

# Israel Journal of Chemistry

Supporting Information

## **Another Torture Track for Quantum Chemistry: Reinvestigation of the Benzaldehyde Amidation by Nitrogen- Atom Transfer from Platinum(II) and Palladium(II) Metallonitrenes**

Hendrik Verplancke, Martin Diefenbach, Jonas N. Lienert, Mihkel Ugandi, Marios-Petros Kitsaras, Michael Roemelt, Stella Stopkowicz, and Max C. Holthausen\*© 2023 The Authors. Israel Journal of Chemistry published by Wiley-VCH GmbH. This is an open access article under the terms of the Creative Commons Attribution Non-Commercial NoDerivs License, which permits use and distribution in any medium, provided the original work is properly cited, the use is non-commercial and no modifications or adaptations are made.

Supporting Information:  
**Another Torture Track for Quantum Chemistry:  
Reinvestigation of the Benzaldehyde Amidation  
by Nitrogen-Atom Transfer from Platinum(II)  
and Palladium(II) Metallonitrenes**

Hendrik Verplancke,<sup>[a]</sup> Martin Diefenbach,<sup>[a,b]</sup> Jonas N. Lienert,<sup>[a]</sup>  
Mihkel Ugandi,<sup>[c]</sup> Marios-Petros Kitsaras,<sup>[d,e]</sup> Michael Roemelt,<sup>[c]</sup>  
Stella Stopkowicz,<sup>[d,e,f]</sup> and Max C. Holthausen<sup>[a]\*</sup>

[a] *H. Verplancke, M. Diefenbach, J. N. Lienert, M. C. Holthausen*  
Institut für Anorganische und Analytische Chemie, Goethe-Universität,  
Max-von-Laue-Str.7, 60438 Frankfurt am Main, Germany;  
E-mail: max.holthausen@chemie.uni-frankfurt.de

[b] *M. Diefenbach*  
Fachbereich Chemie, Theoretische Chemie, Technische Universität Darmstadt,  
Alarich-Weiss-Straße 4, 64287 Darmstadt, Germany

[c] *M. Ugandi, M. Roemelt*  
Institut für Chemie, Humboldt-Universität zu Berlin,  
Brook-Taylor-Straße 2, 12489 Berlin, Germany

[d] *M.-P. Kitsaras, S. Stopkowicz*  
Department Chemie, Johannes Gutenberg-Universität Mainz,  
Duesbergweg 10-14, 55128 Mainz, Germany

[e] *M.-P. Kitsaras, S. Stopkowicz*  
Fachrichtung Chemie, Universität des Saarlandes,  
Campus B2.2, 66123 Saarbrücken, Germany

[f] *S. Stopkowicz*  
Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry,  
University of Oslo, P.O. Box 1033, N-0315 Oslo, Norway

## FCIQMC Calculations:

The FCI/ano-pVDZ energy of imidogen (NH) was obtained with the FCI module of Molpro. For all other species the FCIDUMP files for FCIQMC calculations were generated accordingly. The number of walkers in the FCIQMC calculations was increased stepwise from  $1 \cdot 10^7$  until convergence was achieved. For CH<sub>2</sub>O pleasing accuracy was already obtained with  $5 \cdot 10^7$  walkers. For all isomers of **H<sub>3</sub>** increasing the number of walkers from  $1 \cdot 10^8$  to  $5 \cdot 10^8$  caused a significant change of more than 1 mE<sub>h</sub>. The number of walkers was further increased to  $2 \cdot 10^9$ , to obtain reliable FCI energies. For singlet **H<sub>3</sub>b** the number of walkers was increased even to  $5 \cdot 10^9$ . As these computations were performed on a public computer cluster, depending on availability different time and CPU resources have been used for each computation.

**Table S1.** FCI/ano-pVDZ energies for imidogen.

Species	Reference energy / E <sub>h</sub>	Correlation energy / E <sub>h</sub>
NH (S=1)	-54.975227	-0.142259
NH (S=0)	-54.874616	-0.177109

**Table S2.** FCIQMC/ano-pVDZ results for singlet CH<sub>2</sub>O<sup>[a]</sup>.

Number of walkers	Correlation energy / mE <sub>h</sub> <sup>[b]</sup>	Timesteps for manual blocking analysis
$1 \cdot 10^7$	$-359.620 \pm 0.125$	24740
$5 \cdot 10^7$	$-359.579 \pm 0.003$	9440

[a] Reference energy:  $-113.910978 E_h$

[b] CCSDTQ(P) correlation energy for comparison:  $-359.640 mE_h$

**Table S3.** FCIQMC/ano-pVDZ results for  $^1A''$   $H3a^{[a]}$ .  $J$  value for slater-determinant-spin-purification:  $0.02 E_h$ .

Number of walkers	Correlation energy / $mE_h$	Timesteps for manual blocking analysis
$1*10^8$	$-687.247 \pm 0.012$	42960
$5*10^8$	$-686.464 \pm 0.004$	47590
$1*10^9$	$-687.110 \pm 0.003$	118420
$2*10^9$	$-687.176 \pm 0.003$	83760
$5*10^9$	$-687.306 \pm 0.002$	53980

[a] Reference energy:  $-168.686728 E_h$

**Table S4.** FCIQMC/ano-pVDZ results for  $^1A'$   $H3a^{[a]}$ .

Number of walkers	Correlation energy / $mE_h$	Timesteps for manual blocking analysis
$1*10^7$	$-640.128 \pm 0.379$	315410
$5*10^7$	$-640.747 \pm 0.142$	665460
$1*10^8$	$-640.628 \pm 0.182$	521580
$5*10^8$	$-640.525 \pm 0.006$	87670
$1*10^9$	$-640.440 \pm 0.007$	21800
$2*10^9$	$-639.615 \pm 0.004$	47340
$5*10^9$	$-639.856 \pm 0.003$	52710

[a] Reference energy:  $-168.735542 E_h$

**Table S5.** FCIQMC/ano-pVDZ results for  $^1A'$   $H3b^{[a]}$ .

Number of walkers	Correlation energy / $mE_h^{[b]}$	Timesteps for manual blocking analysis
$1*10^7$	$-635.324 \pm 0.924$	244280
$5*10^7$	$-638.488 \pm 0.162$	340550
$1*10^8$	$-637.569 \pm 0.131$	469050
$5*10^8$	$-635.953 \pm 0.017$	71760
$1*10^9$	$-636.342 \pm 0.004$	105250
$2*10^9$	$-635.778 \pm 0.004$	31150
$5*10^9$	$-635.471 \pm 0.002$	27140

[a] Reference energy:  $-168.755977 E_h$

[b] CCSDTQ(P) correlation energy for comparison:  $-635.860 mE_h$

**Table S6.** FCIQMC/ano-pVDZ results for  $^3A''$  **H3a**<sup>[a]</sup>.

Number of walkers	Correlation energy / mE <sub>h</sub> <sup>[b]</sup>	Timesteps for manual blocking analysis
1*10 <sup>7</sup>	-510.048 ± 0.124	437120
5*10 <sup>7</sup>	-510.201 ± 0.040	318280
1*10 <sup>8</sup>	-509.667 ± 0.052	418030
5*10 <sup>8</sup>	-508.244 ± 0.041	241920
1*10 <sup>9</sup>	-507.985 ± 0.030	74470
2*10 <sup>9</sup>	-507.693 ± 0.004	28200

[a] Reference energy: -168.876032 E<sub>h</sub>

[b] CCSDTQ(P) correlation energy for comparison: -507.960 mE<sub>h</sub>

**Table S7.** FCIQMC/ano-pVDZ results for  $^3A'$  **H3b**<sup>[a]</sup>.

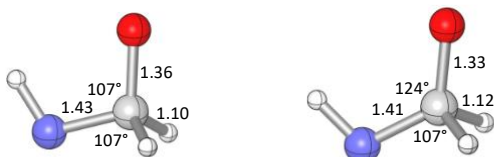
Number of walkers	Correlation energy / mE <sub>h</sub> <sup>[b]</sup>	Timesteps for manual blocking analysis
1*10 <sup>7</sup>	-504.978 ± 0.098	180570
5*10 <sup>7</sup>	-504.919 ± 0.049	290440
1*10 <sup>8</sup>	-504.279 ± 0.043	438690
5*10 <sup>8</sup>	-502.705 ± 0.048	50090
1*10 <sup>9</sup>	-502.434 ± 0.014	40500
2*10 <sup>9</sup>	-502.161 ± 0.002	30010

[a] Reference energy: -168.883392 E<sub>h</sub>

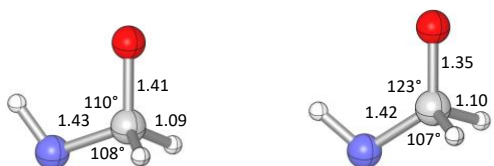
[b] CCSDTQ(P) correlation energy for comparison: -502.372 mE<sub>h</sub>

## Additional Figures and Tables:

PBE0-D/def2-TZVPP (int=superfine):



CASSCF(2,2)-MRAQCC/aug-cc-pVQZ:



**H<sub>3</sub>a (<sup>1</sup>A'')**

**H<sub>3</sub>b (<sup>1</sup>A')**

**Figure S1.** The upper row shows the DFT structures of **H<sub>3</sub>a**, optimized by employing a <sup>1</sup>A'' broken-symmetry determinant (left) and **H<sub>3</sub>b** with <sup>1</sup>A' determinant. CASSCF(2,2)-MRAQCC geometry optimizations (lower row) result in similar structures, when the active space is chosen according to the singly occupied orbitals of the broken-symmetry UKS wavefunction, confirming that the presence of two singlet electromers for **H<sub>3</sub>** is not a DFT artifact.

**Table S8.** CCSD(T) relative energies in kcal mol<sup>-1</sup> for the H system employing the cc-pVTZ, cc-pVQZ basis sets, as well as CBS extrapolation. These calculations were performed using the Molpro program.

Structure	Spin	cc-pVTZ	cc-pVQZ	CBS
<b>H1</b>	1	0.0	0.0	0.0
	0	44.5	43.5	43.1
<b>H<sup>H</sup>TS1</b>	1	13.3	12.7	12.2
<b>H2</b>	0.5	-2.1	-3.3	-3.9
<b>H<sup>H</sup>TS2</b>	1	6.3	5.7	5.1
	0	43.9	42.3	41.2
<b>H3a</b>	1	-1.6	-3.0	-4.2
	0	-201.7	-198.3	-195.1
<b>H3b</b>	1	-3.0	-4.2	-5.3
	0	-16.1	-17.0	-17.1
<b>H<sup>H</sup>TS3</b>	0	-8.9	-11.0	-12.1
<b>H4</b>	0	-105.0	-108.0	-109.9
<b>H<sup>H</sup>TS4</b>	0	-1.8	-3.3	-4.2
<b>H5</b>	0	-35.8	-37.9	-39.5

**Table S9.** SCF, CCSD and CCSD(T) total energies in  $E_h$  obtained with the ano-pVDZ basis set for singlet  $^1\mathbf{H3a}$  with the coupled cluster modules of several quantum chemistry codes. All programs produce basically identical Hartree-Fock energies. However, two branches of CCSD solutions are obtained, for the different implementations.

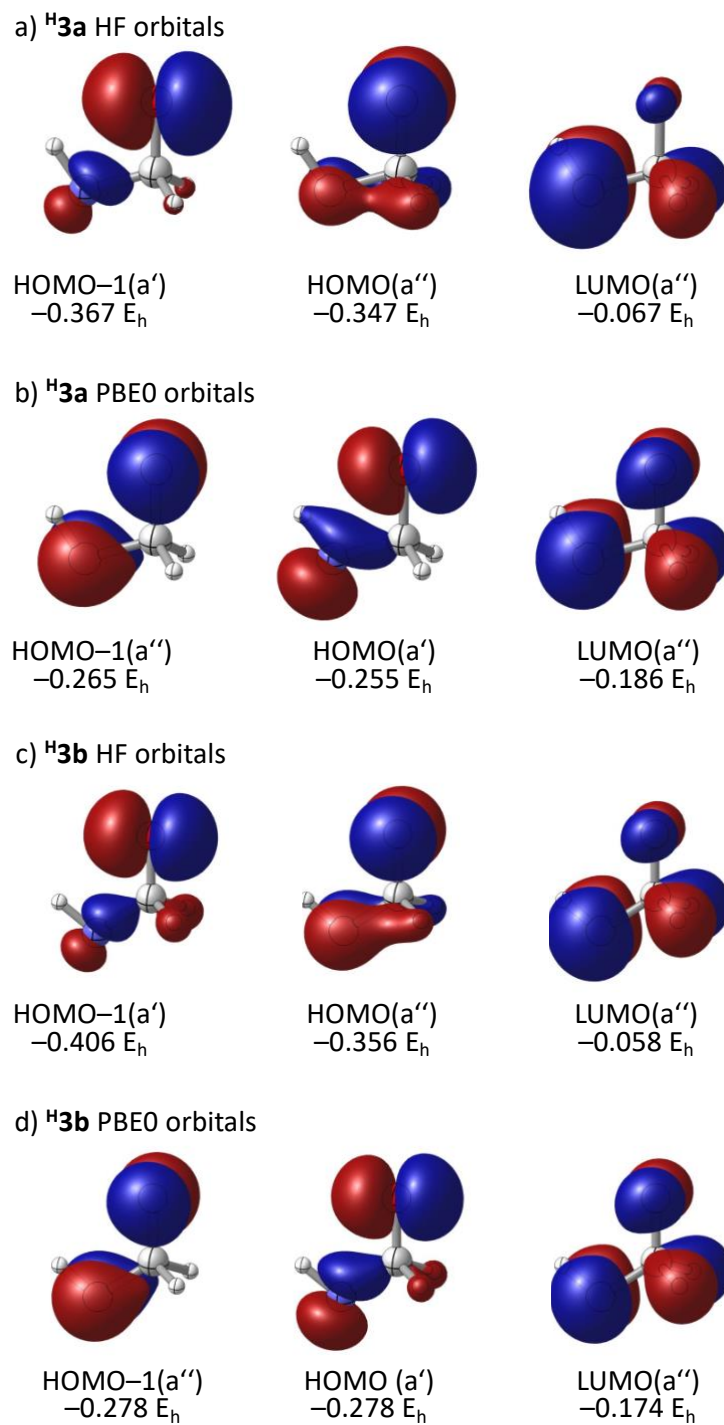
Program	Module	Reference	SCF	MP2	CCSD	CCSD(T)	$\mathcal{T}_1$	$t_{1\max}$	$t_{2\max}$
ORCA		RHF	-168.73554 <b>118</b>	-169.24913 <b>06</b>	-169.3160503	-169.7331848	0.24	1.02	0.91
GAUSSIAN		RHF	-168.73554 <b>234</b>	-169.24913 <b>14</b>	-169.3160539	-169.7332522	0.24	1.02	-0.91
MOLPRO		RHF	-168.73554 <b>240</b>	-169.24913 <b>29</b>	-169.3160537	-169.7332203	0.24	-1.02	-0.91
MRCC	CCSD	RHF	-168.73554 <b>241</b>	-169.24913 <b>14</b>	-169.3160536	-169.7332462	0.24	1.02	0.92
	CCSD	UHF	-168.73554 <b>241</b>	-169.24913 <b>14</b>	-169.2478679	-169.2649965	0.14	0.39	0.08
	MRCC	RHF	-168.73554 <b>241</b>	-169.24913 <b>14</b>	-169.2478677	-169.2649960	-	0.39	-0.08
	MRCC	UHF	-168.73554 <b>241</b>	-169.24913 <b>14</b>	-169.2478677	-169.2649960	-	0.39	-0.08
CFOUR	VCC	RHF	-168.73554 <b>236</b>	-169.24913 <b>14</b>	-169.2478677	-169.2649960	0.10	-0.39	-0.08
	ECC	RHF	-168.73554 <b>236</b>	-169.24913 <b>14</b>	-169.2478677	-169.2649960	0.10	-0.39	-0.08
	NCC	RHF	-168.73554 <b>236</b>	-169.24913 <b>14</b>	-169.2478677	-169.2649960	-	-0.39	-0.08
Qcumbre GAMESS		RHF	-168.73554 <b>236</b>	-	-169.2478677	-169.2649960	-	-	0.08
		RHF	-168.73554 <b>242</b>	-169.24913 <b>14</b>	-169.2478677	-169.2649960	0.10	-0.39	-0.08



**Table S10.** FCI Singlet–Triplet energy differences computed with the cc-pVTZ and cc-pVQZ basis sets, as well as by CBS extrapolation.<sup>[a]</sup>

	$\Delta E_{S-T} / \text{kcal mol}^{-1}$
cc-pVTZ	38.3
cc-pVQZ	37.0
CBS	36.4

[a]  $3\zeta/4\zeta$  extrapolated correlation energy added to the  $4\zeta$  HF energy



**Figure S2.** Molecular orbitals and orbital energies for the occupation pattern 10-2 obtained with the ano-pVDZ basis set. Isosurfaces at  $\pm 0.05 a_0^{-3/2}$ .

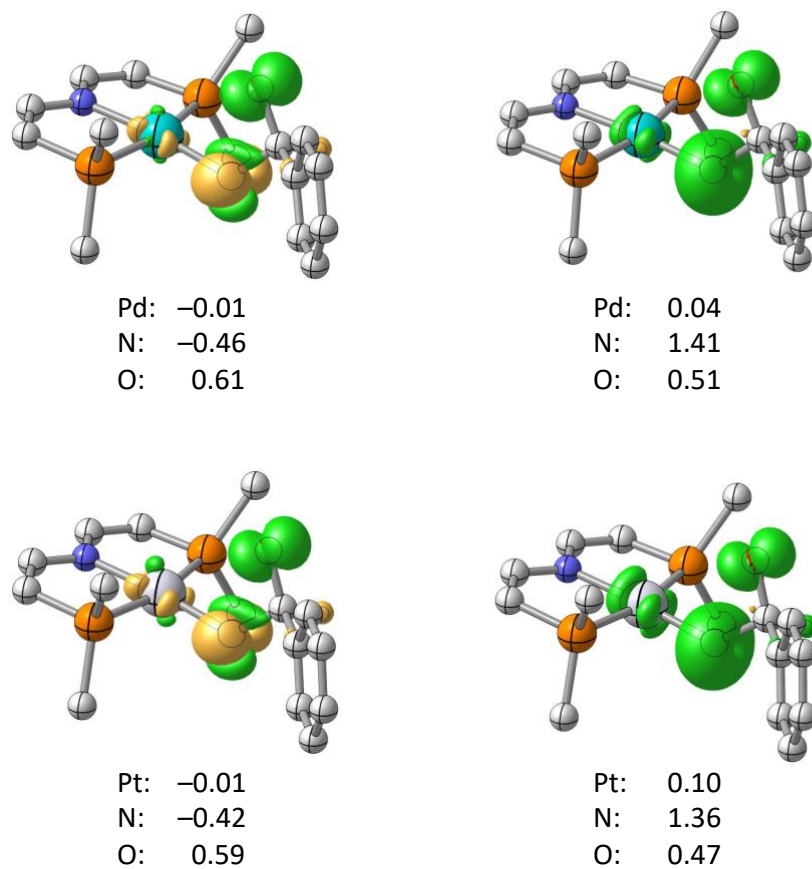
**Table S11.** Selected EOM-CCSD/ano-pVDZ singlet excitation energies for **H3a** and **H3b** in kcal mol<sup>-1</sup> employing UHF references, with either matching  $\alpha$  and  $\beta$  orbital sets or broken-symmetry. The occupation X-Y stands for x doubly occupied a' and y a'' orbitals in the closed shell UHF reference. A' denotes a broken-symmetry 10-2/10-2 occupation in the  $\alpha$  and  $\beta$  parts of the reference wave function. A'' denotes a broken-symmetry 10-2/9-3 occupation in the  $\alpha$  and  $\beta$  parts of the reference wave function.

