	9.630969	9.686097	4.507176	9.796049	9.703965
C	1.388761	14.182567	6.77899	1.240488	14.091903	6.734702	H	3.037261	8.999222	9.043275	2.968329	9.104067	9.134468
H	0.941097	14.451183	7.747075	0.752767	14.331485	7.691103	H	3.544207	10.663111	8.656637	3.45058	10.736117	8.614072
H	0.561392	14.029943	6.068949	0.44086	13.890548	6.005148							
H	1.998622	15.031002	6.429784	1.803159	14.976806	6.396801							

Table S20. Calculated vibrational frequencies of **2** using different functionals with and without dispersion correction.

	2											
	TPSSh; Disp ON		TPSSh; Disp OFF		PBE0; Disp ON		PBE0; Disp OFF		BP86; Disp ON		BP86; Disp OFF	
Mode	freq	T**2	freq	T**2	freq	T**2	freq	T**2	freq	T**2	freq	T**2
	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)
6:	17.56	0.000115	18.27	0.00011	17.98	0.000083	18.06	0.000135	27.5	0.00002	16.95	0.000233
7:	28.67	0.000801	29.34	0.000663	29.22	0.000682	27.64	0.000539	39.41	0.000288	24.34	0.001169
8:	29.41	0.00002	34.56	0.00002	31.53	0.000118	33.58	0.000032	46.52	0.000583	25.74	0.000621
9:	34.81	0.000165	36.8	0.000703	35.81	0.000099	35.25	0.001192	50.37	0.00051	28.91	0.00039
10:	35.97	0.000282	37.38	0.000347	36.37	0.000848	36.64	0.000002	55.53	0.000062	34.77	0.000766
11:	38.92	0.000512	38.5	0.000012	37.42	0.000209	37.63	0.000141	61.82	0.000434	34.88	0.000319
12:	40.34	0.000158	41.27	0.00005	41.28	0.000058	40.98	0.000059	64.99	0.000054	35.28	0.000005
13:	45.15	0.00023	44.63	0.000453	45.08	0.000206	45.38	0.000283	67.12	0.000751	36.67	0.000128
14:	46.92	0.000471	47.2	0.000249	46.64	0.000511	46.66	0.000423	74.61	0.000263	38.66	0.000538
15:	51.88	0.000651	48.96	0.00002	51.59	0.000147	48.46	0.000029	82.04	0.000002	40.01	0.00033
16:	56.96	0.000337	53.24	0.000378	56.76	0.000877	56.77	0.000833	82.68	0.000196	44.72	0.000021
17:	59.78	0.000301	54.07	0.00088	58.64	0.000309	59.61	0.000288	93.34	0.001149	48.6	0.000758
18:	64.44	0.000079	62.25	0.000088	63.99	0.000057	63.18	0.000196	97.1	0.001884	52.54	0.00044
19:	68.6	0.0004	64.66	0.000548	68.05	0.000504	71.74	0.000152	103.01	0.000138	57.68	0.000338
20:	77.34	0.000019	74.07	0.000168	76.59	0.000145	76.54	0.000365	104.45	0.000256	70.7	0.000232
21:	85.77	0.001569	82.36	0.000935	85.62	0.001403	83.33	0.001333	108.78	0.000212	77.43	0.000915
22:	88.01	0.001693	87.05	0.001949	89.63	0.002334	86.83	0.002398	115.42	0.000088	85.17	0.001284
23:	94.9	0.000407	92.59	0.000434	98.21	0.000396	97.21	0.000249	117.8	0.000024	89.08	0.000965
24:	101.57	0.000314	95.88	0.000476	105	0.000185	99.6	0.000393	126.64	0.000052	93.32	0.00042
25:	106.48	0.000034	106.94	0.000031	109.21	0.000006	109.86	0.000022	129.27	0.000106	101.91	0.000036
26:	114.24	0.000336	112.1	0.000318	119.23	0.000039	114.26	0.000313	130.41	0.00022	108.54	0.000291
27:	118.27	0.000013	114.4	0.00001	120.19	0.000246	116.22	0.000006	143.33	0.000875	112.34	0.000007
28:	119.38	0.000011	118	0.000018	121.89	0.000066	118.8	0.000023	144.25	0.000026	115.33	0.000027
29:	127.55	0.000007	124.94	0.000006	131.8	0.000007	128.41	0.000005	158.07	0.000182	123.53	0.000009
30:	139.87	0.000975	138.09	0.00091	143.18	0.00097	140.76	0.000972	166.63	0.00132	134.54	0.000861
31:	155.42	0.000157	153.3	0.000154	158.95	0.000222	156.58	0.000188	180.62	0.00009	150.35	0.000166
32:	159.62	0.000001	158.07	0.000006	161.51	0.000002	160.93	0.000007	198.94	0.00026	155.85	0.000078
33:	162.5	0.001153	160.3	0.001321	166.15	0.001241	163.79	0.001341	199.4	0.00047	157.05	0.001295
34:	163.67	0.000104	162.23	0.000084	168.13	0.000061	166.45	0.000085	206.14	0.000127	158.32	0.000061
35:	180.44	0.000017	178.25	0.00001	185.73	0.000023	179.68	0.000018	209.08	0.000012	175.67	0.000006
36:	193.35	0.000876	190.84	0.000034	198.99	0.000853	193.4	0.000109	218.71	0.000177	188.27	0.000888
37:	195.91	0.00006	192.43	0.0008	200	0.000036	195.5	0.00063	224.94	0.000012	188.89	0.000099
38:	198.94	0.000032	197.96	0.000069	204.59	0.00003	201.92	0.000187	241.08	0.000509	194.47	0.000067
39:	207.44	0.000116	204.19	0.000171	213.13	0.000134	204.11	0.000158	247.9	0.00005	202.19	0.000252
40:	213.49	0.000056	212.94	0.000026	220.2	0.000055	215.44	0.000009	249.06	0.000095	207.38	0.000017
41:	216.49	0.000218	214.68	0.000114	222.29	0.000256	217.91	0.00007	251.06	0.000037	212.24	0.000079
42:	218.66	0.000001	216.78	0.000067	224.84	0.000001	220.04	0.000147	253.8	0.000005	213.01	0.000155
43:	228.02	0.000035	225.42	0.000048	234.75	0.000054	228.6	0.000039	275.96	0.000363	219.38	0.000032
44:	237.15	0.000579	236.07	0.000492	242.71	0.000609	241.21	0.000596	283.45	0.000122	231.33	0.000434

45:	250.45	0.000024	249.91	0.000026	254.58	0.000018	255.02	0.000021	286.25	0.000683	242.8	0.000017
46:	261.64	0.000207	264.1	0.000256	272.5	0.000235	267.41	0.000278	296.33	0	260.05	0.00023
47:	267.96	0.000319	266.21	0.000339	273.82	0.000292	270.52	0.000303	309.7	0.001731	263.17	0.000232
48:	274.49	0.000142	273.32	0.000036	280.72	0.000002	278.73	0.000023	312.52	0.000208	267	0.00007
49:	276.05	0.000403	276.75	0.000836	282.81	0.000794	281.7	0.00079	313.2	0.000066	274.11	0.000727
50:	278.21	0.000293	279.85	0.000017	289.94	0.000074	283.21	0.000052	322.3	0.000572	279.04	0.000137
51:	285.38	0.000005	292.22	0.000025	293.38	0.000011	288.71	0.000057	330.01	0.00046	284.82	0.000052
52:	297.58	0.000014	295.62	0.00002	304.06	0.000009	293.66	0.000039	333.58	0.000224	291.51	0.000036
53:	301.72	0.000027	298.98	0.000017	307.36	0.000049	300.88	0.000063	334.67	0.000271	293.22	0.000001
54:	304.31	0.000259	301.61	0.000283	312.43	0.000283	302.35	0.000261	348.28	0.000986	307.34	0.000295
55:	321.07	0.00188	319.41	0.001798	328.66	0.001873	324.26	0.001836	350.35	0.000305	317.36	0.001895
56:	330.09	0.000424	327.81	0.000678	338.84	0.000484	333.31	0.000733	353.49	0.00013	323.85	0.000293
57:	331.83	0.000328	331.76	0.00036	339.15	0.000537	337.56	0.000432	355.27	0.002032	325.81	0.000879
58:	333.07	0.000507	332.57	0.000305	342.06	0.000322	338.15	0.000184	360.46	0.000931	331.92	0.000384
59:	339.88	0.000504	339.43	0.000549	348.23	0.000581	344.01	0.000406	363.98	0.000152	334.45	0.00079
60:	350.01	0.000394	346.98	0.000265	356.01	0.000424	350.64	0.000111	367.01	0.000367	341.49	0.000382
61:	350.28	0.000306	350.39	0.000353	358.38	0.000482	356.16	0.00011	370.3	0.000085	348.85	0.000604
62:	352.95	0.000348	351.61	0.000388	361.65	0.000352	356.9	0.000632	372.32	0.000033	350.97	0.001935
63:	357.85	0.002584	357.3	0.002519	364.19	0.00264	360.32	0.001133	372.74	0.000118	351.84	0.00021
64:	365.34	0.000029	361.16	0.000258	373.37	0.000017	364.35	0.002141	379.15	0.000014	362.02	0.000013
65:	369.06	0.000015	367.63	0.000011	377.1	0.000004	372.91	0.000013	383.82	0.000034	364.33	0.000016
66:	373.65	0.000009	372.17	0.00001	383.18	0.000004	376.47	0.000032	387.77	0.000233	372.5	0.000025
67:	382.53	0.000264	382.26	0.000187	390.77	0.000258	388.81	0.000252	390.69	0.000264	376.6	0.000094
68:	392.58	0.000343	390.44	0.000337	402.16	0.000492	397.2	0.0006	401.68	0.000213	388.18	0.000335
69:	402.06	0.000638	398.25	0.000573	411.92	0.000645	405.6	0.000583	421.69	0.000998	393.32	0.000535
70:	412.36	0.000028	412.07	0.001024	418.72	0.000004	419.2	0.000015	423.25	0.000495	401.49	0.00007
71:	412.65	0.000062	413.48	0.00117	419.18	0.00003	419.44	0.000112	426.43	0.00013	402.04	0.000025
72:	417.4	0.002289	414.35	0.000501	429.33	0.002448	423.15	0.002367	427.56	0.000488	408.07	0.002525
73:	422.26	0.000077	420.41	0.0002	432.89	0.000165	429.91	0.000275	429.61	0.000018	414.19	0.000698
74:	433.35	0.007124	431.4	0.006994	444.28	0.00754	441.08	0.007037	431.23	0.001147	425.02	0.000248
75:	434.66	0.000399	434.78	0.000147	445.13	0.000401	444.3	0.000236	436.87	0.008553	426.45	0.007884
76:	452.86	0.000514	452.85	0.000626	461.24	0.000498	461.92	0.000545	465.75	0.002122	440.94	0.000607
77:	457.15	0.002145	456.79	0.00185	471.81	0.001807	467.15	0.001158	468.17	0.000323	454.85	0.001352
78:	462.88	0.001005	460.54	0.001219	475.68	0.001119	468.87	0.00198	473.17	0.000604	455.63	0.00098
79:	465.73	0.000558	461.5	0.000797	478.89	0.000602	473.35	0.000616	484.94	0.000015	458.65	0.001295
80:	477.92	0.000004	475.92	0.000025	490.88	0.000023	485.26	0.000009	487.16	0.000736	473.87	0.000052
81:	486.46	0.003542	484.68	0.003683	500.01	0.003718	495.3	0.004171	498.3	0.003403	481.95	0.003548
82:	500.42	0.002269	495.27	0.002238	516.47	0.001802	510.9	0.001948	511.58	0.002399	495.12	0.000523
83:	504.73	0.001322	500.5	0.00148	521.54	0.001298	515.94	0.00148	514.67	0.001037	501.7	0.003023
84:	511.13	0.001092	510.79	0.001069	523.47	0.003328	520.41	0.002005	522.56	0.000173	503.52	0.002573
85:	515.17	0.000185	514.82	0.00011	530.67	0.000449	525.7	0.000459	523.26	0.000261	509.58	0.000926
86:	518.29	0.002439	518.23	0.002699	531.21	0.000974	527.5	0.001826	530.18	0.000212	511.56	0.000076
87:	521.77	0.001054	521.52	0.000987	531.88	0.000828	529.78	0.00091	535.3	0.003741	513.48	0.000597
88:	525.5	0.001573	525.64	0.00136	538.25	0.001577	534.68	0.001616	537.21	0.000567	521.44	0.000632

89:	538.27	0.003209	539.27	0.003227	558.01	0.0034	556.56	0.003427	556.32	0.001922	530.97	0.003226
90:	570.16	0.005736	569.15	0.005667	589.6	0.005159	587.74	0.005298	585.03	0.004359	557.03	0.005408
91:	600.69	0.000322	600.89	0.000314	611.92	0.000278	611.37	0.000308	602.45	0.002003	587.11	0.000319
92:	610.98	0.000006	611.02	0.000007	622.2	0.000008	622.31	0.000007	622.16	0.000003	598.64	0.000008
93:	617.54	0.001208	616.81	0.001179	631.45	0.001425	628.59	0.001394	630.1	0.000889	599.96	0.001045
94:	633.9	0.005592	631.07	0.005803	645.87	0.004144	643.16	0.005779	630.58	0.005173	618.64	0.004491
95:	634.79	0.000334	631.55	0.000103	646.97	0.000552	643.85	0.000074	634.98	0.0008	618.8	0.000652
96:	640.92	0.000127	641.04	0.000069	648.87	0.001163	648.73	0.000325	638.99	0.00005	628.54	0.000091
97:	641.47	0.000067	641.59	0.000048	649.95	0.000334	649.13	0.00005	639.98	0.000176	628.79	0.000022
98:	695.09	0.00055	695.91	0.000532	708.57	0.000591	708.52	0.000578	688.77	0.000585	681.64	0.000532
99:	720.96	0.002361	714.37	0.002588	739.52	0.000001	737.59	0.001916	709.68	0.002378	695.81	0.002675
100:	727.18	0.000001	726.88	0.001405	740.32	0.000142	739.82	0.000001	721.74	0.001366	707.99	0.000061
101:	730.55	0.000116	727.19	0.000012	741.93	0.00001	740.86	0.000462	725.49	0.002119	708.95	0.001137
102:	731.31	0.00031	730.37	0.000235	745.41	0.002168	741.56	0.000055	733.9	0.000005	709.67	0.001983
103:	731.65	0.000873	730.83	0.000432	754.96	0.001015	750.71	0.001193	735.01	0.000014	712.39	0.000201
104:	737.33	0.001629	732.09	0.00124	759.03	0.001363	751.83	0.001395	735.17	0.000011	712.9	0.000404
105:	761.81	0.001013	759	0.001024	781.48	0.001282	777.53	0.001291	756.99	0.000759	739.58	0.00072
106:	768.54	0.000688	763.76	0.000608	785.95	0.000004	783.17	0.000004	758.54	0.000626	741.1	0.00099
107:	768.82	0.000009	767.81	0	790.03	0.000727	785.35	0.000688	762.49	0.000003	755.26	0.000002
108:	784.22	0.001151	781.45	0.001156	800.9	0.001309	798.11	0.001335	778.82	0.00077	761.69	0.000913
109:	811.28	0.000016	810.96	0.000013	823.12	0.000302	822.45	0.000325	806.91	0.000061	792.2	0.000315
110:	812.63	0.000121	812.14	0.000098	827.06	0.000341	826.12	0.000278	807.06	0.000195	795.28	0.000613
111:	823	0.002021	822.79	0.001955	832.39	0.001219	831.1	0.001246	830.92	0.00036	798.42	0.000471
112:	825.6	0.000773	824.46	0.000636	834.9	0.000852	833.59	0.000921	837.42	0.000159	799.66	0.00034
113:	831.29	0.001157	829.53	0.000847	839.7	0.002222	838.02	0.002002	846.61	0.002556	806.11	0.000651
114:	832.53	0.001279	831.64	0.001526	855.13	0.000721	851.01	0.000672	857.08	0.002369	808.82	0.002881
115:	840.51	0.000755	838.2	0.000857	867.45	0.000041	864.65	0.000345	858.25	0.000546	815.31	0.000547
116:	863.89	0.000043	864.82	0.000042	867.92	0.000142	867.18	0.000042	883.26	0.002727	830.58	0.000025
117:	865	0.000059	865.35	0.000133	868.84	0.000265	869.19	0.000059	893.89	0.000043	831.44	0.00004
118:	871.62	0.002462	871.6	0.002459	887.65	0.001363	887.21	0.00156	894.43	0.00002	851.05	0.002369
119:	882.89	0.000486	884.31	0.000432	889.23	0.000961	888.6	0.000603	902.53	0.000447	858.7	0.000551
120:	897	0.000645	896.93	0.000657	900.66	0.000619	901.13	0.000612	916.35	0.005871	862.49	0.000576
121:	903.14	0.000056	902.78	0.000029	907.63	0.000029	908.23	0.000031	924.18	0.000655	869.54	0.000018
122:	904.02	0.006023	903.54	0.005962	915.06	0.005837	913.87	0.005888	927.89	0.000167	877.76	0.005919
123:	918.62	0.000187	917.94	0.000174	928.33	0.000225	925.43	0.000269	930.56	0.00004	891.59	0.000182
124:	921.97	0.000139	921.3	0.000157	931.95	0.000151	929.15	0.000204	931	0.000132	893.77	0.000143
125:	932.94	0.000088	932.83	0.000073	940.32	0.000066	935.45	0.000058	941.74	0.000048	905.9	0.000083
126:	933.03	0.000006	932.99	0.000023	941.27	0.000055	938.58	0.000052	943.1	0.000065	906.14	0.000037
127:	953.45	0.000001	953.11	0.000005	951.31	0.000006	946.48	0.000018	949.71	0.000059	920.72	0.000004
128:	953.68	0.000007	954.02	0.000007	951.54	0.00002	950.6	0.000029	975.86	0.000003	922.83	0.000002
129:	957.15	0.000061	957.62	0.000063	980.07	0.000069	980.17	0.000079	976.16	0.000002	934.21	0.000074
130:	979.25	0.00004	979.19	0.000044	984.87	0.00005	984.73	0.000055	1001.49	0.000038	943.48	0.000045
131:	979.75	0.000014	979.68	0.000006	986.22	0.000012	985.02	0.000009	1002.26	0.000013	944.37	0.00001
132:	1002.48	0.000541	1001.82	0.000528	1000.37	0.000594	997.66	0.000588	1015.04	0.000298	966.03	0.000002

133:	1004.93	0.000364	1004.66	0.000399	1002.43	0.0017	999.29	0.000442	1017.82	0.000195	967.44	0.000004
134:	1005.05	0.001326	1005.62	0.001618	1002.68	0.000328	999.77	0.001574	1019.68	0.001631	967.55	0.000672
135:	1005.48	0.000267	1006.36	0.000027	1010.72	0.000005	1010.77	0.000005	1023.43	0.000597	969.96	0.00046
136:	1006.04	0.000035	1006.64	0.000045	1011.21	0.000002	1012.93	0	1023.92	0.00045	971.54	0.001903
137:	1020.15	0.000034	1020.56	0.000016	1018.65	0.000042	1016.97	0.000026	1026.08	0.000091	985.62	0.000021
138:	1025.18	0.000522	1021.68	0.002504	1031.46	0.000202	1028.14	0.000069	1026.54	0.000082	993.81	0.000127
139:	1026.21	0.000604	1025.92	0.000597	1032.13	0.000009	1029.72	0.00006	1031.77	0.000092	994.52	0.001978
140:	1029.45	0.002082	1026.71	0.000498	1032.34	0.000311	1030.73	0.000215	1033.72	0.00333	995.74	0.000321
141:	1032.05	0.000072	1030.36	0.000076	1032.59	0.000046	1031.36	0.000326	1046.93	0.000075	997.1	0.000124
142:	1034.27	0.000208	1033.65	0.000071	1032.74	0.00045	1031.55	0.000103	1047.59	0.000443	997.85	0.000585
143:	1034.96	0.000115	1035.28	0.000301	1034.32	0.000069	1032.4	0.000012	1049.52	0.000086	998.61	0.000604
144:	1036	0.000218	1035.79	0.000223	1036.64	0.000038	1032.62	0.000381	1051.62	0.000073	999.49	0.000223
145:	1037.65	0.000377	1036.55	0.000255	1051.24	0.00064	1051.8	0.000624	1051.78	0.00022	1001.1	0.000649
146:	1050.25	0.000867	1043.13	0.000733	1052.2	0.000314	1052.05	0.000303	1056.11	0.000591	1011.24	0.000793
147:	1052.67	0.000556	1052.55	0.00058	1058.56	0.000001	1058.58	0.002377	1067.32	0.000609	1011.54	0.000362
148:	1053.64	0.000229	1052.87	0.000224	1065.01	0.002248	1059.16	0.000001	1067.95	0.000233	1014.69	0.001139
149:	1060.74	0.000001	1060.55	0.000001	1080.68	0.000631	1073.51	0.000677	1074.19	0.000001	1019.88	0.000002
150:	1116.08	0.000557	1112.06	0.000824	1135.61	0.002519	1132.81	0.001576	1104.44	0.001252	1082.31	0.00118
151:	1116.39	0.00414	1112.58	0.003663	1136.77	0.002869	1133.56	0.00364	1104.93	0.003251	1083.01	0.003118
152:	1123.08	0.000042	1123.62	0.000047	1140.09	0.000036	1136.2	0.000049	1113.79	0.000038	1092.96	0.000052
153:	1138.67	0.000012	1138.54	0.000061	1142.93	0.000083	1138.74	0.000093	1141.98	0.00004	1110.52	0.000085
154:	1139.39	0.000073	1139.07	0.000008	1143.58	0.000168	1139.45	0.000162	1142.46	0.00004	1111.07	0.000019
155:	1141.79	0.000033	1139.8	0.00005	1174.16	0.000178	1171.23	0.000191	1146.48	0.000096	1112.85	0.000046
156:	1144.87	0.000001	1143.38	0.000002	1180.95	0.000018	1176.39	0.000021	1151.62	0.00002	1116.67	0.000001
157:	1176.7	0.000011	1176.64	0.000012	1190.69	0.000005	1190.41	0.000005	1173.48	0.00001	1145.46	0.000012
158:	1206.42	0.000833	1205.4	0.005817	1205.61	0.000686	1201.99	0.000785	1211.09	0.002371	1159.29	0.00633
159:	1206.78	0.00142	1206.4	0.002772	1206.45	0.000409	1202.51	0.00034	1211.68	0.003853	1161.66	0.00643
160:	1208.06	0.005447	1207.64	0.00196	1220.48	0.006238	1216.94	0.006644	1211.74	0.00165	1173.95	0.002539
161:	1210.94	0.005621	1209.6	0.003165	1222.52	0.006368	1219.01	0.006069	1214.64	0.005014	1175.7	0.001039
162:	1214.92	0.001712	1214.13	0.001562	1231.6	0.001221	1226.93	0.001183	1224.41	0.001864	1177.66	0.000543
163:	1220.34	0.000168	1220.1	0.000026	1238.67	0.000487	1235.61	0.0006	1229.46	0.000035	1182.88	0.000142
164:	1236.9	0.000174	1236.75	0.000151	1252.66	0.000126	1250.61	0.000521	1231.44	0.000153	1199.01	0.00058
165:	1237.13	0.000061	1237.09	0.000086	1252.8	0.000107	1252.04	0.000125	1231.74	0.000105	1200.77	0.000631
166:	1243	0.00048	1241.01	0.000504	1253.84	0.00055	1252.83	0.000057	1242.27	0.000483	1206.49	0.000233
167:	1246.6	0.000535	1243.77	0.000561	1256.79	0.000512	1252.93	0.000504	1242.98	0.000103	1207.27	0.000096
168:	1250.04	0.000052	1249.4	0.000059	1261.75	0.000019	1256.9	0.000205	1244.54	0.000558	1210.1	0.000005
169:	1252.77	0.000006	1252.35	0.000013	1262.53	0.00021	1258.33	0.00003	1258.26	0.000061	1213.72	0.000034
170:	1257.13	0.00009	1256.07	0.000086	1268.94	0.00005	1265.6	0.000039	1263.89	0.0003	1218.47	0.000094
171:	1264.05	0.000257	1264.13	0.00026	1269.08	0.000045	1267.19	0.000022	1267.32	0.000281	1223.91	0.000243
172:	1289.35	0.001068	1287.43	0.000909	1295.15	0.001714	1290.55	0.001636	1297.18	0.000297	1240.87	0.001074
173:	1293.61	0.000099	1294.01	0.000132	1301.5	0.000502	1298.64	0.000635	1299.02	0.000582	1252.4	0.000063
174:	1295.19	0.000743	1296.35	0.000808	1305.4	0.000135	1305.02	0.000021	1304.3	0.000445	1254.7	0.000732
175:	1299.11	0.00047	1300.02	0.000501	1307.34	0.000516	1307	0.000637	1305.17	0.000791	1256.6	0.000642
176:	1315.25	0.000104	1314.35	0.000114	1315.97	0.000165	1315.65	0.000117	1317.67	0.000184	1269.89	0.000216

177:	1318.89	0.00036	1319.3	0.000321	1317.73	0.000041	1317.46	0.000049	1317.87	0.000308	1273.48	0.000263
178:	1320.48	0.00002	1320.99	0.000026	1327.62	0.000153	1321.99	0.000143	1324.48	0.00011	1276.79	0.00003
179:	1325.48	0.000118	1325.4	0.000091	1337.57	0.000086	1333.15	0.000044	1327.86	0.000193	1280.88	0.000041
180:	1356.24	0.000095	1355.3	0.000103	1371.21	0.00012	1370.85	0.000086	1332.3	0.000116	1327.49	0.000078
181:	1356.89	0.000229	1356.32	0.000199	1372.06	0.000189	1371.53	0.000215	1336.09	0.000027	1332.02	0.000157
182:	1361.21	0.000238	1361.73	0.000218	1375.16	0.000084	1375.39	0.000051	1339.3	0.000152	1332.9	0.000564
183:	1371.59	0.000258	1370.9	0.000261	1377.5	0.000336	1376.66	0.00122	1360.38	0.000303	1333.09	0.000202
184:	1391.52	0.000632	1391.04	0.000316	1380.13	0.001227	1377.65	0.000375	1403.78	0.000574	1335.49	0.000841
185:	1392.61	0.000441	1392.2	0.000646	1382.35	0.000994	1380.77	0.001019	1407.22	0.000312	1336.15	0.00084
186:	1394.23	0.000438	1395.4	0.000586	1384.81	0.000725	1380.94	0.000753	1407.51	0.000466	1337.63	0.000364
187:	1394.94	0.000352	1396.54	0.000319	1386.04	0.000717	1385.89	0.000684	1408.3	0.000298	1338.51	0.000498
188:	1401.02	0.000065	1401.84	0.000057	1391.9	0.000072	1391.2	0.000067	1414.2	0.000034	1345.05	0.00006
189:	1403.38	0.000002	1402.8	0.000001	1392.09	0.000061	1391.41	0.000056	1417.26	0.000015	1345.53	0.000045
190:	1403.77	0.000006	1403.87	0.000005	1397.48	0.000017	1396.75	0.000018	1418.45	0.000022	1346.5	0.000086
191:	1408.72	0.000245	1409.06	0.000259	1403.02	0.000091	1403.18	0.000106	1422.48	0.000065	1355.01	0.000004
192:	1418.62	0.000739	1421.24	0.000917	1405.37	0.001267	1404.49	0.001636	1422.77	0.00013	1363.33	0.001106
193:	1419.62	0.000871	1421.65	0.000553	1406.2	0.001354	1405	0.000903	1422.95	0.000728	1363.91	0.000767
194:	1428.41	0.000026	1427.15	0.000192	1427.37	0.000007	1426.65	0.000029	1432.4	0.00076	1377.22	0.00003
195:	1428.71	0.00044	1428.37	0.000291	1429.66	0.000221	1429.29	0.000205	1432.7	0.000803	1380.47	0.000179
196:	1441.08	0.000026	1442.7	0.000006	1438.38	0.000027	1437.65	0.00005	1449.13	0.000055	1389.92	0.00007
197:	1443.9	0.000117	1445.19	0.000126	1438.98	0.000048	1438.12	0.00004	1453.16	0.000092	1390.35	0.000051
198:	1460.4	0.000124	1461.76	0.000116	1444.72	0	1445.09	0.000001	1468.91	0.000131	1399.27	0.000004
199:	1465.24	0.000588	1464.8	0.000523	1448.27	0.000023	1445.59	0.000156	1473.51	0	1399.48	0.000176
200:	1467.57	0	1467.69	0.000001	1450.56	0.000048	1449.15	0.000125	1474.17	0.000541	1401.61	0.000147
201:	1470.93	0.000011	1472.08	0.000129	1451.24	0.000145	1450.78	0.000178	1477.68	0.000012	1403.43	0.000328
202:	1473.52	0.000001	1474.22	0	1453.23	0.000182	1452.26	0.000447	1479.7	0.000008	1405.64	0.000015
203:	1475.49	0.000076	1475.31	0.000235	1453.41	0.000316	1453.23	0.00011	1481.38	0.000923	1407.45	0.00031
204:	1475.78	0.000214	1476.58	0.000558	1454.57	0.000548	1453.44	0.000334	1481.97	0.000198	1409.42	0.000087
205:	1476.14	0.000659	1476.87	0.000403	1456.62	0.000374	1454.46	0.000135	1482.1	0.0001	1410.09	0.000337
206:	1477.19	0.000379	1477.23	0.00009	1457.46	0.000222	1455.34	0.000339	1482.24	0.000592	1412.19	0.000105
207:	1479.97	0.000141	1479.09	0.000117	1459.77	0.000916	1459.28	0.000865	1483.39	0.000368	1412.29	0.00086
208:	1481.7	0.000359	1481.53	0.000241	1461.56	0.000645	1459.35	0.000751	1486.94	0.000125	1417.18	0.000026
209:	1481.86	0.000672	1481.65	0.000827	1465.12	0.000708	1464.37	0.000387	1487.94	0.000359	1417.23	0.000634
210:	1483.97	0.000453	1483.52	0.000443	1465.57	0.000124	1464.52	0.000422	1488.07	0.000562	1418.24	0.00062
211:	1484.51	0.000221	1484.89	0.000186	1465.88	0.000951	1464.99	0.001042	1490	0.000444	1418.61	0.000087
212:	1485.71	0.00003	1485.91	0.000052	1466.62	0.000122	1465.25	0.000059	1491.21	0.000016	1419.18	0.000781
213:	1487.3	0.00006	1486.71	0.000054	1466.73	0.000082	1465.48	0.000122	1492.59	0.000024	1421.46	0.000139
214:	1493.44	0.000819	1493.16	0.00085	1477.72	0.000409	1476.44	0.000235	1494.06	0.000056	1432.74	0.000153
215:	1496.56	0.000281	1497.93	0.000161	1478.01	0.000136	1477.85	0.000281	1501.41	0.000199	1432.89	0.00019
216:	1497.53	0.000152	1499.28	0.000169	1482.03	0.000119	1479.68	0.000141	1502.53	0.000258	1434.54	0.000201
217:	1499.95	0.000112	1499.95	0.00016	1483.82	0.0002	1482.65	0.000221	1505.54	0.000112	1435.72	0.000153
218:	1501.82	0.000168	1501.87	0.00018	1497.16	0.000931	1494.72	0.000855	1508.11	0.000189	1449.55	0.001143
219:	1514.94	0.000744	1514.97	0.000671	1499.16	0.000916	1496.19	0.000945	1520.55	0.00072	1451.07	0.000632
220:	1516.87	0.000741	1516.45	0.000722	1514.93	0.00128	1513.35	0.001269	1522.03	0.000576	1452.64	0.000841

221:	1528.42	0.001025	1527.84	0.000547	1540.97	0.000647	1540.43	0.000648	1523.14	0.001016	1478.71	0.000675
222:	1528.52	0.000018	1529.1	0.000508	1541.49	0.00072	1541.68	0.000738	1523.86	0.00036	1480.47	0.000684
223:	1567.33	0.000025	1567.27	0.000028	1599.8	0.000023	1599.98	0.000025	1542.05	0.000035	1518.93	0.000036
224:	1606	0.000295	1605.45	0.000305	1635.24	0.00029	1635.18	0.000336	1584.63	0.000298	1558.71	0.00035
225:	1606.6	0.000118	1606.21	0.000115	1636.06	0.000177	1635.91	0.000139	1585.17	0.000083	1559.31	0.000102
226:	1637.11	0.000091	1635.94	0.000102	1672.26	0.000078	1671.26	0.000085	1617.11	0.000105	1588.96	0.000131
227:	1653.15	0.000766	1652.19	0.000714	1685.07	0.001033	1684.15	0.000887	1634.51	0.000708	1604.52	0.000692
228:	1653.29	0.00065	1652.86	0.000679	1685.16	0.000698	1684.85	0.000839	1634.8	0.000664	1605.11	0.000586
229:	1900.38	0.023985	1899.65	0.024268	1955.57	0.023896	1955.36	0.024452	1825.71	0.024787	1836.65	0.022295
230:	1951.17	0.03116	1950.44	0.031021	2008.12	0.032461	2007.57	0.032059	1878.82	0.032362	1887.71	0.028654
231:	2980.26	0.000389	2971.51	0.000494	3002.77	0.000397	2997.15	0.00045	2895.66	0.000469	2880.67	0.00049
232:	2982.85	0.000853	2975.33	0.00079	3005.55	0.000656	3000.5	0.000659	2898.98	0.000967	2885.14	0.000951
233:	2989.06	0.000275	2982.19	0.000259	3009.87	0.000214	3007.06	0.000203	2904.37	0.000323	2892.32	0.000271
234:	2991.98	0.000203	2986.52	0.000216	3016.1	0.000185	3010.66	0.000189	2906.57	0.000218	2895.23	0.000269
235:	3016.95	0.002552	3017.16	0.002567	3041.73	0.001922	3043.08	0.001905	2949.82	0.002699	2943.98	0.00255
236:	3017.98	0.000243	3018.12	0.000232	3042.72	0.000185	3044.25	0.000202	2950.73	0.000276	2945.63	0.000219
237:	3026.09	0.000417	3026.57	0.00048	3050.63	0.000278	3052.37	0.000312	2960.42	0.000682	2955.18	0.000608
238:	3026.51	0.000489	3027.22	0.000387	3051.08	0.000331	3052.93	0.000273	2960.68	0.000486	2956.42	0.000545
239:	3027.58	0.000634	3027.95	0.000629	3052.88	0.000406	3054.33	0.0004	2960.91	0.00046	2956.53	0.000419
240:	3028.95	0.000612	3029.32	0.000606	3054.13	0.000409	3055.6	0.000397	2961.55	0.000663	2956.96	0.000351
241:	3032.61	0.000406	3031.49	0.000396	3055.59	0.000305	3056.14	0.0003	2967.42	0.000424	2961.16	0.00036
242:	3035.84	0.00046	3035.05	0.000447	3059.19	0.000313	3060.27	0.000308	2971.58	0.000475	2964.79	0.000378
243:	3037.39	0.000189	3036.67	0.000204	3060.57	0.00011	3061.68	0.000112	2972.76	0.000187	2965.77	0.000179
244:	3041.1	0.000338	3040.39	0.000297	3064.08	0.000206	3065.34	0.000178	2976.68	0.000366	2969.26	0.000239
245:	3081.54	0.000708	3081.48	0.000707	3116.53	0.000439	3116.99	0.000438	3006.27	0.000758	3008.64	0.000564
246:	3084.62	0.000001	3084.55	0	3119.9	0.000001	3120.61	0.000002	3009.55	0.000008	3012.78	0.000001
247:	3102.32	0.000209	3102.3	0.000209	3137.83	0.000135	3138.47	0.000141	3027.48	0.000242	3029.7	0.000161
248:	3102.96	0.000257	3103.1	0.00026	3138.05	0.000108	3138.53	0.000103	3028.37	0.000277	3030.94	0.000192
249:	3112.34	0.000308	3110.83	0.000327	3147.98	0.000193	3147.53	0.000224	3041.99	0.000325	3043.42	0.000267
250:	3112.42	0.000317	3111.79	0.00029	3148.16	0.000197	3148.7	0.000185	3042.1	0.000321	3044.5	0.000223
251:	3115.09	0.000135	3115.09	0.000076	3149.01	0.000164	3149.86	0.000163	3043.54	0.000156	3047.31	0.000097
252:	3117.96	0.000098	3117.35	0.000012	3151.62	0.000092	3152.77	0.000037	3047.29	0.000481	3049.08	0.000014
253:	3118.25	0.000511	3117.7	0.000523	3153.41	0.00028	3153.93	0.000251	3047.44	0.000176	3050.37	0.000367
254:	3120.43	0.000268	3119.62	0.00031	3154.67	0.000204	3154.77	0.000132	3050.49	0.000266	3051.33	0.000214
255:	3122.99	0.001411	3121.85	0.000347	3155.02	0.000064	3155.48	0.000129	3052.19	0.001465	3052.58	0.000259
256:	3123.18	0.00025	3122.49	0.001346	3157.34	0.000313	3156.39	0.000267	3052.52	0.000232	3053.39	0.000113
257:	3124.78	0.000539	3123.4	0.00069	3157.75	0.000672	3158.35	0.000703	3053.6	0.000415	3055.09	0.000986
258:	3127.26	0.0011	3125.64	0.00103	3161.48	0.000887	3161.15	0.000859	3055.29	0.000578	3057.95	0.000512
259:	3127.49	0.000643	3127.51	0.000528	3161.71	0.000244	3162.56	0.000233	3056.24	0.000037	3057.99	0.000907
260:	3128.47	0.00007	3128.59	0.000091	3162.82	0.000127	3163.71	0.000135	3057.83	0.001433	3058.7	0.000079
261:	3135.19	0.000068	3131.99	0.000081	3165.31	0.000054	3164.37	0.000013	3063.31	0.000207	3059.74	0.000383
262:	3136.24	0.000212	3134.62	0.00045	3165.59	0.000216	3166.08	0.000306	3063.58	0.000208	3060.57	0.000284
263:	3136.39	0.000198	3135.08	0.000294	3168.79	0.000385	3166.85	0.000449	3066.73	0.000082	3061.8	0.000039
264:	3138.08	0.000407	3136.77	0.000189	3170.63	0.000102	3167.87	0.000192	3069.36	0.000291	3064.14	0.000541

265:	3142.16	0.000292	3137.08	0.000133	3170.71	0.000105	3171.24	0.000133	3070.39	0.000321	3066.55	0.000145
266:	3142.77	0.00006	3137.14	0.000225	3171.54	0.000172	3171.78	0.000108	3070.48	0.000177	3066.77	0.000145
267:	3148.61	0.000174	3143.28	0.000157	3174.02	0.000128	3172.09	0.000104	3075.96	0.000183	3067.12	0.000212
268:	3149.26	0.000114	3145.43	0.000136	3175.05	0.000116	3173.86	0.000124	3077.47	0.000101	3068.15	0.000043
269:	3158.1	0.000021	3158.94	0.000024	3186.06	0.000109	3188.68	0.000113	3083.68	0.00018	3085	0.000168
270:	3158.88	0.0001	3160.76	0.000055	3186.75	0.000077	3190.44	0.000101	3085.07	0.000087	3085.66	0.000336
271:	3160.13	0.000102	3161.24	0.000169	3189.17	0.000084	3191.65	0.000224	3086.1	0.00042	3086.36	0.000116
272:	3160.98	0.000186	3162.02	0.000406	3189.73	0.000221	3193.42	0.000071	3086.58	0.000123	3087.68	0.000197
273:	3161.8	0.000401	3162.61	0.000183	3190.32	0.000064	3193.76	0.000118	3087.16	0.000042	3088.31	0.000098
274:	3164.58	0.000199	3164.65	0.000197	3191.8	0.000113	3194.87	0.000057	3088.06	0.000179	3089.05	0.000059
275:	3178.21	0.000386	3178.63	0.000373	3204.27	0.000233	3205.79	0.000222	3102.55	0.000442	3102.22	0.000324
276:	3178.8	0.000463	3179.57	0.000434	3204.53	0.000223	3207.09	0.00021	3103.61	0.000443	3103.01	0.000259
277:	3180.67	0.000396	3180.53	0.000216	3207.47	0.000188	3208.99	0.000213	3105.32	0.00019	3103.87	0.000229
278:	3180.7	0.000099	3181.06	0.000291	3207.68	0.00015	3209.25	0.000132	3105.43	0.00031	3104.76	0.000341

Table S21. Calculated vibrational frequencies of **3**, **4** and **5** with and without dispersion correction.

	3					**4**					**5**			
	TPSSh; Disp ON		TPSSh; Disp ON			TPSSh; Disp ON		TPSSh; Disp OFF			TPSSh; Disp ON		TPSSh; Disp OFF	
Mode	freq	T**2	freq	T**2	Mode	freq	T**2	freq	T**2	Mode	freq	T**2	freq	T**2
	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)		cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm**-1	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)
6:	19.54	0.000082	17.1	0.001807	6:	18.98	0.000476	20.85	0.000371	6:	18.3	0.000373	19.27	0.000472
7:	22.51	0.001751	21.87	0.000071	7:	30.07	0.000135	32.06	0.000047	7:	29.27	0.000011	31.34	0.000077
8:	28.83	0.000669	28.63	0.000551	8:	34.46	0.000065	36.86	0.000282	8:	32.76	0.000096	35.23	0.000181
9:	34.54	0.000127	34.9	0.000026	9:	37.22	0.000105	41.97	0.000024	9:	35.14	0.00015	37.47	0.000074
10:	36.15	0.000408	36.7	0.000188	10:	43.77	0.000305	43.97	0.0001	10:	38.81	0.0001	39.19	0.000125
11:	36.82	0.000167	38.33	0.000345	11:	45.8	0.000317	45.35	0.000347	11:	42.76	0.000172	41.65	0.000122
12:	38.69	0.000303	39.08	0.000051	12:	47.54	0.000167	47.1	0.000105	12:	43.94	0.000341	44.33	0.00017
13:	39.52	0.000062	41.29	0.000025	13:	49.15	0.000287	47.92	0.000154	13:	45.83	0.000118	45.68	0.000192
14:	40.26	0.000042	43.59	0.000331	14:	54.72	0.000214	54.84	0.00009	14:	49.73	0.00031	48.89	0.000333
15:	45.58	0.000188	45.76	0.000169	15:	60.05	0.000187	55.1	0.000533	15:	57.88	0.000014	53.34	0.000016
16:	47.14	0.000249	53.31	0.00075	16:	64.69	0.000061	64.07	0.000371	16:	62.83	0.000049	62.15	0.000028
17:	52.86	0.000627	60.07	0.000102	17:	66.32	0.000144	66.99	0.000187	17:	65.59	0.000243	65.37	0.000462
18:	61.62	0.0001	60.38	0.000105	18:	71.17	0.000076	71.72	0.000199	18:	68.24	0.000036	67.05	0.000123
19:	64.52	0.000254	62.2	0.000538	19:	80.73	0.001496	78.4	0.001	19:	83.34	0.001481	81.03	0.001155
20:	77.02	0.000006	72.95	0.000009	20:	92.08	0.00233	91.14	0.002211	20:	91.81	0.001443	90.81	0.001131
21:	87.82	0.001153	84.58	0.001053	21:	96.6	0.000047	94.02	0.000264	21:	96.55	0.000022	93.64	0.000198
22:	89.57	0.00144	87.35	0.00129	22:	99.71	0.000472	97.1	0.000596	22:	98.92	0.000433	96.71	0.000672
23:	97.05	0.000136	92.65	0.000114	23:	110.81	0.000475	109.3	0.000298	23:	116.61	0.000323	113.66	0.000364
24:	102.74	0.000129	97.59	0.000369	24:	119.33	0.00022	117.78	0.0003	24:	118.78	0.000103	116.33	0.0001
25:	112.35	0.000037	104.91	0.000012	25:	126.25	0.000154	125.37	0.000078	25:	125.44	0.000547	125.68	0.000468
26:	116.54	0.000364	116.16	0.00033	26:	128.99	0.000537	129.09	0.000464	26:	131.19	0.000084	130.66	0.00006
27:	118.56	0.000047	117.43	0.000064	27:	135.29	0.000023	134.73	0.000035	27:	133.68	0.000246	132.6	0.00026
28:	124.15	0.000172	122.12	0.000126	28:	138.8	0.000938	136.9	0.000869	28:	143.24	0.000412	141.2	0.000412
29:	130.58	0.000037	131.51	0.000029	29:	159.08	0.000134	156.56	0.000157	29:	150.57	0.001557	148.88	0.001503
30:	142.83	0.000511	140.16	0.000464	30:	161.48	0.000003	159.41	0.000002	30:	160.74	0.000085	158.18	0.000116
31:	148.09	0.001326	145.75	0.001366	31:	166.13	0.000127	164.21	0.000123	31:	171.09	0.000595	169.48	0.000605
32:	157.37	0.000435	154.43	0.000288	32:	169.22	0.00047	168.52	0.000498	32:	172.76	0.000024	173.75	0.000031
33:	166.76	0.001216	164.62	0.00138	33:	176.94	0.000084	176.61	0.000013	33:	192.25	0.000368	193.01	0.000195
34:	180.5	0.000002	171.7	0.000009	34:	193.95	0.000935	193.3	0.001011	34:	197.4	0.000092	196.95	0.000234
35:	190.88	0.000033	183.07	0.000017	35:	199.58	0.00008	196.36	0.000332	35:	202.28	0.000085	203.25	0.000081
36:	195.15	0.000272	190.5	0.000334	36:	200.17	0.000255	198.72	0.000012	36:	209.92	0.000041	211.45	0.000047
37:	209.52	0.00001	204.68	0.000004	37:	209.75	0.000006	205.85	0.000039	37:	213.55	0.000071	214.59	0.00001
38:	214.85	0.000045	207.14	0.000035	38:	212.7	0.000039	210.49	0.000036	38:	217.89	0.000005	218.4	0.000036
39:	215.91	0.000093	211.68	0.000098	39:	214.38	0.000045	212.7	0.000063	39:	226.5	0.000329	225.24	0.000314
40:	225.58	0.00006	219.24	0.000033	40:	217.16	0.000097	214.1	0.000015	40:	240.45	0.00059	239.43	0.000541
41:	227.63	0.000324	226.4	0.000265	41:	222.77	0.000008	220.36	0.000007	41:	248.7	0.000271	246.42	0.00024
42:	248	0.000722	245.29	0.00079	42:	234.74	0.000496	233.33	0.000464	42:	252.41	0.000007	252.46	0.000074
43:	263.86	0.00021	256.49	0.000193	43:	249.71	0.00007	249.02	0.000089	43:	255.18	0.00007	258.22	0.000014
44:	265.4	0.000299	258.59	0.000078	44:	254.62	0.000111	254.06	0.00015	44:	265.12	0.000012	264.84	0.000013

45:	270.46	0.000164	262.72	0.000181	45:	255.64	0.000136	254.61	0.000123	45:	269.7	0.000012	270.72	0.000029
46:	277.36	0.000288	268.14	0.000072	46:	263.22	0.000049	259.88	0.000023	46:	275.47	0.000031	276.66	0.000012
47:	279.13	0.000272	272.34	0.000064	47:	273.41	0.000034	267.77	0.000019	47:	280.79	0.000048	284.48	0.000045
48:	282.62	0.000071	274.7	0.000676	48:	275.44	0.000052	274.58	0.000018	48:	289.22	0.000024	287.86	0.000005
49:	285.32	0.000014	277.15	0.000017	49:	280.62	0.00002	277.64	0.000009	49:	300.59	0.000701	299.99	0.00067
50:	298.18	0.000024	290.25	0.000016	50:	285.62	0.000014	280.23	0.000012	50:	304.25	0.000044	302.23	0.000086
51:	305.93	0.000039	298.74	0.000058	51:	291.57	0.000069	286.19	0.000051	51:	305.87	0.000007	304.56	0.000006
52:	314.96	0.000023	314.14	0.000208	52:	300.51	0.000768	299.47	0.000777	52:	315.72	0.000034	315.38	0.00003
53:	322.59	0.001862	314.91	0.001495	53:	303.38	0.00017	300.64	0.000159	53:	327.25	0.001893	324.29	0.001611
54:	330.73	0.000365	322.94	0.000511	54:	307.26	0.000006	303	0.000004	54:	330.57	0.00041	328.88	0.000541
55:	332.22	0.000246	326.72	0.000091	55:	330.6	0.001398	326.21	0.00167	55:	333.54	0.000042	332.46	0.00001
56:	339.25	0.000959	332.98	0.00069	56:	331.12	0.00069	330.05	0.000538	56:	339.42	0.000313	337.62	0.000365
57:	347.36	0.001365	338.26	0.000422	57:	332.79	0.000637	331.45	0.000348	57:	344.96	0.001295	344.44	0.001427
58:	351	0.000163	344.96	0.000186	58:	336.6	0.000042	334.98	0.000015	58:	355.01	0.000066	352.73	0.000053
59:	353.18	0.000075	347.71	0.001129	59:	341.25	0.00026	337.82	0.00021	59:	355.89	0.00001	354.1	0.000009
60:	364.11	0.000068	350.84	0.000047	60:	350.13	0.000513	350.18	0.000509	60:	364.35	0.000548	362.46	0.000658
61:	368.06	0.0001	362.63	0.000004	61:	355.99	0.002316	354.12	0.000562	61:	372.97	0.000451	371.72	0.000384
62:	369.83	0.00047	363.33	0.000161	62:	356.59	0.000055	354.32	0.000007	62:	376.74	0.000737	373.74	0.000835
63:	375.03	0.000336	370.16	0.000817	63:	357.75	0.000434	356.49	0.002498	63:	392.96	0.000578	390.41	0.000824
64:	392.62	0.000508	386.2	0.000627	64:	368.59	0.000016	367.3	0.000032	64:	398.18	0.000607	395.85	0.000511
65:	400.87	0.000499	392.58	0.000483	65:	376.42	0.000667	373.77	0.000737	65:	405.07	0.001445	401.68	0.001458
66:	411.79	0.000141	408.53	0.002574	66:	381.91	0.000202	381.72	0.000135	66:	410.46	0.003154	408.43	0.003159
67:	413.05	0.00018	412.45	0.000078	67:	395.87	0.00063	393.22	0.000746	67:	427.44	0.000171	426.79	0.000173
68:	416.47	0.002442	413.17	0.000092	68:	399.8	0.000458	395.81	0.000685	68:	435.56	0.000606	434.91	0.000561
69:	419.95	0.000061	416.37	0.000118	69:	406.11	0.001348	402.31	0.001333	69:	437.25	0.000207	436.77	0.000204
70:	428.78	0.000231	427.05	0.001339	70:	412	0.003163	410.74	0.003118	70:	439.16	0.000009	438.52	0.000035
71:	431.79	0.007301	427.76	0.005807	71:	433.87	0.00011	433.79	0.000096	71:	442.91	0.000399	441.43	0.00033
72:	437.18	0.000537	435.59	0.000536	72:	438.42	0.000342	438.74	0.000217	72:	443.72	0.000231	442.19	0.00024
73:	459.01	0.001801	451.45	0.001899	73:	441.73	0.000015	440.89	0.000003	73:	459.45	0.002578	457.43	0.002622
74:	463.06	0.001114	455.61	0.00138	74:	444.58	0.000334	443.28	0.000321	74:	463.06	0.000539	460.02	0.000609
75:	465.7	0.000719	462.44	0.000302	75:	446.15	0.000263	444.85	0.000192	75:	468.69	0.001024	467.46	0.001052
76:	476.91	0.000026	469.91	0.000033	76:	453.31	0.000422	453.6	0.000493	76:	478.93	0.000523	476.19	0.000582
77:	485.97	0.004074	480.91	0.005278	77:	460.04	0.002594	458.7	0.002614	77:	489.09	0.000464	487.12	0.000455
78:	500.88	0.001782	495.34	0.00134	78:	466.97	0.000189	461.97	0.000334	78:	498.59	0.000284	496.69	0.000495
79:	507.97	0.001049	502.49	0.000734	79:	468.1	0.000987	467.69	0.001032	79:	501.84	0.000383	497.18	0.000307
80:	510.15	0.000936	503.84	0.000713	80:	478.19	0.000661	476.27	0.000681	80:	511.61	0.001091	508.53	0.001459
81:	513.63	0.000325	507.71	0.000288	81:	492.46	0.000317	489.26	0.000455	81:	514.38	0.000748	513.39	0.0018
82:	518.77	0.003657	516.99	0.004344	82:	500.1	0.000297	498.09	0.000595	82:	516.28	0.002422	514.38	0.001019
83:	521.45	0.001161	520.39	0.001047	83:	502.51	0.00046	498.63	0.000383	83:	527.06	0.000077	524.84	0.000089
84:	528.51	0.000606	528.78	0.000634	84:	507.96	0.001611	503.93	0.001604	84:	528.98	0.000696	528.76	0.00063
85:	536.98	0.001256	534.11	0.000838	85:	515.18	0.000106	513.51	0.000087	85:	536.7	0.000555	536.27	0.000581
86:	541.9	0.002308	541.72	0.002744	86:	518.32	0.002554	516.15	0.00253	86:	545.66	0.003588	546.25	0.003543
87:	572.5	0.005941	571.79	0.005844	87:	524.5	0.000456	524.14	0.000368	87:	573.26	0.005761	572.65	0.005643
88:	604.93	0.000161	604.32	0.000167	88:	528.23	0.000072	526.34	0.000084	88:	604.62	0.000171	604.97	0.000188