Reference/Excitation	Irrep.	<b>H3a</b>	<b>H3b</b>
10-2 with ORCA	<sup>1</sup> A'	0.0	0.0
	<sup>1</sup> A''	-2.8	17.9
10-2 with CFOUR	<sup>1</sup> A'	0.0	0.0
	HOMO(a'')→LUMO(a'')	-71.4	85.1
	HOMO-1(a')→LUMO(a'')	-67.7	17.8
Broken-Symmetry <sup>1</sup> A' [a]	<sup>1</sup> A'	0.0	0.0
	$\alpha$ :HOMO(a')→LUMO(a'')	-0.3	-
	$\alpha$ :HOMO-1(a')→LUMO(a'')	-	13.1
Broken-Symmetry <sup>1</sup> A'' [b]	<sup>1</sup> A''	0.0	0.0
	$\alpha$ :HOMO(a')→LUMO(a'')	49.8	-
	$\beta$ :HOMO(a'')→LUMO(a') +	1.4	-12.1
	$\beta$ :HOMO-2(a'')→LUMO(a')		
PBE0: 10-2 [c]	<sup>1</sup> A'	0.0	0.0
	HOMO-1(a'')→LUMO(a'')	0.7	-
	HOMO-1(a')→LUMO(a'')	-	19.3

[a] Computations performed with the ORCA program package

[b] Computations performed with the CFOUR program package

[c] Computations performed with the ORCA program package on the basis of PBE0 orbitals.



**Figure S3.** Spin-density plot for the broken-symmetry singlet and triplet solutions of **Pd<sub>3</sub>** (top) and **Pt<sub>3</sub>** (bottom) together with Mulliken spin-populations for selected atoms. Isosurfaces at  $\pm 0.01 a_0^{-3}$ .

**Table S12.** ONIOM relative (free) energies in kcal mol<sup>-1</sup> obtained for the Pt system, as well as the relative energies for the individual ONIOM layers: PBE0-CCSD(T\*)-F12b/VTZ as high-level method and PBE0-D/def2-TZVPP as low-level method.

Structure	Spin	$\Delta E_{\text{KS-CCSD}}^{\text{model}}$	$\Delta E_{\text{KS-CCSD(T)}}^{\text{model}}$	$\Delta E_{\text{DFT}}^{\text{model}}$	$\Delta E_{\text{DFT}}^{\text{full}}$	$\Delta E_{\text{ONIOM}}$	$\Delta G_{\text{ONIOM}}$
<b>Pt1</b>	1	0.0	0.0	0.0	0.0	0.0	0.0
	0	25.5	20.9	27.5	22.8	16.1	17.1
<b>PtTS1</b>	1	18.5	13.5	8.3	5.3	10.5	20.5
<b>Pt2</b>	0.5	7.1	6.0	5.2	7.5	8.3	7.1
<b>PtTS2</b>	1	5.3	1.8	-2.0	-3.4	0.3	16.2
	0	33.0	25.4	17.7	11.9	19.6	36.1
<b>Pt3</b>	1	0.2	-3.0	-10.9	-9.9	-2.0	15.1
	0	29.2	10.0	-2.5	0.5	13.0	30.4
<b>PtTS3</b>	0	14.6	2.0	-4.7	0.0	6.6	22.8
<b>Pt4</b>	0	-97.3	-97.9	-101.0	-97.1	-94.0	-74.6
<b>PtTS4</b>	0	9.2	-1.2	-7.4	-2.8	3.3	20.3
<b>Pt5</b>	0	-24.3	-26.7	-30.0	-24.9	-21.7	-2.9

**Table S13.** ONIOM(KS-CCSD(T\*)-F12:PBE0-D) results for the Pt-system (corresponding HF-CC data taken from reference [5a] for comparison); relative free energies in kcal mol<sup>-1</sup>, relative PBE0-CCSD-F12/VTZ and PBE0-CCSD(T\*)-F12/VTZ energies for the high-level ONIOM layer and differences  $\Delta\Delta(T)$  of the (T) contributions between the KS-CC and HF-CC results.

Structure	Spin	$\Delta G_{\text{ONIOM}}$		$\Delta E_{\text{CCSD-F12}}^{\text{model}}$		$\Delta E_{\text{CCSD(T*)-F12}}^{\text{model}}$		$\Delta\Delta(T)$
		KS-CC	HF-CC	KS-CC	HF-CC	KS-CC	HF-CC	
<b>Pt1</b>	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0	17.1	15.8	25.5	24.8	20.9	19.6	0.5
<b>PtTS1</b>	1	20.5	20.9	18.5	18.3	13.5	13.9	-0.5
<b>Pt2</b>	0.5	7.1	7.2	7.1	7.3	6.0	6.1	0.1
<b>PtTS2</b>	1	16.2	16.8	5.3	4.9	1.8	2.4	-1.0
	0	36.1	35.4	33.0	31.9	25.4	24.7	-0.4
<b>Pt3</b>	1	15.1	16.2	0.2	0.4	-3.0	-1.9	-0.9
	0	30.4	2.3	29.2	25.8	10.0	-18.1	24.7
<b>PtTS3</b>	0	22.8	13.0	14.6	11.4	2.0	-7.9	6.6
<b>Pt4</b>	0	-74.6	-75.9	-97.3	-96.8	-97.9	-99.2	1.8
<b>PtTS4</b>	0	20.3	17.5	9.2	8.5	-1.2	-4.0	2.1
<b>Pt5</b>	0	-2.9	-4.2	-24.3	-23.9	-26.7	-28.1	1.7

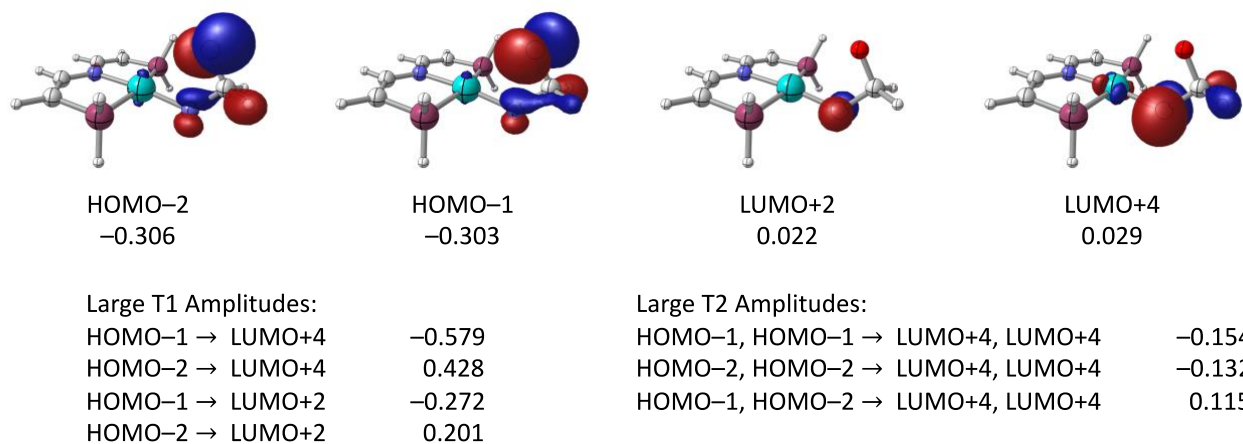
**Table S14.** ONIOM relative (free) energies in kcal mol<sup>-1</sup> obtained for the Pd system, as well as the relative energies for the individual ONIOM layers: PBE0-CCSD(T\*)-F12b/VTZ as high-level method and PBE0-D/def2-TZVPP as low-level method.

Structure	Spin	$\Delta E_{\text{KS-CCSD}}^{\text{model}}$	$\Delta E_{\text{KS-CCSD(T)}}^{\text{model}}$	$\Delta E_{\text{DFT}}^{\text{model}}$	$\Delta E_{\text{DFT}}^{\text{full}}$	$\Delta E_{\text{ONIOM}}$	$\Delta G_{\text{ONIOM}}$
<b>Pd1</b>	1	0.0	0.0	0.0	0.0	0.0	0.0
	0	29.2	24.3	31.5	26.3	19.1	20.1
<b>PdTS1</b>	1	20.4	15.1	9.5	7.2	12.8	21.9
<b>Pd2</b>	0.5	6.1	4.9	3.6	5.3	6.6	5.4
<b>PdTS2</b>	1	5.3	2.0	-2.0	-3.7	0.2	15.6
	0	36.4	28.3	16.7	13.1	24.8	40.8
<b>Pd3</b>	1	-2.6	-5.4	-13.8	-12.8	-4.4	12.3
	0	28.5	4.4	-5.6	-2.6	7.4	24.6
<b>PdTS3</b>	0	15.3	0.3	2.4	-2.8	-4.8	10.6
<b>Pd4</b>	0	-99.2	-99.4	-103.4	-101.2	-97.3	-78.3
<b>PdTS4</b>	0	6.4	-3.5	-9.6	-5.3	0.8	17.5
<b>Pd5</b>	0	-26.3	-28.9	-33.1	-28.6	-24.4	-5.9

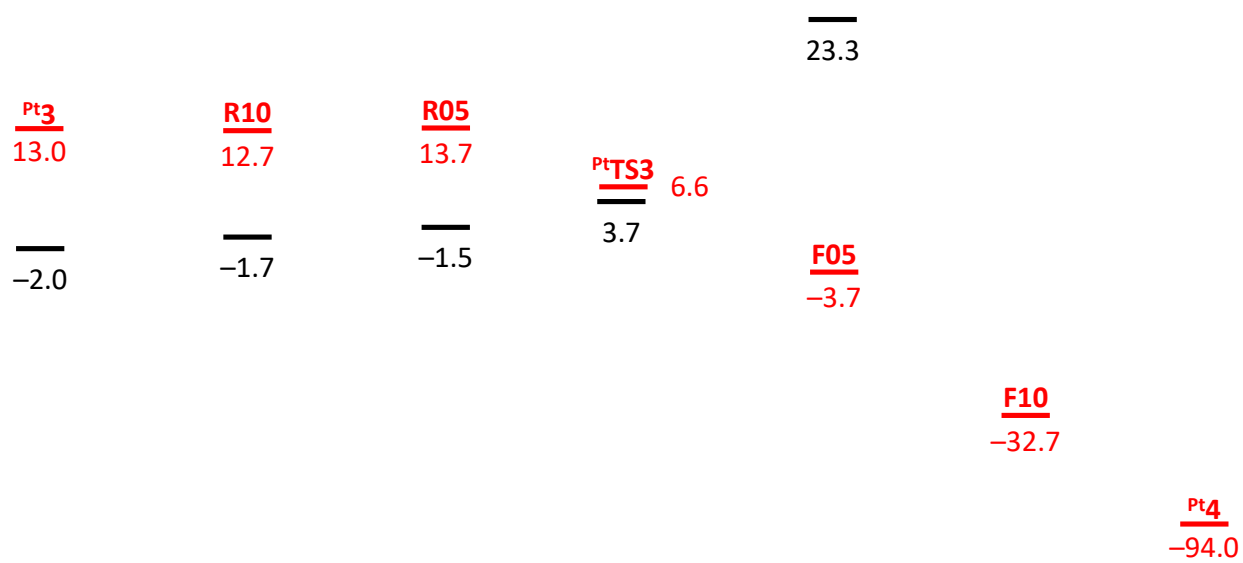
**Table S15.** ONIOM(PBE0-CCSD(T\*)-F12:PBE0-D) results for the Pd-system (corresponding HF-CC based data for comparison); relative free energies in kcal mol<sup>-1</sup>, relative PBE0-CCSD-F12/VTZ and PBE0-CCSD(T\*)-F12/VTZ energies for the high-level ONIOM layer and differences  $\Delta\Delta(T)$  of the (T) contributions between KS-CC and HF-CC results.

Structure	Spin	$\Delta G_{\text{ONIOM}}$		$\Delta E_{\text{CCSD-F12}}^{\text{model}}$		$\Delta E_{\text{CCSD(T*)-F12}}^{\text{model}}$		$\Delta\Delta(T)$
		KS-CC	HF-CC	KS-CC	HF-CC	KS-CC	HF-CC	
<b>Pd1</b>	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	0	20.1	19.3	29.2	28.7	24.3	23.5	0.3
<b>PdTS1</b>	1	21.9	22.1	20.4	19.9	15.1	15.4	-0.7
<b>Pd2</b>	0.5	5.4	5.3	6.1	6.1	4.9	4.8	0.1
<b>PdTS2</b>	1	15.6	16.0	5.3	4.8	2.0	2.4	-0.9
	0	40.8	39.7	36.4	34.6	28.3	27.3	-0.7
<b>Pd3</b>	1	12.3	13.0	-2.6	-2.7	-5.4	-4.7	-0.8
	0	24.6	-28.0	28.5	25.4	4.4	-48.2	49.4
<b>PdTS3</b>	0	10.6	-5.5	15.3	11.6	0.3	-15.8	12.4
<b>Pd4</b>	0	-78.3	-79.9	-99.2	-99.0	-99.4	-101.1	1.9
<b>PdTS4</b>	0	17.5	14.8	6.4	5.6	-3.5	-6.3	2.0
<b>Pd5</b>	0	-5.9	-7.5	-26.3	-26.2	-28.9	-30.5	1.8

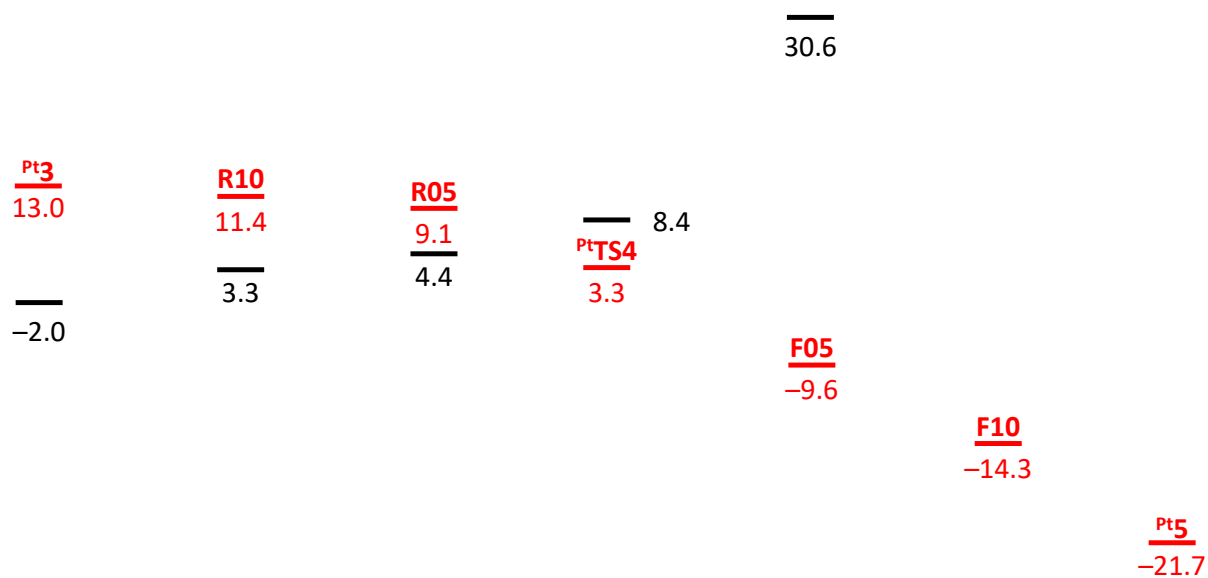




**Figure S4.** Orbitals of restricted HF reference for the CCSD(T\*)-F12/VTZ calculation of singlet  $\text{Pd}_3$  involved in  $t_1$  and  $t_2$  amplitudes exceeding 0.1. Orbital energies in  $E_h$ ; orbital isosurfaces at  $0.05 a_0^{-3/2}$ .



**Figure S5.** Relative singlet and triplet energies along the intrinsic reaction coordinate connected with <sup>Pt</sup>TS3 obtained at the ONIOM(KS-CCSD(T\*)-F12:PBE0-D) level (kcal mol<sup>-1</sup>).



**Figure S6.** Relative singlet and triplet energies along the intrinsic reaction coordinate connected with **PtTTS4** obtained at the ONIOM(KS-CCSD(T\*)-F12:PBE0-D) level (kcal mol<sup>-1</sup>).

## Total Energies:

**Table S16.** Total energies in  $E_h$  obtained with the ano-pVDZ basis set. For BS-CC calculations rigorous  $\langle S^2 \rangle$  expectation values, obtained from a gradient calculation, and projected  $\langle S^2 \rangle$  expectation values are given as well.