89:	616.89	0.000946	614.8	0.000907	89:	543.45	0.004126	545.44	0.003889	89:	617.97	0.000922	616.94	0.000848
90:	633.48	0.004799	628.78	0.003289	90:	570.1	0.005457	570.24	0.005319	90:	712.9	0.001198	706.28	0.001351
91:	634.31	0.001177	629.53	0.002811	91:	601.41	0.000399	601.51	0.000389	91:	722.72	0.001434	717.19	0.001361
92:	640.83	0.000015	640.6	0.000002	92:	609.89	0.000011	609.72	0.000013	92:	734.5	0.000996	728.81	0.001389
93:	641.31	0.000117	641	0.000061	93:	623.04	0.001021	622.51	0.000982	93:	737.74	0.001088	732.73	0.000995
94:	720.83	0.002319	711.5	0.002542	94:	694.65	0.000567	695.46	0.000546	94:	746.66	0.000119	740.43	0.00019
95:	730.37	0.00008	724.76	0.00144	95:	713.36	0.001296	706.62	0.0014	95:	764.6	0.000798	761.87	0.000764
96:	731.46	0.000002	728.87	0.001608	96:	723.61	0.001443	717.43	0.001481	96:	776.39	0.000241	770.84	0.000182
97:	731.94	0.001129	730.29	0.000105	97:	726.62	0.000015	726.57	0.000003	97:	787.58	0.000442	784.15	0.000416
98:	737.04	0.001612	731.11	0.00002	98:	733.73	0.000945	729.08	0.001412	98:	796.38	0.000019	795.98	0.000018
99:	762.23	0.001049	757.44	0.000994	99:	739.52	0.00113	733.97	0.001025	99:	799.89	0.00002	798.83	0.00002
100:	769.11	0.000867	763.53	0.000877	100:	747.85	0.000045	741.12	0.000103	100:	809.69	0.000035	809.06	0.000042
101:	783.87	0.001152	780.48	0.001209	101:	766.01	0.000745	763.33	0.000757	101:	822.97	0.000771	822.1	0.000505
102:	810.72	0.000009	808.78	0.000023	102:	769.15	0.000003	767.86	0.000002	102:	828.13	0.000352	826.83	0.00031
103:	810.89	0.000033	808.9	0.000038	103:	776.13	0.00033	770.63	0.000253	103:	829.53	0.000341	827.96	0.000278
104:	812.27	0.00017	810.66	0.000131	104:	788.05	0.000424	784.27	0.00042	104:	832.45	0.000107	829.93	0.000197
105:	823.01	0.002014	821.03	0.002426	105:	797.86	0.000018	798.26	0.000017	105:	835.09	0.001141	833.14	0.001299
106:	825.79	0.000847	822.94	0.000473	106:	801.68	0.000017	800.08	0.000026	106:	839.78	0.000391	837.41	0.000357
107:	827.82	0.000314	823.47	0.000437	107:	824.79	0.000688	824.32	0.000353	107:	859.91	0.000725	858.37	0.000531
108:	831.64	0.001067	827.54	0.000625	108:	830.27	0.000507	827.35	0.000468	108:	860.33	0.000379	859.62	0.000472
109:	832.59	0.001034	830.09	0.000954	109:	832.62	0.000203	829.19	0.000102	109:	865.96	0.000004	865.35	0.000006
110:	841.52	0.000753	837.36	0.000974	110:	834.93	0.001288	833.24	0.001538	110:	872.12	0.002108	871.86	0.002092
111:	865.73	0.000033	864.4	0.000004	111:	840.54	0.000388	837.46	0.000409	111:	883.98	0.000666	884.85	0.0006
112:	866.46	0.000069	865.43	0.000033	112:	860.44	0.000545	860.34	0.00051	112:	902.19	0.000349	900.4	0.00032
113:	867.5	0.000009	866.54	0.000093	113:	862.07	0.000618	861.94	0.000511	113:	903.23	0.000715	901.3	0.000552
114:	871.6	0.001756	870.1	0.001723	114:	871.56	0.002664	872.03	0.002802	114:	905.35	0.000332	903.96	0.00043
115:	885.18	0.000603	884.74	0.000552	115:	885.39	0.000056	886.19	0.000056	115:	905.69	0.000763	904.75	0.000662
116:	904.64	0.005956	903.55	0.005885	116:	898.42	0.00058	898.61	0.000577	116:	907.46	0.003573	906.84	0.003927
117:	908.86	0.000005	904.25	0.000007	117:	902.17	0.001224	900.97	0.000818	117:	909.63	0.000002	908.94	0.000002
118:	919.11	0.000025	915.39	0.0001	118:	904.01	0.00108	902.92	0.000865	118:	917.38	0.000068	916.39	0.000152
119:	920.44	0.000243	916.86	0.00022	119:	904.96	0.000966	904.68	0.00108	119:	919.48	0.000359	918.66	0.000242
120:	932.52	0.000064	928.25	0.000067	120:	905.28	0.000067	905.35	0.000063	120:	929.54	0.000004	926.72	0.000023
121:	933.07	0.000033	929.23	0.000037	121:	906.47	0.0003	905.88	0.000355	121:	930.66	0.000299	929.21	0.000238
122:	953.03	0.000009	947.65	0.000008	122:	907.97	0.00286	907.58	0.003297	122:	931.47	0.000514	929.88	0.000608
123:	957.69	0.000007	952.69	0.00001	123:	917.6	0.00019	916.9	0.000259	123:	932.07	0.000048	933.53	0.000037
124:	962.78	0.000028	960.12	0.000028	124:	920.05	0.000275	920.07	0.000143	124:	952.05	0.000004	952.67	0.000004
125:	978.46	0.00004	977.93	0.000035	125:	929.49	0.000015	928.07	0.000022	125:	955.25	0.000007	954.36	0.000008
126:	980.1	0.000031	979.83	0.000031	126:	931.29	0.000397	930.79	0.00037	126:	961.22	0.000032	961.51	0.000029
127:	993.21	0.000064	991.87	0.000079	127:	933.35	0.00038	932.12	0.00039	127:	991.09	0.000047	990.32	0.000057
128:	1002.94	0.000315	999.32	0.000296	128:	935.85	0.000044	934.29	0.000049	128:	1017.54	0.000803	1015.24	0.001134
129:	1003.83	0.00009	1000.86	0.00011	129:	953.91	0.000007	953.33	0.000001	129:	1019.54	0.000765	1017.08	0.000814
130:	1007.96	0.000001	1007.77	0.000008	130:	956.2	0.00005	953.93	0.000009	130:	1028.23	0.001745	1022.02	0.001772
131:	1008.31	0.000018	1008.45	0.000019	131:	956.35	0.000004	956.43	0.000056	131:	1029.06	0.000192	1029.56	0.000257
132:	1024.77	0.000886	1017.46	0.002649	132:	1004.22	0.001735	1003.62	0.00174	132:	1031.22	0.000086	1030.5	0.000075

133:	1026.14	0.000427	1024.43	0.000343	133:	1018.55	0.000513	1016.04	0.000813	133:	1032.7	0.000037	1031.77	0.00007
134:	1028.53	0.001767	1024.63	0.000451	134:	1018.71	0.00003	1017.24	0.000727	134:	1037.01	0.000388	1035.28	0.000295
135:	1032.51	0.000163	1026.63	0.000404	135:	1018.94	0.000786	1018.39	0.000019	135:	1042.46	0.000338	1039.49	0.000362
136:	1032.76	0.000076	1029.35	0.000092	136:	1031.07	0.001331	1025.69	0.00189	136:	1043.83	0.000096	1042.73	0.000105
137:	1034.57	0.000115	1029.89	0.000065	137:	1031.84	0.000067	1027.76	0.000402	137:	1046.41	0.000333	1044.2	0.000219
138:	1038.55	0.000295	1033.38	0.000208	138:	1034.93	0.000271	1030.85	0.000091	138:	1047.08	0.000202	1046.3	0.000049
139:	1044.54	0.000797	1036.93	0.000596	139:	1035.11	0.000076	1031.96	0.000124	139:	1062.59	0.000024	1062.2	0.000003
140:	1048.23	0.000059	1046.93	0.000046	140:	1035.95	0.000218	1035.65	0.000216	140:	1063.72	0.000118	1062.87	0.000162
141:	1051.04	0.00055	1052.11	0.000531	141:	1039.08	0.000607	1036.23	0.000088	141:	1087.58	0.000012	1087.15	0.000019
142:	1052	0.00054	1052.19	0.000496	142:	1043.43	0.000623	1039.83	0.00074	142:	1088.19	0.000183	1087.29	0.000169
143:	1088.2	0.000011	1085.22	0.000006	143:	1043.76	0.000095	1042.81	0.000129	143:	1089.35	0.000203	1088.16	0.000233
144:	1091.5	0.000017	1089.19	0.000022	144:	1046.9	0.000589	1044.4	0.000209	144:	1090.7	0.000024	1091.55	0.00002
145:	1115.12	0.001973	1110.37	0.001682	145:	1060.91	0	1060.63	0	145:	1103.44	0.000036	1103.03	0.000023
146:	1116.63	0.002818	1111.85	0.002946	146:	1062.4	0.000042	1061.97	0.000073	146:	1103.82	0.000116	1103.33	0.00009
147:	1136.54	0.000197	1132.21	0.000047	147:	1064.85	0.000111	1064.21	0.000129	147:	1131.21	0.000214	1129.27	0.000166
148:	1137.61	0.000038	1132.74	0.000206	148:	1089.76	0.000203	1090.39	0.000206	148:	1134.73	0.000165	1134.07	0.000204
149:	1139.08	0.000063	1133.29	0.00008	149:	1091.76	0.000196	1091.76	0.000211	149:	1135.46	0.000465	1134.41	0.00041
150:	1140.73	0.000061	1136.69	0.000037	150:	1103.69	0.000049	1103.08	0.000063	150:	1143.91	0.000179	1141.71	0.000209
151:	1144.01	0.000019	1140.45	0.000024	151:	1104.19	0.00017	1103.53	0.000114	151:	1144.65	0.000052	1142.04	0.000036
152:	1145.91	0.000031	1143.99	0.000039	152:	1122.85	0.000039	1123.24	0.000043	152:	1145.09	0.00005	1144.75	0.000028
153:	1189.92	0.00011	1187.56	0.000107	153:	1131.57	0.000184	1129.83	0.000125	153:	1190.27	0.000106	1191.06	0.00011
154:	1205.7	0.000905	1200.43	0.000744	154:	1135.96	0.000381	1134.85	0.000431	154:	1195.79	0.000129	1195.02	0.000189
155:	1206.94	0.001709	1201.25	0.000882	155:	1145.4	0.000235	1142.86	0.000182	155:	1196.6	0.000318	1196.81	0.000295
156:	1208.05	0.005142	1203.28	0.005879	156:	1146.01	0.000007	1143.7	0.000041	156:	1208.46	0.005129	1206.12	0.005782
157:	1210.94	0.005245	1205.96	0.005437	157:	1175.52	0.000012	1175.57	0.000013	157:	1210.97	0.005164	1208.83	0.004699
158:	1214.29	0.001532	1209.63	0.0019	158:	1197.86	0.000227	1199.07	0.000172	158:	1216.19	0.00144	1215.79	0.001295
159:	1218.65	0.000126	1214.58	0.000029	159:	1200.08	0.000278	1199.79	0.000381	159:	1221.76	0.000028	1222.08	0.000021
160:	1236.43	0.000135	1235.97	0.000141	160:	1208.49	0.004724	1206.41	0.005339	160:	1231	0.000108	1229.32	0.000065
161:	1237.07	0.000086	1236.46	0.000082	161:	1212.22	0.005931	1208.85	0.005597	161:	1231.94	0.000094	1230.07	0.000185
162:	1243.6	0.000454	1239.82	0.000428	162:	1220.03	0.001327	1219.15	0.001255	162:	1243.56	0.000497	1241.6	0.000509
163:	1245.58	0.000453	1242.95	0.000447	163:	1223.27	0.000212	1223.7	0.000068	163:	1245.26	0.000414	1243.64	0.000441
164:	1250.28	0.000027	1246.42	0.000022	164:	1229.53	0.000128	1229.73	0.000193	164:	1251.65	0.000005	1252.02	0.000002
165:	1256.31	0.000076	1252.11	0.000075	165:	1232.1	0.000111	1232.24	0.000131	165:	1256.84	0.000107	1256.17	0.000137
166:	1258.66	0.000529	1256.07	0.000521	166:	1244.61	0.00042	1242.27	0.000457	166:	1259.24	0.000545	1259.48	0.000555
167:	1282.96	0.000078	1280.69	0.000094	167:	1244.86	0.000503	1242.85	0.000493	167:	1279.19	0.000026	1278.43	0.000021
168:	1284.85	0.001039	1284.04	0.000877	168:	1249.26	0.00005	1248.67	0.000058	168:	1281.07	0.00001	1280.21	0.000008
169:	1292.51	0.000237	1290.84	0.000157	169:	1254.63	0	1254	0.000003	169:	1283.28	0.000115	1283.54	0.00012
170:	1297.5	0.00055	1293.18	0.000702	170:	1259.04	0.000108	1258.02	0.00014	170:	1287.93	0.000612	1287.59	0.000278
171:	1299.78	0.000478	1297.17	0.000476	171:	1263.1	0.000238	1263.38	0.00024	171:	1289.58	0.000133	1289.8	0.000292
172:	1313.84	0.000125	1306.97	0.000074	172:	1279.82	0.000022	1279.68	0.000009	172:	1293.81	0.000382	1293.14	0.000515
173:	1317.23	0.00032	1314.98	0.000295	173:	1282.8	0.000014	1282.54	0.00001	173:	1295.87	0.000618	1295.32	0.00032
174:	1320.34	0.00006	1318.19	0.000029	174:	1290.54	0.000159	1290.21	0.000128	174:	1297.18	0.000181	1296.22	0.000191
175:	1323.77	0.000101	1320.1	0.000112	175:	1292.08	0.000488	1292.77	0.000218	175:	1298.54	0.000664	1298.41	0.000795
176:	1345.89	0.000062	1345.18	0.000072	176:	1295.24	0.000722	1296.44	0.000351	176:	1302.6	0.000001	1302.49	0.000077

177:	1356.19	0.000267	1355.08	0.000251	177:	1296.98	0.000375	1297.71	0.000235	177:	1305.98	0.000606	1305.8	0.000597
178:	1356.92	0.000316	1355.97	0.000402	178:	1298.16	0.000139	1298.47	0.000841	178:	1313.04	0.000188	1310.85	0.000173
179:	1358.9	0.000101	1357.2	0.000325	179:	1301.39	0.00041	1301.09	0.000611	179:	1315.53	0.000118	1313.37	0.000139
180:	1360.35	0.000402	1359.01	0.000093	180:	1303.07	0.001001	1302.63	0.000843	180:	1320.62	0.000135	1319.07	0.000134
181:	1378.01	0.000462	1376.27	0.00054	181:	1304.36	0.000137	1304.94	0.000182	181:	1325.82	0.000188	1325.28	0.000184
182:	1389.88	0.000672	1384.83	0.000655	182:	1316.21	0.000116	1316.84	0.000127	182:	1345.51	0.000065	1345.54	0.000075
183:	1390.46	0.000517	1389.24	0.000489	183:	1317.5	0.000056	1318.48	0.000066	183:	1351.29	0.000026	1351.36	0.000015
184:	1394.01	0.000358	1391.29	0.000361	184:	1324.08	0.000122	1321.71	0.000077	184:	1352.79	0.000042	1351.78	0.00007
185:	1398.31	0.000317	1396.23	0.000313	185:	1330.23	0.00022	1329.94	0.000206	185:	1358.68	0.000336	1358.74	0.000496
186:	1401.59	0.000009	1401.05	0.000007	186:	1351.87	0.000024	1351.67	0.000031	186:	1360.01	0.000215	1360.52	0.000049
187:	1402.27	0.000033	1402.04	0.000029	187:	1352.25	0.000043	1352.42	0.000038	187:	1364.03	0.000007	1362.35	0.000003
188:	1417.99	0.000724	1416.21	0.000706	188:	1359.94	0.000277	1360.29	0.000233	188:	1365.33	0.000071	1363.51	0.000064
189:	1421.16	0.000787	1417.98	0.000744	189:	1366.93	0.000028	1365.75	0.000027	189:	1377.96	0.000457	1376.63	0.000037
190:	1428.08	0.000086	1425.87	0.000077	190:	1369.39	0.000313	1368.91	0.000304	190:	1379.13	0.000174	1378.45	0.000471
191:	1428.48	0.000392	1426.22	0.000431	191:	1370.98	0.000064	1369.07	0.000075	191:	1379.33	0.000071	1379.27	0.000038
192:	1437.94	0.000083	1438.23	0.000059	192:	1379.31	0.000153	1376.62	0.000126	192:	1381.36	0.000033	1381.19	0.00026
193:	1448.91	0.000073	1449.1	0.000066	193:	1380.55	0.000063	1381.75	0.000093	193:	1382.28	0.000188	1381.74	0.000253
194:	1455.96	0.000034	1455.95	0.00003	194:	1382.19	0.000027	1382.51	0.000123	194:	1383.7	0.000195	1383.05	0.000159
195:	1460.39	0.000129	1459.22	0.000129	195:	1382.42	0.000231	1382.77	0.000165	195:	1384.98	0.000144	1384.53	0.000094
196:	1464.13	0.000139	1464.04	0.000136	196:	1385.57	0.00024	1386.32	0.000271	196:	1387.69	0.000469	1386.05	0.000707
197:	1467.02	0.000273	1468.02	0.000459	197:	1385.83	0.000102	1386.6	0.000075	197:	1389.01	0.0007	1390.3	0.000381
198:	1472.84	0.000136	1470.58	0.00004	198:	1387.57	0.00066	1387.75	0.000674	198:	1390.28	0.000452	1393.26	0.000497
199:	1473.21	0.000112	1472.59	0.000018	199:	1389.38	0.000409	1392.28	0.000379	199:	1394.93	0.000361	1394.62	0.000359
200:	1474.12	0.000085	1473.88	0.000087	200:	1395.59	0.000372	1393.69	0.000496	200:	1414.23	0.00076	1417.36	0.000816
201:	1475.73	0.000333	1474.02	0.000138	201:	1396.11	0.000509	1395.81	0.000355	201:	1418.35	0.0008	1418.21	0.000683
202:	1475.83	0.000311	1475.8	0.000282	202:	1401.11	0.000038	1400.91	0.000057	202:	1439.52	0.000085	1440.92	0.000062
203:	1475.87	0.000154	1476.06	0.000084	203:	1408.06	0.000284	1407.82	0.000272	203:	1447.59	0.000054	1450.14	0.000042
204:	1477.11	0.000115	1476.29	0.000287	204:	1417.83	0.000871	1417.96	0.000801	204:	1456.8	0.000033	1457.32	0.00003
205:	1480.41	0.000451	1479.46	0.000504	205:	1419.19	0.000698	1419.32	0.000745	205:	1461.65	0.000146	1461.52	0.000148
206:	1481.74	0.000476	1481.33	0.00049	206:	1443.63	0.000056	1445.25	0.000045	206:	1466.52	0.000087	1466.96	0.000107
207:	1485.68	0.000038	1484.4	0.000023	207:	1448.5	0.000057	1450.69	0.000057	207:	1466.95	0.00003	1468.31	0.000117
208:	1488.01	0.000042	1486.39	0.00002	208:	1461.43	0.000169	1462.75	0.000153	208:	1467.65	0.00014	1469.35	0.000031
209:	1489.11	0.000027	1487.43	0.000022	209:	1467.02	0.000138	1467.69	0.000005	209:	1469.16	0.000025	1471.27	0.000058
210:	1495.85	0.000296	1493.94	0.00027	210:	1467.69	0.000024	1469.07	0.000181	210:	1471.22	0.000019	1471.77	0.000012
211:	1496.31	0.000145	1494.26	0.000162	211:	1467.8	0.000005	1469.43	0.000032	211:	1471.52	0.000038	1472.53	0.00006
212:	1499.11	0.000096	1497.67	0.000109	212:	1470.99	0.000074	1471.32	0.00003	212:	1473.47	0.000062	1473.74	0.000111
213:	1502.09	0.000184	1500.68	0.000187	213:	1471.73	0.00007	1472.35	0.000021	213:	1473.54	0.00026	1473.97	0.000114
214:	1514.7	0.000754	1511.96	0.000766	214:	1473.57	0.000052	1472.49	0.000076	214:	1474.24	0.000171	1474.53	0.00008
215:	1517.3	0.000666	1514.02	0.000662	215:	1473.65	0.000188	1474.3	0.000217	215:	1475.16	0.000461	1475.34	0.000569
216:	1527.31	0.000559	1526.4	0.000561	216:	1474.69	0.000402	1474.83	0.000227	216:	1475.61	0.000085	1477.63	0.000118
217:	1529.14	0.000566	1527.93	0.000571	217:	1476.34	0.00062	1475.66	0.000406	217:	1477.31	0.000054	1478.1	0.000042
218:	1593.01	0.000875	1592.39	0.000931	218:	1476.45	0.000041	1476.46	0.000395	218:	1480.26	0.000058	1480.57	0.000064
219:	1606.03	0.000244	1605.39	0.000247	219:	1477.39	0.000122	1476.8	0.000074	219:	1481.1	0.000191	1481.49	0.000166
220:	1606.63	0.000064	1606.01	0.000061	220:	1477.52	0.000048	1478.39	0.000128	220:	1483.19	0.000278	1483.35	0.000275

221:	1652.61	0.000725	1651.26	0.00071	221:	1481.01	0.000069	1481.6	0.000065	221:	1485.6	0.000153	1485.46	0.000192
222:	1652.92	0.000617	1651.68	0.000632	222:	1481.86	0.000189	1482.67	0.000089	222:	1487	0.000064	1486.07	0.000075
223:	1893.29	0.024196	1892.63	0.024316	223:	1483.45	0.00036	1483.01	0.000383	223:	1487.35	0.000026	1487.73	0.000027
224:	1944.11	0.029912	1943.12	0.030077	224:	1483.66	0.000368	1484.14	0.000369	224:	1493.13	0.000161	1493.01	0.000166
225:	2973.95	0.000602	2970.19	0.000609	225:	1485.32	0.000306	1485.12	0.000211	225:	1495.21	0.000228	1495.89	0.000009
226:	2982.22	0.000669	2976.28	0.000713	226:	1485.56	0.000209	1485.31	0.000273	226:	1495.72	0.000051	1497.79	0.000197
227:	2987.88	0.000281	2983.9	0.000262	227:	1489.44	0.000057	1487.33	0.000042	227:	1498.02	0.000015	1498.16	0.000035
228:	2989.26	0.00021	2984.52	0.000222	228:	1492.57	0.000796	1492.04	0.000837	228:	1498.85	0.000087	1499.56	0.000178
229:	3006.24	0.000565	3007.25	0.00064	229:	1494.63	0.000171	1494.59	0.000187	229:	1499.72	0.000187	1501	0.000121
230:	3006.76	0.000657	3007.71	0.000584	230:	1496.52	0.00003	1496.69	0.00019	230:	1514.02	0.000616	1513.96	0.000586
231:	3022.02	0.000826	3022.93	0.000819	231:	1496.82	0.000224	1497.6	0.000018	231:	1515.81	0.000749	1515.13	0.000763
232:	3022.32	0.000455	3025.24	0.000601	232:	1498.04	0.000004	1498.59	0.000028	232:	1592.4	0.000819	1591.91	0.000877
233:	3023.77	0.000585	3026.16	0.00049	233:	1499.31	0.000101	1498.77	0.000104	233:	1877.13	0.022799	1877.17	0.023065
234:	3026.16	0.000474	3027.89	0.000435	234:	1502.52	0.000202	1501.33	0.000174	234:	1930.7	0.03037	1930.64	0.030376
235:	3027.06	0.000461	3029.45	0.000597	235:	1514.25	0.000671	1514.07	0.000675	235:	2976.81	0.000509	2971.35	0.000622
236:	3027.4	0.000624	3029.75	0.000445	236:	1517.12	0.000735	1516.08	0.000684	236:	2979.14	0.000775	2975.53	0.000708
237:	3028	0.000579	3030.5	0.000577	237:	1565.7	0.000025	1565.58	0.000029	237:	2991.11	0.000254	2987.04	0.000247
238:	3034.94	0.000209	3036	0.000411	238:	1635.89	0.000089	1634.64	0.000105	238:	2993.91	0.000279	2989.05	0.000279
239:	3035.06	0.000432	3036.59	0.000231	239:	1884.81	0.022409	1884.85	0.022736	239:	3000.48	0.000842	3005.41	0.000622
240:	3041.33	0.000321	3042.28	0.000288	240:	1938.18	0.031657	1938.22	0.031443	240:	3005.45	0.000475	3007.06	0.000593
241:	3064.58	0.000789	3065.55	0.000798	241:	2977.91	0.0005	2970.74	0.000592	241:	3014.59	0.000574	3015.11	0.000603
242:	3065.38	0.000154	3066.3	0.000145	242:	2980.73	0.000736	2975.72	0.000679	242:	3014.67	0.00058	3015.26	0.000578
243:	3079.15	0.001772	3078.61	0.001728	243:	2991.4	0.000248	2987.21	0.000229	243:	3018.31	0.000321	3019.15	0.000031
244:	3083.4	0.000867	3083.19	0.000873	244:	2994.45	0.000276	2988.97	0.000277	244:	3018.63	0.000356	3019.27	0.000617
245:	3101.92	0.000258	3103.23	0.000258	245:	3014.68	0.000571	3014.93	0.000562	245:	3020.26	0.000763	3020.43	0.000639
246:	3102.99	0.000241	3104.45	0.000228	246:	3015.05	0.000526	3015.52	0.000533	246:	3020.33	0.000631	3020.68	0.000632
247:	3111.65	0.000311	3111.52	0.000314	247:	3016.68	0.002419	3016.87	0.002472	247:	3020.98	0.00082	3020.99	0.000139
248:	3112.88	0.000244	3112.26	0.000274	248:	3017.73	0.000392	3017.9	0.000372	248:	3021.11	0.000131	3021.72	0.000185
249:	3115.41	0.000121	3116.31	0.000069	249:	3019.01	0.000345	3018.72	0.000189	249:	3022.08	0.000204	3021.91	0.000916
250:	3117.66	0.000119	3117.84	0.000004	250:	3019.89	0.000454	3019.49	0.000489	250:	3023.03	0.000561	3023.46	0.000592
251:	3118.13	0.000512	3118.78	0.00051	251:	3020.43	0.000601	3020.2	0.000076	251:	3024.7	0.000163	3025.39	0.000314
252:	3119.34	0.000446	3120.2	0.000288	252:	3020.8	0.000568	3020.5	0.000614	252:	3025.46	0.000259	3025.47	0.000019
253:	3120.36	0.000184	3122.26	0.000391	253:	3021.48	0.000188	3020.59	0.000586	253:	3025.67	0.000622	3025.56	0.000445
254:	3122.95	0.001419	3123.21	0.000501	254:	3023.41	0.000173	3020.96	0.00026	254:	3026.93	0.000405	3027.28	0.000392
255:	3123.01	0.000259	3123.29	0.001282	255:	3025.1	0.000451	3025.7	0.000422	255:	3030.7	0.000426	3030.9	0.000439
256:	3126.41	0.001354	3125.41	0.001242	256:	3027.31	0.000228	3026.19	0.000092	256:	3034.35	0.000402	3032.71	0.000441
257:	3133.29	0.000193	3130.96	0.000232	257:	3027.44	0.000389	3026.55	0.00022	257:	3034.45	0.000262	3032.91	0.000157
258:	3134.63	0.000241	3135.26	0.000253	258:	3028.99	0.000385	3027.07	0.000356	258:	3035.83	0.000128	3033.36	0.000452
259:	3135.27	0.000197	3136.11	0.00023	259:	3031.22	0.000409	3030.96	0.000463	259:	3036.53	0.000245	3036.64	0.000221
260:	3138.82	0.000291	3136.19	0.000315	260:	3034.58	0.000316	3032.38	0.000482	260:	3039.57	0.000281	3038.79	0.000257
261:	3139.21	0.000226	3137.13	0.000202	261:	3034.65	0.000389	3032.94	0.000406	261:	3056.19	0.000633	3062.86	0.000599
262:	3143.83	0.000126	3138.64	0.000182	262:	3036.81	0.000192	3033.98	0.000414	262:	3063.03	0.000369	3065.72	0.000362
263:	3149.79	0.000173	3147.7	0.000225	263:	3038.54	0.000194	3036.52	0.000214	263:	3073.29	0.001502	3071.99	0.001677
264:	3151.07	0.000121	3148.16	0.00008	264:	3039.85	0.000293	3039.19	0.000242	264:	3073.46	0.001145	3072.2	0.000995

265:	3158.37	0.000034	3163.78	0.000135	265:	3073.4	0.001894	3072.41	0.001535	265:	3075.7	0.000566	3074.88	0.000389
266:	3158.78	0.000039	3164.12	0.000192	266:	3073.52	0.000722	3072.44	0.001009	266:	3075.8	0.001088	3074.96	0.001188
267:	3160.61	0.000244	3165.13	0.000075	267:	3076.32	0.000637	3075.43	0.000517	267:	3078.63	0.001797	3077.46	0.001783
268:	3160.74	0.000104	3165.41	0.000083	268:	3076.5	0.001047	3075.5	0.001117	268:	3079.21	0.000252	3079.02	0.00077
269:	3177.72	0.000297	3179.95	0.000277	269:	3079.89	0.000291	3079.41	0.000365	269:	3079.45	0.000307	3079.03	0.000021
270:	3178.21	0.000452	3180.53	0.000375	270:	3080.18	0.000194	3079.65	0.000276	270:	3082.86	0.000896	3082.38	0.00092
271:	3179.5	0.000328	3182.14	0.000339	271:	3081.07	0.000711	3081.25	0.000708	271:	3084.47	0.000069	3085.98	0.000567
272:	3179.77	0.000299	3182.21	0.000308	272:	3084.27	0.000012	3084.41	0.000013	272:	3085.22	0.000517	3086.42	0.000127
					273:	3085.45	0.000078	3086.38	0.00007	273:	3087.03	0.001015	3088.64	0.000882
					274:	3086.1	0.00013	3086.42	0.000231	274:	3089.03	0.000544	3090.49	0.000441
					275:	3088	0.000798	3088.46	0.000701	275:	3111.39	0.000285	3109.64	0.000316
					276:	3088.82	0.001125	3089.04	0.001087	276:	3113.07	0.000261	3110.87	0.000279
					277:	3110.98	0.000318	3109.59	0.000324	277:	3113.88	0.000109	3113.92	0.000076
					278:	3113.45	0.000149	3111.29	0.000275	278:	3116.93	0.000496	3116.48	0.000029
					279:	3113.96	0.000238	3113.25	0.000127	279:	3117.82	0.000008	3116.64	0.000496
					280:	3116.77	0.000442	3116.15	0.000425	280:	3120.17	0.000366	3120.26	0.00027
					281:	3117.88	0.000035	3116.69	0.000058	281:	3121.26	0.001284	3120.86	0.001261
					282:	3120.42	0.000455	3119.99	0.00032	282:	3122.6	0.000222	3122.35	0.000706
					283:	3121.41	0.001278	3120.93	0.001242	283:	3122.97	0.000802	3122.93	0.000673
					284:	3121.55	0.000337	3121.25	0.000546	284:	3126.6	0.001068	3125.31	0.000775
					285:	3124.29	0.000507	3123.66	0.000646	285:	3132.03	0.000036	3127.87	0.000107
					286:	3126.17	0.000475	3125.73	0.000841	286:	3134.97	0.000526	3131.02	0.000557
					287:	3127.08	0.00116	3126.28	0.000531	287:	3140.06	0.000296	3135.78	0.000356
					288:	3127.33	0.000106	3127.31	0.000083	288:	3140.91	0.000009	3136.7	0.000007
					289:	3132.5	0.000015	3128.46	0.00001	289:	3149.56	0.000125	3141.84	0.000183
					290:	3135.16	0.000548	3131.05	0.00065	290:	3150.23	0.000068	3142.62	0.000054
					291:	3138.77	0.000273	3134.69	0.000355					
					292:	3140.25	0.000043	3136.02	0.000026					
					293:	3146.93	0.000112	3139.06	0.000141					
					294:	3155.37	0.000071	3145.28	0.000089					
					295:	3162.66	0.000357	3163.05	0.00036					
					296:	3165.32	0.000215	3165.62	0.000212					

Table S22. Calculated vibrational frequencies of the mono reduced complex $\mathbf{2}^{1-}$ using different functionals with and without dispersion correction.

	$\mathbf{2}^{1-}$											
	TPSSh; Disp ON*		TPSSh; Disp OFF*		PBE0; Disp ON*		PBE0; Disp OFF*		BP86; Disp ON		BP86; Disp OFF	
Mode	freq	T**2	freq	T**2	freq	T**2	freq	T**2	freq	T**2	freq	T**2
	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)
8:	20.88	0.000306	12.81	0.000953	16.17	0.001234	28.07	0.000538	50.6	0.001145	48.13	0.000519
9:	28.12	0.000985	21.82	0.00005	23.92	0.00043	33.48	0.002537	57.92	0.001437	51.9	0.00188
10:	30.46	0.001063	26.43	0.000189	28.39	0.000395	36.64	0.000568	62.94	0.000857	57.93	0.001666
11:	31.12	0.000417	27.85	0.000892	29.45	0.000419	39.1	0.000556	69.7	0.00036	62.12	0.001263
12:	35.47	0.001413	30.51	0.00053	35.13	0.001329	42.58	0.000284	76.14	0.000204	66.01	0.000197
13:	38.21	0.000979	33.47	0.001446	36.66	0.001117	45.09	0.000286	77.37	0.000224	76.81	0.000053
14:	45.57	0.000768	37.47	0.000774	40.31	0.00027	46.08	0.001275	85.08	0.000888	79.55	0.000669
15:	46.02	0.000054	38.17	0.000403	44.37	0.000051	48.47	0.000816	99.18	0.000201	92.08	0.001524
16:	48.08	0.00028	41.21	0.001595	49.27	0.000117	52.68	0.000386	99.73	0.000287	97.81	0.000803
17:	53.33	0.000154	45.81	0.000451	52.78	0.001073	56.79	0.000178	104.09	0.000333	98.48	0.000184
18:	54.85	0.000217	49.69	0.000251	57.63	0.00028	70.65	0.000593	104.7	0.000098	103.86	0.000294
19:	64.35	0.000407	55.72	0.000203	59.57	0.000597	75.04	0.001119	112.08	0.000111	105.55	0.000047
20:	68.22	0.000468	67.62	0.000986	63.78	0.000664	78.53	0.000228	113.77	0.000417	110	0.000204
21:	75.8	0.000635	77.38	0.000975	79.84	0.000282	80.9	0.000458	119.43	0.000959	114.62	0.000062
22:	87.85	0.000049	84.05	0.000446	85.99	0.001221	83.88	0.000305	120.79	0.000702	116.46	0.000178
23:	90.54	0.001116	85.36	0.000807	90.41	0.000827	89.5	0.001571	126.38	0.00145	120.91	0.001655
24:	93.8	0.000211	95.99	0.000312	98.58	0.001234	99.33	0.000592	133.97	0.000049	127.79	0.000994
25:	105.11	0.001275	97.65	0.000264	106.15	0.000454	101.86	0.000442	140.84	0.000513	128.55	0.000216
26:	107	0.001442	99.88	0.000711	107.35	0.000224	104.24	0.000668	143.23	0.000614	132.3	0.00094
27:	114.13	0.00015	104.17	0.001109	110.56	0.001215	106.06	0.00048	147.6	0.000036	143.37	0.000329
28:	119.62	0.000746	114.95	0.000605	120.67	0.000408	118.22	0.000569	151.47	0.001542	151.25	0.00071
29:	127.34	0.000707	122.88	0.001175	126.86	0.001123	127.01	0.001466	162.31	0.000505	160.03	0.000981
30:	135.53	0.00051	128.15	0.000021	140.82	0.000686	136.56	0.000706	171.35	0.000911	165.25	0.000873
31:	141.91	0.000307	135.69	0.000616	147.01	0.000141	144.17	0.000069	186.54	0.000617	185.26	0.000235
32:	148.16	0.000422	138.88	0.000083	155.5	0.00045	145.9	0.000106	195.64	0.000298	188.91	0.000243
33:	156.81	0.001075	150.58	0.000922	159.77	0.0012	156.96	0.000823	199.14	0.000109	191.67	0.000158
34:	163.17	0.000039	156.56	0.000932	167.15	0.000085	164.66	0.00098	206.04	0.000077	200.27	0.000624
35:	167.81	0.00011	162.51	0.000057	170.63	0.000035	167.36	0.000042	213.73	0.000376	215.95	0.000209
36:	176.98	0.001211	173.59	0.001143	181.16	0.001268	179.65	0.001209	219.07	0.000171	219.95	0.000245
37:	188.52	0.000267	180.44	0.000118	189.75	0.000095	188.09	0.000145	229.58	0.000041	223.98	0.000045
38:	192.18	0.000223	184.12	0.000122	198.99	0.000157	195.44	0.000021	229.91	0.000066	228.35	0.000002
39:	197.93	0.000036	189.46	0.000066	203.13	0.000088	202.82	0.000337	252.51	0.000627	247.73	0.000547
40:	204.12	0.000471	198.57	0.000153	211.3	0.000641	206.12	0.000049	265.11	0.000003	260.36	0.000006
41:	211.19	0.000071	204.6	0.000579	218.54	0.00007	215.34	0.000646	272.32	0.000287	265.65	0.000184
42:	213.82	0.000093	212.03	0.000174	221.39	0.000089	219.73	0.000094	273.71	0.000538	266.2	0.000375
43:	214.45	0.000037	215.38	0.000062	222.37	0.000012	222.39	0.000027	293.89	0.001322	272.18	0.000134
44:	219	0.000192	220.04	0.000035	224.62	0.000166	226.74	0.000087	294.96	0.000781	290.01	0.001819
45:	247.47	0.00097	243.68	0.000032	254.46	0.001158	248.83	0.000014	298.72	0.000322	295.7	0.000594
46:	251.15	0.000106	246.38	0.001292	255.47	0.000159	257.26	0.001328	310.78	0.000053	304.57	0.000263

47:	253.58	0.000209	251.28	0.000031	264.4	0.00009	267.86	0.000028	313.79	0.000165	307.31	0.000912
48:	264	0.000036	260.69	0.000075	268.61	0.000008	273.57	0.000397	316.02	0.000889	310.91	0.000021
49:	264.84	0.000066	267.47	0.000152	272.3	0.000072	277.83	0.000408	322.13	0.000284	313.01	0.000496
50:	267	0.000403	274.53	0.000434	278.85	0.000494	283.05	0.000359	326.94	0.000826	314.01	0.000059
51:	278.91	0.000297	280.25	0.000494	287.75	0.000265	292.68	0.000293	328.92	0.000034	325.62	0.000987
52:	281.13	0.000218	283.49	0.000062	290.38	0.000188	295.25	0.000063	332.68	0.000709	329.31	0.000274
53:	294.45	0.000388	287.84	0.000145	299.57	0.000166	299.83	0.000089	335.34	0.000257	335.09	0.001002
54:	296.19	0.000252	292.42	0.000408	305.63	0.000681	302.21	0.000669	345.54	0.000261	337.6	0.000444
55:	302.07	0.000029	304.96	0.000414	313.47	0.0006	308.45	0.000317	351.76	0.000012	348.09	0.000356
56:	307.66	0.000463	310.06	0.000914	314.36	0.000164	316.87	0.001027	357.42	0.000363	353.43	0.000015
57:	321.97	0.001887	322.42	0.001164	332.12	0.001887	331.93	0.001228	359.36	0.000082	355.36	0.000228
58:	328.76	0.000429	327.33	0.000098	334.84	0.000555	335.67	0.000424	369.51	0.0023	362.86	0.003141
59:	330.51	0.000411	332.43	0.002277	337.57	0.000703	339.82	0.001513	369.9	0.000054	368	0.000313
60:	333.02	0.00032	333.96	0.000474	342.17	0.000584	343.69	0.0011	373.05	0.000043	369.32	0.000408
61:	338.71	0.000475	337.2	0.000466	347.45	0.000285	345.39	0.000326	376.47	0.000145	374.53	0.000081
62:	348.16	0.000944	342.68	0.000912	352.41	0.000977	348.87	0.000779	382.1	0.00113	375.26	0.0001
63:	354.19	0.000172	351.71	0.0003	360.87	0.000158	359.6	0.000061	382.82	0.000145	377.14	0.000386
64:	356.53	0.00017	351.98	0.000006	363.33	0.000015	362.32	0.000315	385.68	0.000058	384.27	0.000277
65:	361.07	0.00049	365.42	0.000499	370.69	0.000655	374.38	0.000587	395.54	0.000149	385.14	0.000048
66:	364.36	0.000101	368.69	0.000153	375	0.000054	378.09	0.00008	396.52	0.00027	394.59	0.000124
67:	371.62	0.000172	370.55	0.000079	380.86	0.000161	380.43	0.000059	399.65	0.000245	396.54	0.000156
68:	378.65	0.000146	378.09	0.000398	389.02	0.000151	388.56	0.000321	408.55	0.000083	404.9	0.000237
69:	401.12	0.002943	397.62	0.003991	410.64	0.002683	409.19	0.003674	418.25	0.000768	416.2	0.00201
70:	404.49	0.0003	402.69	0.000277	413.71	0.000448	412.05	0.000007	422.89	0.001038	423.84	0.000294
71:	406.08	0.000743	404.21	0.000321	416.2	0.000715	415.76	0.000553	433.77	0.000475	429.15	0.001019
72:	411.65	0.000023	410.35	0.000034	419.99	0.000063	421.53	0.000077	435.52	0.001382	432.48	0.000402
73:	415.47	0.000072	413.85	0.000154	424.94	0.000073	425.24	0.000169	438.91	0.00104	433.99	0.000186
74:	421	0.000204	424.06	0.000083	432.84	0.000126	434.66	0.000127	441.3	0.000461	437.94	0.004683
75:	429.97	0.005323	427.59	0.004931	439.01	0.005282	438.69	0.0048	444.78	0.003656	443.39	0.001195
76:	449.59	0.0003	448.6	0.000221	458.34	0.000405	459.44	0.000348	473.75	0.000914	474.12	0.001332
77:	451.55	0.001746	450.29	0.001821	465.19	0.001423	463.99	0.001612	477.5	0.001446	478.84	0.00086
78:	462.68	0.001302	462.34	0.001236	476.06	0.001461	477.01	0.001208	481.84	0.000915	480.48	0.00082
79:	474.99	0.00048	474.67	0.000431	487.8	0.00063	484.69	0.000482	486.62	0.001187	485.91	0.000998
80:	477.87	0.000901	476.37	0.000487	490.46	0.000709	489.85	0.001364	496.62	0.000669	493.11	0.000743
81:	482.01	0.000185	478.14	0.000066	493.25	0.000203	491.99	0.000145	500.28	0.000205	496.48	0.000927
82:	498.66	0.002083	485.54	0.003597	498.97	0.00344	496.23	0.002181	504.86	0.001599	510.74	0.000802
83:	504.82	0.001606	503.07	0.003042	516.09	0.005706	515.38	0.006685	532.75	0.000532	530.78	0.000779
84:	509.5	0.002285	507.17	0.004089	518.89	0.000647	520.04	0.000813	535.14	0.000166	532.78	0.000124
85:	511.01	0.002844	509.39	0.000656	526.09	0.001155	525.91	0.00126	536.13	0.000342	536.26	0.002244
86:	513.28	0.000195	510.92	0.000564	528.73	0.00043	527.35	0.000675	542.03	0.003739	538.9	0.000964
87:	516.7	0.001561	516.55	0.002845	530.66	0.001839	529.5	0.002278	549.87	0.003455	540.71	0.004238
88:	521.4	0.002408	520.91	0.001048	533.44	0.001315	532.76	0.001247	554.66	0.001097	549.53	0.002795
89:	535.29	0.002648	533.97	0.003303	551.84	0.003234	546.25	0.003858	572.41	0.00232	574.47	0.002776
90:	574.54	0.002739	582.35	0.001724	594.81	0.00173	599.39	0.001018	594.51	0.000406	595.84	0.000161

91:	595.63	0.000259	600.3	0.000064	610.93	0.000596	614.54	0.000021	619.43	0.001425	623.31	0.000692
92:	602.36	0.000137	602.35	0.000661	616.67	0.000289	618.34	0.001306	630.59	0.001056	627.3	0.001736
93:	625.82	0.000519	621.2	0.000292	639.51	0.000747	635.64	0.000608	632.07	0.000555	630.72	0.000008
94:	628.3	0.002909	624.04	0.001449	641.88	0.002727	640.45	0.002364	634.08	0.003049	637.66	0.002953
95:	629.46	0.001738	625.5	0.002895	647.05	0.0014	642.39	0.001862	645.9	0.000042	645.8	0.000004
96:	640.92	0.000032	641.43	0.000026	649.01	0.000027	649.35	0.000041	647.26	0.000072	645.96	0.000029
97:	642.84	0.000009	641.51	0.000014	650.65	0.000101	650.4	0.000019	665.22	0.001113	667.12	0.000901
98:	688.57	0.000368	690.16	0.000514	703.04	0.000549	703.6	0.000704	689.99	0.000383	692.53	0.000616
99:	717.15	0.002443	709.25	0.003614	731.4	0.000037	731.97	0.000001	710.82	0.003233	703.43	0.003574
100:	717.7	0.000572	718.16	0.000007	734.14	0.000047	733.7	0.00004	724.93	0.001455	717.75	0.00188
101:	721.22	0.000179	720.61	0.000566	738.65	0.002395	736.72	0.003076	730.1	0.001402	727.14	0.001809
102:	731.21	0.00006	726.48	0.001584	744.34	0.000557	744.14	0.000353	741.57	0.000208	741.78	0.000003
103:	731.92	0.001552	729.16	0.000833	751.89	0.001166	749.84	0.001404	741.91	0.000057	743.61	0.000264
104:	737.34	0.001459	732.05	0.000825	756.97	0.001266	754.8	0.001518	747.07	0.000095	746.97	0.000144
105:	758.02	0.000857	751.96	0.00056	775.51	0.001021	775.44	0.001231	758.85	0.000329	755.81	0.000179
106:	765.06	0.000208	758.73	0.000731	784.59	0.000098	782.05	0.000162	764.17	0.000856	764.83	0.000107
107:	767.6	0.00007	765.61	0.000086	785.78	0.000142	783.39	0.000136	768.05	0.000126	766.01	0.001186
108:	781.47	0.000794	775.24	0.00066	798.24	0.000865	795.65	0.000645	783.03	0.000439	780.13	0.000474
109:	805.56	0.000828	805.44	0.000188	812.86	0.001383	815.58	0.000544	811.04	0.00028	808.8	0.000045
110:	808.51	0.000165	808.18	0.000157	818.06	0.000458	820.42	0.000314	811.89	0.000065	810.15	0.00043
111:	812.86	0.000915	812.81	0.00054	825.49	0.000705	825.35	0.000552	838.62	0.000421	834.21	0.000082
112:	818.19	0.000563	817.61	0.000632	828.57	0.000604	828.35	0.000419	842.16	0.002071	840.59	0.000124
113:	821.13	0.001615	821.76	0.001826	832.45	0.00116	832.4	0.001655	846.16	0.000029	846.58	0.001513
114:	827.53	0.000472	824.97	0.000566	848.38	0.000296	848.5	0.000283	849.53	0.001242	852.6	0.001299
115:	837.47	0.00017	833.42	0.000276	851.45	0.000208	852.13	0.000183	855.15	0.000946	856.09	0.001039
116:	844.72	0.000109	845.71	0.000073	865.19	0.000116	863.28	0.000222	877.64	0.000129	880.78	0.000105
117:	862.82	0.000837	862.93	0.000368	870.78	0.000119	870.23	0.000062	883.08	0.001298	885.3	0.00139
118:	865.75	0.000648	866.02	0.001096	878.43	0.00098	883.06	0.000919	896.29	0.000169	898.49	0.000096
119:	879.07	0.000691	883.16	0.000538	884.61	0.00049	889.54	0.000539	902.51	0.001137	908.83	0.000566
120:	891.28	0.000224	891.51	0.000371	897.81	0.000394	898.34	0.000483	914.07	0.005652	916.91	0.006463
121:	896.38	0.006346	897.39	0.000519	902.24	0.000107	902.62	0.000076	922.68	0.000621	924.01	0.000512
122:	900.33	0.000349	897.94	0.006567	906.06	0.006785	911.53	0.006785	928	0.000059	926.55	0.000195
123:	913.7	0.000188	913.45	0.00023	922.19	0.000227	924.4	0.000254	929.2	0.000132	928.38	0.00008
124:	917.4	0.00005	918.1	0.000063	928.02	0.000049	928.97	0.000078	929.72	0.000271	930.1	0.000123
125:	929.77	0.000039	927.41	0.000035	936.25	0.000046	937.48	0.000071	944.59	0.000077	941.33	0.000073
126:	936.07	0.000038	930.67	0.000031	941.07	0.000051	937.66	0.000038	945.56	0.000073	943.4	0.000065
127:	945.86	0.000166	947.27	0.000137	946.37	0.000034	951.42	0.000017	950.45	0.000172	951.19	0.000152
128:	949.23	0.000004	949.56	0.000008	948.92	0.000006	951.9	0.000028	969.9	0.000001	970.2	0.000009
129:	951.9	0.000017	952.99	0.000003	969.51	0.000164	968.7	0.000158	975.38	0.000023	972.78	0.000007
130:	961.27	0.000239	965.29	0.000146	970.71	0.00019	972.27	0.000129	989.64	0.000286	993.84	0.000124
131:	965.35	0.00014	966.99	0.000153	974.17	0.000149	973.56	0.000156	994.06	0.000103	996.3	0.000127
132:	981.78	0.000014	984.12	0.000028	990.4	0.000018	991.52	0.000032	1007.24	0.000034	1010.95	0.000097
133:	997.71	0.001998	997.75	0.002917	997.4	0.0001	994.95	0.002956	1010.1	0.002188	1011.32	0.003182
134:	999.01	0.00011	999.77	0.000064	998.92	0.000095	997.54	0.000067	1013.38	0.00016	1012.27	0.000064

135:	1001.28	0.000064	1001.27	0.000285	1001.49	0.002308	1000.3	0.000243	1013.84	0.000092	1014.88	0.000145
136:	1008.65	0.000017	1011.3	0.000012	1014.81	0.000068	1009.63	0.000034	1022.08	0.000018	1022.62	0.000318
137:	1012.6	0.000104	1011.67	0.000051	1017.7	0.000006	1018.64	0.000015	1024.31	0.000222	1022.86	0.000012
138:	1021.52	0.001369	1022.12	0.00118	1027.01	0.000011	1027.17	0.000269	1026.63	0.00023	1023.9	0.000251
139:	1026.05	0.000343	1024.86	0.000441	1030.2	0.00031	1028.23	0.000006	1030.46	0.000009	1036.37	0.000576
140:	1026.64	0.000131	1026.05	0.000345	1031.15	0.000037	1029.56	0.00012	1041.66	0.000244	1037.23	0.000623
141:	1029.06	0.000184	1029.21	0.000057	1031.41	0.000352	1030.93	0.000112	1042.17	0.000817	1040.14	0.000205
142:	1030.2	0.00013	1029.4	0.000135	1031.95	0.000019	1033.04	0.000212	1044.07	0.000291	1042.22	0.00017
143:	1033.63	0.000325	1030.87	0.00033	1032.33	0.000074	1034.32	0.000056	1044.75	0.000076	1044.98	0.000226
144:	1034.15	0.000174	1032.89	0.000759	1032.96	0.000034	1036.12	0.000045	1051.14	0.000112	1045.74	0.000278
145:	1034.86	0.000455	1033.46	0.000178	1046.25	0.000617	1046.59	0.000536	1051.6	0.001181	1046.01	0.000796
146:	1045.1	0.000438	1041.96	0.000615	1048.89	0.000915	1048.36	0.000857	1061.44	0.001129	1054.51	0.000612
147:	1047.65	0.001241	1047.3	0.000412	1055.52	0.000005	1053.07	0.000001	1063.14	0.000305	1062.57	0.000411
148:	1048.56	0.000585	1048.96	0.000846	1063.39	0.001602	1062.84	0.001552	1063.33	0.000802	1064.36	0.000864
149:	1053.13	0	1054.38	0	1077.71	0.000633	1070.82	0.000775	1066.99	0.000024	1068.85	0
150:	1112.55	0.000529	1102.65	0.00048	1129.64	0.000596	1124.15	0.000377	1109.88	0.000199	1100.94	0.000229
151:	1112.73	0.000143	1108.86	0.00068	1131.52	0.00022	1131.19	0.000817	1110.29	0.0013	1105.48	0.000959
152:	1113.3	0.000846	1111.71	0.00067	1133.65	0.001333	1132.68	0.001067	1113.22	0.000277	1110.57	0.000843
153:	1136.18	0.000105	1136.19	0.000112	1139.69	0.000141	1141.56	0.000116	1137.76	0.000121	1138.42	0.000091
154:	1141.29	0.000113	1139.32	0.000148	1145.83	0.000181	1144.3	0.000208	1143.88	0.000125	1143.45	0.000269
155:	1143.81	0.000012	1139.81	0.000045	1177.19	0.000016	1174.7	0.000029	1160.71	0.000022	1154.29	0.000016
156:	1146.25	0.00007	1144.32	0.000076	1181.78	0.000004	1181.72	0.000006	1162.37	0.000076	1158.05	0.00012
157:	1170.95	0.000025	1170.75	0.000023	1184.35	0.000016	1185.01	0.000012	1172.77	0.000013	1172.14	0.000017
158:	1204.86	0.001384	1203.87	0.005542	1203.62	0.000644	1206.06	0.000204	1204.61	0.000751	1206.38	0.001709
159:	1206.81	0.004672	1205.43	0.003286	1207.29	0.000224	1206.2	0.000724	1209.82	0.000669	1208.04	0.005033
160:	1208.17	0.002439	1206.47	0.000893	1219.33	0.006239	1218.25	0.006209	1212.2	0.004751	1208.96	0.002511
161:	1210.18	0.002874	1207.75	0.00218	1221.61	0.005232	1219.98	0.005861	1215.38	0.00565	1211.01	0.003086
162:	1217.44	0.000778	1213.25	0.000944	1231.82	0.000669	1228.65	0.000677	1229.02	0.000584	1231.58	0.000847
163:	1229.06	0.000482	1227.34	0.000561	1242.46	0.000436	1240.6	0.0005	1233.46	0.00022	1233.24	0.000091
164:	1236.89	0.000036	1236.37	0.000131	1249.9	0.000539	1249.23	0.000656	1236.35	0.000083	1236.31	0.000115
165:	1239.14	0.000124	1237.66	0.000506	1251.89	0.000111	1251.15	0.000646	1238.74	0.000194	1237.92	0.000598
166:	1239.73	0.000519	1238.87	0.000149	1253.39	0.00015	1252.17	0.000095	1241.3	0.000433	1239.01	0.000312
167:	1242.34	0.000691	1241.01	0.000616	1253.69	0.000782	1253.58	0.000055	1241.66	0.000929	1240.02	0.000791
168:	1248.67	0.000118	1245.64	0.00007	1254.39	0.000166	1255.42	0.000222	1245.62	0.000137	1242.1	0.00008
169:	1251	0.000022	1250.24	0.000033	1258.37	0.000173	1259.14	0.000131	1257.59	0.000283	1252.94	0.000319
170:	1257.39	0.000411	1255.07	0.000315	1265.85	0.00035	1265.34	0.000311	1260.68	0.00008	1260.22	0.000027
171:	1259.18	0.00022	1256.38	0.00035	1269.11	0.000303	1268.12	0.000296	1268.63	0.000751	1265.57	0.000637
172:	1290.99	0.000522	1288.81	0.001041	1296.87	0.001399	1296.26	0.001204	1294.37	0.00006	1297.39	0.000383
173:	1294.33	0.000921	1293.45	0.000309	1301.33	0.000083	1301.61	0.000252	1300.17	0.001176	1298.58	0.000889
174:	1297.39	0.000223	1302.01	0.000326	1305.74	0.000391	1305.67	0.000462	1301.94	0.000344	1303.14	0.000124
175:	1302.65	0.000286	1302.72	0.000299	1308.55	0.000278	1309.46	0.000377	1306.05	0.000579	1304.25	0.000492
176:	1315.3	0.00001	1316.66	0.000023	1314.61	0.000124	1317.01	0.000072	1308.47	0.000905	1308.55	0.000116
177:	1319.15	0.000332	1318.97	0.000232	1320.17	0.000164	1320.1	0.000173	1309.6	0.000424	1310.2	0.002398
178:	1324.27	0.000121	1322.43	0.000108	1327.56	0.000206	1329.01	0.000268	1310.54	0.000407	1313.77	0.000494