Program	Method	Molecule	State	Reference	Total energy
Molpro	FCI	<b>H1</b>	S=1	ROHF	-55.117486
			S=0	RHF	-55.051725
NECI	FCIQMC	CH <sub>2</sub> O	S=0		-114.270557
		<b>H3a</b>	<sup>1</sup> A'		-169.375398
		<b>H3a</b>	<sup>1</sup> A''		-169.374033
		<b>H3a</b>	<sup>3</sup> A''		-169.383724
		<b>H3b</b>	<sup>1</sup> A'		-169.391448
		<b>H3b</b>	<sup>3</sup> A'		-169.385553
MOLBLOCK	HCI	<b>H3a</b>	<sup>1</sup> A'		-169.375780
		<b>H3a</b>	<sup>1</sup> A''		-169.375114
		<b>H3a</b>	<sup>3</sup> A''		-169.383428
		<b>H3b</b>	<sup>1</sup> A'		-169.391412
		<b>H3b</b>	<sup>3</sup> A'		-169.385322
MRCC	CCSD	<b>H1</b>	S=1	UHF	-55.117486
		<b>H1</b>	S=0	RHF	-55.035532
		CH <sub>2</sub> O	S=0	RHF	-114.258287
		<b>H3a</b>	<sup>1</sup> A'	RHF	-169.247868
		<b>H3a</b>	<sup>3</sup> A''	UHF	-169.368156
		<b>H3b</b>	<sup>1</sup> A'	RHF	-169.342288
		<b>H3b</b>	<sup>3</sup> A'	UHF	-169.371584
	CCSD(T)	<b>H1</b>	S=1	UHF	-55.117071
		<b>H1</b>	S=0	RHF	-55.042741
		CH <sub>2</sub> O	S=0	RHF	-114.270194
		<b>H3a</b>	<sup>1</sup> A'	RHF 10-2	-169.264996
		<b>H3a</b>	<sup>3</sup> A''	UHF	-169.381581
		<b>H3b</b>	<sup>1</sup> A'	RHF 10-2	-169.405954
		<b>H3b</b>	<sup>3</sup> A'	UHF	-169.383934
	CCSDT	<b>H1</b>	S=1	UHF	-55.117413
		<b>H1</b>	S=0	RHF	-55.051193
		CH <sub>2</sub> O	S=0	RHF	-114.269630
		<b>H3a</b>	<sup>1</sup> A'	RHF 10-2	-169.264070
		<b>H3a</b>	<sup>3</sup> A''	UHF	-169.382948
		<b>H3b</b>	<sup>1</sup> A'	RHF 10-2	-169.386239
		<b>H3b</b>	<sup>3</sup> A'	UHF	-169.384890
	CCSDT(Q)	<b>H1</b>	S=1	UHF	-55.117550
		<b>H1</b>	S=0	RHF	-55.051945

		CH <sub>2</sub> O	S=0	RHF	-114.270721
		<b>H3a</b>	<sup>1</sup> A'	RHF 10-2	-169.268651
		<b>H3a</b>	<sup>3</sup> A''	UHF	-169.384052
		<b>H3b</b>	<sup>1</sup> A'	RHF 10-2	-169.397485
		<b>H3b</b>	<sup>3</sup> A'	UHF	-169.385791
	CCSDTQ	<b>H1</b>	S=1	UHF	-55.117566
		<b>H1</b>	S=0	RHF	-55.051701
		CH <sub>2</sub> O	S=0	RHF	-114.270565
		<b>H3a</b>	<sup>1</sup> A'	RHF 10-2	-169.265327
		<b>H3a</b>	<sup>3</sup> A''	UHF	-169.383955
		<b>H3b</b>	<sup>1</sup> A'	RHF 10-2	-169.391351
		<b>H3b</b>	<sup>3</sup> A'	UHF	-169.385736
	CCSDTQ(P)	<b>H1</b>	S=1	UHF	-55.117569
		<b>H1</b>	S=0	RHF	-55.051722
		CH <sub>2</sub> O	S=0	RHF	-114.270618
		<b>H3a</b>	<sup>1</sup> A'	RHF 10-2	-169.264664
		<b>H3a</b>	<sup>3</sup> A''	UHF	-169.383992
		<b>H3b</b>	<sup>1</sup> A'	RHF 10-2	-169.391837
		<b>H3b</b>	<sup>3</sup> A'	UHF	-169.385764
GAMESS	CR-CC(2,3)	<b>H1</b>	S=1	UHF	-55.117461
		<b>H1</b>	S=0	RHF	-55.044079
		CH <sub>2</sub> O	S=0	RHF	-114.269978
		<b>H3a</b>	<sup>1</sup> A'	RHF 10-2	-169.264734
		<b>H3a</b>	<sup>3</sup> A''	UHF	-169.382591
		<b>H3b</b>	<sup>1</sup> A'	RHF 10-2	-169.381948
		<b>H3b</b>	<sup>3</sup> A'	UHF	-169.384605
Molpro	CCSD	<b>H1</b>	S=1	ROHF	-55.114998
		<b>H1</b>	S=0	RHF	-55.035533
		CH <sub>2</sub> O	S=0	RHF	-114.258287
		<b>H3a</b>	<sup>1</sup> A'	RHF 10-2	-169.316054
		<b>H3a</b>	<sup>3</sup> A''	ROHF	-169.367910
		<b>H3b</b>	<sup>1</sup> A'	RHF 10-2	-169.342288
		<b>H3b</b>	<sup>3</sup> A'	ROHF	-169.371078
	CCSD(T)	<b>H1</b>	S=1	ROHF	-55.116973
		<b>H1</b>	S=0	RHF	-55.042738
		CH <sub>2</sub> O	S=0	RHF	-114.269255
		<b>H3a</b>	<sup>1</sup> A'	RHF 10-2	-169.733220
		<b>H3a</b>	<sup>3</sup> A''	ROHF	-169.381541
		<b>H3b</b>	<sup>1</sup> A'	RHF 10-2	-169.405950
		<b>H3b</b>	<sup>3</sup> A'	ROHF	-169.383665
CFOUR	BS-CCSD				
$\langle S^2 \rangle_{\text{rig.}} = 1.61$	$\langle S^2 \rangle_{\text{proj.}} = 1.35$	<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.093379
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H1</b>	S=1@BSS	UHF	-55.115165
		<b>H1</b>	S=0	Yamaguchi	-55.047888
$\langle S^2 \rangle_{\text{rig.}} = 1.00$	$\langle S^2 \rangle_{\text{proj.}} = 1.00$	<b>H3a</b>	<sup>1</sup> A'	UHF 10-2/10-2	-169.362655
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3a</b>	<sup>3</sup> A'@BSS	UHF 10-3/10-1	-169.363242

		<b>H3a</b>	<sup>1</sup> A'	Yamaguchi	-169.362073
		<b>H3a</b>	<sup>1</sup> A''	UHF 10-2/9-3	-169.364271
$\langle S^2 \rangle_{\text{rig.}} = 1.05$	$\langle S^2 \rangle_{\text{proj.}} = 1.02$	<b>H3a</b>	<sup>3</sup> A''@BSS	UHF 10-3/9-2	-169.368445
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3a</b>	<sup>1</sup> A''	Yamaguchi	-169.359914
		<b>H3b</b>	<sup>1</sup> A'	UHF 10-2/10-2	-169.372421
$\langle S^2 \rangle_{\text{rig.}} = 0.89$	$\langle S^2 \rangle_{\text{proj.}} = 0.94$	<b>H3b</b>	<sup>3</sup> A''@BSS	UHF 10-3/10-1	-169.368259
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3b</b>	<sup>1</sup> A'	Yamaguchi	-169.376071
		BS-CCSD(T)			
		<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.102470
$\langle S^2 \rangle_{\text{rig.}} = 1.96$		<b>H1</b>	S=1@BSS	UHF	-55.117062
$\langle S^2 \rangle_{\text{rig.}} = 2.00$		<b>H1</b>	S=0	Yamaguchi	-54.369209
		<b>H3a</b>	<sup>1</sup> A'	UHF 10-2/10-2	-169.374952
$\langle S^2 \rangle_{\text{rig.}} = 1.00$		<b>H3a</b>	<sup>3</sup> A''@BSS	UHF 10-3/10-1	-169.375355
$\langle S^2 \rangle_{\text{rig.}} = 2.00$		<b>H3a</b>	<sup>1</sup> A'	Yamaguchi	-169.374550
		<b>H3a</b>	<sup>1</sup> A''	UHF 10-2/9-3	-169.377385
$\langle S^2 \rangle_{\text{rig.}} = 1.09$		<b>H3a</b>	<sup>3</sup> A''@BSS	UHF 10-3/9-2	-169.381702
$\langle S^2 \rangle_{\text{rig.}} = 2.00$		<b>H3a</b>	<sup>1</sup> A''	Yamaguchi	-169.372233
		<b>H3b</b>	<sup>1</sup> A'	UHF 10-2/10-2	-169.385663
$\langle S^2 \rangle_{\text{rig.}} = 0.83$		<b>H3b</b>	<sup>3</sup> A''@BSS	UHF 10-3/10-1	-169.380691
$\langle S^2 \rangle_{\text{rig.}} = 2.00$		<b>H3b</b>	<sup>1</sup> A'	Yamaguchi	-169.389167
		BS-CCSDT			
		<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.116295
$\langle S^2 \rangle_{\text{proj.}} = 1.97$		<b>H1</b>	S=1@BSS	UHF	-55.117404
$\langle S^2 \rangle_{\text{proj.}} = 2.00$		<b>H1</b>	S=0	Yamaguchi	-55.051993
		<b>H3a</b>	<sup>1</sup> A'	UHF 10-2/10-2	-169.376015
$\langle S^2 \rangle_{\text{proj.}} = 1.03$		<b>H3a</b>	<sup>3</sup> A''@BSS	UHF 10-3/10-1	-169.376302
$\langle S^2 \rangle_{\text{proj.}} = 2.00$		<b>H3a</b>	<sup>1</sup> A'	Yamaguchi	-169.375710
		<b>H3a</b>	<sup>1</sup> A''	UHF 10-2/9-3	-169.380125
$\langle S^2 \rangle_{\text{proj.}} = 1.34$		<b>H3a</b>	<sup>3</sup> A''@BSS	UHF 10-3/9-2	-169.383069
$\langle S^2 \rangle_{\text{proj.}} = 2.00$		<b>H3a</b>	<sup>1</sup> A''	Yamaguchi	-169.374121
		<b>H3b</b>	<sup>1</sup> A'	UHF 10-2/10-2	-169.388374
$\langle S^2 \rangle_{\text{proj.}} = 0.58$		<b>H3b</b>	<sup>3</sup> A''@BSS	UHF 10-3/10-1	-169.381638
$\langle S^2 \rangle_{\text{proj.}} = 2.00$		<b>H3b</b>	<sup>1</sup> A'	Yamaguchi	-169.391100
QCumbe	EOM-EE-CCSD	<b>H3a</b>	<sup>1</sup> A'	RHF-CCSD 10-2	-169.361619
		<b>H3a</b>	<sup>1</sup> A''	RHF-CCSD 10-2	-169.355789
	EOM-SF-CCSD	<b>H1</b>	S=0	UHF-CCSD S=1	-55.049164
		<b>H3a</b>	<sup>1</sup> A'	UHF-CCSD <sup>3</sup> A'	-169.361405
		<b>H3a</b>	<sup>1</sup> A''	UHF-CCSD <sup>3</sup> A''	-169.359759
		<b>H3b</b>	<sup>1</sup> A'	UHF-CCSD <sup>3</sup> A'	-169.375438
	CCSD(T)(a)	<b>H1</b>	S=1	UHF	-55.116778
		CH <sub>2</sub> O	S=0	RHF	-114.270079
	EOM-SFCCSD(T)(a)*	<b>H1</b>	S=0	UHF-CCSD(T)(a)	-55.050847
		<b>H3a</b>	<sup>1</sup> A'	UHF-CCSD(T)(a)	-169.373886
		<b>H3a</b>	<sup>1</sup> A''	UHF-CCSD(T)(a)	-169.372777
		<b>H3b</b>	<sup>1</sup> A'	UHF-CCSD(T)(a)	-169.388909
Molpro	PBE0-CCSD	<b>H1</b>	S=1	ROKS	-55.114518

		H1	S=0	RKS	-55.034988
		CH <sub>2</sub> O	S=0	RKS	-114.256236
		H3a	<sup>1</sup> A'	RKS 10-2	-169.314001
		H3a	<sup>3</sup> A''	ROKS	-169.364310
		H3b	<sup>1</sup> A'	RKS 10-2	-169.338897
		H3b	<sup>3</sup> A'	ROKS	-169.368005
	PBE0-CCSD(T)	H1	S=1	ROKS	-55.116536
		H1	S=0	RKS	-55.042278
		CH <sub>2</sub> O	S=0	RKS	-114.267931
		H3a	<sup>1</sup> A'	RKS 10-2	-169.374791
		H3a	<sup>3</sup> A''	ROKS	-169.380474
		H3b	<sup>1</sup> A'	RKS 10-2	-169.384861
		H3b	<sup>3</sup> A'	ROKS	-169.382444
	BP86-CCSD	H1	S=1	ROKS	-55.114255
		H1	S=0	RKS	-55.034701
		CH <sub>2</sub> O	S=0	RKS	-114.255228
		H3a	<sup>1</sup> A'	RKS 10-2	-169.312522
		H3a	<sup>3</sup> A''	ROKS	-169.362049
		H3b	<sup>1</sup> A'	RKS 10-2	-169.337134
		H3b	<sup>3</sup> A'	ROKS	-169.365645
	BP86-CCSD(T)	H1	S=1	ROKS	-55.116290
		H1	S=0	RKS	-55.042028
		CH <sub>2</sub> O	S=0	RKS	-114.267202
		H3a	<sup>1</sup> A'	RKS 10-2	-169.371096
		H3a	<sup>3</sup> A''	ROKS	-169.379349
		H3b	<sup>1</sup> A'	RKS 10-2	-169.383167
		H3b	<sup>3</sup> A'	ROKS	-169.380653
	CAS-CCSD	H1	S=1	CASSCF(6,5)	-55.115259
		H1	S=0	CASSCF(6,5)	-55.033748
		CH <sub>2</sub> O	S=0	CASSCF(12,10)	-114.257295
		H3a	<sup>1</sup> A'	CASSCF(18,15)	-169.319268
		H3a	<sup>3</sup> A''	CASSCF(18,15)	-169.367263
		H3b	<sup>1</sup> A'	CASSCF(18,15)	-169.342116
		H3b	<sup>3</sup> A'	CASSCF(18,15)	-169.370621
	CAS-CCSD(T)	H1	S=1	CASSCF(6,5)	-55.117231
		H1	S=0	CASSCF(6,5)	-55.041431
		CH <sub>2</sub> O	S=0	CASSCF(12,10)	-114.268665
		H3a	<sup>1</sup> A'	CASSCF(18,15)	-169.373063
		H3a	<sup>3</sup> A''	CASSCF(18,15)	-169.382087
		H3b	<sup>1</sup> A'	CASSCF(18,15)	-169.386193
		H3b	<sup>3</sup> A'	CASSCF(18,15)	-169.383916
ORCA	OOMP2-CCSD	H1	S=1	UHF-OOMP2	-55.115107
		H1	S=0	RHF-OOMP2	-55.035463
		CH <sub>2</sub> O	S=0	RHF-OOMP2	-114.257328
		H3a	<sup>1</sup> A'	RHF-OOMP2	-169.316437
		H3a	<sup>3</sup> A''	UHF-OOMP2	-169.366006

Gaussian	OOMP2-CCSD(T)	H3b	<sup>1</sup> A'	RHF-OOMP2	-169.339773	
		H3b	<sup>3</sup> A'	UHF-OOMP2	-169.369827	
		H1	S=1	UHF-OOMP2	-55.117061	
		H1	S=0	RHF-OOMP2	-55.042709	
		CH <sub>2</sub> O	S=0	RHF-OOMP2	-114.268934	
		H3a	<sup>1</sup> A'	RHF-OOMP2	-169.372775	
		H3a	<sup>3</sup> A''	UHF-OOMP2	-169.381845	
		H3b	<sup>1</sup> A'	RHF-OOMP2	-169.385783	
		H3b	<sup>3</sup> A'	UHF-OOMP2	-169.383839	
		BD	H1	S=1	UHF	-55.115107
	H1		S=0	RHF	-55.035457	
	CH <sub>2</sub> O		S=0	RHF	-114.257404	
	H3a		<sup>1</sup> A'	RHF	-169.317347	
	H3a		<sup>3</sup> A''	UHF	-169.366788	
	H3b		<sup>1</sup> A'	RHF	-169.340923	
	H3b		<sup>3</sup> A'	UHF	-169.370257	
	BD(T)		H1	S=1	UHF	-55.117046
			H1	S=0	RHF	-55.042697
			CH <sub>2</sub> O	S=0	RHF	-114.268895
		H3a	<sup>1</sup> A'	RHF	-169.370870	
H3a		<sup>3</sup> A''	UHF	-169.381640		
H3b		<sup>1</sup> A'	RHF	-169.385171		
H3b		<sup>3</sup> A'	UHF	-169.383632		
ORCA		CASSCF	H1	S=1	CASSCF(6,5)	-55.001324
			H1	S=0	CASSCF(6,5)	-54.928261
			CH <sub>2</sub> O	S=0	CASSCF(12,10)	-114.044184
	H3a		<sup>1</sup> A'	CASSCF(18,15)	-169.007101	
	H3a		<sup>1</sup> A''	CASSCF(18,15)	-169.005323	
	H3a		<sup>3</sup> A''	CASSCF(18,15)	-169.012961	
	H3b		<sup>1</sup> A'	CASSCF(18,15)	-169.019838	
	H3b		<sup>3</sup> A'	CASSCF(18,15)	-169.016544	
	NEVPT2		H1	S=1	CASSCF(6,5)	-55.095886
			H1	S=0	CASSCF(6,5)	-55.027480
CH <sub>2</sub> O		S=0	CASSCF(12,10)	-114.230143		
H3a		<sup>1</sup> A'	CASSCF(18,15)	-169.313647		
H3a		<sup>1</sup> A''	CASSCF(18,15)	-169.312696		
H3a		<sup>3</sup> A''	CASSCF(18,15)	-169.321621		
H3b		<sup>1</sup> A'	CASSCF(18,15)	-169.330056		
H3b		<sup>3</sup> A'	CASSCF(18,15)	-169.322966		
MRCC		PBE0-CCSD	H1	S=1	UKS	-55.114717
			H1	S=0	RKS	-55.035051
	CH <sub>2</sub> O		S=0	RKS	-114.256291	
	H3a		<sup>1</sup> A'	RKS 10-2	-169.314093	
	H3a		<sup>3</sup> A''	UKS	-169.364702	
	H3b		<sup>1</sup> A'	RKS 10-2	-169.338987	
	H3b		<sup>3</sup> A'	UKS	-169.368784	



PBE0-CCSD(T)	H1	S=1	UKS	-55.116672
	H1	S=0	RKS	-55.042340
	CH <sub>2</sub> O	S=0	RKS	-114.267988
	H3a	<sup>1</sup> A'	RKS 10-2	-169.374928
	H3a	<sup>3</sup> A''	UKS	-169.380224
	H3b	<sup>1</sup> A'	RKS 10-2	-169.384958
PBE0-CCSDT	H3b	<sup>3</sup> A'	UKS	-169.382448
	H1	S=1	UKS	-55.117041
	H1	S=0	RKS	-55.050819
	CH <sub>2</sub> O	S=0	RKS	-114.268547
	H3a	<sup>1</sup> A'	RKS 10-2	-169.368985
	H3a	<sup>3</sup> A''	UKS	-169.381325
PBE0-CCSDT(Q)	H3b	<sup>1</sup> A'	RKS 10-2	-169.384393
	H3b	<sup>3</sup> A'	UKS	-169.383385
	H1	S=1	UKS	-55.117181
	H1	S=0	RKS	-55.051578
	CH <sub>2</sub> O	S=0	RKS	-114.269721
	H3a	<sup>1</sup> A'	RKS 10-2	-169.378396
PBE0-CCSDTQ	H3a	<sup>3</sup> A''	UKS	-169.382590
	H3b	<sup>1</sup> A'	RKS 10-2	-169.392121
	H3b	<sup>3</sup> A'	UKS	-169.384358
	H1	S=1	UKS	-55.117197
	H1	S=0	RKS	-55.051356
	CH <sub>2</sub> O	S=0	RKS	-114.269639
PBE0-CCSDTQ(P)	H3a	<sup>1</sup> A'	RKS 10-2	-169.374620
	H3a	<sup>3</sup> A''	UKS	-169.382579
	H3b	<sup>1</sup> A'	RKS 10-2	-169.389950
	H3b	<sup>3</sup> A'	UKS	-169.384374
	H1	S=1	UKS	-55.117200
	H1	S=0	RKS	-55.051379
PBE0-CCSDTQ(P)	CH <sub>2</sub> O	S=0	RKS	-114.269707
	H3a	<sup>1</sup> A'	RKS 10-2	-169.375295
	H3a	<sup>3</sup> A''	UKS	-169.3826473
	H3b	<sup>1</sup> A'	RKS 10-2	-169.3906752
	H3b	<sup>3</sup> A'	UKS	-169.3844096

**Table S17.** Total energies in  $E_h$  used for complete basis set extrapolation. For BS-CC calculations rigorous  $\langle S^2 \rangle$  expectation values, obtained from a gradient calculation, and projected  $\langle S^2 \rangle$  expectation values are given as well.