179:	1326.47	0.000132	1324.91	0.000206	1334.6	0.000177	1332.97	0.000061	1323.81	0.000109	1327.32	0.000047
180:	1350.64	0.00167	1349.04	0.000426	1364.37	0.002378	1364.34	0.000078	1328.15	0.000231	1328.19	0.000161
181:	1351.95	0.000214	1349.21	0.00014	1365.71	0.000061	1364.56	0.000479	1332.73	0.000171	1333.49	0.000075
182:	1355.18	0.000012	1351.82	0.002081	1367.89	0.00033	1366.9	0.00128	1333.69	0.000052	1343.76	0.000378
183:	1363.56	0.000365	1360.71	0.00052	1369.77	0.000195	1367.6	0.001771	1358.34	0.000287	1354.98	0.00031
184:	1382.84	0.000645	1384.33	0.000582	1371.56	0.00124	1373	0.001099	1382.13	0.000923	1383.74	0.000936
185:	1389.52	0.000053	1390.16	0.000288	1378.75	0.000681	1379.77	0.000945	1385.6	0.000696	1388.86	0.000557
186:	1390.37	0.000302	1390.81	0.000355	1379.23	0.000922	1382.65	0.000661	1390.2	0.000791	1390	0.000843
187:	1391.42	0.000511	1392.6	0.000077	1382.43	0.000679	1383.8	0.000711	1390.58	0.00041	1390.04	0.000537
188:	1391.53	0.000267	1393.08	0.000517	1385.55	0.000059	1387.63	0.000033	1390.9	0.000048	1395.98	0.00009
189:	1393.66	0.000068	1398.88	0.000785	1388.68	0.000023	1388.48	0.000074	1396.28	0.000071	1399.59	0.000546
190:	1397.11	0.000435	1399.17	0.000227	1392.21	0.00006	1388.9	0.000098	1398.81	0.000038	1399.71	0.000044
191:	1398.5	0.000125	1399.39	0.000288	1397.4	0.001702	1397.41	0.000199	1399.63	0.000166	1400.48	0.000071
192:	1413.7	0.001156	1414.3	0.001059	1399.22	0.000175	1401.15	0.001772	1411.44	0.001803	1411.24	0.001438
193:	1416.46	0.000769	1417.43	0.000742	1402.61	0.001181	1403.06	0.001186	1411.86	0.001199	1412.84	0.001003
194:	1425.3	0.000188	1424	0.000218	1417.07	0.000147	1420.63	0.000143	1419.54	0.000188	1418.92	0.000232
195:	1428.43	0.000111	1426.08	0.000139	1427.1	0.000265	1435.42	0.000082	1421.34	0.000143	1423.36	0.000279
196:	1431.54	0.000098	1435.91	0.000133	1436.01	0.000072	1437.53	0.000072	1424.5	0.000168	1433.7	0.000121
197:	1440.05	0.000201	1453.78	0.000099	1439.61	0.000026	1439.53	0.000075	1436.53	0.000263	1446.13	0.000163
198:	1451.22	0.000247	1457.7	0.000221	1443.81	0.000222	1442.07	0.000001	1446.39	0.000252	1450.68	0.000006
199:	1465.75	0.000027	1464.39	0.000005	1445.48	0.00005	1445.34	0.000066	1449.56	0.00011	1452.4	0.000043
200:	1466.52	0.000244	1466.61	0.000031	1445.9	0.000056	1446.21	0.000218	1452.28	0.000032	1456.28	0.000202
201:	1468.4	0.000027	1470.57	0.000021	1448.04	0.000008	1449.9	0.000035	1459.3	0.000134	1457.09	0.000003
202:	1470.59	0.000007	1474.36	0.000176	1451.82	0.000082	1452.27	0.000051	1459.87	0.000903	1459.93	0.00005
203:	1472.89	0.000344	1475.01	0.000138	1452.98	0.000266	1453.23	0.000246	1460.5	0.000017	1461.48	0.000246
204:	1474.82	0.000087	1475.47	0.000579	1453.89	0.000067	1454.32	0.000057	1462.11	0.000024	1462.56	0.000232
205:	1475.72	0.0005	1476.26	0.000187	1455.12	0.000254	1454.77	0.000242	1462.54	0.000463	1462.94	0.000063
206:	1476.15	0.000028	1477.07	0.000068	1457.18	0.000807	1456.91	0.000933	1463.9	0.000137	1463.49	0.00078
207:	1477.78	0.000235	1478.65	0.000234	1458.24	0.000291	1457.86	0.000601	1464.94	0.000243	1465.67	0.000417
208:	1477.89	0.000388	1479.25	0.000316	1461.56	0.000464	1462.56	0.000183	1465.62	0.000277	1467.92	0.000607
209:	1479.66	0.000405	1479.87	0.00043	1463.82	0.000737	1464.16	0.000544	1467.9	0.000544	1468.86	0.000455
210:	1480.83	0.000063	1480.14	0.000256	1464.45	0.000446	1464.23	0.000159	1471.23	0.000499	1470.54	0.000234
211:	1485.37	0.000043	1482.58	0.000287	1465.63	0.000027	1465.37	0.000266	1473.63	0.000014	1471.5	0.000083
212:	1485.86	0.000485	1483.91	0.000048	1466	0.000077	1466.43	0.000543	1476.02	0.000246	1471.63	0.000259
213:	1489.28	0.000028	1488.15	0.000055	1471.22	0.000144	1468.02	0.000041	1478.12	0.000097	1475.33	0.000036
214:	1490.58	0.000255	1489.31	0.000428	1471.45	0.000369	1472.49	0.000138	1478.71	0.000287	1477.53	0.00014
215:	1491.27	0.000115	1491.75	0.000069	1473.71	0.000222	1474.26	0.000208	1480.85	0.000072	1479.25	0.000263
216:	1492.21	0.000168	1492.85	0.000163	1478.76	0.000083	1481.03	0.000083	1483.18	0.000101	1483.17	0.000966
217:	1496.46	0.000077	1498.17	0.000142	1479.07	0.000151	1481.86	0.000167	1484.34	0.000541	1485.15	0.000071
218:	1498.23	0.000148	1498.36	0.000084	1496.28	0.000635	1495.05	0.000954	1490.79	0.00019	1486.23	0.000192
219:	1514.15	0.000633	1512.48	0.000704	1498.07	0.00068	1498.4	0.000537	1502.29	0.00084	1500.31	0.001008
220:	1517.04	0.000276	1517.38	0.000386	1509.88	0.001012	1511.52	0.001191	1505.57	0.000282	1503.83	0.000615
221:	1526.81	0.000963	1527.62	0.000641	1540.32	0.001055	1539.48	0.001872	1520.89	0.001193	1521.81	0.001066
222:	1529.68	0.000859	1527.8	0.001643	1541.39	0.001269	1541.3	0.001035	1525.17	0.000939	1523.55	0.001617

223:	1560.07	0.000113	1556.81	0.00029	1591.18	0.000287	1591.16	0.000454	1546.94	0.000079	1544.12	0.000293
224:	1603.04	0.000069	1599.71	0.000098	1631.94	0.000007	1629.39	0.000038	1592.25	0.000082	1588.7	0.000075
225:	1603.98	0.000061	1602.61	0.000113	1632.85	0.000133	1632.68	0.000111	1593.79	0.000057	1591.3	0.000143
226:	1625.11	0.000056	1623.68	0.000043	1658.19	0.000052	1658.74	0.000043	1621.48	0.000061	1617.86	0.000033
227:	1651.37	0.000061	1647.51	0.000703	1682.72	0.000133	1679.62	0.000633	1646.16	0.000179	1642.39	0.000311
228:	1652.33	0.000077	1651.37	0.000116	1684.87	0.00019	1684.7	0.00021	1646.73	0.000035	1645.2	0.000237
229:	1790.85	0.030358	1798.09	0.028292	1847.6	0.030959	1853.58	0.03005	1712	0.034467	1722.6	0.031943
230:	1855.67	0.053967	1857.67	0.050841	1914.67	0.053517	1915.13	0.049245	1785.3	0.059215	1787.76	0.053833
231:	2955.34	0.001181	2952.97	0.00108	2979.79	0.001031	2976.85	0.000977	2900.93	0.001117	2903.59	0.000902
232:	2975.03	0.000859	2966.34	0.001007	3004.48	0.00065	2993.4	0.000765	2922.36	0.000703	2915.35	0.000797
233:	2985.75	0.000261	2979.91	0.000216	3014.12	0.000212	2999.71	0.000217	2927.62	0.000265	2924.69	0.00019
234:	2999.83	0.000155	2984.53	0.00028	3021.67	0.000196	3008.03	0.000251	2945.27	0.000165	2928.07	0.000279
235:	3004.2	0.002225	2994.03	0.00316	3027.4	0.00204	3031.45	0.002475	2956.86	0.002612	2958.22	0.002703
236:	3005.06	0.002347	3005.81	0.002765	3031.84	0.002117	3031.8	0.002266	2958	0.001221	2958.5	0.002184
237:	3019.87	0.001485	3021.97	0.001507	3047.03	0.001144	3045.7	0.001132	2974.01	0.001152	2974.75	0.001051
238:	3021.42	0.001265	3022.46	0.001365	3047.56	0.000826	3047.38	0.000485	2974.31	0.000958	2975.29	0.000973
239:	3022.66	0.000653	3022.53	0.000771	3048.45	0.000454	3047.98	0.000832	2975.13	0.00048	2977.73	0.000483
240:	3024.12	0.000579	3024.78	0.000505	3049.35	0.00039	3050.08	0.000357	2979.43	0.000415	2980.22	0.000362
241:	3030.46	0.000416	3028.7	0.000377	3054.59	0.000317	3053.73	0.000338	2984.73	0.000347	2983.06	0.000343
242:	3031.54	0.000507	3030.99	0.000471	3055.2	0.000377	3055.38	0.000396	2986.38	0.000446	2986.02	0.000403
243:	3036.19	0.000484	3034.67	0.000599	3060.12	0.000288	3059.58	0.000349	2990.47	0.000363	2989.33	0.000387
244:	3037.2	0.000736	3036.47	0.000706	3060.46	0.000581	3061.03	0.000496	2991.68	0.000591	2991.55	0.000499
245:	3063.2	0.001418	3060.68	0.001038	3100.48	0.000934	3099.97	0.000887	3020.57	0.001005	3020.3	0.000983
246:	3065.84	0.000009	3064.67	0.000225	3104.12	0.000012	3103.56	0.000025	3024.57	0.000118	3023.82	0.000005
247:	3092.09	0.000529	3092.12	0.000455	3129.66	0.00029	3129.74	0.000282	3050.7	0.000346	3051.37	0.000286
248:	3094.93	0.00042	3094.61	0.000424	3131.1	0.000237	3132.23	0.000248	3052.9	0.000279	3053.05	0.000282
249:	3104.33	0.000471	3101.79	0.000486	3141.66	0.000306	3139.17	0.000364	3064.63	0.000376	3064.54	0.000386
250:	3106.49	0.000402	3104.73	0.000339	3142.88	0.000272	3142.04	0.000253	3069.12	0.000306	3067.48	0.000264
251:	3109.84	0.000035	3108.3	0.000015	3145.6	0.000025	3146.01	0.000015	3070.18	0.00009	3071.61	0.00001
252:	3113.37	0.000017	3109.84	0.000023	3147.37	0.000392	3146.53	0.000033	3073.35	0.000436	3072.51	0.000016
253:	3114.12	0.00059	3112.98	0.00064	3148.67	0.000013	3149.14	0.000465	3074.43	0.000364	3074.46	0.000423
254:	3115.09	0.000642	3114.91	0.000684	3149.16	0.000463	3151.25	0.000446	3075.67	0.000048	3074.54	0.000518
255:	3116.26	0.000125	3115.12	0.002028	3151.08	0.000246	3151.91	0.000139	3076.2	0.000164	3075.22	0.000139
256:	3116.72	0.001925	3115.9	0.000132	3152.22	0.001197	3152.1	0.000449	3077.79	0.001312	3078.21	0.001362
257:	3118.3	0.000258	3117.35	0.002119	3152.94	0.000182	3152.62	0.001227	3079.22	0.000205	3078.81	0.000972
258:	3120.27	0.001653	3118.56	0.000225	3155.51	0.000789	3153.56	0.000292	3081.78	0.000236	3080.09	0.000362
259:	3123	0.000475	3120.42	0.000159	3156.24	0.000433	3155.16	0.000667	3082.21	0.000768	3081.24	0.000227
260:	3124.16	0.000315	3120.8	0.000207	3157.55	0.000543	3156.08	0.000626	3083.87	0.000632	3082.42	0.000592
261:	3124.37	0.000503	3122.24	0.000551	3158.91	0.000262	3159.35	0.000207	3084.77	0.000536	3085.99	0.000227
262:	3126.61	0.000321	3125.71	0.00033	3160.93	0.000198	3162.24	0.000219	3085.03	0.000199	3086.85	0.000115
263:	3128.52	0.000167	3127.72	0.000311	3162.59	0.000195	3163.6	0.000277	3091.79	0.000055	3087.27	0.000213
264:	3132.56	0.000308	3128.84	0.000231	3164.23	0.000233	3164	0.000309	3095.11	0.000149	3089.75	0.000294
265:	3140.95	0.000258	3131.42	0.000318	3167.66	0.000186	3164.28	0.000212	3100.6	0.000196	3091.24	0.000343
266:	3142.67	0.000303	3132.61	0.000399	3169.74	0.000345	3167.46	0.000153	3102.7	0.000411	3094.27	0.00017

267:	3143.51	0.000212	3139.05	0.000209	3170.15	0.000068	3168.19	0.000186	3102.86	0.000184	3095.93	0.000176
268:	3146.67	0.000596	3146	0.000757	3175.19	0.000475	3175.31	0.000533	3107.02	0.000184	3101.55	0.000543
269:	3148.58	0.000188	3148.29	0.00031	3178.06	0.000159	3177.79	0.000208	3108.91	0.0002	3103.9	0.000199
270:	3151.49	0.000271	3153.24	0.000155	3181.47	0.000168	3182.43	0.000129	3110.52	0.000363	3109.72	0.000127
271:	3155.96	0.000376	3155.97	0.000654	3184.87	0.00023	3185.46	0.00031	3112.82	0.000031	3111.88	0.000425
272:	3156.83	0.000645	3159.56	0.000565	3184.98	0.000382	3187.18	0.0003	3112.89	0.000453	3114.44	0.000388
273:	3163.09	0.000244	3159.81	0.000403	3190.24	0.000251	3187.82	0.000418	3118.7	0.000171	3115.88	0.000305
274:	3164.55	0.000406	3162.74	0.000233	3191.08	0.000154	3188.3	0.000238	3122.65	0.000288	3118.21	0.000193
275:	3173.83	0.000287	3177.16	0.000395	3201.85	0.000205	3199.93	0.000414	3128	0.000137	3131.32	0.000426
276:	3178.37	0.000295	3179.51	0.000228	3204.45	0.000306	3205.42	0.000147	3133.93	0.000195	3135.05	0.000091
277:	3183.57	0.000459	3184.6	0.000465	3208.83	0.000324	3212.58	0.00029	3139.71	0.000266	3140.29	0.000277
278:	3201.73	0.000133	3190.21	0.000172	3217.67	0.000077	3217.46	0.000097	3162.4	0.000057	3149.72	0.000054

*: A maximum of two imaginary modes in the range of -5 to -75 cm^{-1} related to the rotational freedom of the methyl substituent of the *p*-tolyl group have been observed.

Table S23. Calculated vibrational frequencies of the mono reduced complex $\mathbf{3}^{1-}$, $\mathbf{4}^{1-}$ and $\mathbf{5}^{1-}$with and without dispersion correction.

	$\mathbf{3}^{1-}$				$\mathbf{4}^{1-}$				$\mathbf{5}^{1-}$			
	TPSSh; Disp on*		TPSSh; Disp OFF*		TPSSh; Disp ON		TPSSh; Disp OFF		TPSSh; Disp ON		TPSSh; Disp OFF	
Mode	freq	T**2	freq	T**2	freq	T**2	freq	T**2	freq	T**2	freq	T**2
	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)
8:	25.16	0.000449	25.69	0.000091	28.8	0.000278	27.69	0.000346	27.57	0.000066	31.32	0.000078
9:	30.17	0.001482	27.67	0.000298	34.37	0.000515	30.68	0.000389	31.25	0.000443	34.31	0.000425
10:	30.93	0.000247	29.87	0.000732	37.44	0.001025	36.83	0.000144	33.56	0.000298	40.99	0.000789
11:	33.5	0.001872	30.93	0.000824	39.86	0.000132	39.53	0.000834	41.34	0.00094	44.08	0.00059
12:	36.84	0.000541	34.16	0.000896	41.43	0.00018	40.97	0.000508	44.11	0.000334	46.55	0.000817
13:	39.9	0.00097	39.29	0.000616	46.61	0.000432	46.5	0.000618	45.09	0.00031	47.94	0.000338
14:	45.56	0.000324	39.64	0.000614	48.37	0.000314	50.32	0.000654	50.12	0.000362	49.17	0.000076
15:	47.54	0.000466	41.9	0.001647	52.69	0.00058	51.63	0.000365	54.8	0.000256	56.59	0.000224
16:	50.51	0.000116	48.31	0.000123	61.43	0.000119	54.45	0.000334	63.54	0.000014	60.23	0.000188
17:	51.01	0.000063	54.82	0.000093	67.59	0.000198	61.21	0.000327	71.67	0.000181	70.29	0.000338
18:	57.38	0.000405	56.39	0.00031	72.23	0.00028	68.34	0.000454	74.94	0.000706	75.26	0.000584
19:	61.45	0.000249	58.23	0.000493	80.25	0.001005	78.71	0.00105	81.97	0.000908	81.35	0.001326
20:	70.67	0.000303	68.88	0.001028	84.35	0.000774	81.22	0.001405	85.19	0.000835	84.79	0.000703
21:	83.1	0.00131	82.56	0.00128	91.99	0.000785	86.9	0.000879	90.7	0.00041	90.36	0.000577
22:	87.9	0.000234	85.25	0.000312	95.45	0.000671	95.15	0.000252	97.87	0.000423	97.09	0.000567
23:	95.32	0.000665	86.54	0.000243	104.81	0.001384	101.81	0.000866	103.85	0.001468	102.93	0.001636
24:	98.65	0.000541	98.76	0.000629	106.44	0.000398	103.73	0.000518	107.14	0.000418	111.94	0.000445
25:	100.68	0.000306	101.16	0.000622	113.77	0.001307	104.77	0.001253	122.14	0.000315	127.12	0.000191
26:	105.57	0.0016	105.29	0.001457	125.74	0.001017	124.53	0.00055	127.94	0.000066	130.81	0.000582
27:	117.55	0.00023	117.22	0.000234	132.85	0.000035	128.08	0.000464	134.53	0.000922	132.47	0.000131
28:	121.71	0.000519	120.3	0.000593	138.53	0.000369	134.76	0.000006	137.11	0.001321	137.13	0.001437
29:	131.28	0.000172	126.82	0.000263	139.95	0.000508	135.06	0.001192	141.27	0.000925	140.36	0.001063
30:	136.07	0.000558	130.96	0.000654	148.95	0.000184	141.22	0.00032	155.23	0.000396	153.46	0.000559
31:	145.43	0.000416	141.99	0.000442	155.53	0.000663	151.6	0.000577	163.64	0.000801	162.38	0.000667
32:	156.11	0.000546	153.32	0.000825	160.57	0.000751	157.32	0.000781	170.55	0.000662	169.57	0.000477
33:	160.77	0.001122	159.6	0.001272	170.54	0.000712	165.58	0.000791	178.71	0.000461	175.11	0.000463
34:	161.81	0.000417	165.73	0.00002	183.93	0.00019	177.29	0.000235	194.64	0.000708	192.58	0.000529
35:	179.76	0.00134	173.98	0.001081	188.07	0.000143	185.69	0.000066	205.96	0.000084	206.91	0.000042
36:	190.94	0.000295	185.66	0.000475	193.2	0.000237	187.34	0.000054	208.62	0.000021	209.06	0.000142
37:	196.02	0.000164	200.72	0.000057	196.99	0.000518	194.17	0.000512	210.96	0.00009	213.67	0.000076
38:	205.61	0.000685	203.68	0.000703	211.55	0.000051	208.58	0.000157	214.82	0.000045	216.17	0.000031
39:	209.16	0.000174	208.29	0.000174	213.53	0.000066	209.29	0.000045	218.53	0.000039	219.16	0.000029
40:	215.08	0.000111	213.53	0.000141	217.67	0.000019	214.23	0.00003	229.9	0.000137	229.17	0.000198
41:	217.54	0.000011	219.04	0.000065	222.06	0.000051	215.56	0.000019	242.06	0.000719	233.46	0.000292
42:	227.87	0.000257	227.06	0.000285	224.62	0.000062	222.62	0.000069	253.17	0.000179	252.77	0.000293
43:	247.73	0.001336	243.18	0.001234	244.51	0.000452	234.77	0.000377	255.03	0.000102	258.63	0.000338
44:	256.4	0.000134	254.33	0.000085	245.58	0.000006	245.36	0.000009	263.61	0.000021	265.6	0.000161
45:	263.36	0.00004	265.26	0.000138	251.46	0.000264	248.57	0.000247	270.38	0.000029	274.92	0.00004
46:	265.52	0.000076	270.58	0.000046	257.92	0.00017	259	0.000274	273.66	0.000114	281.75	0.000011

47:	269.69	0.000431	278.05	0.000131	259.73	0.000072	260.89	0.000084	281.95	0.000068	284.02	0.000029
48:	279.78	0.000216	279.56	0.000868	274.76	0	272.08	0.000062	283.25	0.000225	288.5	0.00055
49:	282.71	0.00028	283.97	0.000358	281.71	0.00003	277.99	0.000006	295.52	0.000769	294.44	0.000449
50:	292.87	0.000149	292.16	0.000051	283.07	0.000119	281.09	0.000033	301.25	0.00005	299.95	0.000042
51:	299.18	0.000734	298.69	0.000461	290.87	0.00032	289.07	0.00038	303.85	0.000048	303.03	0.000273
52:	302.86	0.000165	302.68	0.000003	295.27	0.000216	293.08	0.000217	307.76	0.001255	303.47	0.000128
53:	307.8	0.000622	310.66	0.001159	300.13	0.000951	294.38	0.000749	310.33	0.001132	310.05	0.002174
54:	320.98	0.001765	320.04	0.001393	303.45	0.000176	300.29	0.000146	317.54	0.001405	317.9	0.001453
55:	325.19	0.001073	322.83	0.001204	307.02	0.000061	303.56	0.00017	331.9	0.000269	330.2	0.000489
56:	329.77	0.000128	328.63	0.000188	317.13	0.001343	316.3	0.001488	333.8	0.000286	335.37	0.000232
57:	332.85	0.000792	333.56	0.001688	330.79	0.000883	329.39	0.000732	339.62	0.000368	336.59	0.000653
58:	338.18	0.000093	341.58	0.000303	332.98	0.000033	329.97	0.000324	342.63	0.000513	342.98	0.000664
59:	343.23	0.000584	344.85	0.000686	337.54	0.000206	333.45	0.00043	343.3	0.000982	344.17	0.000187
60:	352.65	0.000144	350.69	0.000088	339.9	0.000305	336.74	0.000482	349.07	0.000283	346.3	0.000352
61:	354.58	0.000003	352.63	0.000122	342.08	0.000419	338.42	0.000458	368.04	0.000127	363.52	0.000425
62:	359.47	0.000738	363.76	0.000697	347.62	0.001179	341.59	0.00102	370.33	0.000733	370.05	0.00112
63:	371.53	0.000167	371.02	0.000189	351.19	0.000374	346.89	0.000396	389.12	0.002336	386.1	0.002807
64:	379.85	0.000215	378.2	0.00027	367.6	0.000099	362.51	0.00038	396.35	0.001505	393.31	0.000843
65:	400.8	0.003816	397.88	0.004136	370.29	0.000544	367.3	0.000837	399.61	0.00092	397.41	0.001281
66:	404.64	0.000431	402.79	0.000461	372.69	0.00038	368.85	0.00008	407.36	0.00269	405.57	0.002721
67:	406.3	0.000274	406.9	0.000078	390.82	0.002759	386.49	0.002549	416.94	0.000097	417.11	0.000119
68:	412.08	0.00001	411.57	0.000005	395.14	0.000744	394.36	0.000957	431.08	0.00014	431.05	0.000147
69:	414.94	0.000064	413.88	0.000133	401.97	0.00124	397.72	0.00151	438.5	0.000514	432.9	0.0008
70:	418.1	0.000273	417.8	0.00016	408.6	0.002409	405.22	0.002827	440.2	0.000292	437.18	0.000611
71:	428.59	0.003172	427.19	0.005216	423.61	0.000059	423.61	0.000065	441.82	0.000132	439.64	0.000246
72:	430.69	0.0021	431.31	0.000258	437.1	0.000811	432.63	0.000507	446.4	0.000976	446.24	0.000439
73:	451.19	0.001583	450.31	0.00171	440.16	0.000192	436.47	0.000337	452.41	0.003329	453.13	0.003222
74:	461.38	0.00158	462.71	0.001303	441.23	0.000045	438.6	0.00037	471.03	0.000523	467.14	0.000573
75:	476.13	0.000622	475.14	0.000654	446.51	0.000704	443.3	0.000767	478.13	0.000487	477.46	0.000503
76:	478.05	0.000923	477.36	0.000617	450.35	0.000393	449.79	0.000277	479.16	0.00022	481.1	0.000195
77:	480.97	0.000129	479.57	0.000228	453.83	0.003179	451.9	0.003043	488.55	0.000908	486.35	0.000744
78:	500.88	0.003299	492.21	0.004262	470.61	0.00056	466.21	0.000701	495.03	0.00125	490.52	0.001594
79:	505.73	0.003189	504.63	0.003839	477.73	0.000579	475.61	0.00059	497.39	0.00056	496.67	0.000438
80:	508.19	0.002956	507.7	0.003438	478.34	0.000202	478.94	0.000167	503.45	0.000094	504.78	0.000328
81:	510.8	0.001212	510.04	0.000776	487.49	0.001128	484.15	0.000823	511.77	0.000667	510.22	0.001601
82:	512.74	0.001138	511.9	0.000592	490.87	0.000852	487.64	0.000948	513.99	0.00201	512.95	0.001143
83:	517.2	0.000092	517.63	0.000087	496.46	0.000335	493.33	0.000259	515.11	0.000214	517.4	0.000008
84:	520.49	0.003246	519.96	0.003078	502.37	0.000088	503.67	0.000231	522.79	0.000242	520.81	0.000198
85:	529.53	0.001056	531.44	0.001678	511.42	0.000451	508.26	0.00176	532.33	0.001542	531.62	0.001399
86:	539.6	0.002327	539.63	0.002205	512.99	0.000827	511.44	0.000363	543.24	0.003336	545.58	0.003788
87:	588.25	0.003073	591.99	0.002667	520.22	0.001578	518.77	0.00016	590.88	0.003302	593.5	0.002514
88:	597.04	0.00011	596.91	0.000199	523.43	0.000489	521.05	0.001014	596.86	0.000087	597.63	0.000401
89:	626.29	0.00052	621.14	0.000381	538.31	0.004118	540.46	0.004413	624.48	0.001114	627.36	0.000981
90:	627.16	0.002396	624.12	0.002375	582.49	0.002084	583.76	0.00172	711.32	0.002076	703.95	0.002037

91:	629.61	0.002588	625.39	0.002141	601.02	0.000519	601.15	0.000048	719.01	0.001922	712.92	0.002159
92:	640.84	0.000014	641.4	0.000019	602.06	0.000529	602.38	0.000971	733.74	0.001025	727.01	0.001826
93:	642.76	0.000008	641.91	0.000016	622.44	0.000994	625.59	0.000872	735.87	0.001333	728.89	0.000951
94:	714.54	0.003094	708.28	0.003448	688.85	0.000544	690.18	0.000587	745.21	0.000095	737.89	0.000187
95:	722.37	0.000119	720.26	0.000627	711.26	0.002128	703.56	0.002023	761.47	0.000707	759.9	0.000691
96:	730.45	0.001141	726.65	0.001403	717.51	0.000071	712.35	0.00193	765.65	0.000022	761.77	0.000006
97:	730.95	0.000666	729.15	0.001008	719.56	0.00162	717.89	0.000009	780.55	0.000491	778.44	0.000473
98:	734.89	0.001247	732.62	0.000692	734.65	0.001005	726.43	0.001736	796.61	0.000028	787.4	0.000013
99:	754.96	0.000817	752.03	0.000519	736.51	0.001252	729.55	0.000954	799.03	0.000026	798.66	0.000151
100:	763.72	0.000327	759.43	0.000694	746.69	0.000126	737.48	0.000212	799.38	0.000109	800.07	0.000013
101:	780.53	0.000706	776.16	0.000657	762.31	0.000703	759.08	0.000744	809.7	0.00103	812.29	0.001008
102:	800.91	0.000224	800.8	0.00017	767.22	0.00003	761.44	0.000025	823.6	0.000234	823.42	0.000428
103:	804.35	0.000489	806.52	0.000138	767.45	0.000092	766.42	0.000076	826.75	0.000538	826.33	0.000497
104:	807.43	0.000383	807.43	0.000139	783.15	0.000506	779.1	0.00049	830.64	0.000208	826.48	0.000236
105:	812.4	0.001166	811.84	0.000537	796.18	0.000007	790.53	0.000013	831.96	0.000294	830.42	0.000284
106:	817.71	0.000592	818.34	0.000965	797.33	0.000019	793.77	0.000007	838.49	0.000336	835.5	0.000346
107:	821.09	0.001492	820.18	0.001562	814.12	0.000986	811.59	0.000794	855.99	0.000984	856.33	0.001169
108:	823.63	0.00019	824.84	0.000265	828.16	0.00039	823.53	0.000285	857.77	0.000537	858.45	0.000271
109:	826.81	0.000445	825.29	0.00049	831.43	0.00044	827.7	0.000149	861.66	0.00115	861.7	0.001506
110:	836.68	0.000179	833.84	0.00029	831.68	0.000291	828.44	0.000667	866.47	0.000013	865.33	0.000011
111:	846.65	0.000088	846.6	0.000056	839.69	0.000426	835.34	0.000363	878.1	0.000243	879.64	0.000237
112:	861.36	0.001072	862.89	0.000654	857.63	0.00101	857.28	0.000807	891.98	0.004882	892.77	0.003814
113:	865.54	0.000199	865.39	0.000341	859.34	0.000232	858.25	0.000486	899.81	0.001029	897.29	0.000613
114:	866.56	0.000035	865.82	0.000152	863.95	0.001931	863.54	0.001721	902.54	0.001242	899.24	0.000497
115:	875.52	0.000516	881.27	0.000723	880.76	0.001042	880.64	0.001265	903.23	0.000117	900.77	0.00182
116:	892.7	0.006499	895.42	0.00655	893.04	0.000583	893.35	0.000546	904.37	0.000093	906.68	0.000039
117:	906.93	0.000002	908.61	0.000007	895.41	0.00001	895.24	0.0008	909.79	0.000007	909.31	0.000005
118:	912.31	0.000175	913.22	0.000193	898.05	0.002791	895.93	0.000029	914.14	0.000069	913.54	0.000148
119:	917.61	0.000043	917.55	0.000052	899.73	0.000029	898.05	0.00123	915.03	0.000112	917.66	0.00003
120:	929.19	0.000038	927.77	0.000041	902.08	0.000333	898.44	0.000118	925.68	0.000311	924.14	0.000415
121:	932	0.00003	931.78	0.000033	903.44	0.000896	901.08	0.00089	929.59	0.000128	928.49	0.000131
122:	949.1	0.000012	949.45	0.000008	904.82	0.002347	902.9	0.003192	929.75	0.00001	929.1	0.000352
123:	950.76	0.000001	952.42	0.000004	914.72	0.000102	913.71	0.000138	930.25	0.000428	929.56	0.000078
124:	958.02	0.000069	957.67	0.000063	916.02	0.000163	916.37	0.000088	947.02	0.000002	952.25	0.000021
125:	962.74	0.000208	963.43	0.000128	926.51	0.000278	923.6	0.000437	951.03	0.000019	952.72	0.000002
126:	964.87	0.000147	966.57	0.000138	928.46	0.000177	926.99	0.000297	958.05	0.000057	957.35	0.000059
127:	982.07	0.000034	980.46	0.000239	929.31	0.000357	927.44	0.000305	982.8	0.000087	982.36	0.000085
128:	983.07	0.000342	985.22	0.000051	929.78	0.000088	931.21	0.000025	1016.71	0.000542	1011.93	0.000611
129:	999.5	0.000065	996.89	0.000335	945.7	0.000154	946.27	0.000148	1018.53	0.000611	1016.97	0.000651
130:	1000.95	0.000066	1000.81	0.000071	948.61	0.000005	949.66	0.000004	1024.33	0.000109	1020.15	0.0006
131:	1011.17	0.000011	1011.48	0.000009	954.22	0.000026	954.13	0.000024	1025.87	0.001212	1023.64	0.000843
132:	1023.21	0.000838	1022.45	0.001047	996.96	0.002677	996.98	0.002864	1031.64	0.000077	1030.83	0.000061
133:	1025.59	0.000321	1025.03	0.000528	1010.97	0.000051	1011.31	0.000035	1034.29	0.000257	1032.62	0.000388
134:	1026.38	0.000313	1026.25	0.000623	1015.86	0.000458	1013.43	0.000463	1034.78	0.000233	1034.65	0.000181

135:	1030.29	0.000115	1028.77	0.000149	1017.59	0.000811	1014.42	0.000816	1040.91	0.000287	1039.26	0.000326
136:	1032.45	0.000263	1031.43	0.00025	1026.25	0.000566	1021.35	0.000828	1042.01	0.00028	1041.42	0.000198
137:	1032.78	0.000149	1031.99	0.000019	1027.4	0.000498	1024.88	0.000521	1043.08	0.000201	1042.02	0.000104
138:	1034.72	0.000834	1032.72	0.000732	1030.66	0.000184	1029.96	0.000165	1044.67	0.000273	1043.62	0.000213
139:	1042.62	0.000162	1041.19	0.00066	1031.67	0.000082	1031.07	0.000071	1055.49	0.000028	1054.6	0.000049
140:	1045.02	0.000938	1043.38	0.000133	1035.95	0.000264	1033.77	0.000144	1058.46	0.000066	1057.85	0.000073
141:	1046.34	0.000662	1047.69	0.000187	1036.76	0.00046	1034.82	0.00064	1081.93	0.00011	1082.93	0.000164
142:	1048.87	0.000841	1049.08	0.000839	1041.66	0.000207	1040.88	0.000453	1083.27	0.000155	1083.75	0.000143
143:	1083.63	0.00013	1083.27	0.000162	1043.58	0.000334	1043.13	0.000204	1086.81	0.000162	1087.17	0.000017
144:	1087	0.000039	1087.34	0.000023	1045.87	0.000439	1044	0.000171	1087.16	0.000018	1087.39	0.000182
145:	1110.34	0.000428	1101.15	0.000654	1054.87	0.000026	1054.74	0.000001	1100.25	0.000045	1101.88	0.000051
146:	1111.55	0.000587	1107.43	0.000693	1055.42	0.000001	1055.08	0.000053	1103.08	0.00008	1102.61	0.00009
147:	1128.62	0.000276	1125.96	0.000299	1057.2	0.000072	1056.65	0.000086	1125.95	0.000384	1122.55	0.000395
148:	1135.18	0.000098	1135.2	0.000095	1082.99	0.000058	1082.8	0.000122	1126.35	0.000338	1126	0.000371
149:	1139.63	0.00007	1138.37	0.000029	1084.04	0.000198	1084.1	0.00022	1131.35	0.000629	1130.19	0.000538
150:	1140.42	0.000084	1139.1	0.000139	1099.26	0.00004	1100.19	0.000054	1138.22	0.000083	1136.02	0.000134
151:	1141.43	0.000073	1139.61	0.000066	1102.29	0.000084	1101.5	0.00008	1140.43	0.000048	1139.82	0.000038
152:	1145.65	0.00008	1144.83	0.000098	1111.91	0.000859	1113.47	0.000863	1150.99	0.000099	1149.24	0.000136
153:	1182.16	0.000039	1181.7	0.000042	1127.3	0.000325	1123.9	0.000287	1180.96	0.000022	1181.17	0.000025
154:	1203.87	0.000959	1203.55	0.00422	1130.68	0.000662	1128.11	0.000648	1189.72	0.000195	1191.38	0.000258
155:	1206.29	0.00359	1204.69	0.002921	1140.06	0.000033	1136.78	0.000046	1193.56	0.000177	1194.57	0.000187
156:	1207.39	0.003003	1205.63	0.001948	1151.94	0.000106	1147.54	0.000129	1207.08	0.004821	1204.9	0.00496
157:	1209.55	0.003905	1207.3	0.002454	1170.43	0.000019	1170.68	0.000022	1209	0.004667	1206.95	0.004729
158:	1218.3	0.000884	1215.85	0.000954	1192.27	0.000198	1192.58	0.000165	1215.09	0.000385	1214.68	0.000015
159:	1226.69	0.000374	1227.79	0.000486	1193.15	0.000226	1193.93	0.000246	1218.1	0.000938	1220.45	0.001055
160:	1236.06	0.000033	1235.88	0.000051	1207.67	0.004563	1205.14	0.005018	1222.99	0.000228	1223.14	0.000125
161:	1239	0.000131	1238.02	0.000581	1209.7	0.00484	1207.15	0.004986	1225.09	0.000013	1228.61	0.000216
162:	1239.36	0.000526	1238.4	0.00012	1217.31	0.000069	1216.58	0.000222	1239.57	0.000598	1238.64	0.000702
163:	1242.59	0.000709	1241.23	0.000678	1219.38	0.000837	1219.06	0.000249	1243.01	0.000552	1240.7	0.000586
164:	1249.92	0.000071	1249.34	0.000029	1221.48	0.000816	1220.37	0.001092	1251.37	0.000019	1253.09	0.000021
165:	1253.3	0.000458	1253.67	0.000672	1225.29	0.000226	1225.85	0.000106	1253.5	0.000609	1253.46	0.000679
166:	1256.51	0.00043	1255.82	0.000372	1241.22	0.000628	1239.24	0.000603	1257.11	0.000437	1257.23	0.000421
167:	1276.28	0.000035	1276.33	0.000047	1242.47	0.000531	1241.07	0.000605	1273.97	0.000055	1275.63	0.000041
168:	1290.13	0.000169	1288.79	0.000952	1246.49	0.00014	1246.25	0.000141	1274.84	0.000036	1275.99	0.000026
169:	1293.61	0.001211	1293.06	0.000337	1253.35	0.000014	1252.59	0.000012	1277.55	0.000015	1278.13	0.000014
170:	1297.4	0.000256	1301	0.000163	1255.62	0.00032	1255.85	0.000332	1283.83	0.000025	1283.34	0.000054
171:	1302.75	0.000122	1301.71	0.000319	1257.71	0.000342	1256.65	0.000299	1286.26	0.000318	1286.84	0.000056
172:	1313.44	0.000016	1315.36	0.000025	1272.71	0.000049	1275.45	0.000019	1288.7	0.000238	1288.71	0.00016
173:	1317.13	0.000435	1317.59	0.000335	1275.93	0.000008	1277.48	0.000023	1289.53	0.000546	1292.52	0.00016
174:	1320	0.000096	1321.32	0.000007	1284.63	0.000024	1285.59	0.00012	1292.27	0.000471	1295.43	0.000889
175:	1324.9	0.000137	1323.51	0.000254	1286.76	0.000236	1285.69	0.000163	1295.04	0.000415	1299.11	0.000633
176:	1338.03	0.000126	1336.64	0.000151	1289.75	0.000105	1289.3	0.000038	1304.14	0.000446	1306	0.000508
177:	1352.16	0.000501	1351.21	0.000646	1292.05	0.000091	1291.82	0.000211	1307.43	0.000172	1310.6	0.000176
178:	1352.82	0.000022	1351.46	0.000479	1295.44	0.001213	1296.38	0.00078	1312.15	0.000244	1311.77	0.000261

179:	1353.25	0.000477	1351.6	0.000356	1297.87	0.000371	1298.59	0.000712	1315.45	0.000041	1315.75	0.000138
180:	1354.15	0.000363	1354.42	0.000178	1301.46	0.000747	1302.23	0.000817	1317.58	0.000231	1316.6	0.000077
181:	1369.06	0.000259	1372.39	0.00039	1307.81	0.000136	1307.3	0.00015	1325.13	0.000235	1328.72	0.000215
182:	1382.64	0.000677	1383.93	0.00062	1310.79	0.000083	1312.22	0.000194	1336.84	0.000163	1335.77	0.000162
183:	1387.56	0.000363	1388.89	0.000308	1313.97	0.000128	1320.13	0.000044	1345.14	0.000028	1346.54	0.00004
184:	1388.22	0.000291	1389.49	0.000289	1320.76	0.000222	1320.9	0.000137	1348.88	0.000032	1349.16	0.000029
185:	1392	0.000462	1392.52	0.000509	1331.53	0.00022	1329.4	0.000166	1351.59	0.000684	1351.45	0.00094
186:	1395.86	0.000223	1397.22	0.000369	1347.09	0.000052	1347.58	0.000016	1354.47	0.00027	1354.35	0.000114
187:	1398.89	0.000136	1399.47	0.000128	1347.73	0.000108	1347.84	0.00009	1356.84	0.000035	1359.04	0.000039
188:	1411.97	0.001108	1413.33	0.001034	1350.3	0.002117	1351.64	0.002159	1365.44	0.000035	1364.49	0.000033
189:	1415.86	0.000768	1416.77	0.000745	1357.9	0.000014	1357.18	0.00001	1370.97	0.000341	1370.71	0.000396
190:	1424.73	0.00018	1423.85	0.000202	1360.51	0.000583	1359.68	0.000582	1373.92	0.000082	1371.94	0.000077
191:	1427.28	0.000054	1426.54	0.000133	1361.75	0.000072	1360.26	0.000119	1376.68	0.000022	1374.97	0.000269
192:	1429.94	0.000222	1434.54	0.000108	1373.7	0.00009	1372.34	0.000075	1378.19	0.00022	1376.73	0.000068
193:	1438.32	0.000168	1452.16	0.000133	1376.16	0.00007	1375.85	0.00005	1379.26	0.000235	1377.7	0.00002
194:	1452.54	0.000011	1455.39	0.000017	1377.4	0.000098	1376.34	0.000057	1379.6	0.000045	1378.59	0.000107
195:	1453.54	0.000172	1456.46	0.000208	1377.7	0.000007	1377.77	0.000259	1380.88	0.000078	1381.68	0.000164
196:	1463.77	0.000038	1466.05	0.00002	1378.16	0.000197	1377.91	0.000416	1385.24	0.000621	1383.79	0.000653
197:	1464.7	0.000279	1466.45	0.000027	1379.43	0.000192	1377.98	0.000357	1385.5	0.000501	1389.24	0.0005
198:	1467.72	0.000128	1470.54	0.000029	1381.88	0.000625	1381.67	0.00013	1388.89	0.000328	1390.52	0.000231
199:	1467.76	0.000041	1471.02	0.000053	1385.45	0.000492	1388.97	0.00036	1389.51	0.000294	1391.05	0.000393
200:	1469.91	0.000006	1472.4	0.000158	1390.32	0.000313	1391.09	0.000403	1412.88	0.000811	1414.24	0.001075
201:	1474.76	0.000222	1475.23	0.000063	1391.52	0.000346	1393.09	0.000317	1413.81	0.001144	1416.06	0.00075
202:	1474.79	0.000013	1476.88	0.000177	1392.75	0.000105	1393.3	0.000028	1428.62	0.000047	1436.74	0.000038
203:	1476.62	0.000054	1477.4	0.000231	1399.25	0.000716	1399.46	0.000868	1444.92	0.000014	1444.28	0.00007
204:	1476.97	0.000178	1478.21	0.000052	1414.36	0.000846	1414.86	0.001104	1447.04	0.000167	1457.85	0.000033
205:	1480.38	0.000395	1480.52	0.000414	1414.91	0.001138	1416.23	0.000732	1453.86	0.000032	1460.88	0.000064
206:	1480.62	0.000289	1482.48	0.000319	1429.02	0.000049	1428.25	0.000059	1464.14	0.000013	1461.23	0.000051
207:	1484.61	0.000043	1485	0.000034	1447.48	0.000048	1448.28	0.000059	1466.05	0.000159	1467.34	0.000178
208:	1485.26	0.000023	1488.16	0.000051	1449.64	0.000193	1450.6	0.00017	1466.97	0.000054	1467.95	0.000083
209:	1487.37	0.000033	1489.25	0.00003	1465.29	0.000032	1460.93	0.000048	1468.02	0.000056	1469.49	0.000118
210:	1490.85	0.000094	1492.21	0.000066	1465.55	0.000044	1465.6	0.000001	1469.15	0.000023	1469.91	0.000184
211:	1492.54	0.000168	1492.8	0.000169	1467.02	0.00008	1466.13	0.000063	1469.55	0.000103	1470.96	0.000049
212:	1496.5	0.000059	1497.16	0.000063	1467.63	0.000006	1467.68	0.000035	1469.9	0.000021	1471.53	0.000019
213:	1497.19	0.000148	1497.89	0.000141	1471.24	0.000033	1470.29	0.000037	1471.2	0.00023	1471.99	0.000059
214:	1514.21	0.000584	1513.8	0.000709	1471.45	0.000057	1470.8	0.000075	1472.08	0.000037	1472.65	0.000069
215:	1516.31	0.000415	1518.13	0.00038	1471.8	0.000093	1471.87	0.000027	1474.7	0.000061	1473.24	0.000059
216:	1526.53	0.000946	1526.68	0.00125	1473.96	0.000071	1472.48	0.000037	1476.2	0.000105	1474.43	0.000177
217:	1528.97	0.001191	1526.82	0.001242	1475.14	0.000388	1473.9	0.000423	1478.24	0.000076	1476.48	0.000051
218:	1563.21	0.001103	1568.07	0.001215	1475.75	0.000077	1474.9	0.00032	1478.59	0.00005	1478.78	0.000094
219:	1601.69	0.000037	1599	0.000038	1475.84	0.00035	1475.49	0.000354	1479.38	0.000085	1480.7	0.000054
220:	1602.87	0.00007	1602.55	0.00008	1476.05	0.000078	1475.63	0.000192	1481.7	0.000148	1486.18	0.000213
221:	1648.68	0.000261	1647.36	0.000886	1476.83	0.000288	1476.77	0.000055	1485.6	0.000029	1486.76	0.000013
222:	1651.74	0.000074	1650.93	0.000089	1479.15	0.000405	1477.15	0.00002	1485.88	0.000056	1487.09	0.000024

223:	1784.6	0.030217	1789.19	0.02861	1480.34	0.00017	1479	0.00035	1486.97	0.000051	1490.18	0.000056
224:	1844.1	0.051794	1847.14	0.050445	1481.19	0.000354	1479.32	0.000227	1492.65	0.000137	1491.9	0.000015
225:	2951.23	0.001248	2955.7	0.000941	1481.75	0.000068	1480.69	0.000271	1493.32	0.000086	1492.91	0.000096
226:	2975.85	0.0008	2964.58	0.001151	1486.23	0.000052	1485.85	0.000063	1494.37	0.000014	1496.3	0.000122
227:	2978.82	0.001029	2979.85	0.000216	1488.52	0.000068	1487.8	0.000065	1496.42	0.00006	1498.18	0.000136
228:	2986.32	0.00024	2983.76	0.000289	1490.33	0.000458	1489.69	0.00048	1497.22	0.000113	1499.3	0.00015
229:	2988.07	0.001287	2984.08	0.001125	1493.51	0.000125	1490.87	0.000096	1498.36	0.000122	1500.03	0.000014
230:	2994.86	0.000266	2987.36	0.001319	1493.94	0.000053	1493.47	0.000063	1514.64	0.000673	1516.29	0.000291
231:	3011.19	0.000747	3004.92	0.001116	1495.43	0.000035	1494.38	0.000023	1517.21	0.000376	1519.23	0.000685
232:	3014.1	0.001087	3012.2	0.000955	1496.68	0.000025	1495.81	0.000153	1575.6	0.000459	1577.71	0.000519
233:	3019.62	0.001747	3020	0.000708	1498.43	0.000117	1499.72	0.000109	1776.26	0.031313	1777.63	0.029901
234:	3020.37	0.001153	3021.64	0.001821	1500.49	0.000152	1499.74	0.000141	1837.88	0.048246	1838.19	0.047595
235:	3022.89	0.000661	3021.99	0.001318	1514.57	0.000661	1514.62	0.000735	2949.27	0.000932	2947.78	0.000925
236:	3024.2	0.000575	3024.67	0.000556	1518.03	0.000315	1517.68	0.000346	2963.11	0.001274	2959.29	0.001267
237:	3029.69	0.000485	3028.8	0.000469	1556.89	0.000355	1557.36	0.000391	2984.22	0.00111	2980.33	0.000266
238:	3030.86	0.000495	3030.63	0.000491	1624.4	0.000066	1622.77	0.000065	2986.8	0.001176	2982.27	0.001176
239:	3036	0.000523	3035.46	0.00059	1784.94	0.031031	1786	0.029918	2990.11	0.000221	2983.78	0.000283
240:	3036.68	0.000822	3036.65	0.000711	1848.35	0.050496	1848.35	0.049338	2991.48	0.000369	2986.46	0.001182
241:	3046.35	0.001262	3046.67	0.001129	2948.35	0.00102	2946.22	0.000972	3007.13	0.000729	3006.02	0.000027
242:	3048.04	0.000357	3048.61	0.000504	2971.62	0.001067	2963.06	0.001157	3007.68	0.000672	3007.95	0.000608
243:	3060.86	0.002935	3060.48	0.003204	2985.88	0.000306	2981.32	0.000274	3008.21	0.000603	3008.05	0.000669
244:	3067.17	0.001548	3065.3	0.001481	2994.2	0.000284	2986.03	0.00028	3010.79	0.00056	3009.1	0.000673
245:	3092.65	0.000495	3090.84	0.000421	3005.16	0.003019	3005.16	0.002162	3011.78	0.001159	3011.83	0.000444
246:	3094.59	0.000438	3095.16	0.000432	3006.01	0.002398	3005.56	0.003557	3012.71	0.00077	3012.38	0.001022
247:	3104.33	0.000463	3101.88	0.000527	3007.76	0.000667	3008.2	0.000669	3013.37	0.000892	3013.03	0.00124
248:	3106.32	0.000396	3105.16	0.000356	3008.3	0.00075	3008.77	0.0002	3014.33	0.000333	3013.71	0.000471
249:	3109.66	0.000061	3108.93	0.000032	3012.59	0.00037	3009.57	0.00057	3014.78	0.000322	3013.93	0.0006
250:	3112.93	0.000047	3110.8	0.000019	3013.01	0.000742	3012.8	0.000506	3016.61	0.000124	3016.54	0.000546
251:	3114.29	0.000616	3112.87	0.000612	3014.23	0.000453	3013.62	0.000958	3016.82	0.000684	3016.74	0.000157
252:	3116.55	0.002	3115.82	0.002027	3014.59	0.00062	3014.11	0.000448	3019.69	0.000027	3019.81	0.000023
253:	3118.62	0.00028	3118.06	0.002187	3016.89	0.000463	3016.48	0.000427	3022.13	0.000637	3021.55	0.000613
254:	3120.02	0.001957	3119.13	0.000221	3017.4	0.000648	3017.01	0.000561	3022.16	0.00051	3022.35	0.000733
255:	3122.74	0.000313	3121.19	0.000161	3019.24	0.000024	3019.55	0.000012	3024.86	0.000565	3023.67	0.000523
256:	3124.82	0.000413	3123.02	0.000426	3020	0.000032	3020.6	0.000026	3025.81	0.000521	3026.4	0.00062
257:	3125.08	0.000348	3125.67	0.000331	3021.47	0.000689	3021.27	0.000664	3028.08	0.000432	3028.63	0.000357
258:	3126.69	0.00033	3127.75	0.000324	3022.86	0.000562	3024.25	0.000538	3029.71	0.000513	3029.77	0.000496
259:	3127.77	0.000204	3127.87	0.000075	3027.78	0.000461	3024.93	0.000736	3031.99	0.00064	3034.81	0.000604
260:	3132.4	0.000271	3130.46	0.000407	3027.84	0.000642	3027.46	0.000604	3035.48	0.000817	3035.52	0.000785
261:	3139.33	0.000613	3133.66	0.000495	3029.32	0.000371	3028.47	0.000388	3045.41	0.00125	3044.93	0.001127
262:	3139.94	0.000032	3136.5	0.000264	3030.35	0.000517	3030.5	0.000497	3048.45	0.00059	3046.97	0.000751
263:	3141.3	0.000199	3136.99	0.000189	3034.4	0.000575	3034.79	0.000587	3059.88	0.003124	3058.82	0.00321
264:	3153.61	0.000196	3152.6	0.000159	3036.36	0.0008	3036.21	0.000765	3061.01	0.003445	3059.78	0.002683
265:	3155.71	0.000688	3155.77	0.000675	3061.76	0.00204	3061.66	0.003657	3061.34	0.001009	3060.46	0.00178
266:	3157.47	0.000399	3158.09	0.000463	3062.81	0.002051	3061.74	0.000398	3064.3	0.001434	3063.55	0.0011

267:	3160.8	0.000451	3159.49	0.000596	3063.24	0.001408	3062.56	0.00147	3065.45	0.00121	3064.57	0.001219
268:	3162.69	0.000247	3162.19	0.00024	3066.46	0.000045	3065.32	0.000019	3065.59	0.001314	3065.22	0.001541
269:	3176.14	0.000315	3176.9	0.00042	3066.52	0.000242	3065.69	0.001178	3071.18	0.000865	3070.69	0.000773
270:	3177.77	0.000334	3178.36	0.000213	3066.56	0.002118	3066.37	0.001145	3073.21	0.000761	3072.2	0.000849
271:	3182.74	0.000465	3184.15	0.00045	3074.02	0.000751	3073.19	0.000782	3081.08	0.000781	3081.78	0.000724
272:	3189.81	0.000197	3189.74	0.000201	3075.05	0.000537	3074.34	0.000773	3082.87	0.000912	3083.31	0.000896
260:					3081.32	0.000893	3085.23	0.000732	3093.75	0.00015	3088	0.000196
261:					3084.13	0.000837	3088.27	0.000806	3102.37	0.000488	3095.84	0.000132
262:					3092.8	0.000156	3095.03	0.000146	3103.79	0.00021	3101.12	0.000484
263:					3102.33	0.000558	3095.48	0.000125	3104.06	0.000379	3102.43	0.000389
264:					3104.82	0.000376	3101.09	0.000534	3107.56	0.00003	3106.99	0.00002
265:					3109.28	0.000004	3103.63	0.000364	3110.61	0.000023	3109.04	0.000077
266:					3111.35	0.000038	3108.69	0.000016	3113.1	0.000508	3113.09	0.00062
267:					3112.65	0.00056	3109.62	0.000061	3114.05	0.001981	3113.28	0.00174
268:					3115.31	0.000629	3113.08	0.000529	3116.51	0.001765	3116.54	0.002092
269:					3115.45	0.000326	3115.05	0.002043	3117.58	0.000341	3118.08	0.000187
270:					3115.84	0.00194	3115.22	0.000745	3119.71	0.000491	3119.14	0.00034
271:					3116.55	0.000137	3116.45	0.000143	3121.41	0.000268	3119.4	0.000308
272:					3117.66	0.000423	3116.95	0.00199	3123.43	0.000384	3122.53	0.000165
260:					3118.33	0.001337	3118.45	0.000315	3125.7	0.00038	3123.13	0.000631
261:					3119.42	0.000886	3119.99	0.000304	3131.23	0.000563	3128.91	0.000522
262:					3123.45	0.000304	3122.87	0.000214	3132.93	0.000071	3130.95	0.000121
263:					3125.51	0.000046	3123.56	0.000195	3134.07	0.000291	3132.45	0.000352
264:					3127.07	0.00052	3125.47	0.000454	3142.79	0.000384	3137.43	0.000405
265:					3133.05	0.000604	3130.44	0.000454				
266:					3133.52	0.000247	3131.25	0.000469				
267:					3134.75	0.000021	3132.73	0.000061				
268:					3139.56	0.000408	3137.43	0.000392				
269:					3146.57	0.00077	3146.01	0.000793				
270:					3148.97	0.00027	3148.35	0.000278				

*: A maximum of two imaginary modes in the range of -5 to -75 cm^{-1} related to the rotational freedom of the methyl substituent of the *p*-tolyl group have been observed.