Program	Method	Molecule	State	Reference	Total energy	
Molpro	HF/cc-pVTZ	H1	S=1	ROHF	-54.973495	
		H1	S=0	RHF	-54.874288	
	FCI/cc-pVTZ	H1	S=1	ROHF	-55.141126	
		H1	S=0	RHF	-55.080102	
	HF/cc-pVQZ	H1	S=1	ROHF	-54.977234	
		H1	S=0	RHF	-54.878745	
	FCI/cc-pVQZ	H1	S=1	ROHF	-55.155037	
		H1	S=0	RHF	-55.096089	
	FCI/CBS	H1	S=1	ROHF	-55.162279	
		H1	S=0	RHF	-55.104297	
	MRCC	HF/cc-pVTZ	CH <sub>2</sub> O	S=0	RHF	-113.912330
			H1	S=1	UHF	-54.981169
H1			S=0	RHF	-54.874288	
H3a			<sup>1</sup> A'	RHF	-168.738778	
H3a			<sup>3</sup> A''	UHF	-168.889317	
H3b			<sup>1</sup> A'	RHF	-168.757991	
H3b			<sup>3</sup> A'	UHF	-168.896201	
CCSD/cc-pVTZ			CH <sub>2</sub> O	S=0	RHF	-114.317171
			H1	S=1	UHF	-55.136904
			H1	S=0	RHF	-55.060863
			H3a	<sup>1</sup> A'	RHF	-169.340497
			H3a	<sup>3</sup> A''	UHF	-169.455707
		H3b	<sup>1</sup> A'	RHF	-169.429178	
		H3b	<sup>3</sup> A'	UHF	-169.459247	
		CCSD(T)/cc-pVTZ	CH <sub>2</sub> O	S=0	RHF	-114.333560
			H1	S=1	UHF	-55.140687
			H1	S=0	RHF	-55.069623
			H3a	<sup>1</sup> A'	RHF	-169.367327
			H3a	<sup>3</sup> A''	UHF	-169.476772
H3b			<sup>1</sup> A'	RHF	-169.499838	
H3b			<sup>3</sup> A'	UHF	-169.479085	
CCSDT/cc-pVTZ			CH <sub>2</sub> O	S=0	RHF	-114.333735
			H1	S=1	UHF	-55.141132
			H1	S=0	RHF	-55.079151
			H3a	<sup>1</sup> A'	RHF	-169.364721
			H3a	<sup>3</sup> A''	UHF	-169.478223
		H3b	<sup>1</sup> A'	RHF	-169.481709	
		H3b	<sup>3</sup> A'	UHF	-169.480060	
		CCSDT(Q)/cc-pVTZ	CH <sub>2</sub> O	S=0	RHF	-114.334719
			H1	S=1	UHF	-55.141229
	H1		S=0	RHF	-55.080604	

	<b>H3a</b>	<sup>1</sup> A'	RHF	-169.373157
	<b>H3a</b>	<sup>3</sup> A''	UHF	-169.479314
	<b>H3b</b>	<sup>1</sup> A'	RHF	-169.494580
	<b>H3b</b>	<sup>3</sup> A'	UHF	-169.480874
HF/cc-pVQZ	CH <sub>2</sub> O	S=0	RHF	-113.921366
	<b>H1</b>	S=1	UHF	-54.985079
	<b>H1</b>	S=0	RHF	-54.878745
	<b>H3a</b>	<sup>1</sup> A'	RHF	-168.753372
	<b>H3a</b>	<sup>3</sup> A''	UHF	-168.901983
	<b>H3b</b>	<sup>1</sup> A'	RHF	-168.771976
	<b>H3b</b>	<sup>3</sup> A'	UHF	-168.908644
CCSD/cc-pVQZ	CH <sub>2</sub> O	S=0	RHF	-114.350637
	<b>H1</b>	S=1	UHF	-55.150104
	<b>H1</b>	S=0	RHF	-55.075787
	<b>H3a</b>	<sup>1</sup> A'	RHF	-169.393209
	<b>H3a</b>	<sup>3</sup> A''	UHF	-169.504311
	<b>H3b</b>	<sup>1</sup> A'	RHF	-169.478206
	<b>H3b</b>	<sup>3</sup> A'	UHF	-169.507582
CCSD(T)/cc-pVQZ	CH <sub>2</sub> O	S=0	RHF	-114.368803
	<b>H1</b>	S=1	UHF	-55.154577
	<b>H1</b>	S=0	RHF	-55.085160
	<b>H3a</b>	<sup>1</sup> A'	RHF	-169.423558
	<b>H3a</b>	<sup>3</sup> A''	UHF	-169.528132
	<b>H3b</b>	<sup>1</sup> A'	RHF	-169.550368
	<b>H3b</b>	<sup>3</sup> A'	UHF	-169.530055
CCSDT/cc-pVQZ	CH <sub>2</sub> O	S=0	RHF	-114.368841
	<b>H1</b>	S=1	UHF	-55.155028
	<b>H1</b>	S=0	RHF	-55.094907
	<b>H3a</b>	<sup>1</sup> A'	RHF	-169.419418
	<b>H3a</b>	<sup>3</sup> A''	UHF	-169.529525
	<b>H3b</b>	<sup>1</sup> A'	RHF	-169.533144
	<b>H3b</b>	<sup>3</sup> A'	UHF	-169.530933
CCSDT(Q)/cc-pVQZ	CH <sub>2</sub> O	S=0	RHF	-114.369925
	<b>H1</b>	S=1	UHF	-55.155146
	<b>H1</b>	S=0	RHF	-55.096711
	<b>H3a</b>	<sup>1</sup> A'	RHF	-169.436715
	<b>H3a</b>	<sup>3</sup> A''	UHF	-169.530802
	<b>H3b</b>	<sup>1</sup> A'	RHF	-169.546677
	<b>H3b</b>	<sup>3</sup> A'	UHF	-169.531885
CCSD/CBS	CH <sub>2</sub> O	S=0	RHF	-114.368029
	<b>H1</b>	S=1	UHF	-55.156717
	<b>H1</b>	S=0	RHF	-55.083238
	<b>H3a</b>	<sup>1</sup> A'	RHF	-169.420346
	<b>H3a</b>	<sup>3</sup> A''	UHF	-169.529895
	<b>H3b</b>	<sup>1</sup> A'	RHF	-169.503154
	<b>H3b</b>	<sup>3</sup> A'	UHF	-169.533133

	CCSD(T)/CBS	CH <sub>2</sub> O	S=0	RHF	-114.387460
		H <sub>1</sub>	S=1	UHF	-55.161682
		H <sub>1</sub>	S=0	RHF	-55.093047
		H <sub>3a</sub>	<sup>1</sup> A'	RHF	-169.453199
		H <sub>3a</sub>	<sup>3</sup> A''	UHF	-169.555678
		H <sub>3b</sub>	<sup>1</sup> A'	RHF	-169.576384
		H <sub>3b</sub>	<sup>3</sup> A'	UHF	-169.557483
	CCSDT/CBS	CH <sub>2</sub> O	S=0	RHF	-114.387401
		H <sub>1</sub>	S=1	UHF	-55.162137
		H <sub>1</sub>	S=0	RHF	-55.102950
		H <sub>3a</sub>	<sup>1</sup> A'	RHF	-169.447966
		H <sub>3a</sub>	<sup>3</sup> A''	UHF	-169.557030
		H <sub>3b</sub>	<sup>1</sup> A'	RHF	-169.559804
		H <sub>3b</sub>	<sup>3</sup> A'	UHF	-169.558292
	CCSDT(Q)/CBS	CH <sub>2</sub> O	S=0	RHF	-114.388554
		H <sub>1</sub>	S=1	UHF	-55.162271
		H <sub>1</sub>	S=0	RHF	-55.105004
		H <sub>3a</sub>	<sup>1</sup> A'	RHF	-169.471573
		H <sub>3a</sub>	<sup>3</sup> A''	UHF	-169.558438
		H <sub>3b</sub>	<sup>1</sup> A'	RHF	-169.573809
		H <sub>3b</sub>	<sup>3</sup> A'	UHF	-169.559341
CFOUR	BS-CCSD/cc-pVDZ	CH <sub>2</sub> O	S=0	RHF	-114.208363
		H <sub>1</sub>	S=1	UHF	-55.089869
$\langle S^2 \rangle_{\text{rig.}} = 1.66$	$\langle S^2 \rangle_{\text{proj.}} = 1.39$	H <sub>1</sub>	S=0	UHF 3-1-0-0/3-0-1-0	-55.068806
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	H <sub>1</sub>	S=1@BSS	UHF	-55.089877
		H <sub>1</sub>	S=0	Yamaguchi	-55.021240
$\langle S^2 \rangle_{\text{rig.}} = 1.00$	$\langle S^2 \rangle_{\text{proj.}} = 1.00$	H <sub>3a</sub>	<sup>1</sup> A'	UHF 10-2/10-2	-169.289433
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	H <sub>3a</sub>	<sup>3</sup> A'@BSS	UHF 10-3/10-1	-169.289970
		H <sub>3a</sub>	<sup>1</sup> A'	Yamaguchi	-169.288900
$\langle S^2 \rangle_{\text{rig.}} = 1.05$	$\langle S^2 \rangle_{\text{proj.}} = 1.03$	H <sub>3a</sub>	<sup>1</sup> A''	UHF 10-2/9-3	-169.290170
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	H <sub>3a</sub>	<sup>3</sup> A''@BSS	UHF 10-3/9-2	-169.294343
		H <sub>3a</sub>	<sup>1</sup> A''	Yamaguchi	-169.285798
$\langle S^2 \rangle_{\text{rig.}} = 0.89$	$\langle S^2 \rangle_{\text{proj.}} = 0.94$	H <sub>3b</sub>	<sup>1</sup> A'	UHF 10-2/10-2	-169.298972
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	H <sub>3b</sub>	<sup>3</sup> A'@BSS	UHF 10-3/10-1	-169.295014
		H <sub>3b</sub>	<sup>1</sup> A'	Yamaguchi	-169.302449
	BS-CCSD(T)/cc-pVDZ	CH <sub>2</sub> O	S=0	RHF	-114.218117
		H <sub>1</sub>	S=1	UHF	-55.091389
$\langle S^2 \rangle_{\text{rig.}} = 2.02$		H <sub>1</sub>	S=0	UHF 3-1-0-0/3-0-1-0	-55.078296
$\langle S^2 \rangle_{\text{rig.}} = 2.00$		H <sub>1</sub>	S=1@BSS	UHF	-55.091397
		H <sub>1</sub>	S=0	Yamaguchi	-56.581214
$\langle S^2 \rangle_{\text{rig.}} = 1.00$		H <sub>3a</sub>	<sup>1</sup> A'	UHF 10-2/10-2	-169.300124
$\langle S^2 \rangle_{\text{rig.}} = 2.00$		H <sub>3a</sub>	<sup>3</sup> A'@BSS	UHF 10-3/10-1	-169.300488
		H <sub>3a</sub>	<sup>1</sup> A'	Yamaguchi	-169.299762
$\langle S^2 \rangle_{\text{rig.}} = 1.09$		H <sub>3a</sub>	<sup>1</sup> A''	UHF 10-2/9-3	-169.301596
$\langle S^2 \rangle_{\text{rig.}} = 2.00$		H <sub>3a</sub>	<sup>3</sup> A''@BSS	UHF 10-3/9-2	-169.305872
		H <sub>3a</sub>	<sup>1</sup> A''	Yamaguchi	-169.296422

$\langle S^2 \rangle_{\text{rig.}} = 0.83$	<b>H3b</b>	$^1A'$	UHF 10-2/10-2	-169.310503	
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	<b>H3b</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.305805	
	<b>H3b</b>	$^1A'$	Yamaguchi	-169.313828	
	BS-CCSDT/cc-pVDZ	CH <sub>2</sub> O	S=0	RHF	-114.218583
		<b>H1</b>	S=1	UHF	-55.091673
		<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.090909
$\langle S^2 \rangle_{\text{proj.}} = 1.98$		<b>H1</b>	S=1@BSS	UHF	-55.091682
$\langle S^2 \rangle_{\text{proj.}} = 2.00$		<b>H1</b>	S=0	Yamaguchi	-55.025028
		<b>H3a</b>	$^1A'$	UHF 10-2/10-2	-169.301148
$\langle S^2 \rangle_{\text{proj.}} = 1.03$		<b>H3a</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.301408
$\langle S^2 \rangle_{\text{proj.}} = 2.00$		<b>H3a</b>	$^1A'$	Yamaguchi	-169.300871
		<b>H3a</b>	$^1A''$	UHF 10-2/9-3	-169.304445
$\langle S^2 \rangle_{\text{proj.}} = 1.38$		<b>H3a</b>	$^3A''@BSS$	UHF 10-3/9-2	-169.307195
$\langle S^2 \rangle_{\text{proj.}} = 2.00$		<b>H3a</b>	$^1A''$	Yamaguchi	-169.298255
		<b>H3b</b>	$^1A'$	UHF 10-2/10-2	-169.313183
$\langle S^2 \rangle_{\text{proj.}} = 0.56$		<b>H3b</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.306734
$\langle S^2 \rangle_{\text{proj.}} = 2.00$		<b>H3b</b>	$^1A'$	Yamaguchi	-169.315665
	BS-CCSD/cc-pVTZ	CH <sub>2</sub> O	S=0	RHF	-114.317171
		<b>H1</b>	S=1	UHF	-55.136904
$\langle S^2 \rangle_{\text{rig.}} = 1.53$		<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.115079
$\langle S^2 \rangle_{\text{proj.}} = 1.30$		<b>H1</b>	S=1@BSS	UHF	-55.136903
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H1</b>	S=0	Yamaguchi	-55.074922
		<b>H3a</b>	$^1A'$	UHF 10-2/10-2	-169.450947
$\langle S^2 \rangle_{\text{rig.}} = 0.99$	$\langle S^2 \rangle_{\text{proj.}} = 1.00$	<b>H3a</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.451441
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3a</b>	$^1A'$	Yamaguchi	-169.450459
		<b>H3a</b>	$^1A''$	UHF 10-2/9-3	-169.451987
$\langle S^2 \rangle_{\text{rig.}} = 1.04$	$\langle S^2 \rangle_{\text{proj.}} = 1.02$	<b>H3a</b>	$^3A''@BSS$	UHF 10-3/9-2	-169.455911
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3a</b>	$^1A''$	Yamaguchi	-169.447923
		<b>H3b</b>	$^1A'$	UHF 10-2/10-2	-169.460586
$\langle S^2 \rangle_{\text{rig.}} = 0.89$	$\langle S^2 \rangle_{\text{proj.}} = 0.94$	<b>H3b</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.456251
$\langle S^2 \rangle_{\text{rig.}} = 2.00$	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3b</b>	$^1A'$	Yamaguchi	-169.464403
	BS-CCSD(T)/cc-pVTZ	CH <sub>2</sub> O	S=0	RHF	-114.333560
		<b>H1</b>	S=1	UHF	-55.140688
$\langle S^2 \rangle_{\text{rig.}} = 1.88$		<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.125004
$\langle S^2 \rangle_{\text{rig.}} = 2.00$		<b>H1</b>	S=1@BSS	UHF	-55.140688
		<b>H1</b>	S=0	Yamaguchi	-54.887743
$\langle S^2 \rangle_{\text{rig.}} = 0.99$		<b>H3a</b>	$^1A'$	UHF 10-2/10-2	-169.470776
$\langle S^2 \rangle_{\text{rig.}} = 2.00$		<b>H3a</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.471036
		<b>H3a</b>	$^1A'$	Yamaguchi	-169.470520
$\langle S^2 \rangle_{\text{rig.}} = 1.07$		<b>H3a</b>	$^1A''$	UHF 10-2/9-3	-169.472636
$\langle S^2 \rangle_{\text{rig.}} = 2.00$		<b>H3a</b>	$^3A''@BSS$	UHF 10-3/9-2	-169.476784
		<b>H3a</b>	$^1A''$	Yamaguchi	-169.467818
$\langle S^2 \rangle_{\text{rig.}} = 0.83$		<b>H3b</b>	$^1A'$	UHF 10-2/10-2	-169.481497
$\langle S^2 \rangle_{\text{rig.}} = 2.00$		<b>H3b</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.476166
		<b>H3b</b>	$^1A'$	Yamaguchi	-169.485263
	BS-CCSDT/cc-pVTZ	CH <sub>2</sub> O	S=0	RHF	-114.333735