Table S24. Calculated vibrational frequencies of the bis reduced complexes $\mathbf{2}^{2-}$, $\mathbf{3}^{2-}$, $\mathbf{4}^{2-}$ and $\mathbf{5}^{2-}$ with and without dispersion correction.

	$\mathbf{2}^{2-}$				$\mathbf{3}^{2-}$				$\mathbf{4}^{2-}$				$\mathbf{5}^{2-}$			
	TPSSh; Disp ON*		TPSSh; Disp OFF*		TPSSh; Disp ON*		TPSSh; Disp OFF*		TPSSh; Disp ON*		TPSSh; Disp OFF*		TPSSh; Disp ON*		TPSSh; Disp OFF*	
Mode	freq	T**2	freq	T**2	freq	T**2	freq	T**2	freq	T**2	freq	T**2	freq	T**2	freq	T**2
	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)	cm^{-1}	L/(mol·cm)
9:	18.21	0.000049	20.27	0.000062	19.44	0.001625	15.34	0.000425	24.47	0.000851	26.54	0.001256	34.35	0.000425	33.76	0.001687
10:	24.08	0.001801	24.16	0.00075	23.23	0.001692	22.86	0.000133	36.04	0.001192	31.66	0.000256	35.74	0.000342	39.13	0.001991
11:	27.23	0.003197	25.59	0.001152	24.52	0.00079	26.19	0.000473	38.98	0.000637	36.74	0.000238	37.48	0.001219	39.6	0.001032
12:	31.95	0.000711	29.82	0.001227	28.07	0.002316	28.66	0.003682	43.69	0.000952	37.79	0.00147	41.89	0.000684	43.36	0.001029
13:	36.31	0.000642	31.63	0.000066	31.31	0.001838	30.46	0.001846	47.44	0.000519	41.2	0.001407	51.82	0.00002	46.31	0.000934
14:	37.93	0.002693	32.8	0.002728	38.02	0.00015	32.41	0.000683	49.81	0.000147	46.63	0.000813	53.17	0.000756	50.36	0.000104
15:	41.71	0.000336	38.25	0.002456	46.55	0.000507	38.23	0.002164	51.17	0.000536	47.58	0.001977	54.78	0.000352	54.58	0.000661
16:	47.58	0.000664	41.1	0.000414	48.53	0.000324	44.35	0.000653	57.79	0.000198	55.02	0.000226	59.69	0.000137	58.14	0.000176
17:	52.52	0.000481	47.13	0.000941	51.15	0.000054	50.24	0.000183	62.63	0.000096	61.74	0.000024	64.84	0.000165	63.91	0.000022
18:	60.63	0.001179	49.22	0.000197	55.35	0.000156	51.36	0.000519	71.21	0.001131	71.45	0.001328	72.94	0.00198	71.68	0.00197
19:	67.22	0.000291	55.9	0.001061	59.83	0.000168	59.85	0.002022	77.16	0.001207	78.57	0.001257	80.4	0.001179	78.37	0.001579
20:	69.58	0.000237	66	0.001311	60.61	0.002417	67.01	0.000717	80.75	0.001573	79.5	0.001817	84.5	0.000768	83.1	0.000632
21:	72.44	0.002091	70	0.000468	80.38	0.001161	75.79	0.001033	82.33	0.00057	83.52	0.000401	94.04	0.000673	95.23	0.000528
22:	85.41	0.000679	74.92	0.000705	84.8	0.000578	84.8	0.000165	93.8	0.000631	92.2	0.000762	97.26	0.000264	98.42	0.001479
23:	89.24	0.000122	84.89	0.000125	95.4	0.000413	90.07	0.00071	96.04	0.000361	93.51	0.000175	106.51	0.00264	106.86	0.002725
24:	93.59	0.000058	89.3	0.000571	95.76	0.000724	91.74	0.000035	104.89	0.000478	104.65	0.001654	112.02	0.000411	114.42	0.000543
25:	96.56	0.00014	92.12	0.000071	99.86	0.001084	98.91	0.00104	108.26	0.002608	107.07	0.001707	122.18	0.000321	123.14	0.000555
26:	101.92	0.001243	95.81	0.000916	106.18	0.001209	105.47	0.00163	116.14	0.000161	112.54	0.000541	128.55	0.001285	127.87	0.001456
27:	107.28	0.001038	106.22	0.001806	115.87	0.00041	115.08	0.000417	121.42	0.000596	117.35	0.000949	132.48	0.002104	131.31	0.0005
28:	111.2	0.000972	107.98	0.000625	118.54	0.000731	119.4	0.000834	125.79	0.000926	123.55	0.000505	137.13	0.001131	135.31	0.001649
29:	115.85	0.000229	109.08	0.00073	131.02	0.000603	129.08	0.000555	129.69	0.002345	126.75	0.001213	141	0.000602	137.58	0.000973
30:	123.74	0.001593	113.88	0.000089	139.14	0.001592	130.62	0.000999	138.55	0.000539	131.47	0.001238	148.92	0.000288	145.87	0.000463
31:	132.04	0.001321	122.24	0.002577	141.23	0.000497	132.87	0.001274	147.44	0.000618	144.05	0.001168	157.35	0.002136	155.34	0.002085
32:	134.44	0.000823	127.96	0.000695	150.34	0.001249	147.79	0.000802	156.05	0.001514	152.19	0.001662	164.31	0.001829	160.68	0.001249
33:	150.25	0.000874	145.17	0.000962	157.28	0.00129	156.39	0.002399	161.65	0.002157	156.36	0.001275	172	0.000708	170.8	0.000147
34:	156.35	0.001342	149.09	0.001416	165.5	0.00179	161.71	0.001467	168.17	0.000242	167.38	0.000334	190.92	0.000207	186.62	0.000394
35:	163.08	0.000048	156.73	0.000631	177.28	0.0006	168.32	0.001118	176.53	0.000637	171.93	0.000528	195.38	0.00012	194.87	0.000087
36:	172.98	0.001958	166.61	0.001511	181.06	0.000445	175.31	0.000082	183.02	0.000042	182.39	0.000042	203.66	0.000147	204.1	0.000015
37:	174.6	0.000802	170.25	0.001378	189.74	0.000101	183.22	0.000328	194.02	0.000296	195.88	0.00029	205.7	0.000008	207.11	0.000071
38:	178.6	0.000294	175.59	0.000087	197.95	0.000461	195.89	0.000423	202.22	0.000114	201.09	0.000135	211.2	0.000067	209.4	0.000016
39:	185.74	0.001073	181.29	0.000485	202.31	0.000245	199.14	0.000131	205.16	0.00011	206.48	0.00006	213.88	0.000038	211.08	0.000091
40:	191.44	0.000106	187.23	0.000079	211.99	0.000043	207.19	0.000068	212.67	0.000045	210.55	0.000046	225.43	0.000311	222.88	0.000365
41:	206	0.000048	198.68	0.000201	214.21	0.00016	210.45	0.00011	216.12	0.000008	212.82	0.000008	240.54	0.000204	235.85	0.000135
42:	209.32	0.000069	206.51	0.000053	221.4	0.000644	221.05	0.001072	222.64	0.000237	221.04	0.000202	243.97	0.00002	245.45	0.000038
43:	211.65	0.000097	211.15	0.000083	244.49	0.000553	238.82	0.000019	235.03	0.000141	231.62	0.000158	249.65	0.000016	250.18	0.000018
44:	217.08	0.000645	216.13	0.001012	246.26	0.000284	243.26	0.000418	237.58	0.000003	237.25	0.000007	256.21	0.000066	251.34	0.000053
45:	239.36	0.000251	238.37	0.000022	251.51	0.000249	246.09	0.000202	246.85	0.00004	246.78	0.000109	256.66	0.000026	260.43	0.000135
46:	242.75	0.000038	239.98	0.000041	258.54	0.000138	255.88	0.000035	250.92	0.000017	254.12	0.000008	261.82	0.000185	271.77	0.000596
47:	250.55	0.000553	242.64	0.000721	264.4	0.00029	258.56	0.000124	261.34	0.000046	261.67	0.000276	273.24	0.000669	274.73	0.000581

48:	253.76	0.000351	244.15	0.000148	270.89	0.000271	270.96	0.000201	265.33	0.000182	264.12	0.000186	282.7	0.000678	285.37	0.000464
49:	257.79	0.000155	253.42	0.00006	277.29	0.000172	275.88	0.001014	269.12	0.000046	268.52	0.000133	288.73	0.000337	288.97	0.001363
50:	260.16	0.000246	256.65	0.000096	285.12	0.002334	281.98	0.000429	272.7	0.000798	270.71	0.000518	291.57	0.001644	290.82	0.000253
51:	273.49	0.000746	269.72	0.00037	292.76	0.000398	286.98	0.000822	283.51	0.000479	278.92	0.000366	296.55	0.000026	295.12	0.000962
52:	275.5	0.000401	273.66	0.001181	296.85	0.000061	293.57	0.002652	284.94	0.000487	280.47	0.000563	300.09	0.000498	299.3	0.000527
53:	282.06	0.000211	277.23	0.000171	299.32	0.000412	297.79	0.000391	287.97	0.00037	286	0.000223	304.61	0.000712	299.7	0.000016
54:	283.27	0.000024	281.63	0.000174	306.87	0.000681	303.04	0.000104	291.96	0.00021	290.08	0.000126	312.48	0.000746	312.71	0.000869
55:	292.45	0.000235	287.85	0.000174	323.39	0.000083	317.94	0.001138	298.16	0.000161	296.18	0.000213	324.61	0.000046	323.46	0.000036
56:	293.67	0.000512	298.08	0.000729	325.87	0.000526	323.77	0.000126	304.5	0.000064	303.12	0.000062	330.15	0.001093	326.19	0.001773
57:	301.46	0.000117	302.5	0.000357	327.77	0.000617	324.62	0.000568	314.31	0.000683	311.03	0.001034	333.17	0.000477	330.86	0.000116
58:	312.34	0.000832	313.73	0.000839	331.57	0.000519	331.26	0.000593	328.56	0.000238	326.96	0.00035	336.65	0.000604	336.24	0.000682
59:	322.46	0.000502	320.68	0.000698	340.71	0.000564	337.83	0.000471	329.56	0.00072	327.73	0.001838	344.36	0.000119	342.83	0.000109
60:	327.83	0.000064	326.59	0.000304	346.06	0.000061	347.95	0.000088	333.6	0.00041	329.49	0.000155	351.53	0.000623	349.59	0.000821
61:	334.94	0.000176	329.9	0.000196	353.11	0.000171	349.71	0.000085	336.34	0.001222	332.05	0.000508	371.57	0.001044	363.54	0.000184
62:	341.88	0.000409	331.96	0.000448	364.65	0.000349	359.31	0.000783	344.8	0.0001	340.76	0.000333	375.63	0.000663	371.82	0.001507
63:	346.79	0.000277	342.86	0.000205	371.95	0.000264	367.09	0.000141	349.68	0.000387	344.73	0.000241	388.79	0.001008	385.77	0.001507
64:	350.38	0.000695	344.09	0.000123	376.43	0.000145	374.74	0.000184	360.89	0.00003	358.48	0.000693	397.13	0.003618	392.6	0.0025
65:	351.83	0.000139	352.71	0.000793	400.68	0.001326	398.36	0.00262	363.54	0.000425	360.98	0.00004	397.5	0.000871	396.71	0.002116
66:	357.71	0.000184	359.69	0.000059	402.56	0.001615	399.67	0.00112	371.59	0.001253	369.96	0.001532	409.16	0.003149	407.48	0.003598
67:	364.82	0.000157	363.73	0.000153	404.78	0.000522	407.08	0.000053	389.83	0.001074	385.5	0.00229	410.13	0.000486	408.92	0.000502
68:	371.63	0.000378	370.19	0.000189	409.39	0.000051	407.84	0.000266	395.33	0.002	392.08	0.001322	427.17	0.000068	426.92	0.000038
69:	398.46	0.000396	395.47	0.001917	410.47	0.001233	409.86	0.000502	398.72	0.003198	395.91	0.003055	435.12	0.000864	434.15	0.001887
70:	401.67	0.003326	397.29	0.00263	411.05	0.000081	411.58	0.000212	408.79	0.003516	405.8	0.003888	436.67	0.00036	435.67	0.000477
71:	406.53	0.000267	405.73	0.00036	425.34	0.004591	425.36	0.004654	419.19	0.000334	418.47	0.000416	439.07	0.001	436.55	0.000267
72:	408.3	0.000484	407.31	0.000069	427.01	0.000317	427.25	0.000151	435.25	0.001377	431.05	0.002227	444.43	0.001403	442.69	0.001012
73:	412.37	0.000139	412.19	0.000079	448.14	0.001488	448.15	0.0015	435.85	0.000277	435.55	0.000237	453.95	0.003301	453.28	0.003134
74:	416.44	0.000423	417.71	0.000374	461.23	0.001446	460.85	0.001071	438.01	0.000503	438.17	0.000132	469.95	0.000557	465.99	0.000637
75:	425.93	0.004768	423.69	0.005089	473.54	0.00151	471.78	0.001968	443.95	0.001205	442.65	0.000864	477.22	0.00065	475.28	0.000781
76:	444.4	0.002257	442.03	0.001955	480.27	0.001126	476.47	0.000331	446.16	0.000657	445.57	0.000385	485.33	0.000268	484.39	0.000391
77:	449.43	0.00047	447.66	0.000434	492.34	0.001172	492.73	0.003311	454.05	0.003354	452.2	0.003598	488.22	0.000817	489.02	0.00093
78:	453.61	0.000976	454.64	0.000855	501.04	0.007126	497.95	0.006108	465.74	0.000596	463.56	0.000789	497.99	0.000212	500.15	0.0007
79:	471.32	0.001652	468.78	0.001686	503.18	0.000637	503.56	0.000492	477.1	0.000545	476.84	0.000567	503.21	0.004397	501.57	0.003942
80:	476.31	0.000451	472.24	0.000806	503.24	0.000333	505.87	0.000297	485.6	0.000616	483.44	0.000604	504.78	0.00017	508.12	0.000255
81:	491.84	0.000144	490.94	0.000942	509.11	0.000824	507.72	0.000694	489.89	0.000767	488.75	0.000997	507.45	0.00092	508.6	0.000732
82:	496.67	0.000645	498.69	0.000815	515.53	0.000613	512.56	0.002741	497.33	0.000172	499.81	0.000395	514.42	0.000141	513.84	0.000043
83:	500.18	0.000135	500.08	0.003279	516.66	0.003115	517.75	0.001788	503.91	0.003659	500.89	0.004022	522.88	0.0003	524.38	0.000304
84:	504.91	0.000361	501.86	0.005142	522.4	0.000066	523.07	0.000087	506.65	0.001483	506.53	0.000648	526.66	0.000756	529.45	0.000723
85:	506.54	0.006133	508.55	0.000211	546.9	0.000455	543.82	0.000573	511.83	0.000069	511.43	0.000082	552.79	0.000416	551.17	0.000245
86:	515.16	0.003551	513.36	0.002426	571.82	0.004372	571.87	0.004549	516.74	0.000026	514.58	0.000136	577.08	0.00233	579.15	0.002576
87:	518.04	0.001676	518.01	0.001557	585.39	0.00018	585.7	0.000252	526.85	0.000801	526.91	0.000759	585.06	0.000159	586.4	0.000182
88:	548.02	0.000585	542.17	0.00057	606.88	0.001558	603.14	0.001354	556.13	0.000449	550.74	0.000474	618.39	0.003083	618.99	0.002745
89:	567.78	0.003468	571.52	0.004298	615.4	0.00139	611.12	0.000687	577.2	0.002178	580.79	0.00226	654.43	0.000828	658.55	0.000696
90:	586.45	0.000236	586.61	0.00047	623.57	0.005655	618.45	0.004649	587.14	0.000264	587.45	0.000217	707.76	0.002305	698.66	0.002052
91:	592.04	0.000102	593.4	0.000038	641.06	0.000008	642.1	0.000002	592.08	0.000014	592.11	0.000024	713.77	0.003699	704.96	0.004446

92:	609.86	0.000405	603.94	0.000565	643.25	0.000185	642.27	0.000075	619.37	0.003092	620.63	0.002826	727.22	0.001798	717.67	0.001723
93:	615.28	0.0006	611.07	0.000768	649.53	0.002482	649.31	0.002477	656.79	0.000754	659.14	0.000807	728.05	0.001392	722.13	0.001498
94:	623.12	0.005655	618.71	0.005844	707.15	0.00348	700.64	0.003711	680.75	0.001044	681.87	0.001148	736.71	0.000144	728.96	0.000253
95:	641.46	0.000016	641.99	0.000072	713.99	0.001007	713.31	0.000556	706.71	0.000156	699.81	0.002541	757.64	0.000343	751.47	0.000124
96:	642.76	0.000017	642.48	0.000016	717.37	0.001671	718.34	0.002497	707.14	0.002423	706.26	0.004211	761.63	0.000389	757.35	0.000552
97:	649.73	0.001984	649.48	0.002492	726.98	0.000854	723.83	0.000852	713.14	0.003558	708	0.000014	777.28	0.000633	772.87	0.000651
98:	682.53	0.000902	681.85	0.001236	730.2	0.000572	727.84	0.000537	727.67	0.002221	718.12	0.002125	782.99	0.000458	785.3	0.000368
99:	708.4	0.00272	699.52	0.003947	744.26	0.000017	742.85	0.000058	728.59	0.001093	722.69	0.001263	787.95	0.000036	787.9	0.000028
100:	709.85	0.000508	710.69	0.000049	754.69	0.000634	754.38	0.000698	738.06	0.000116	729.79	0.000212	789.52	0.000016	788.65	0.00001
101:	718.4	0.00034	712.43	0.001477	775.03	0.000959	772.09	0.000876	758.68	0.000228	750.2	0.000129	806.79	0.000828	808.93	0.000813
102:	724.15	0.002325	718.71	0.001514	785.57	0.00045	785.44	0.000417	759.61	0.000555	756.55	0.00059	820.52	0.000393	818.81	0.000498
103:	727.1	0.000212	722.47	0.00118	793.86	0.000086	796.85	0.000118	765.92	0.000545	764.71	0.000562	820.76	0.00036	822.64	0.000411
104:	731.8	0.001665	728.57	0.000406	801.51	0.00023	802.08	0.000233	777.47	0.000678	773.85	0.000661	825.37	0.000371	824.59	0.00079
105:	749.38	0.000103	741.53	0.000096	807.82	0.000482	806.01	0.000527	789.25	0.00002	785.96	0.000022	827.2	0.000525	826.07	0.000152
106:	758.57	0.000848	752.91	0.000799	812.25	0.003056	807.79	0.001258	791.12	0.000008	791.97	0.000006	833.24	0.000307	830.21	0.000309
107:	763.86	0.000475	762.43	0.000518	815.49	0.001477	812.89	0.003371	806.07	0.001124	806.24	0.000981	852.57	0.00054	853.38	0.000748
108:	773.2	0.000908	770.1	0.000887	820.05	0.000159	817.57	0.000442	819.72	0.000772	817.41	0.00052	853.64	0.001432	854.05	0.001186
109:	800.45	0.000234	799.37	0.000051	820.6	0.000485	821.92	0.000145	825.63	0.000243	822.35	0.000441	856.67	0.000996	857.3	0.001388
110:	802.7	0.000091	802.4	0.000079	829.98	0.000044	828.13	0.000238	827.33	0.000588	824.29	0.000666	864.77	0.000171	863.78	0.000185
111:	807.76	0.000213	806.42	0.000297	832.34	0.000328	832.87	0.000018	833.28	0.000372	830.49	0.00033	876.69	0.000697	877.63	0.000345
112:	809.08	0.001065	809.37	0.001824	854.87	0.000905	855.58	0.000607	850.68	0.001452	851.27	0.001405	887.39	0.002952	885.76	0.002833
113:	814.77	0.002708	814.26	0.002776	860.28	0.000419	856.57	0.000573	854.02	0.0003	853.57	0.000614	895.23	0.000928	894.28	0.001175
114:	819.83	0.000483	816.15	0.000481	865.05	0.000162	864.47	0.000153	857.52	0.001973	856.93	0.001774	897.14	0.001682	896.41	0.001502
115:	830.83	0.00027	826.57	0.000274	871.52	0.000965	873.78	0.001185	874.6	0.000257	874.75	0.000413	898.3	0.000123	897.42	0.000796
116:	834.73	0.000087	836.97	0.000024	883.71	0.006289	886.96	0.004962	880.73	0.000176	881.27	0.000179	898.85	0.001271	898.07	0.000395
117:	853.94	0.000074	855.84	0.001139	905.84	0.000043	906.9	0.000204	882.78	0.000398	883.17	0.000405	907.15	0.000036	909.89	0.000021
118:	859.4	0.000911	857.93	0.000339	908.02	0.000221	907.12	0.000034	885.91	0.003678	884.28	0.003151	910.08	0.00013	910.08	0.000185
119:	877.85	0.001409	875.75	0.001189	914.14	0.000027	912.82	0.000027	895.04	0.000646	893.01	0.000611	910.76	0.000109	912.01	0.000026
120:	884.29	0.000156	884.24	0.000133	925.77	0.000024	924.28	0.000013	896.16	0.001933	894.5	0.002171	921.76	0.000498	921.57	0.00053
121:	888.49	0.000163	885.98	0.000405	929.37	0.00002	927.89	0.000021	899.81	0.000643	898.35	0.00093	923.98	0.000519	923.24	0.000529
122:	892.35	0.005039	888.94	0.005496	946.68	0.000006	943.53	0.00001	900.95	0.000193	901.07	0.000012	926.08	0.000006	925.8	0.000063
123:	906.43	0.000138	905.67	0.000286	948.53	0.000006	947.89	0.000002	910.66	0.000005	908.15	0.000201	926.87	0.00005	929.04	0.000008
124:	907.72	0.000194	911.59	0.000019	949.43	0.0004	950.44	0.000214	913.14	0.000183	911.54	0.000016	943.84	0.000001	945.68	0.000012
125:	923.7	0.000056	921.7	0.000025	949.94	0.000365	952.13	0.000568	921.12	0.000383	919.66	0.000566	947.77	0.000009	946.89	0.000004
126:	923.95	0.000004	924.75	0.000016	963.97	0.000013	952.22	0.000355	924.05	0.00059	922.91	0.000586	950.27	0.000275	949.88	0.000258
127:	935.44	0.000422	934.57	0.000424	965.31	0.000103	970.57	0.000097	926.78	0.000009	927.26	0.000046	978.14	0.000959	977.34	0.000934
128:	941.97	0.000024	938.92	0.000018	976.95	0.000968	976.06	0.000849	927.76	0.000041	928.01	0.000007	1012.47	0.000277	1009.76	0.000495
129:	945.17	0.000012	944.47	0.000004	992.63	0.000804	990.68	0.0004	934.66	0.000626	934.64	0.000603	1013.52	0.000535	1011.52	0.00049
130:	954.21	0.000416	955.8	0.000505	993.26	0.000081	993.11	0.000058	946.31	0.000001	946.02	0.000002	1016.95	0.000698	1013.62	0.000488
131:	954.62	0.000386	955.93	0.000353	1014.44	0.000022	1009.01	0.000043	951.12	0.000014	946.97	0.000015	1020.09	0.00014	1018.41	0.000397
132:	971.38	0.000015	973.86	0.000029	1021.03	0.00042	1016.99	0.000982	989.19	0.004923	987.23	0.005169	1026.54	0.000362	1026.72	0.000298
133:	984.08	0.003396	984.85	0.004997	1023.65	0.000052	1022.06	0.000202	1001.69	0.000156	1000.32	0.000144	1027.96	0.000172	1027.27	0.000438
134:	988.65	0.000073	989.57	0.000197	1024.02	0.000357	1023.57	0.000539	1013.15	0.000404	1010.8	0.000384	1032.25	0.000131	1031.97	0.00013
135:	990.58	0.000102	990.11	0.000087	1027.15	0.000056	1024.65	0.000127	1014.83	0.000566	1012.93	0.000549	1032.69	0.000545	1032.78	0.000424

136:	998.78	0.000151	999.6	0.000164	1029.63	0.000238	1026.3	0.00007	1020.78	0.000222	1015.31	0.000274	1038.81	0.000133	1037.23	0.000053
137:	1002.29	0.000063	1008.44	0.000054	1030	0.000037	1027.13	0.00023	1021.53	0.000129	1018.31	0.00054	1039.86	0.000332	1037.94	0.000413
138:	1015.1	0.000845	1015.97	0.001014	1031.99	0.001255	1028.23	0.000833	1022.62	0.000772	1020.94	0.000128	1041.42	0.000412	1039.89	0.000413
139:	1019.16	0.000128	1021.03	0.000117	1032.4	0.000651	1032.52	0.000335	1028.25	0.000103	1028.08	0.000259	1051.1	0.000015	1050.77	0.000042
140:	1020.61	0.000096	1021.15	0.000104	1041.06	0.001832	1038.04	0.000856	1031.42	0.000358	1028.71	0.000561	1051.85	0.000097	1051.23	0.000098
141:	1022.75	0.000226	1022.23	0.000372	1042.3	0.000707	1039.76	0.001287	1034.76	0.000106	1032.54	0.000116	1078.64	0.000285	1078.24	0.000071
142:	1022.86	0.000072	1023.05	0.000034	1045.06	0.000468	1043.15	0.001546	1039.29	0.000144	1036.81	0.000246	1079.26	0.000042	1078.84	0.000209
143:	1024.46	0.000052	1024.66	0.000067	1079.31	0.000236	1078.36	0.000313	1039.93	0.00048	1038.95	0.000551	1080.04	0.000227	1081.27	0.000013
144:	1026.39	0.000587	1025.14	0.000218	1081.19	0.000363	1081.62	0.000807	1042.13	0.00034	1040.11	0.00027	1082.19	0.000256	1085.28	0.000452
145:	1032.07	0.000361	1026.46	0.000869	1092.09	0.001461	1084.17	0.004461	1045.8	0	1045.53	0.000001	1098.56	0.00007	1098.09	0.000071
146:	1041.85	0.000908	1036.44	0.000709	1094.15	0.001805	1090.24	0.000277	1049.6	0.000028	1051.37	0.00003	1100.04	0.0001	1099.46	0.000104
147:	1043.57	0.001363	1041.41	0.00143	1115.52	0.000514	1113.49	0.000501	1053.13	0.000092	1053.01	0.000109	1112.89	0.00063	1113.6	0.000657
148:	1044.08	0.001114	1045.12	0.001344	1126.92	0.000137	1127.51	0.000101	1076.05	0.000152	1079.08	0.000122	1120.31	0.000673	1116.44	0.00057
149:	1046.82	0.000024	1046.86	0.000002	1129.56	0.000083	1129.76	0.000027	1080.38	0.000135	1080.06	0.000187	1124.08	0.00106	1121.08	0.001052
150:	1094.15	0.000175	1086.64	0.002747	1133.62	0.000116	1133.11	0.00013	1098.4	0.000092	1099.12	0.000082	1131.01	0.000054	1129.63	0.00009
151:	1097.24	0.000827	1090.38	0.000032	1134.67	0.000104	1133.63	0.000114	1099.66	0.000101	1099.57	0.000118	1134.37	0.000059	1141.86	0.000057
152:	1106.85	0.004484	1105.82	0.005362	1147.1	0.000094	1142.7	0.000066	1106.22	0.005807	1108.36	0.006115	1152.72	0.000129	1147.61	0.000129
153:	1123.1	0.000077	1120.45	0.000094	1170.98	0.000057	1169.91	0.000027	1120.24	0.000539	1117.59	0.000478	1168.65	0.000024	1170.63	0.000017
154:	1130.13	0.000175	1127.61	0.000204	1193.17	0.000705	1195.83	0.000205	1123.86	0.000994	1122.23	0.000931	1184.15	0.000283	1184.24	0.000227
155:	1139.95	0.000032	1134.32	0.000034	1199.69	0.000539	1199.22	0.001816	1134.99	0.000048	1131	0.000085	1184.6	0.000208	1186.97	0.000363
156:	1147.83	0.000069	1142.42	0.000061	1203.49	0.005085	1200.65	0.004384	1153.8	0.000128	1148.09	0.000124	1203.11	0.004355	1200.96	0.004374
157:	1164.08	0.00004	1163.15	0.000035	1206	0.004225	1203.18	0.004269	1162.67	0.000027	1162.36	0.000027	1205.62	0.004425	1202.99	0.004469
158:	1190.27	0.000267	1188.33	0.000284	1215.5	0.000732	1212.23	0.000604	1183.79	0.000249	1184.13	0.000223	1211.7	0.000034	1208.35	0.000031
159:	1196.45	0.000295	1194.11	0.000446	1228.44	0.000382	1229.14	0.000288	1186.18	0.000275	1188.43	0.000346	1215.3	0.000069	1210.74	0.000035
160:	1201.51	0.004196	1199.11	0.00527	1233.34	0.000029	1232.75	0.000131	1203.17	0.003821	1201.7	0.004236	1224.66	0.000724	1223.78	0.000677
161:	1203.32	0.004742	1201.99	0.004413	1234.18	0.000058	1234.29	0.000693	1205.84	0.005207	1204.1	0.005035	1229.37	0.000038	1230.99	0.000225
162:	1208.13	0.000673	1205.21	0.001078	1235.35	0.000702	1235.77	0.000064	1210.98	0.000011	1210.36	0.00004	1234.83	0.000894	1234.73	0.000798
163:	1226.32	0.000373	1225.83	0.000456	1239.98	0.000819	1237.99	0.00077	1212.63	0.000082	1213.99	0.000071	1239.33	0.000609	1237.72	0.000713
164:	1232.71	0.000126	1231.98	0.000189	1243.82	0.000413	1244.6	0.000792	1221.8	0.000684	1220.91	0.00082	1244.73	0.000721	1248.26	0.000079
165:	1234.85	0.000493	1232.87	0.00056	1246.14	0.000143	1244.68	0.00012	1230.65	0.000215	1230.32	0.000207	1248.86	0.000037	1248.56	0.000628
166:	1236.66	0.000101	1235.64	0.000095	1253.87	0.000586	1251.52	0.000406	1236.31	0.000939	1235.04	0.000903	1254.16	0.000417	1253.22	0.000453
167:	1238.19	0.00066	1236.82	0.00069	1265.66	0.000011	1265.56	0.000007	1238.65	0.000574	1237.61	0.000646	1263.74	0.000011	1269.4	0.000008
168:	1240.96	0.001098	1239.42	0.001082	1284.05	0.001506	1282.04	0.001072	1241.72	0.001921	1241.66	0.001999	1272.7	0.000037	1270.95	0.000045
169:	1244.41	0.000235	1241.7	0.000208	1286.29	0.000094	1289.52	0.000268	1245.49	0.000433	1245.21	0.000079	1274.15	0.000037	1273.09	0.000037
170:	1245.23	0.000869	1242.49	0.001204	1297.07	0.000092	1296.19	0.00017	1247.25	0.000191	1246.49	0.000472	1282.27	0.000087	1280.4	0.000108
171:	1251.44	0.000322	1248.88	0.000397	1300.19	0.000157	1299.9	0.000172	1253.29	0.000232	1250.42	0.000254	1283.48	0.000043	1282.51	0.000109
172:	1281.6	0.000894	1279.63	0.001195	1308.66	0.000136	1308.74	0.000333	1269.24	0.000022	1274.78	0.000071	1285.02	0.000104	1283.36	0.000028
173:	1290.82	0.000258	1288.72	0.000163	1311.58	0.000425	1314.37	0.000367	1275.64	0.000062	1275.82	0.000021	1286.04	0.000109	1285.39	0.000055
174:	1294.68	0.000508	1293.53	0.00028	1320.21	0.000157	1317.07	0.000108	1281.71	0.000147	1281.21	0.000177	1288.88	0.001149	1291.59	0.00096
175:	1303.55	0.000202	1296.81	0.000359	1321.21	0.000329	1319.48	0.000279	1282.4	0.000008	1281.6	0.000046	1291.31	0.001031	1293.28	0.001197
176:	1308.92	0.000189	1306.02	0.000195	1324.62	0.000459	1323.47	0.000415	1283.98	0.000028	1283.92	0.000023	1295.94	0.000245	1298.04	0.000111
177:	1313.41	0.000192	1311.57	0.000462	1343.35	0.000866	1341.75	0.00121	1285.53	0.000196	1285.6	0.00035	1308.48	0.000028	1306.74	0.000033
178:	1318.61	0.000539	1313.33	0.00007	1346.06	0.000117	1346.72	0.000093	1290.09	0.001397	1291.84	0.001084	1310.69	0.000122	1308.68	0.000249
179:	1321.7	0.000082	1316.85	0.000172	1356.27	0.000152	1353.99	0.000385	1291.51	0.000928	1294.4	0.00127	1314.79	0.000241	1311.84	0.000293

180:	1353.15	0.000309	1351.37	0.001105	1357.16	0.000442	1355.96	0.000195	1293.94	0.000447	1296.53	0.00016	1319.33	0.000347	1315.7	0.000333
181:	1354.3	0.000753	1352.23	0.003949	1362.32	0.000077	1365.21	0.000222	1307.16	0.000009	1304.99	0.000035	1322.05	0.000191	1323.5	0.000081
182:	1355.31	0.000692	1353.76	0.000251	1374.56	0.000701	1375.14	0.000641	1309.18	0.000144	1310.83	0.000279	1322.94	0.000641	1324.12	0.000654
183:	1357.63	0.001079	1353.9	0.000125	1383.17	0.000365	1381.44	0.000262	1315.68	0.000195	1313.05	0.000336	1340.54	0.00078	1343.07	0.000067
184:	1369.7	0.000628	1373.2	0.000653	1383.54	0.000183	1384.05	0.000228	1315.86	0.000335	1315.53	0.000134	1342.92	0.000049	1344.67	0.001005
185:	1373.87	0.00045	1380.25	0.000254	1386.92	0.000464	1385.76	0.000456	1325.18	0.000306	1321.38	0.000211	1345	0.000009	1345.14	0.000012
186:	1378.8	0.000284	1380.63	0.000029	1390.1	0.001692	1386.03	0.002069	1342.91	0.000115	1343.94	0.000041	1346.1	0.000199	1351.33	0.000148
187:	1379.27	0.000055	1382.15	0.000317	1390.21	0.000024	1390.16	0.000919	1345.5	0.000003	1345.9	0.000002	1354.23	0.000135	1354.16	0.000024
188:	1383.31	0.000635	1383.75	0.00036	1405.84	0.001222	1404.91	0.001091	1350.14	0.000797	1349.27	0.000806	1356.3	0.000024	1355.05	0.000062
189:	1385.5	0.000282	1385.28	0.001883	1410.8	0.00083	1409.87	0.000828	1351.07	0.003576	1351.41	0.004127	1361.94	0.000176	1368.3	0.000015
190:	1387.53	0.000779	1387	0.001514	1419.94	0.000155	1419.27	0.000144	1351.59	0.000673	1355.31	0.000033	1369.16	0.000033	1370.25	0.000048
191:	1389.27	0.00072	1390.25	0.00058	1424.35	0.000074	1423.78	0.00008	1358.57	0.00001	1357.75	0.000009	1371.56	0.000185	1371.15	0.000295
192:	1399.59	0.000879	1403.77	0.001183	1428.69	0.000061	1432.63	0.000127	1369.3	0.000007	1368.83	0.000029	1373.07	0.00026	1372.7	0.000174
193:	1406.8	0.001097	1407.57	0.00085	1445.53	0.000058	1450.57	0.000057	1369.44	0.000064	1370.38	0.000091	1373.84	0.000186	1374.25	0.000155
194:	1419.79	0.000141	1418.26	0.000145	1449.81	0.000088	1452.34	0.00015	1372.66	0.000341	1372.72	0.000227	1375.8	0.000072	1375.25	0.000109
195:	1425.44	0.000113	1422.74	0.00008	1451.02	0.000383	1455.51	0.00027	1374.95	0.00017	1374.71	0.000146	1378.42	0.00044	1375.97	0.000106
196:	1431.03	0.000092	1431.65	0.000124	1460.42	0.000078	1462.26	0.000059	1375.87	0.000063	1377.13	0.000166	1378.93	0.000584	1378.37	0.000634
197:	1445.64	0.00015	1452.14	0.00025	1462.81	0.000004	1463.53	0.000024	1379.01	0.00017	1377.73	0.000697	1382.24	0.000073	1382.95	0.000282
198:	1450.36	0.000298	1453.2	0.000102	1463.18	0.000046	1464.28	0.000024	1379.39	0.00036	1378.05	0.000058	1383.55	0.000356	1385.47	0.000257
199:	1458.51	0.000127	1460.03	0.000002	1465.16	0.000004	1464.77	0.000007	1381.39	0.000625	1379.46	0.000073	1384.51	0.000294	1385.93	0.000496
200:	1460.76	0.000027	1464.51	0.000023	1469.84	0.00018	1467.65	0.000282	1381.62	0.000035	1383.51	0.000367	1407.03	0.001105	1409.28	0.001307
201:	1468.57	0.000015	1465.55	0.00001	1471.48	0.000438	1472.09	0.00014	1384.29	0.000315	1384.87	0.000294	1407.71	0.001044	1410.42	0.000797
202:	1468.95	0.000185	1469.1	0.000196	1473.39	0.000131	1472.76	0.000026	1387.62	0.000337	1385.23	0.001853	1433.23	0.000019	1435.63	0.00001
203:	1469.57	0.00046	1471.82	0.000117	1474.23	0.000029	1476.15	0.000049	1387.84	0.001799	1386.43	0.000309	1450.35	0.000149	1454.48	0.000031
204:	1470.46	0.000165	1472	0.000541	1475.51	0.000025	1476.58	0.000286	1407.06	0.000858	1409.56	0.000995	1452.42	0.000139	1454.81	0.000139
205:	1470.83	0.000611	1473.09	0.000056	1479.41	0.00023	1479.1	0.00023	1411.03	0.001449	1410.01	0.001176	1454.05	0.000025	1456.84	0.000127
206:	1471.58	0.000504	1473.37	0.000434	1481.34	0.000156	1480.53	0.000268	1436.85	0.000015	1438.04	0.000008	1458.13	0.000044	1460.54	0.000038
207:	1474.15	0.000387	1474.42	0.000511	1481.58	0.00001	1481.94	0.000037	1443.54	0.000042	1450.23	0.000014	1459.2	0.000037	1461.71	0.000054
208:	1475.61	0.000008	1475.78	0.000193	1482.91	0.000004	1483.21	0.000017	1454.31	0.000191	1455.26	0.000173	1461.44	0.000065	1462.63	0.000095
209:	1476.9	0.000031	1477.24	0.000036	1483.39	0.000062	1483.82	0.000079	1459.21	0.000041	1459.12	0.000025	1461.57	0.00003	1465.32	0.000032
210:	1479.8	0.000247	1479.92	0.000234	1488.97	0.000102	1488.06	0.000144	1460.17	0.000002	1460.03	0.000003	1464.04	0.000013	1465.66	0.000039
211:	1481.17	0.000023	1480.8	0.000214	1490.01	0.00004	1488.19	0.000017	1462.55	0.000144	1463.91	0.000042	1464.57	0.000009	1466.04	0.00006
212:	1482.2	0.000089	1481.5	0.000039	1491.76	0.000148	1490.91	0.000123	1464.11	0.000076	1464.43	0.00012	1465.01	0.000049	1466.36	0.000023
213:	1484.19	0.00007	1482.59	0.000037	1494.24	0.000057	1492.97	0.000071	1465.08	0.000009	1466.94	0.000053	1465.43	0.000096	1467.56	0.000007
214:	1484.62	0.000072	1487.49	0.000144	1511.43	0.000721	1511.4	0.000694	1466.47	0.000056	1467.44	0.000009	1469.19	0.000057	1470.3	0.000063
215:	1486.81	0.001204	1487.77	0.000126	1515.16	0.00027	1513.67	0.000312	1467.17	0.000092	1468.35	0.000012	1470.66	0.000052	1472.24	0.000138
216:	1490.96	0.000058	1487.8	0.001244	1522.96	0.000662	1520.19	0.001181	1467.58	0.000008	1468.86	0.000076	1471.55	0.000092	1474.35	0.000156
217:	1491.99	0.000101	1491.72	0.000147	1523.91	0.00174	1521.39	0.002308	1468.31	0.000368	1470.68	0.0007	1471.99	0.00011	1475.68	0.000104
218:	1495.23	0.00012	1493.38	0.000053	1586.89	0.001817	1582.54	0.000321	1472.69	0.000516	1472.21	0.000145	1474.54	0.000142	1475.95	0.000049
219:	1509.08	0.000563	1508.79	0.00073	1601.59	0.000039	1594.36	0.000418	1473.46	0.000122	1472.91	0.000396	1477.05	0.000033	1476.96	0.000058
220:	1514.83	0.000297	1512.28	0.000329	1606.88	0.001337	1608.4	0.001777	1473.83	0.000004	1474.59	0.000184	1479.34	0.000228	1479.6	0.000156
221:	1520.41	0.001357	1519.67	0.00122	1633.71	0.004762	1636	0.00887	1474.35	0.000233	1474.8	0.000111	1481.75	0.000005	1483.68	0.00003
222:	1524.82	0.001223	1521.47	0.001955	1644.93	0.000186	1641.07	0.000795	1474.96	0.000459	1475.01	0.000496	1483	0.000048	1483.96	0.00003
223:	1561.31	0.000957	1555.26	0.002188	1698.19	0.037248	1701.11	0.03449	1476.04	0.00023	1475.96	0.000005	1485.45	0.000027	1484.42	0.000079

224:	1596.16	0.000559	1589.86	0.000143	1758.25	0.059233	1764.63	0.057033	1476.91	0.000181	1477.81	0.000107	1487.94	0.000012	1491.3	0.000073
225:	1596.23	0.000159	1596.77	0.000153	2935.97	0.001474	2927.81	0.001668	1479.02	0.000045	1478.8	0.000039	1489.1	0.000074	1491.82	0.000044
226:	1609.75	0.000276	1609.34	0.000257	2951.55	0.001593	2955.61	0.001631	1483.12	0.000022	1483.47	0.000021	1489.83	0.000083	1491.89	0.000173
227:	1640.29	0.00221	1638.93	0.005533	2955.42	0.001545	2956.08	0.001591	1486.2	0.00004	1485.26	0.000032	1490.95	0.00013	1492.17	0.000057
228:	1642.72	0.000656	1642.35	0.000427	2963.17	0.002205	2964.21	0.002109	1488.3	0.001063	1487.74	0.001285	1492.41	0.00003	1493.42	0.000065
229:	1703.33	0.034233	1706.13	0.035702	2981.71	0.000292	2967.16	0.000216	1489.07	0.000087	1489.39	0.000095	1492.59	0.000197	1495.62	0.000133
230:	1765.24	0.057727	1768.91	0.057384	2988.54	0.000208	2967.97	0.000298	1490.12	0.000104	1491.61	0.000094	1513.36	0.000789	1511.73	0.000809
231:	2922.83	0.001851	2930.38	0.00173	2995.13	0.00055	2995.59	0.000507	1492.52	0.000126	1493.37	0.000062	1517.46	0.00021	1518.13	0.000212
232:	2966.8	0.000922	2958.15	0.001204	3002.62	0.002828	3003.96	0.002194	1492.82	0.000081	1493.57	0.000162	1605.89	0.00236	1608.76	0.002172
233:	2970.77	0.000382	2968.08	0.000239	3004.23	0.003066	3010.08	0.005858	1493.15	0.000175	1494.08	0.000062	1683.01	0.038102	1683.36	0.036889
234:	2989.67	0.003194	2969.98	0.000309	3015.75	0.002402	3013.65	0.00278	1495	0.000041	1495.64	0.000119	1748.96	0.052878	1751	0.05338
235:	2991.89	0.003824	2992.95	0.002082	3017.81	0.000975	3018.62	0.000933	1511.32	0.000724	1512.24	0.000784	2932.54	0.001576	2926.22	0.001733
236:	2995.76	0.000401	2995.1	0.008173	3020.09	0.000211	3020.6	0.000695	1519.08	0.000195	1517.53	0.000241	2947.6	0.001761	2945.59	0.001565
237:	3014.59	0.004508	3014.5	0.004311	3020.38	0.003236	3022.52	0.002379	1553.55	0.002189	1553.06	0.002326	2958.16	0.003088	2958.54	0.003236
238:	3015.13	0.001432	3016.28	0.002214	3025.02	0.000493	3025.15	0.000458	1609.21	0.000348	1607.21	0.000342	2960.07	0.000952	2959.54	0.000822
239:	3019.66	0.000907	3020.41	0.000911	3026.56	0.000487	3026.39	0.000448	1688.69	0.038109	1689.66	0.037911	2970.37	0.000412	2961.85	0.000377
240:	3020.89	0.000759	3022.56	0.000742	3027.43	0.000742	3026.99	0.001129	1754.76	0.055299	1755.76	0.054518	2978.76	0.000328	2966.56	0.000451
241:	3026.67	0.000454	3027.13	0.000464	3031.87	0.001313	3032.02	0.001304	2934	0.001485	2930.27	0.001488	2993.38	0.000588	2991.05	0.000018
242:	3029.16	0.00052	3028.96	0.000499	3033.12	0.001587	3032.96	0.001558	2947.06	0.001836	2943.68	0.00183	2998.61	0.000675	2993.57	0.000535
243:	3033.61	0.001257	3034.31	0.00127	3041.66	0.003966	3041.49	0.004644	2970.41	0.000391	2966.2	0.000271	2999.54	0.000603	2999.06	0.000687
244:	3035.78	0.001426	3035.52	0.001505	3051.41	0.002279	3051.31	0.002072	2977.36	0.000287	2967.5	0.000378	3000.15	0.00015	2999.71	0.000579
245:	3043.34	0.001841	3042.85	0.001889	3079.06	0.000816	3076.7	0.000777	2990.76	0.001134	2988.3	0.003844	3001.51	0.001837	3002.68	0.002288
246:	3049.12	0.000652	3046.17	0.000234	3084.16	0.000623	3084.08	0.000686	2992.4	0.008793	2991.83	0.006911	3004.94	0.000806	3004	0.000355
247:	3083.32	0.000795	3082.12	0.000742	3095.93	0.000657	3095.42	0.000613	2998.87	0.000731	2993.14	0.000014	3005.37	0.00183	3005.34	0.001725
248:	3085.54	0.000677	3086.76	0.000644	3098.88	0.000454	3097.99	0.000416	2999.84	0.000074	2994.59	0.00092	3007.14	0.000399	3007.23	0.000164
249:	3096.41	0.000685	3096.3	0.000673	3102.95	0.000105	3101.93	0.000077	3000.05	0.000624	3000.2	0.000703	3007.52	0.001149	3007.28	0.001527
250:	3099.56	0.000476	3099.64	0.000402	3104.39	0.000033	3102.75	0.000008	3005.68	0.001207	3002.69	0.000836	3009.67	0.000452	3009.69	0.000396
251:	3104.69	0.000654	3104.05	0.000091	3110.05	0.00282	3108.99	0.002942	3005.84	0.001404	3004.9	0.000329	3010.27	0.000303	3010.95	0.000565
252:	3104.83	0.000138	3104.44	0.000017	3111.46	0.000544	3110.71	0.003062	3008.39	0.000758	3006.02	0.00135	3012.83	0.000418	3012.86	0.000476
253:	3105.52	0.000026	3105.35	0.000889	3111.98	0.002942	3112.47	0.000438	3008.74	0.000536	3007.57	0.000807	3015.34	0.000987	3014.67	0.000707
254:	3107.38	0.000318	3107.1	0.000315	3113.89	0.000624	3115.52	0.000488	3011.04	0.000557	3011.36	0.000551	3018.5	0.000808	3017.58	0.00096
255:	3111.74	0.002702	3110.88	0.002903	3118.83	0.000135	3116.16	0.000199	3011.59	0.000089	3011.57	0.000193	3018.85	0.000915	3018.77	0.000691
256:	3112.83	0.002493	3112.31	0.002981	3120.09	0.000242	3118.43	0.000403	3013.33	0.000264	3013.25	0.000227	3020.25	0.000639	3019.98	0.000615
257:	3113.09	0.00082	3112.87	0.000477	3120.85	0.000371	3119.22	0.000187	3018.63	0.000668	3016.96	0.00062	3024.05	0.002791	3020.7	0.002234
258:	3114.96	0.000565	3118	0.000504	3122.08	0.000412	3120	0.000367	3019.03	0.001147	3017.68	0.001008	3024.23	0.000427	3023.91	0.000458
259:	3118.31	0.000187	3118.26	0.000191	3125.97	0.000056	3121.75	0.000196	3019.38	0.000681	3019.23	0.000786	3025.38	0.000528	3025.95	0.000547
260:	3119.04	0.000487	3120.64	0.000197	3127.93	0.000294	3126.86	0.000254	3020.86	0.000669	3020.14	0.000802	3025.81	0.000712	3026.72	0.001761
261:	3120.18	0.000242	3121.03	0.000418	3137.65	0.000346	3130.02	0.000623	3024.26	0.000475	3024.51	0.000446	3030.88	0.001262	3030.93	0.001451
262:	3122.96	0.000362	3122.06	0.000413	3139.64	0.000607	3130.71	0.00027	3025.83	0.000524	3025.91	0.00051	3032.03	0.001853	3032.58	0.001679
263:	3125.55	0.000122	3124.36	0.000196	3140.19	0.001443	3136.27	0.000325	3031.07	0.00123	3031.41	0.001303	3040.17	0.004886	3039.4	0.004809
264:	3128.76	0.000305	3128.17	0.000296	3142.62	0.000321	3141.79	0.000255	3032.55	0.001697	3032.53	0.00158	3047.97	0.003489	3047.01	0.003826
265:	3134.54	0.000923	3131.06	0.000609	3146.65	0.001244	3142.37	0.001644	3041.56	0.002076	3040.23	0.001985	3048.76	0.002916	3048.26	0.002933
266:	3134.77	0.000373	3132.64	0.001299	3147.79	0.000018	3145.97	0.00084	3044.35	0.000104	3043.65	0.000284	3049.1	0.002957	3049.36	0.002278
267:	3138.91	0.000414	3132.87	0.000276	3149.51	0.000833	3147.99	0.001212	3048.78	0.003603	3048.18	0.003646	3053.39	0.001651	3052.94	0.001896

268:	3139.54	0.000422	3135.24	0.000357	3156.53	0.000755	3154.62	0.000613	3050.07	0.003119	3049.04	0.003093	3054.43	0.001826	3053.76	0.001742
269:	3140.71	0.00037	3140.46	0.000326	3166.72	0.000732	3168.5	0.000451	3054.76	0.001564	3053	0.001795	3062.65	0.001034	3063.16	0.000931
270:	3145.27	0.001542	3145.01	0.001426	3168.52	0.000431	3176.89	0.000686	3055.25	0.001827	3055	0.00178	3064.71	0.00135	3064.01	0.001432
271:	3146.73	0.000766	3145.38	0.000418	3184.79	0.000259	3178.01	0.000466	3065.33	0.001248	3063.88	0.001239	3073.43	0.001084	3073.83	0.001087
272:	3147.45	0.000416	3149.15	0.000787	3195.99	0.00079	3183.68	0.000284	3066.71	0.000758	3066.37	0.000972	3083.2	0.000834	3078.79	0.000348
273:	3156.25	0.000649	3151.71	0.001055					3074.44	0.001075	3080.99	0.000252	3094.52	0.000469	3082.97	0.000867
274:	3156.66	0.000708	3157.68	0.00059					3081.6	0.0009	3081.29	0.001562	3095.65	0.000482	3093.17	0.000631
275:	3167.38	0.000419	3171.12	0.000432					3095.68	0.000598	3088.71	0.000241	3096.6	0.000461	3096.22	0.000183
276:	3178.14	0.000306	3179.25	0.000651					3097.91	0.000417	3093.39	0.000635	3097.82	0.000104	3096.4	0.000282
277:	3182.9	0.000567	3182.59	0.000452					3099.33	0.000115	3096.86	0.000391	3098.44	0.000029	3099.33	0.000019
278:	3201.6	0.000169	3187.1	0.000261					3100.09	0.000041	3098.27	0.000121	3102.45	0.00006	3100.35	0.000055
279:									3103.2	0.000028	3099.66	0.000018	3103.71	0.001864	3105.8	0.002566
280:									3103.25	0.00087	3101.28	0.000006	3109.46	0.000312	3108.13	0.003347
281:									3104.94	0.000276	3102.81	0.000846	3110.08	0.003108	3110.96	0.000117
282:									3106.67	0.002439	3104.71	0.000334	3112.61	0.001136	3112.75	0.000966
283:									3110.81	0.003039	3106.41	0.00259	3113.04	0.001055	3113.29	0.000114
284:									3112.16	0.000032	3109.21	0.003315	3116.04	0.000229	3114.31	0.000767
285:									3113.42	0.000906	3111.35	0.000191	3117.79	0.000282	3116.78	0.000418
286:									3115.25	0.00076	3113.43	0.00075	3119.26	0.00041	3119.93	0.000187
287:									3116.91	0.000065	3114.52	0.000127	3126.19	0.00053	3126.92	0.000568
288:									3118.08	0.000173	3114.97	0.000521	3128.35	0.000129	3127.22	0.000557
289:									3118.59	0.000707	3116.58	0.00063	3131.19	0.000761	3129.06	0.000692
290:									3119.04	0.000259	3120.01	0.000205	3134.13	0.00065	3129.36	0.000205
291:									3127.03	0.000544	3126.84	0.000561				
292:									3129.34	0.000135	3128.94	0.000154				
293:									3129.57	0.001347	3129.45	0.001152				
294:									3131.82	0.0006	3129.52	0.00131				
295:									3132.17	0.000439	3129.7	0.000197				
296:									3133.15	0.000629	3132.01	0.000326				

*: A maximum of two imaginary modes in the range of -5 to -75 cm^{-1} related to the rotational freedom of the methyl substituent of the *p*-tolyl group have been observed.

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