		<b>H1</b>	S=1	UHF	-55.141132
	$\langle S^2 \rangle_{\text{proj.}} = 1.94$	<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.139349
	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H1</b>	S=1@BSS	UHF	-55.141133
		<b>H1</b>	S=0	Yamaguchi	-55.079812
	$\langle S^2 \rangle_{\text{proj.}} = 1.00$	<b>H3a</b>	$^1A'$	UHF 10-2/10-2	-169.471883
	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3a</b>	$^3A'$ @BSS	UHF 10-3/10-1	-169.472001
		<b>H3a</b>	$^1A'$	Yamaguchi	-169.471764
	$\langle S^2 \rangle_{\text{proj.}} = 1.25$	<b>H3a</b>	$^1A''$	UHF 10-2/9-3	-169.475053
	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3a</b>	$^3A''$ @BSS	UHF 10-3/9-2	-169.478239
		<b>H3a</b>	$^1A''$	Yamaguchi	-169.469724
	$\langle S^2 \rangle_{\text{proj.}} = 0.63$	<b>H3b</b>	$^1A'$	UHF 10-2/10-2	-169.484166
	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3b</b>	$^3A'$ @BSS	UHF 10-3/10-1	-169.477135
		<b>H3b</b>	$^1A'$	Yamaguchi	-169.487390
	BS-CCSD/cc-pVQZ	CH <sub>2</sub> O	S=0	RHF	-114.350637
		<b>H1</b>	S=1	UHF	-55.150104
	$\langle S^2 \rangle_{\text{rig.}} = 1.50$ $\langle S^2 \rangle_{\text{proj.}} = 1.28$	<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.128443
	$\langle S^2 \rangle_{\text{rig.}} = 2.00$ $\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H1</b>	S=1@BSS	UHF	-55.150102
		<b>H1</b>	S=0	Yamaguchi	-55.090345
	$\langle S^2 \rangle_{\text{rig.}} = 0.99$ $\langle S^2 \rangle_{\text{proj.}} = 1.00$	<b>H3a</b>	$^1A'$	UHF 10-2/10-2	-169.499541
	$\langle S^2 \rangle_{\text{rig.}} = 2.00$ $\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3a</b>	$^3A'$ @BSS	UHF 10-3/10-1	-169.499998
		<b>H3a</b>	$^1A'$	Yamaguchi	-169.499089
	$\langle S^2 \rangle_{\text{rig.}} = 1.04$ $\langle S^2 \rangle_{\text{proj.}} = 1.02$	<b>H3a</b>	$^1A''$	UHF 10-2/9-3	-169.500603
	$\langle S^2 \rangle_{\text{rig.}} = 2.00$ $\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3a</b>	$^3A''$ @BSS	UHF 10-3/9-2	-169.504472
		<b>H3a</b>	$^1A''$	Yamaguchi	-169.496606
	$\langle S^2 \rangle_{\text{rig.}} = 0.89$ $\langle S^2 \rangle_{\text{proj.}} = 0.94$	<b>H3b</b>	$^1A'$	UHF 10-2/10-2	-169.509281
	$\langle S^2 \rangle_{\text{rig.}} = 2.00$ $\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3b</b>	$^3A'$ @BSS	UHF 10-3/10-1	-169.504730
		<b>H3b</b>	$^1A'$	Yamaguchi	-169.513281
	BS-CCSD(T)/cc-pVQZ	CH <sub>2</sub> O	S=0	RHF	-114.368803
		<b>H1</b>	S=1	UHF	-55.154577
	$\langle S^2 \rangle_{\text{rig.}} = 1.84$	<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.138611
	$\langle S^2 \rangle_{\text{rig.}} = 2.00$	<b>H1</b>	S=1@BSS	UHF	-55.154576
		<b>H1</b>	S=0	Yamaguchi	-54.957303
	$\langle S^2 \rangle_{\text{rig.}} = 0.99$	<b>H3a</b>	$^1A'$	UHF 10-2/10-2	-169.522038
	$\langle S^2 \rangle_{\text{rig.}} = 2.00$	<b>H3a</b>	$^3A'$ @BSS	UHF 10-3/10-1	-169.522232
		<b>H3a</b>	$^1A'$	Yamaguchi	-169.521847
	$\langle S^2 \rangle_{\text{rig.}} = 1.07$	<b>H3a</b>	$^1A''$	UHF 10-2/9-3	-169.523953
	$\langle S^2 \rangle_{\text{rig.}} = 2.00$	<b>H3a</b>	$^3A''$ @BSS	UHF 10-3/9-2	-169.528087
		<b>H3a</b>	$^1A''$	Yamaguchi	-169.519190
	$\langle S^2 \rangle_{\text{rig.}} = 0.82$	<b>H3b</b>	$^1A'$	UHF 10-2/10-2	-169.532940
	$\langle S^2 \rangle_{\text{rig.}} = 2.00$	<b>H3b</b>	$^3A'$ @BSS	UHF 10-3/10-1	-169.527277
		<b>H3b</b>	$^1A'$	Yamaguchi	-169.536893
	BS-CCSDT/cc-pVQZ	CH <sub>2</sub> O	S=0	RHF	-114.368841
		<b>H1</b>	S=1	UHF	-55.155028
	$\langle S^2 \rangle_{\text{proj.}} = 1.93$	<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.152976
	$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H1</b>	S=1@BSS	UHF	-55.155028
			S=0	Yamaguchi	-55.096313

$\langle S^2 \rangle_{\text{proj.}} = 1.00$	<b>H3a</b>	$^1A'$	UHF 10-2/10-2	-169.523067
$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3a</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.523099
	<b>H3a</b>	$^1A'$	Yamaguchi	-169.523036
$\langle S^2 \rangle_{\text{proj.}} = 1.23$	<b>H3a</b>	$^1A''$	UHF 10-2/9-3	-169.526217
$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3a</b>	$^3A''@BSS$	UHF 10-3/9-2	-169.529486
	<b>H3a</b>	$^1A''$	Yamaguchi	-169.521027
$\langle S^2 \rangle_{\text{proj.}} = 0.64$	<b>H3b</b>	$^1A'$	UHF 10-2/10-2	-169.535581
$\langle S^2 \rangle_{\text{proj.}} = 2.00$	<b>H3b</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.528146
	<b>H3b</b>	$^1A'$	Yamaguchi	-169.539049
BS-CCSD/CBS	CH <sub>2</sub> O	S=0	RHF	-114.369492
	<b>H1</b>	S=1	UHF	-55.157397
	<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.135874
	<b>H1</b>	S=1@BSS	UHF	-55.157395
	<b>H1</b>	S=0	Yamaguchi	-55.09891
	<b>H3a</b>	$^1A'$	UHF 10-2/10-2	-169.526796
	<b>H3a</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.527230
	<b>H3a</b>	$^1A'$	Yamaguchi	-169.526367
	<b>H3a</b>	$^1A''$	UHF 10-2/9-3	-169.527862
	<b>H3a</b>	$^3A''@BSS$	UHF 10-3/9-2	-169.531701
	<b>H3a</b>	$^1A''$	Yamaguchi	-169.523899
	<b>H3b</b>	$^1A'$	UHF 10-2/10-2	-169.536602
	<b>H3b</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.531917
	<b>H3b</b>	$^1A'$	Yamaguchi	-169.540713
BS-CCSD(T)/CBS	CH <sub>2</sub> O	S=0	RHF	-114.388629
	<b>H1</b>	S=1	UHF	-55.162258
	<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.146190
	<b>H1</b>	S=1@BSS	UHF	-55.162257
	<b>H1</b>	S=0	Yamaguchi	-55.063424
	<b>H3a</b>	$^1A'$	UHF 10-2/10-2	-169.550779
	<b>H3a</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.550933
	<b>H3a</b>	$^1A'$	Yamaguchi	-169.550629
	<b>H3a</b>	$^1A''$	UHF 10-2/9-3	-169.552719
	<b>H3a</b>	$^3A''@BSS$	UHF 10-3/9-2	-169.556847
	<b>H3a</b>	$^1A''$	Yamaguchi	-169.547980
	<b>H3b</b>	$^1A'$	UHF 10-2/10-2	-169.561792
	<b>H3b</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.555926
	<b>H3b</b>	$^1A'$	Yamaguchi	-169.565857
BS-CCSDT/CBS	CH <sub>2</sub> O	S=0	RHF	-114.388585
	<b>H1</b>	S=1	UHF	-55.162708
	<b>H1</b>	S=0	UHF 3-1-0-0/3-0-1-0	-55.160509
	<b>H1</b>	S=1@BSS	UHF	-55.162707
	<b>H1</b>	S=0	Yamaguchi	-55.105570
	<b>H3a</b>	$^1A'$	UHF 10-2/10-2	-169.551754
	<b>H3a</b>	$^3A'@BSS$	UHF 10-3/10-1	-169.551731
	<b>H3a</b>	$^1A'$	Yamaguchi	-169.551776
	<b>H3a</b>	$^1A''$	UHF 10-2/9-3	-169.554894

	<b>H3a</b>	<sup>3</sup> A''@BSS	UHF 10-3/9-2	-169.558204
	<b>H3a</b>	<sup>1</sup> A''	Yamaguchi	-169.549768
	<b>H3b</b>	<sup>1</sup> A'	UHF 10-2/10-2	-169.564415
	<b>H3b</b>	<sup>3</sup> A''@BSS	UHF 10-3/10-1	-169.556727
	<b>H3b</b>	<sup>1</sup> A'	Yamaguchi	-169.568022
QCumbre				
EOM-EE-CCSD/cc-pVDZ	<b>H3a</b>	<sup>1</sup> A'	RHF-CCSD 10-2	-169.290422
	<b>H3a</b>	<sup>1</sup> A''	RHF-CCSD 10-2	-169.282718
EOM-SF-CCSD/cc-pVDZ	<b>H1</b>	S=0	UHF-CCSD S=1	-55.022401
	<b>H3a</b>	<sup>1</sup> A'	UHF-CCSD <sup>3</sup> A'	-169.288275
	<b>H3a</b>	<sup>1</sup> A''	UHF-CCSD <sup>3</sup> A''	-169.285671
	<b>H3b</b>	<sup>1</sup> A'	UHF-CCSD <sup>3</sup> A'	-169.301843
CCSD(T)(a) /cc-pVDZ	<b>H1</b>	S=1	UHF	-55.091122
	CH <sub>2</sub> O	S=0	RHF	-114.218847
EOM-SFCCSD(T)(a)*	<b>H1</b>	S=0	UHF-CCSD(T)(a)	-55.023794
	<b>H3a</b>	<sup>1</sup> A'	UHF-CCSD(T)(a)	-169.299080
	<b>H3a</b>	<sup>1</sup> A''	UHF-CCSD(T)(a)	-169.296922
	<b>H3b</b>	<sup>1</sup> A'	UHF-CCSD(T)(a)	-169.313522
EOM-EE-CCSD/cc-pVTZ	<b>H3a</b>	<sup>1</sup> A'	RHF-CCSD 10-2	-169.446215
	<b>H3a</b>	<sup>1</sup> A''	RHF-CCSD 10-2	-169.440384
EOM-SF-CCSD/cc-pVTZ	<b>H1</b>	S=0	UHF-CCSD S=1	-55.075280
	<b>H3a</b>	<sup>1</sup> A'	UHF-CCSD <sup>3</sup> A'	-169.449593
	<b>H3a</b>	<sup>1</sup> A''	UHF-CCSD <sup>3</sup> A''	-169.447491
	<b>H3b</b>	<sup>1</sup> A'	UHF-CCSD <sup>3</sup> A'	-169.463512
CCSD(T)(a) /cc-pVTZ	<b>H1</b>	S=1	UHF	-55.140268
	CH <sub>2</sub> O	S=0	RHF	-114.334819
EOM-SFCCSD(T)(a)*	<b>H1</b>	S=0	UHF-CCSD(T)(a)	-55.078997
	<b>H3a</b>	<sup>1</sup> A'	UHF-CCSD(T)(a)	-169.469927
	<b>H3a</b>	<sup>1</sup> A''	UHF-CCSD(T)(a)	-169.468389
	<b>H3b</b>	<sup>1</sup> A'	UHF-CCSD(T)(a)	-169.484985
EOM-EE-CCSD/cc-pVQZ	<b>H3a</b>	<sup>1</sup> A'	RHF-CCSD 10-2	-169.493225
	<b>H3a</b>	<sup>1</sup> A''	RHF-CCSD 10-2	-169.487712
EOM-SF-CCSD/cc-pVQZ	<b>H1</b>	S=0	UHF-CCSD S=1	-55.090380
	<b>H3a</b>	<sup>1</sup> A'	UHF-CCSD <sup>3</sup> A'	-169.498141
	<b>H3a</b>	<sup>1</sup> A''	UHF-CCSD <sup>3</sup> A''	-169.496072
	<b>H3b</b>	<sup>1</sup> A'	UHF-CCSD <sup>3</sup> A'	-169.512273
CCSD(T)(a) /cc-pVQZ	<b>H1</b>	S=1	UHF	-55.154139
	CH <sub>2</sub> O	S=0	RHF	-114.370292
EOM-SFCCSD(T)(a)*	<b>H1</b>	S=0	UHF-CCSD(T)(a)	-55.094895
	<b>H3a</b>	<sup>1</sup> A'	UHF-CCSD(T)(a)	-169.521365
	<b>H3a</b>	<sup>1</sup> A''	UHF-CCSD(T)(a)	-169.519901
	<b>H3b</b>	<sup>1</sup> A'	UHF-CCSD(T)(a)	-169.536711
EOM-EE-CCSD/CBS	<b>H3a</b>	<sup>1</sup> A'	RHF-CCSD 10-2	-169.519607
	<b>H3a</b>	<sup>1</sup> A''	RHF-CCSD 10-2	-169.514244
EOM-SF-CCSD/CBS	<b>H1</b>	S=0	UHF-CCSD S=1	-55.098756
	<b>H3a</b>	<sup>1</sup> A'	UHF-CCSD <sup>3</sup> A'	-169.525372



		<b>H3a</b>	<sup>1</sup> A''	UHF-CCSD <sup>3</sup> A''	-169.523308
		<b>H3b</b>	<sup>1</sup> A'	UHF-CCSD <sup>3</sup> A'	-169.539636
	CCSD(T)(a)/CBS	<b>H1</b>	S=1	UHF	-55.161812
		CH <sub>2</sub> O	S=0	RHF	-114.390255
	EOM-SFCCSD(T)(a)*/CBS	<b>H1</b>	S=0	UHF-CCSD(T)(a)	-55.103729
		<b>H3a</b>	<sup>1</sup> A'	UHF-CCSD(T)(a)	-169.550219
		<b>H3a</b>	<sup>1</sup> A''	UHF-CCSD(T)(a)	-169.548784
		<b>H3b</b>	<sup>1</sup> A'	UHF-CCSD(T)(a)	-169.565738
Molpro	PBE0-HF/cc-pVTZ	CH <sub>2</sub> O	S=0	RKS	-113.900882
		<b>H1</b>	S=1	ROKS	-54.970892
		<b>H1</b>	S=0	RKS	-54.870703
		<b>H3a</b>	<sup>1</sup> A'	RKS 10-2	-168.701665
		<b>H3a</b>	<sup>3</sup> A''	ROKS	-168.843826
		<b>H3b</b>	<sup>1</sup> A'	RKS 10-2	-168.732078
		<b>H3b</b>	<sup>3</sup> A'	ROKS	-168.859352
	PBE0-CCSD/cc-pVTZ	CH <sub>2</sub> O	S=0	RKS	-114.314669
		<b>H1</b>	S=1	ROKS	-55.135944
		<b>H1</b>	S=0	RKS	-55.060083
		<b>H3a</b>	<sup>1</sup> A'	RKS 10-2	-169.399143
		<b>H3a</b>	<sup>3</sup> A''	ROKS	-169.451150
		<b>H3b</b>	<sup>1</sup> A'	RKS 10-2	-169.424918
		<b>H3b</b>	<sup>3</sup> A'	ROKS	-169.455070
	PBE0-CCSD(T)/cc-pVTZ	CH <sub>2</sub> O	S=0	RKS	-114.331981
		<b>H1</b>	S=1	ROKS	-55.139987
		<b>H1</b>	S=0	RKS	-55.069008
		<b>H3a</b>	<sup>1</sup> A'	RKS 10-2	-169.466806
		<b>H3a</b>	<sup>3</sup> A''	ROKS	-169.475668
		<b>H3b</b>	<sup>1</sup> A'	RKS 10-2	-169.479745
		<b>H3b</b>	<sup>3</sup> A'	ROKS	-169.477624
	PBE0-HF/cc-pVQZ	CH <sub>2</sub> O	S=0	RKS	-113.909355
		<b>H1</b>	S=1	ROKS	-54.974329
		<b>H1</b>	S=0	RKS	-54.874849
		<b>H3a</b>	<sup>1</sup> A'	RKS 10-2	-168.714579
		<b>H3a</b>	<sup>3</sup> A''	ROKS	-168.855158
		<b>H3b</b>	<sup>1</sup> A'	RKS 10-2	-168.745021
		<b>H3b</b>	<sup>3</sup> A'	ROKS	-168.870582
	PBE0-CCSD/cc-pVQZ	CH <sub>2</sub> O	S=0	RKS	-114.347946
		<b>H1</b>	S=1	ROKS	-55.149039
		<b>H1</b>	S=0	RKS	-55.074924
		<b>H3a</b>	<sup>1</sup> A'	RKS 10-2	-169.447030
		<b>H3a</b>	<sup>3</sup> A''	ROKS	-169.499339
		<b>H3b</b>	<sup>1</sup> A'	RKS 10-2	-169.473448
		<b>H3b</b>	<sup>3</sup> A'	ROKS	-169.503049
	PBE0-CCSD(T)/cc-pVQZ	CH <sub>2</sub> O	S=0	RKS	-114.367058
		<b>H1</b>	S=1	ROKS	-55.153805
		<b>H1</b>	S=0	RKS	-55.084493

	<b>H3a</b>	<sup>1</sup> A'	RKS 10-2	-169.516220
	<b>H3a</b>	<sup>3</sup> A''	ROKS	-169.526793
	<b>H3b</b>	<sup>1</sup> A'	RKS 10-2	-169.530917
	<b>H3b</b>	<sup>3</sup> A'	ROKS	-169.528391
PBE0-CCSD/CBS	CH <sub>2</sub> O	S=0	RKS	-114.365604
	<b>H1</b>	S=1	ROKS	-55.155914
	<b>H1</b>	S=0	RKS	-55.082537
	<b>H3a</b>	<sup>1</sup> A'	RKS 10-2	-169.471927
	<b>H3a</b>	<sup>3</sup> A''	ROKS	-169.525577
	<b>H3b</b>	<sup>1</sup> A'	RKS 10-2	-169.498782
	<b>H3b</b>	<sup>3</sup> A'	ROKS	-169.529210
PBE0-CCSD(T)/CBS	CH <sub>2</sub> O	S=0	RKS	-114.385998
	<b>H1</b>	S=1	ROKS	-55.161195
	<b>H1</b>	S=0	RKS	-55.092565
	<b>H3a</b>	<sup>1</sup> A'	RKS 10-2	-169.542204
	<b>H3a</b>	<sup>3</sup> A''	ROKS	-169.555122
	<b>H3b</b>	<sup>1</sup> A'	RKS 10-2	-169.558132
	<b>H3b</b>	<sup>3</sup> A'	ROKS	-169.556538

---

**Table S18.** PBE0-D/def2-TZVPP total energies and free energy contributions in E<sub>h</sub>.

Molecule	State	Total energy	$\Delta G_{\text{contr.}}$
CH <sub>2</sub> O	S=0	-114.420185	0.005721
CHO	S=0.5	-113.772443	-0.008518
<b>H1</b>	S=1	-55.180171	-0.009700
<b>H1</b>	S=0	-55.090880	-0.008594
<b>H<sup>H</sup>TS1</b>	S=1	-169.592693	0.003619
<b>H2</b>	S=0.5	-55.836915	0.000879
<b>H<sup>H</sup>TS2</b>	S=1	-169.598818	0.011918
<b>H<sup>H</sup>TS2</b>	$\langle S^2 \rangle = 1.02$	-169.580302	0.011713
S=1@BS	$\langle S^2 \rangle = 2.02$	-169.599840	
Yamaguchi	S=0	-169.560717	
<b>H3a</b>	S=1	-169.622797	0.015551
<b>H3a</b>	$\langle S^2 \rangle = 2.01$	-169.618614	0.015362
S=1@BS	$\langle S^2 \rangle = 2.01$	-169.622588	
Yamaguchi	S=0	-169.614651	
<b>H3b</b>	S=1	-169.623744	0.014697
<b>H3b</b>	$\langle S^2 \rangle = 0.88$	-169.628791	0.015025
S=1@BS	$\langle S^2 \rangle = 2.01$	-169.612381	
Yamaguchi	S=0	-169.641430	
<b>H<sup>H</sup>TS3</b>	$\langle S^2 \rangle = 0.61$	-169.624787	0.014068
S=1@BS	$\langle S^2 \rangle = 2.01$	-169.592577	
Yamaguchi	S=0	-169.638582	
<b>H4</b>	S=0	-169.781172	0.021211
<b>H<sup>H</sup>TS4</b>	$\langle S^2 \rangle = 0.88$	-169.617158	0.017258
S=1@BS	$\langle S^2 \rangle = 2.01$	-169.612806	
Yamaguchi	S=0	-169.620476	
<b>H5</b>	S=0	-169.668190	0.022213

**Table S19.** PBE0-CCSD-F12/VTZ and PBE0-CCSD(T\*)-F12/VTZ total energies in E<sub>h</sub>.

Molecule	State	PBE0-CCSD-F12	PBE0-CCSD(T*)-F12
CH <sub>2</sub> O	S=0	-114.361101	-114.381107
CHO	S=0.5	-113.708879	-113.730330
<sup>H</sup> 1	S=1	-55.153966	-55.158941
<sup>H</sup> 1	S=0	-55.081088	-55.091386
<sup>H</sup> TS1	S=1	-169.489232	-169.521341
<sup>H</sup> 2	S=0.5	-55.809431	-55.816663
<sup>H</sup> TS2	S=1	-169.502811	-169.532668
<sup>H</sup> TS2	S=0	-169.442498	-169.475002
<sup>H</sup> 3a	S=1	-169.518610	-169.547418
<sup>H</sup> 3a	S=0	-169.467626	-169.540259
<sup>H</sup> 3b	S=1	-169.522221	-169.548746
<sup>H</sup> 3b	S=0	-169.493885	-169.553817
<sup>H</sup> TS3	S=0	-169.508914	-169.557664
<sup>H</sup> 4	S=0	-169.683136	-169.714863
<sup>H</sup> TS4	S=0	-169.495597	-169.545778
<sup>H</sup> 5	S=0	-169.570075	-169.602852

**Table S20.** Total energies for the individual ONIOM layers in E<sub>h</sub>: PBE0-CCSD(T\*)-F12b/VTZ as high-level method and PBE0-D/def2-TZVPP as low-level method.

Structure	State	$E_{\text{KS-CCSD}}^{\text{model}}$	$E_{\text{KS-CCSD(T)}}^{\text{model}}$	$E_{\text{DFT}}^{\text{model}}$	$E_{\text{DFT}}^{\text{full}}$	$E_{\text{ONIOM}}$
PhCHO	S=0	-114.360610	-114.380966	-114.419571	-345.307574	-345.268970
PhCO	S=0.5	-113.707936	-113.729866	-113.771552	-344.656542	-344.614856
Pt <sub>1</sub>	S=1	-1067.036337	-1067.161131	-1068.314521	-1696.891852	-1695.738461
	S=0	-1066.995634	-1067.127902	-1068.270629	-1696.855517	-1695.712790
Pt <sup>tr</sup> TS1	S=1	-1181.367200	-1181.520347	-1182.720938	-2042.191054	-2040.990463
Pt <sub>2</sub>	S=0.5	-1067.677431	-1067.802403	-1068.954329	-1697.530906	-1696.378980
Pt <sup>tr</sup> TS2	S=1	-1181.388246	-1181.539006	-1182.737225	-2042.204923	-2041.006704
	S=0	-1181.344069	-1181.501300	-1182.705841	-2042.180392	-2040.975851
Pt <sub>3</sub>	S=1	-1181.396376	-1181.546610	-1182.751456	-2042.215177	-2041.010331
	S=0	-1181.350094	-1181.525791	-1182.738036	-2042.198701	-2040.986456
Pt <sup>tr</sup> TS3	S=0	-1181.373350	-1181.538691	-1182.741510	-2042.199367	-2040.996548
Pt <sub>4</sub>	S=0	-1181.551752	-1181.697785	-1182.895074	-2042.354203	-2041.156914
Pt <sup>tr</sup> TS4	S=0	-1181.382050	-1181.543717	-1182.745833	-2042.203969	-2041.001852
Pt <sub>5</sub>	S=0	-1181.435454	-1181.584427	-1182.781928	-2042.239181	-2041.041681
Pd <sub>1</sub>	S=1	-1075.077216	-1075.204623	-1076.832183	-1705.405924	-1703.778364
	S=0	-1075.030671	-1075.165830	-1076.781933	-1705.363997	-1703.747894
Pd <sup>tr</sup> TS1	S=1	-1189.405389	-1189.561450	-1191.236594	-2050.702099	-2049.026956
Pd <sub>2</sub>	S=0.5	-1075.720214	-1075.847950	-1077.474415	-1706.048483	-1704.422019
Pd <sup>tr</sup> TS2	S=1	-1189.429365	-1189.582398	-1191.254871	-2050.719422	-2049.046948
	S=0	-1189.379889	-1189.540465	-1191.225143	-2050.692564	-2049.007886
Pd <sub>3</sub>	S=1	-1189.441996	-1189.594224	-1191.273713	-2050.733860	-2049.054371
	S=0	-1189.392375	-1189.578648	-1191.260682	-2050.717601	-2049.035567
Pd <sup>tr</sup> TS3	S=0	-1189.413457	-1189.585039	-1191.247950	-2050.717894	-2049.054983
Pd <sub>4</sub>	S=0	-1189.595975	-1189.744050	-1191.416459	-2050.874729	-2049.202319
Pd <sup>tr</sup> TS4	S=0	-1189.427593	-1189.591177	-1191.267126	-2050.721985	-2049.046036
Pd <sub>5</sub>	S=0	-1189.479715	-1189.631592	-1191.304524	-2050.759154	-2049.086221

**Table S21.** HF based CCSD-F12b/VTZ and CCSD(T\*)-F12b/VTZ total energies in E<sub>h</sub>.

Structure	State	$E_{\text{HF-CCSD}}^{\text{model}}$	$E_{\text{HF-CCSD(T)}}^{\text{model}}$
PhCHO	S=0	-114.363161	-114.382534
PhCO	S=0.5	-113.711079	-113.731244
Pt1	S=1	-1067.057531	-1067.171293
	S=0	-1067.018084	-1067.140127
PtTS1	S=1	-1181.391482	-1181.531739
Pt2	S=0.5	-1067.697917	-1067.812868
PtTS2	S=1	-1181.412845	-1181.550055
	S=0	-1181.369864	-1181.514520
Pt3	S=1	-1181.420135	-1181.556907
	S=0	-1181.379604	-1181.582634
PtTS3	S=0	-1181.402488	-1181.566392
Pt4	S=0	-1181.575001	-1181.711904
PtTS4	S=0	-1181.407180	-1181.560142
Pt5	S=0	-1181.458861	-1181.598567
Pd1	S=1	-1075.098518	-1075.213740
	S=0	-1075.052729	-1075.176217
PdTS1	S=1	-1189.429955	-1189.571780
Pd2	S=0.5	-1075.740817	-1075.857354
PdTS2	S=1	-1189.454077	-1189.592445
	S=0	-1189.406563	-1189.552817
Pd3	S=1	-1189.465968	-1189.603703
	S=0	-1189.421258	-1189.673163
PdTS3	S=0	-1189.443228	-1189.621414
Pd4	S=0	-1189.619392	-1189.757329
PdTS4	S=0	-1189.452687	-1189.606235
Pd5	S=0	-1189.503418	-1189.644923

**Table S22.** BS-CC total energies in  $E_h$  obtained with the ORCA program.

Basis Set	Molecule	State	Reference	BS-CCSD	BS-CCSD(T)
def2-SVP	CH <sub>2</sub> O	S=0	RHF	-114.110076	-114.120021
	Pd <sub>1</sub>	S=1	UHF	-1074.502412	-1074.569476
	Pd <sub>3</sub>	S=0	UHF	-1188.607285	-1188.685948
	S=1@BS	S=1	UHF	-1188.615342	-1188.693785
	Yamaguchi	S=0		-1188.599228	-1188.678111
	Pd <sub>3</sub>	S=1	UHF	-1188.613898	-1188.692282
def2-TZVPP	CH <sub>2</sub> O	S=0	RHF	-114.320651	-114.337155
	Pd <sub>1</sub>	S=1	UHF	-1075.600665	-1075.707608
	Pd <sub>3</sub>	S=0	UHF	-1189.917268	-1190.042923
	S=1@BS	S=1	UHF	-1189.925306	-1190.051017
	Yamaguchi	S=0		-1189.909230	-1190.034829
	Pd <sub>3</sub>	S=1	UHF	-1189.924423	-1190.050111
def2-QZVPP	CH <sub>2</sub> O	S=0	RHF	-114.350552	-114.369015
	Pd <sub>1</sub>	S=1	UHF	-1075.784111	-1075.905159
	Pd <sub>3</sub>	S=0	UHF	-1190.132408	-1190.274097
	S=1@BS	S=1	UHF	-1190.140347	-1190.282188
	Yamaguchi	S=0		-1190.124470	-1190.266007
	Pd <sub>3</sub>	S=1	UHF	-1190.139530	-1190.281357
CBS	CH <sub>2</sub> O	S=0	RHF	-114.363446	-114.383005
	Pd <sub>1</sub>	S=1	UHF	-1075.869965	-1075.999168
	Pd <sub>3</sub>	S=0	UHF	-1190.232330	-1190.383232
	S=1@BS	S=1	UHF	-1190.240202	-1190.391311
	Yamaguchi	S=0		-1190.224459	-1190.375153
	Pd <sub>3</sub>	S=1	UHF	-1190.239411	-1190.390510

## XYZ-Coordinates:

All cartesian coordinates are given in Å.

**CH<sub>2</sub>O ! 1-A1 (C2V): E(RPBE1PBE-D3(BJ)/def2TZVPP) = -114.420185329**

C	0.000000000000	-0.000000000000	-0.524329845231
H	-0.000000000000	0.939453752953	-1.111292730217
O	0.000000000000	0.000000000000	0.671070566478
H	-0.000000000000	-0.939453752953	-1.111292730217

**CHO ! 2-A' (CS): E(UPBE1PBE-D3(BJ)/def2TZVPP) = -113.772442643**

C	0.061544400418	0.580561656981	0.000000000000
H	-0.861621605852	1.221609985650	-0.000000000000
O	0.061544400418	-0.588122490942	0.000000000000

**H<sub>1</sub>\_bs ! (C\*V): E(UPBE1PBE-D3(BJ)/def2TZVPP) = -55.1580958240**

H	0.000000000000	0.000000000000	-0.908906365623
N	0.000000000000	0.000000000000	0.129843766518

**H<sub>1</sub>\_s ! (C\*V): E(RPBE1PBE-D3(BJ)/def2TZVPP) = -55.0908798609**

H	0.000000000000	0.000000000000	-0.908040298296
N	0.000000000000	0.000000000000	0.129720042614

**H<sub>1</sub>\_t ! 3-SG (C\*V): E(UPBE1PBE-D3(BJ)/def2TZVPP) = -55.1801711285**

H	-0.000000000000	-0.000000000000	-0.908585208029
N	0.000000000000	-0.000000000000	0.129797886861

**H<sub>2</sub>\_d ! 2-B1 (C2V): E(UPBE1PBE-D3(BJ)/def2TZVPP) = -55.8369150069**

H	-0.000000000000	0.802227103451	-0.497313475906
N	0.000000000000	-0.000000000000	0.142089564545
H	-0.000000000000	-0.802227103451	-0.497313475906

**H<sub>3a</sub>\_bs ! 1-A" (CS): E(UPBE1PBE/def2TZVPP) = -169.618613825**

H	-0.795075491578	-1.300732565347	0.000000000000
N	-1.135196573550	-0.331731735095	0.000000000000
C	0.000000000000	0.539852322804	0.000000000000
H	-0.078577543439	1.184646898303	0.893269823742
O	1.112325824164	-0.248194127802	0.000000000000
H	-0.078577543439	1.184646898303	-0.893269823742

**H<sub>3a</sub>\_t ! 3-A" (CS): E(UPBE1PBE-D3(BJ)/def2TZVPP) = -169.622796816**

H	-0.755078798903	-1.320406330496	0.000000000000
N	-1.119253543019	-0.358625959494	0.000000000000
C	-0.000000000000	0.549952296958	0.000000000000
H	-0.103858269841	1.189777823757	0.895327682104
O	1.099696267464	-0.231060172788	0.000000000000



H -0.103858269841 1.189777823757 -0.895327682104

**H3b\_bs ! 1-A' (CS): E(UPBE1PBE/def2TZVPP) = -169.628790761**

H -0.984460514148 -1.299539345580 0.000000000000

N -1.213552594669 -0.300338271632 0.000000000000

C 0.000000000000 0.413714101043 0.000000000000

H -0.039016191324 1.135254754514 0.850058150000

O 1.194670132435 -0.168860858535 0.000000000000

H -0.039016191324 1.135254754514 -0.850058150000

**H3b\_t ! 3-A (C1): E(UPBE1PBE/def2TZVPP) = -169.623744447**

H -1.072855676033 -1.140407229816 -0.247897389235

N -1.219819499808 -0.172715216447 0.055831196041

C 0.051382713440 0.467506182410 -0.021848077770

H 0.110084552690 1.263236237544 0.743124034446

O 1.133189788656 -0.343358754638 0.028854101723

H 0.127693032106 1.028010450044 -0.985789364666

**H4\_s ! 1-A' (CS): E(RPBE1PBE-D3(BJ)/def2TZVPP) = -169.781171629**

H -0.640226941022 -1.522411579307 0.000000000000

N -0.933228264211 -0.560784192625 0.000000000000

O 1.191866833672 0.233706857643 -0.000000000000

C -0.000000000000 0.416141157124 0.000000000000

H -1.912264221567 -0.345299723648 0.000000000000

H -0.449845657309 1.426698847435 0.000000000000

**H5\_s ! 1-A (C1): E(RPBE1PBE-D3(BJ)/def2TZVPP) = -169.668190104**

H -1.101933619384 -0.679404268468 0.754084368442

N -0.701598574040 -0.471666914473 -0.162186380540

O -0.083737061498 0.846811071485 0.022995977677

C 0.701743602869 -0.295348530278 0.016310394024

H 1.158999977401 -0.564801940500 0.966632377271

H 1.313558535034 -0.456522779936 -0.867242267492

**H<sup>+</sup>TS1\_t ! 3-A" (CS): E(UPBE1PBE-D3(BJ)/def2TZVPP) = -169.592693199**

H 1.666109190894 1.369058859355 0.000000000000

N 0.729790156456 1.808347204268 0.000000000000

H -1.761981880240 -0.281426636865 -0.000000000000

C -0.656369604002 -0.426429280118 -0.000000000000

H 0.000000000000 0.695235596193 0.000000000000

O -0.134305097729 -1.485340320982 0.000000000000

**H<sup>+</sup>TS2\_bs ! 1-A" (CS): E(UPBE1PBE/def2TZVPP) = -169.580301957**

H -0.302387802267 -1.741215296691 0.000000000000

N -1.101986721001 -1.081765505120 0.000000000000

C 0.000000000000 0.769429545255 0.000000000000

H	-0.511431438947	1.060894825419	0.933921969985
O	1.129894715896	0.321900863770	0.000000000000
H	-0.511431438947	1.060894825419	-0.933921969985

**<sup>1</sup>H**TS2\_t ! 3-A" (CS): E(UPBE1PBE-D3(BJ)/def2TZVPP) = -169.598818333

H	-0.351653737467	-1.667663381356	0.000000000000
N	-1.094216301853	-0.945911786504	0.000000000000
C	0.000000000000	0.724244766790	0.000000000000
H	-0.471242834583	1.082293884916	0.931091760751
O	1.119206689950	0.222373689539	0.000000000000
H	-0.471242834583	1.082293884916	-0.931091760751

**<sup>1</sup>H**TS3\_bs ! 1-A (C1): E(UPBE1PBE-D3(BJ)/def2TZVPP) = -169.624787275

H	1.149703201404	-1.146517432454	0.065710452576
N	1.229462791735	-0.129925412058	-0.055320147832
C	-0.069944679027	0.386220107208	-0.027669444964
H	-0.113076835010	1.409059709403	-0.445052510688
O	-1.170203587826	-0.285504966567	-0.020012580501
H	0.138430868232	0.613654696743	1.092700406732

**<sup>1</sup>H**TS4\_bs ! 1-A (C1): E(UPBE1PBE/def2TZVPP) = -169.617158164

H	0.967287281139	-1.034645646630	0.523245712040
N	1.101516734203	-0.233515177367	-0.105792671798
O	-1.006685493582	-0.407968116916	-0.033526683582
C	-0.074634788010	0.584936371482	0.042799540607
H	-0.044236599515	1.117737151062	1.010159690538
H	-0.132375144329	1.305641443578	-0.781440474976

**<sup>107</sup>Pd**1\_s ! 1-A' (CS): E(RPBE1PBE-D3(BJ)/def2SVP) = -1704.13023254

Pd	-0.002944747537	-0.137198302609	0.000000000000
N	0.085608970197	-1.912083890432	-0.000000000000
P	-0.010933681904	0.211494280194	2.301847923044
N	-0.091491698751	1.997652811291	0.000000000000
P	-0.010933681904	0.211494280194	-2.301847923044
C	-0.078218432692	1.995869625071	2.381171214989
H	-0.088334378743	2.549029153401	3.321941751541
C	-0.078218432692	1.995869625071	-2.381171214989
H	-0.088334378743	2.549029153401	-3.321941751541
C	-0.107102837261	2.649659932463	1.181959801607
H	-0.144558245272	3.750601391039	1.157437419103
C	-0.107102837261	2.649659932463	-1.181959801607
H	-0.144558245272	3.750601391039	-1.157437419103
C	-1.564564251789	-0.435761955256	3.144159861870
C	1.600916200399	-0.353170219569	-3.099761161680
C	1.600916200399	-0.353170219569	3.099761161680
C	-1.564564251789	-0.435761955256	-3.144159861870

C	-1.523675832728	-1.958948278602	3.236267939792
H	-1.252400948546	-2.409064137165	2.266759877982
H	-2.522913070534	-2.332359972196	3.514562020361
H	-0.817592122680	-2.309470986038	4.002134635358
C	-2.711252044454	-0.021156500980	2.215098783308
H	-2.631321112603	-0.525150665373	1.241068279522
H	-2.720232395520	1.065547871790	2.040315551447
H	-3.670703420498	-0.305058081456	2.678243668361
C	-1.781069113155	0.200748780555	4.516944257880
H	-1.821265443060	1.298183500410	4.449564763366
H	-1.003007808536	-0.074899482063	5.240606773999
H	-2.747065097906	-0.141186721188	4.924151712461
C	1.822429277020	-1.843589717588	-2.840312760003
H	1.160565733651	-2.477758552518	-3.444103464570
H	1.662133624366	-2.088885717103	-1.775787284234
H	2.860697123532	-2.104416815615	-3.103922990578
C	1.653069380673	-0.039102220621	-4.593529820407
H	0.961736004576	-0.668359585095	-5.171647014006
H	2.669373077447	-0.239083500292	-4.971771105783
H	1.424197360772	1.017309004090	-4.803078778986
C	2.691033687228	0.437552944741	-2.367942772145
H	2.576054968523	1.522145453633	-2.507816294928
H	3.676225774820	0.135182248707	-2.758913631932
H	2.671338148607	0.228736785838	-1.287243161463
C	1.822429277020	-1.843589717588	2.840312760003
H	1.662133624366	-2.088885717103	1.775787284234
H	1.160565733651	-2.477758552518	3.444103464570
H	2.860697123532	-2.104416815615	3.103922990578
C	2.691033687228	0.437552944741	2.367942772145
H	2.671338148607	0.228736785838	1.287243161463
H	3.676225774820	0.135182248707	2.758913631932
H	2.576054968523	1.522145453633	2.507816294928
C	1.653069380673	-0.039102220621	4.593529820407
H	1.424197360772	1.017309004090	4.803078778986
H	2.669373077447	-0.239083500292	4.971771105783
H	0.961736004576	-0.668359585095	5.171647014006
C	-1.781069113155	0.200748780555	-4.516944257880
H	-1.003007808536	-0.074899482063	-5.240606773999
H	-1.821265443060	1.298183500410	-4.449564763366
H	-2.747065097906	-0.141186721188	-4.924151712461
C	-2.711252044454	-0.021156500980	-2.215098783308
H	-2.720232395520	1.065547871790	-2.040315551447
H	-2.631321112603	-0.525150665373	-1.241068279522
H	-3.670703420498	-0.305058081456	-2.678243668361
C	-1.523675832728	-1.958948278602	-3.236267939792
H	-0.817592122680	-2.309470986038	-4.002134635358

H	-2.522913070534	-2.332359972196	-3.514562020361
H	-1.252400948546	-2.409064137165	-2.266759877982

Pd1\_t ! 3-A" (CS): E(UPBE1PBE-D3(BJ)/def2SVP) = -1704.17577701

Pd	-0.051738949250	-0.105821325158	-0.000000000000
N	-0.167522192047	-1.993669720487	-0.000000000000
P	-0.008027604184	0.189072175505	2.311192938162
N	-0.013103621294	1.984106894572	-0.000000000000
P	-0.008027604184	0.189072175505	-2.311192938162
C	-0.027589531863	1.981694896230	2.387181402278
H	-0.026112030850	2.543719185991	3.323038886982
C	-0.027589531863	1.981694896230	-2.387181402278
H	-0.026112030850	2.543719185991	-3.323038886982
C	-0.022355083286	2.633459462084	1.187735675764
H	-0.026324764814	3.735012523930	1.161248302306
C	-0.022355083286	2.633459462084	-1.187735675764
H	-0.026324764814	3.735012523930	-1.161248302306
C	-1.550087434011	-0.400384856987	3.212460417966
C	1.604362640142	-0.385780956926	-3.099438169762
C	1.604362640142	-0.385780956926	3.099438169762
C	-1.550087434011	-0.400384856987	-3.212460417966
C	-1.510938086916	-1.916663809151	3.395293172081
H	-1.250863122153	-2.429061402714	2.455485229452
H	-2.506103658267	-2.269957468561	3.712738856192
H	-0.794056947864	-2.219648978192	4.172040285927
C	-2.701379238079	-0.037233867445	2.267165483112
H	-2.625197829778	-0.590928818365	1.319400470579
H	-2.709833360172	1.039183259227	2.036008166917
H	-3.661493013810	-0.294397665387	2.744700503600
C	-1.760078748915	0.310111678322	4.548864817012
H	-1.822502320712	1.400542461595	4.418026478417
H	-0.964384552705	0.093262906648	5.273837020607
H	-2.712554683406	-0.025736817542	4.992246491189
C	1.813134042944	-1.877590680153	-2.829715584903
H	1.123843818442	-2.510624195157	-3.402614868547
H	1.676994100261	-2.113383587018	-1.763349149498
H	2.839323173134	-2.156934479488	-3.121318749934
C	1.678328086773	-0.086173649890	-4.594381462777
H	0.975748669796	-0.702785923883	-5.173152090906
H	2.692635530315	-0.311996098590	-4.964444455731
H	1.474612079525	0.973515819164	-4.812548912216
C	2.696236785108	0.396929209658	-2.361805104796
H	2.604970381065	1.480451619795	-2.523808508684
H	3.684084115345	0.069140756859	-2.724964724183
H	2.652014067469	0.211700083996	-1.276866805063
C	1.813134042944	-1.877590680153	2.829715584903

H	1.676994100261	-2.113383587018	1.763349149498
H	1.123843818442	-2.510624195157	3.402614868547
H	2.839323173134	-2.156934479488	3.121318749934
C	2.696236785108	0.396929209658	2.361805104796
H	2.652014067469	0.211700083996	1.276866805063
H	3.684084115345	0.069140756859	2.724964724183
H	2.604970381065	1.480451619795	2.523808508684
C	1.678328086773	-0.086173649890	4.594381462777
H	1.474612079525	0.973515819164	4.812548912216
H	2.692635530315	-0.311996098590	4.964444455731
H	0.975748669796	-0.702785923883	5.173152090906
C	-1.760078748915	0.310111678322	-4.548864817012
H	-0.964384552705	0.093262906648	-5.273837020607
H	-1.822502320712	1.400542461595	-4.418026478417
H	-2.712554683406	-0.025736817542	-4.992246491189
C	-2.701379238079	-0.037233867445	-2.267165483112
H	-2.709833360172	1.039183259227	-2.036008166917
H	-2.625197829778	-0.590928818365	-1.319400470579
H	-3.661493013810	-0.294397665387	-2.744700503600
C	-1.510938086916	-1.916663809151	-3.395293172081
H	-0.794056947864	-2.219648978192	-4.172040285927
H	-2.506103658267	-2.269957468561	-3.712738856192
H	-1.250863122153	-2.429061402714	-2.455485229452

Pd<sub>2</sub>\_d ! 2-A (C1): E(UPBE1PBE-D3(BJ)/def2SVP) = -1704.81581956

Pd	0.000000935910	-0.073029852800	-0.083970035072
N	-0.000033442385	-0.461130265146	-1.988454478792
P	2.300236719576	0.005282352675	0.200301076613
N	0.000000423154	0.069678284626	1.985515182735
P	-2.300231991316	0.005302202792	0.200322164577
C	2.386103323549	0.041843145042	1.990983109153
H	3.322245502330	0.060034231733	2.552229754804
C	-2.386102480084	0.041915588894	1.991004401179
H	-3.322242137230	0.060141568722	2.552253071632
C	1.185710788540	0.077191854567	2.638919126539
H	1.153041631720	0.111826598832	3.739394859430
C	-1.185703495205	0.077224354595	2.638933322631
H	-1.153017415387	0.111862436333	3.739408433434
C	3.196887010693	-1.552435753814	-0.353122889786
C	-3.094650292643	1.601125121950	-0.418174230176
C	3.094662641851	1.601141802944	-0.418117953956
C	-3.196888316669	-1.552420981725	-0.353066653023
C	3.349000915540	-1.561484730407	-1.873032111353
H	2.386540225184	-1.349059204135	-2.366739721878
H	3.683169363713	-2.560896879539	-2.197919420268
H	4.101827575469	-0.837798270006	-2.218744742271

C	2.257671446852	-2.692042198332	0.060914167395
H	1.302945422036	-2.633675831197	-0.482241221027
H	2.044896093582	-2.667556533398	1.140923621834
H	2.734274543452	-3.658442690845	-0.173740100527
C	4.544809038731	-1.739763442142	0.341742086077
H	4.433802813190	-1.754173385898	1.436226032712
H	5.272149551178	-0.961078271016	0.077190046128
H	4.974708697501	-2.709726314163	0.040254381394
C	-2.767883116144	1.804773688582	-1.898010846426
H	-3.237164228641	1.053299656212	-2.545670039533
H	-1.681574480870	1.762331081172	-2.063500484361
H	-3.127787618310	2.796578426243	-2.218531751640
C	-4.602585000520	1.647675344092	-0.185530775872
H	-5.140883705490	0.935029837522	-0.826606708697
H	-4.980640124418	2.655590845449	-0.426513418611
H	-4.863322977850	1.438805670750	0.863355341782
C	-2.414207233510	2.716100008983	0.383040508995
H	-2.651492394515	2.653213897108	1.454330879781
H	-2.753856974416	3.694219355416	0.004359273267
H	-1.318522273373	2.667864192578	0.278502842047
C	2.767798777734	1.804946593203	-1.897911713835
H	1.681471042469	1.762628086967	-2.063310338050
H	3.236955368231	1.053489518673	-2.545679695181
H	3.127760131442	2.796748771603	-2.218377362954
C	2.414310489059	2.716067489227	0.383238122520
H	1.318616300375	2.667855171525	0.278792532541
H	2.753943268758	3.694208919492	0.004598153121
H	2.651688195660	2.653098420658	1.454502753070
C	4.602613678402	1.647644867949	-0.185572978984
H	4.863423964208	1.438646518943	0.863268878782
H	4.980663916016	2.655585072126	-0.426461684494
H	5.140855173043	0.935072230043	-0.826775856247
C	-4.544956668549	-1.739541236396	0.341566781893
H	-5.272169307499	-0.960811279915	0.076785673993
H	-4.434160557162	-1.753837231025	1.436073019100
H	-4.974894490104	-2.709496119610	0.040107722048
C	-2.257839501993	-2.692052062573	0.061284098278
H	-2.045262404911	-2.667454939224	1.141330033276
H	-1.303007471086	-2.633830032516	-0.481700746621
H	-2.734476569491	-3.658441861607	-0.173344976276
C	-3.348717605733	-1.561638349691	-1.873003103292
H	-4.101414690618	-0.837922980559	-2.218940385130
H	-3.682916595521	-2.561057911768	-2.197837182991
H	-2.386142706295	-1.349352792107	-2.366549900767
H	-0.000118896891	0.429624151182	-2.517348306517

Pd<sub>3</sub>\_bs ! 1-A (C1): E(UPBE1PBE/def2SVP) = -2049.12956540

Pd	0.496308672901	-0.532239073110	-0.033814773456
P	2.746935634786	0.142108126626	0.002963019163
P	-1.504716208201	-1.750805110643	-0.156136325976
N	1.319617450128	-2.329850734129	-0.593410329481
N	-0.276952152782	1.089418275301	0.722565237191
C	2.669086893416	-2.464310256778	-0.614675272531
H	3.063120940705	-3.460474555564	-0.866800113369
C	3.518354481169	-1.439403391197	-0.338747186581
H	4.598827541918	-1.585993079810	-0.374870075464
C	3.361940490634	1.270404146692	-1.380618337032
C	3.305259193335	0.664277493904	1.725722397030
C	0.506309457153	-3.390404363174	-0.824331319716
H	0.993654522234	-4.333834426686	-1.113596146356
C	-0.846075501284	-3.324375033570	-0.703476328715
H	-1.466794520292	-4.200282071298	-0.896814130770
C	-2.780258593796	-1.251242844097	-1.447889920304
C	-2.247385908898	-2.052376652521	1.552031064393
C	-0.502144279807	2.281867771034	-0.045681792890
H	0.193820647992	3.058398740713	0.373611386398
O	-0.185231359841	1.928421666153	-1.308775564410
C	-2.643599346089	-0.727317605202	2.204573816187
H	-1.810153191136	-0.009546222641	2.178747549859
H	-2.913272604032	-0.913373845536	3.257663983348
H	-3.506216243516	-0.253832764817	1.719864148031
C	-1.115382133208	-2.678684926076	2.373262280564
H	-0.238087427095	-2.014456809046	2.414826493310
H	-0.790623874790	-3.642805549044	1.956417174249
H	-1.467247070919	-2.844135500519	3.404706463233
C	-3.433646983090	-3.013124107874	1.500569600538
H	-3.173036236231	-3.962901558911	1.008720116187
H	-4.297989739367	-2.575984059481	0.980749364524
H	-3.755007516490	-3.250167993619	2.528732416915
C	-3.743773374135	-0.196817412444	-0.911056972275
H	-3.219186288055	0.649447659366	-0.448751002962
H	-4.451836747084	-0.615622300218	-0.181495179950
H	-4.335721274899	0.207361222517	-1.748351785227
C	-3.559526324937	-2.465558606263	-1.957504973095
H	-2.896307992061	-3.197855233291	-2.439282851417
H	-4.285370922324	-2.125736559181	-2.714870690257
H	-4.124027418751	-2.975472962818	-1.164427324549
C	-1.954109714528	-0.663478519134	-2.597558740717
H	-1.437388643715	0.259028584584	-2.292123726760
H	-2.625151483041	-0.431983406915	-3.441777271237
H	-1.199483102974	-1.383014207744	-2.953869050884
C	2.938096087657	-0.515505478464	2.632085625314

H	3.185175191908	-0.260797298397	3.675753239655
H	3.484015676409	-1.429172694864	2.356047830923
H	1.860221036750	-0.735377511511	2.580970931457
C	2.524028368290	1.894787261143	2.188428526074
H	2.786130349817	2.113919240132	3.236891658970
H	1.438909086431	1.716040164388	2.134467825362
H	2.755430895588	2.789338639143	1.595534287812
C	4.808731555674	0.921176936126	1.801986977859
H	5.100486032591	1.825616488370	1.249715295502
H	5.394182727942	0.072114936389	1.417458180940
H	5.098323115447	1.073270355939	2.855297130580
C	3.029040699892	2.735506773558	-1.111968573013
H	3.292507856841	3.327273051019	-2.004306661409
H	3.601855705080	3.146423563657	-0.268006441212
H	1.953040341572	2.868289532792	-0.936619260650
C	4.863380299972	1.102604370172	-1.621542244428
H	5.474536957336	1.422972094074	-0.767449054132
H	5.151063292947	1.725315228204	-2.484934730033
H	5.122060638554	0.062619323514	-1.866666258938
C	2.600275632510	0.793155389579	-2.623099476921
H	2.961098504912	1.354269752195	-3.501214780060
H	1.522261088447	0.972590535118	-2.510747257232
H	2.771559298298	-0.277985263118	-2.811587659801
C	-1.923761891057	2.798792669714	0.132028106003
C	-4.544814392869	3.730920172658	0.413351831152
C	-2.510434272191	2.874076028357	1.397114012769
C	-2.648004729900	3.205787526454	-0.988279186172
C	-3.954613007216	3.671963190391	-0.848259277313
C	-3.818312566924	3.332990237199	1.536911099237
H	-1.939169421871	2.551071456339	2.271056200788
H	-2.176231516088	3.128294062131	-1.970328807310
H	-4.518277711166	3.984974026373	-1.730908712991
H	-4.276483948653	3.378171047811	2.528239949134
H	-5.571473948727	4.088847555037	0.523272275753

Pd<sub>3</sub>\_t! 3-A (C1): E(UPBE1PBE-D3(BJ)/def2SVP) = -2049.13823316

Pd	0.506883539112	-0.545002927745	-0.022637757228
P	2.748147361438	0.153370055100	0.010736659543
P	-1.486860941631	-1.767760797132	-0.155491652929
N	1.341937525184	-2.334820578073	-0.559610800594
N	-0.289805081779	1.096956901834	0.666000923821
C	2.693461879525	-2.457842725997	-0.584288067323
H	3.093997859548	-3.452312769444	-0.832023812581
C	3.534214437682	-1.424062242140	-0.318345968497
H	4.615836933305	-1.561566181314	-0.355120329543
C	3.339460456110	1.276752430571	-1.385921496437



C	3.306972715127	0.695763775173	1.726362078683
C	0.535814687470	-3.399778365460	-0.798881079446
H	1.031599278136	-4.339877974844	-1.083977477557
C	-0.817879001733	-3.340481113029	-0.692259912194
H	-1.432780416358	-4.219430970176	-0.890289254479
C	-2.738044135556	-1.258364954360	-1.466487505969
C	-2.254634362903	-2.069520514376	1.540771380773
C	-0.521979683357	2.324432129226	-0.067247005730
H	0.160023060704	3.085534525588	0.403652973002
O	-0.192317114381	2.010816033558	-1.321751437079
C	-2.651554285491	-0.744188688420	2.192468842700
H	-1.808886573782	-0.037494603552	2.196909799852
H	-2.952243242002	-0.934344765104	3.236325730979
H	-3.493163076912	-0.253807320838	1.688276397412
C	-1.139506645045	-2.706718778888	2.376548388957
H	-0.255431352986	-2.052023308686	2.428076809043
H	-0.819769419528	-3.674557442036	1.964638114923
H	-1.505620166406	-2.867497246961	3.403759308709
C	-3.447159162397	-3.021224617966	1.467531049926
H	-3.185115794825	-3.971591285576	0.977637439669
H	-4.299368066401	-2.576793660021	0.934109033686
H	-3.787281139112	-3.258700495051	2.489513906873
C	-3.715067284653	-0.212258254217	-0.938083000431
H	-3.201878416002	0.634736538813	-0.464400160907
H	-4.432660024020	-0.638144007907	-0.222019776146
H	-4.295473192105	0.193840462374	-1.782406200644
C	-3.502318305473	-2.471452912559	-2.000780078603
H	-2.826857290805	-3.196534854104	-2.476495372085
H	-4.216174612606	-2.128486912006	-2.767976283020
H	-4.078327846998	-2.990708865143	-1.221949875807
C	-1.891469273081	-0.654867548054	-2.593261562490
H	-1.388618077620	0.270623689998	-2.271172874298
H	-2.546612045587	-0.421868872390	-3.449476131940
H	-1.124574142567	-1.366134669074	-2.940156683807
C	2.969233990682	-0.484374440692	2.643573811831
H	3.211962797827	-0.215271268442	3.684653838190
H	3.535898274737	-1.387299301298	2.374325861032
H	1.896783454877	-0.730925903645	2.596128129285
C	2.506278826671	1.914865402645	2.186204908795
H	2.778493815401	2.152179393894	3.228064454636
H	1.424936125740	1.714033284273	2.150590689672
H	2.707964516024	2.806823197957	1.578953131084
C	4.805685506086	0.982785125574	1.789179937172
H	5.075903729775	1.886412468678	1.224716483377
H	5.404604116594	0.141006271676	1.409469130735
H	5.099871940941	1.151666832160	2.838648053864

C	3.001411813654	2.741686255625	-1.122250311737
H	3.267236425184	3.329691256321	-2.016402471350
H	3.570486898526	3.158172791788	-0.278396337813
H	1.922620218708	2.869182162446	-0.957201678803
C	4.838427696707	1.112468005056	-1.643495303810
H	5.458496094572	1.437692939834	-0.797497051295
H	5.113816972664	1.733575687160	-2.511951015868
H	5.097718654602	0.072530017376	-1.888368314989
C	2.560703815142	0.789737001788	-2.613998732037
H	2.908153709016	1.345732242133	-3.500699286530
H	1.484678185147	0.972775239032	-2.484981891716
H	2.730275716486	-0.282458365504	-2.798834624427
C	-1.953430828729	2.808625353760	0.132672650480
C	-4.592418255699	3.679051063336	0.438665750079
C	-2.532470909545	2.862318128920	1.402300380275
C	-2.694101238671	3.206336964761	-0.979698372369
C	-4.009716669043	3.642423001353	-0.827425310749
C	-3.849578520426	3.289930704200	1.554793119089
H	-1.948521221407	2.548900914398	2.271872139293
H	-2.221799442124	3.143880860259	-1.962560342314
H	-4.586664959314	3.949479712317	-1.703634210658
H	-4.301855690144	3.318445932772	2.549486528570
H	-5.626035432281	4.013186778839	0.558234326373

Pd<sub>4</sub>\_s ! 1-A (C1): E(RPBE1PBE-D3(BJ)/def2SVP) = -2049.27953202

Pd	0.075104367141	-0.825169079465	-0.149040970274
N	0.070476241353	1.178526118838	-0.362727009850
P	2.382082410356	-1.008435492128	-0.038453241680
N	0.148335220428	-2.851100471718	-0.136093389473
P	-2.247660009644	-1.181777953293	-0.091959881054
C	2.536920623857	-2.789424501907	-0.143988434388
H	3.488564708298	-3.323175194829	-0.141759565064
C	-2.234679754366	-2.973738413070	-0.223633251213
H	-3.138770183102	-3.581818252537	-0.282421918943
C	1.356399000896	-3.468016873950	-0.160929637009
H	1.346835881663	-4.567793723979	-0.196692773264
C	-1.009866581697	-3.560047513504	-0.210323579584
H	-0.913495092709	-4.654812227816	-0.262590695687
C	3.348334462316	-0.304459132446	-1.494432355111
C	-3.111963285680	-0.828760471617	1.551013999363
C	3.068769821465	-0.499628210210	1.641656736232
C	-3.192095686813	-0.550285408847	-1.593184733569
C	3.561464087765	1.201057638087	-1.342324607517
H	2.627873660019	1.726132689820	-1.092966703554
H	3.942810687809	1.612324237816	-2.291705840652
H	4.301256911244	1.435230394802	-0.563686458281

C	2.460229910650	-0.580481490675	-2.713395516701
H	1.507022650948	-0.034242313599	-2.655462778059
H	2.225641113412	-1.652501897662	-2.802866541184
H	2.984716760005	-0.265257764498	-3.630715896853
C	4.687563556634	-1.014954633652	-1.695395265228
H	4.548980903845	-2.093370629932	-1.859614922027
H	5.370685563416	-0.878181976003	-0.846882422250
H	5.183566456120	-0.603529668534	-2.590529433264
C	-3.599535368852	0.614419679405	1.654366904922
H	-4.436142022093	0.820586303798	0.971021200508
H	-2.783685994476	1.330681722884	1.483355295714
H	-3.968614363558	0.783945359905	2.679639944170
C	-4.273875249906	-1.795804405712	1.785613482818
H	-5.067281605437	-1.702120329958	1.030733573372
H	-4.724350074056	-1.573923936371	2.767390247916
H	-3.933762231124	-2.841029237996	1.804678954326
C	-2.024974731364	-1.071691872029	2.605058518995
H	-1.590919905886	-2.080119131395	2.511877689633
H	-2.471846159199	-0.987697552376	3.609935338946
H	-1.229195703252	-0.317118421299	2.511689368814
C	2.719330249612	0.955606139845	1.958544322554
H	1.631541467969	1.112596515413	1.993259367285
H	3.151349361037	1.667649964504	1.243865717078
H	3.124679750948	1.203083449851	2.953996374411
C	2.341550621699	-1.394912253866	2.651444318471
H	1.249184577457	-1.284349510997	2.566322250438
H	2.633124796178	-1.092758702641	3.670465466748
H	2.592215050905	-2.456728435219	2.516746221400
C	4.575203710403	-0.732145460150	1.738673741550
H	4.855871531567	-1.760022159965	1.461298656883
H	4.899497555910	-0.570477421475	2.780296497551
H	5.143530679340	-0.031853993372	1.109511721932
C	-4.645446875925	-1.018391146777	-1.611950533409
H	-5.234360819783	-0.564523587492	-0.802152499462
H	-4.727304652670	-2.113053603843	-1.531463038588
H	-5.113948800445	-0.720705803837	-2.565285786204
C	-2.444355724020	-1.134399917938	-2.796595636664
H	-2.473666935075	-2.233727443589	-2.801979095217
H	-1.386366565002	-0.826688532553	-2.795036277374
H	-2.907728365073	-0.767618438010	-3.727348655790
C	-3.115921982010	0.976202811629	-1.663945882464
H	-3.694808870764	1.465792897023	-0.871148830692
H	-3.522780336810	1.313928035840	-2.631681443543
H	-2.077362116460	1.324478589693	-1.579731464646
O	-0.556780027673	1.775520383896	1.729707289437
C	-0.252373786908	2.072762838001	0.566658988301

H	0.357213903586	1.568457498315	-1.252367232682
C	-0.226681746051	3.534264240652	0.179055212009
C	-0.180116855215	3.998325273111	-1.140936895495
C	-0.271742093020	4.468464492356	1.219057337361
C	-0.164366125557	5.364760188964	-1.413629605997
C	-0.249712893378	5.833680015632	0.950499450683
C	-0.194407693371	6.286327449307	-0.367899060719
H	-0.175748416427	3.295755707986	-1.978836969434
H	-0.329549887465	4.079654902623	2.237644314113
H	-0.134581705699	5.711824038199	-2.449399495135
H	-0.279438893587	6.551603111006	1.774036726349
H	-0.180928848763	7.357936844139	-0.581740345523

Pd<sub>5</sub>\_s ! 1-A (C1): E(RPBE1PBE-D3(BJ)/def2SVP) = -2049.16038914

Pd	0.523735886564	-0.572386821161	-0.041034608145
N	-0.403587116432	1.141393125017	0.382505261437
P	-1.409587204125	-1.907320672904	-0.007607382746
N	1.457215403699	-2.391095960023	-0.273408090128
P	2.726248613701	0.230937952133	-0.064122315224
C	-0.640166520447	-3.519923474928	-0.139981045567
H	-1.200415748038	-4.456068179084	-0.137182690097
C	3.587501155663	-1.319560745504	-0.336439679707
H	4.672266086553	-1.400304186665	-0.418414787958
C	0.715624114127	-3.523612675788	-0.264550302767
H	1.260290731148	-4.475449971454	-0.362650632208
C	2.808201092961	-2.433145843014	-0.381282051322
H	3.265703860123	-3.427007503750	-0.504233168639
C	-2.305240202579	-1.857530871280	1.649360596416
C	3.277914269102	1.362777519152	-1.477703308660
C	-2.584532143920	-1.821675153971	-1.485207470930
C	3.292826660996	0.837869609674	1.629432960634
C	-2.830658247037	-0.446273181978	1.922551667854
H	-2.044359825033	0.309820596361	1.770544681958
H	-3.169358287641	-0.386409484770	2.970393147555
H	-3.686036010072	-0.180458180711	1.288510192743
C	-1.218690906766	-2.178403373535	2.681609849430
H	-0.397515184654	-1.446239271559	2.631962336833
H	-0.791177574963	-3.180249399278	2.529995098065
H	-1.655897923329	-2.132710951211	3.692506067043
C	-3.425995418700	-2.889349813862	1.744666045610
H	-3.069760363209	-3.907159524422	1.522716431222
H	-4.260656070223	-2.655853876571	1.068007321410
H	-3.830169542765	-2.896173730219	2.770984903137
C	3.163865617239	2.848506902611	-1.141201204185
H	3.900622940776	3.159648038627	-0.386790569769
H	2.157063391378	3.107658123583	-0.790588505679

H	3.369791513194	3.431047145173	-2.054928720822
C	4.710635317721	1.041501893009	-1.908279770573
H	5.437426615133	1.190686485182	-1.096623597608
H	4.993977937528	1.714629871103	-2.734708506862
H	4.803982524561	0.008108136858	-2.270402884988
C	2.317491652274	1.026058549697	-2.623610007662
H	2.313997654677	-0.053126948289	-2.844180321824
H	2.627545213729	1.561340140092	-3.536806089871
H	1.292768805506	1.334457926797	-2.370516533074
C	-3.623430635838	-0.716515440196	-1.321029437755
H	-3.177248174654	0.240604782593	-1.021347694482
H	-4.388777931440	-0.979003201709	-0.576881598942
H	-4.141554195454	-0.557215503775	-2.281432043140
C	-1.672416600064	-1.508793403520	-2.676683498911
H	-1.191083792200	-0.525270660557	-2.572134077591
H	-2.264577848544	-1.510329553969	-3.607061783093
H	-0.874554444345	-2.260900376184	-2.776635670514
C	-3.282378924717	-3.158569760619	-1.740301367217
H	-2.557219840824	-3.957540816821	-1.949704334223
H	-3.935046769006	-3.060080044099	-2.624010241601
H	-3.912363313192	-3.474219843158	-0.897551058009
C	4.786154128632	1.157631468079	1.654881378942
H	5.038539035585	2.021937671316	1.024271919064
H	5.393188230639	0.299122368726	1.328601986176
H	5.090364625956	1.404247617185	2.686145354834
C	3.003098506304	-0.322762869431	2.587012241190
H	3.587892512447	-1.219102585203	2.335376745050
H	1.936632952764	-0.596900873000	2.568100480118
H	3.258567447037	-0.015169405795	3.614333460852
C	2.460100493828	2.043656806748	2.068635786074
H	2.632447377308	2.929699016793	1.445889494769
H	2.730726727543	2.304159093501	3.105686417537
H	1.384474346242	1.817557280776	2.036308563392
O	0.178309633243	2.376080318775	-0.183306969432
C	-1.051937600322	1.901316820841	-0.623109680825
H	-1.056837764955	1.524943125407	-1.659897036367
C	-2.259807662360	2.698533039468	-0.267349258599
C	-3.251758013191	2.952823636070	-1.215292803166
C	-2.402708983552	3.200678270075	1.030356478004
C	-4.385929406820	3.688645878474	-0.871344657058
C	-3.531184860814	3.936750748695	1.373770959856
C	-4.527458373207	4.179556992783	0.424503535959
H	-3.136010705390	2.568456548200	-2.232935888230
H	-1.612333473108	2.994806360006	1.755406942305
H	-5.159396215076	3.881175809436	-1.618776353456
H	-3.639631200462	4.326191517342	2.389098064367

H -5.414646384707 4.756309130518 0.697372450725

Pd<sup>d</sup>TS1\_t! 3-A (C1): E(UPBE1PBE-D3(BJ)/def2SVP) = -2049.10129037

Pd	-0.000016662631	-0.755182927190	-0.057933600166
N	-0.000129063406	0.080603205207	1.671941311288
P	2.321979550601	-0.987235927041	-0.268894724849
N	0.000017434163	-1.920757679120	-1.783053202253
P	-2.321978573801	-0.987252937179	-0.268829387460
C	2.384490376729	-2.017836491852	-1.734658985568
H	3.316562618336	-2.367281591587	-2.182688638621
C	-2.384422664624	-2.018547044987	-1.734106310913
H	-3.316481381403	-2.368307258940	-2.181910464377
C	1.183225812298	-2.344052315857	-2.289235348956
H	1.145014744412	-2.985422677180	-3.183911744431
C	-1.183176064716	-2.344499975067	-2.288885492602
H	-1.144979140952	-2.986009024060	-3.183463352783
C	3.315057432402	0.562216723220	-0.675818346938
C	-3.068033562006	-2.006884458124	1.129065700180
C	3.067685081516	-2.007780733361	1.128536110790
C	-3.314823719254	0.562119888289	-0.676770688477
C	3.140493562923	1.602755143931	0.430377043852
H	2.085209093992	1.719204549418	0.706892658574
H	3.508493410973	2.580629653500	0.079462185008
H	3.697565900211	1.343308991850	1.339304804896
C	2.689261724326	1.086737465406	-1.973473283449
H	1.600150842700	1.206262486286	-1.877600022931
H	2.874853057365	0.404141914072	-2.814819918374
H	3.120802172061	2.071772215247	-2.214918267144
C	4.797897657383	0.283267480674	-0.912518342169
H	4.957768675572	-0.517618729697	-1.650417059316
H	5.319967592946	0.013152354977	0.016002184502
H	5.279834422986	1.194860913224	-1.304183422444
C	-3.250124622484	-1.144283942210	2.376625367224
H	-4.090066399287	-0.442262089097	2.275915215935
H	-2.333472226075	-0.578133450094	2.608184176993
H	-3.471043245686	-1.796254872280	3.238001210453
C	-4.376759417365	-2.686085790369	0.727932689173
H	-5.182891764794	-1.970542129116	0.521112350523
H	-4.714006114241	-3.332946266073	1.555083757126
H	-4.242580711999	-3.324601757229	-0.157845865019
C	-2.019225042049	-3.086115446690	1.418657542247
H	-1.772046863990	-3.666143975994	0.515988120944
H	-2.414855575775	-3.782075236478	2.176870969201
H	-1.093999922502	-2.639682461386	1.809380622893
C	3.249138978448	-1.146025860160	2.376777334455
H	2.332320752489	-0.580137186971	2.608332831469

H	4.089034309310	-0.443823324533	2.276919688215
H	3.469781473809	-1.798560692292	3.237797699659
C	2.018939981333	-3.087394471250	1.416940050722
H	1.093349193073	-2.641417285022	1.807309879048
H	2.414268664809	-3.783649487145	2.175039064623
H	1.772454522586	-3.667010492983	0.513818827761
C	4.376663387808	-2.686525431971	0.727456878485
H	4.242985867985	-3.324247987150	-0.158970918159
H	4.713521778285	-3.334118967473	1.554192236935
H	5.182856190760	-1.970741684795	0.521715060985
C	-4.797595264299	0.283123835320	-0.913857533882
H	-5.320004569123	0.013386517024	0.014586038805
H	-4.957221477269	-0.518042650287	-1.651508044058
H	-5.279375343917	1.194575214325	-1.306047857379
C	-2.688558129961	1.085988472412	-1.974463634507
H	-2.873892046721	0.402987027708	-2.815537442715
H	-1.599469620650	1.205501657966	-1.878288197245
H	-3.119983072797	2.070919563263	-2.216539083163
C	-3.140595150563	1.603181212058	0.428990078684
H	-3.698202470003	1.344331769688	1.337756550603
H	-3.508194766589	2.580958425677	0.077386022636
H	-2.085435741918	1.719565097161	0.706011926026
C	-0.000017760419	3.635863783454	0.839259070502
C	-0.000020522238	3.124562735451	-0.459907453660
C	0.000271164067	5.021001606896	1.049148545953
H	-0.000260511535	2.037822057352	-0.590691919931
H	0.000266337965	5.393195407302	2.076517820279
C	0.000257452778	3.988000441663	-1.551104335819
C	0.000560910292	5.883600133184	-0.041039928932
H	0.000247343928	3.586317174878	-2.567179183346
H	0.000795137181	6.965095355012	0.115619752071
C	0.000552153602	5.367016651657	-1.340020624029
H	0.000778364738	6.048197787178	-2.194752513033
C	-0.000313297467	2.704112749378	1.997351519774
H	-0.000300814628	1.310135360820	1.737008948265
O	-0.000446025456	3.043055068598	3.143763513281

**Pd**TS2\_bs ! 1-A (C1): E(UPBE1PBE/def2SVP) = -2049.10609566

Pd	0.508133251110	-0.556744280110	-0.023977437966
P	2.763104240870	0.142625726155	0.006561744937
P	-1.474677687543	-1.780738180226	-0.211816946440
N	1.349434967712	-2.316388039422	-0.736937482789
N	-0.297909398373	0.950572492314	0.734014434459
C	2.699834007771	-2.428363247799	-0.791359923105
H	3.109274963603	-3.396585081931	-1.118739182175
C	3.536800782675	-1.409207614435	-0.458948532327

H	4.618406123541	-1.537286251392	-0.522912352624
C	3.354228758917	1.372871705173	-1.297756302576
C	3.345537677135	0.546238779040	1.750985181910
C	0.534323320522	-3.352628179489	-1.047627690468
H	1.012378193946	-4.270148820765	-1.424689901074
C	-0.819180748878	-3.297131265169	-0.904220614373
H	-1.442565376974	-4.154485190290	-1.162444962841
C	-2.733101884185	-1.122632368149	-1.445663362170
C	-2.219510427889	-2.224745184685	1.461651847748
C	-0.540572670493	2.776007764756	-0.084596501013
H	0.113264021498	3.150805802241	0.738709436912
O	-0.102732160161	2.665645310393	-1.232168183430
C	-2.603315215724	-0.958845019672	2.231168514930
H	-1.771232090456	-0.238124192580	2.252749712410
H	-2.852255939882	-1.233584661038	3.269747916628
H	-3.474680576970	-0.447346398649	1.804940165975
C	-1.091071510646	-2.930520698010	2.221058156655
H	-0.210428171912	-2.277050286299	2.322810231372
H	-0.771283890870	-3.853425906445	1.716435226104
H	-1.443479148030	-3.188986028414	3.232962084157
C	-3.413081040246	-3.167800164904	1.323069571452
H	-3.153203747672	-4.075770169997	0.757412558576
H	-4.268979590266	-2.683802537522	0.831390941723
H	-3.746752658173	-3.486335347056	2.324913638498
C	-3.708573224953	-0.151781662200	-0.788113170266
H	-3.191548842101	0.626888632978	-0.211971879957
H	-4.423958958515	-0.664969807153	-0.129662293181
H	-4.290998414207	0.357952014236	-1.572148426948
C	-3.495752184115	-2.267819148167	-2.114600822131
H	-2.820205432244	-2.927963484655	-2.677070413646
H	-4.221335965888	-1.843510535531	-2.828281909716
H	-4.058425422992	-2.879271885296	-1.394610187699
C	-1.900048168876	-0.382756942912	-2.499266624090
H	-1.410138251612	0.510314885043	-2.081968995030
H	-2.560537896357	-0.061399114402	-3.321903190315
H	-1.122035130605	-1.035415522633	-2.926705566628
C	3.003028263652	-0.693871395091	2.582862043621
H	3.274941919129	-0.510935135182	3.635405095759
H	3.543361583321	-1.584853833120	2.231624831278
H	1.924219588697	-0.912961629261	2.543030560340
C	2.555419469745	1.735593067638	2.300554065077
H	2.803521228164	1.872468336606	3.366266940049
H	1.471150412822	1.562218888440	2.216816218528
H	2.790238707960	2.673673806970	1.781510525620
C	4.847651203276	0.812342141761	1.819120685433
H	5.127149751587	1.737382001438	1.295232999931



H	5.432199371203	-0.018831083914	1.395860101030
H	5.151083478179	0.927343027074	2.873288597955
C	3.132737754669	2.821816991424	-0.872063330000
H	3.392362178588	3.477680784549	-1.719600873105
H	3.774074941257	3.112534600936	-0.027407251923
H	2.076970559195	3.010726882219	-0.635573518315
C	4.826328383787	1.145128028523	-1.648055287301
H	5.499743614758	1.302373781906	-0.794141649442
H	5.114903319023	1.863598678432	-2.433083431245
H	4.997262119395	0.134819083700	-2.045768618441
C	2.488625964865	1.063098274805	-2.525121905031
H	2.847747321473	1.661838723541	-3.378767450197
H	1.438347452513	1.327282813601	-2.337496478955
H	2.554980847248	0.000047432531	-2.805953421829
C	-2.006873160710	2.953728611722	0.171599246881
C	-4.746940905671	3.318629688832	0.575432101241
C	-2.544413662593	2.868639834807	1.459467369486
C	-2.844663814468	3.238571075096	-0.908868403368
C	-4.210579926062	3.425145424539	-0.707330794018
C	-3.910766718335	3.040856612219	1.659826041349
H	-1.882171455037	2.636951157413	2.297694097080
H	-2.395216077513	3.303693888872	-1.902362297340
H	-4.862374268098	3.651130324783	-1.555131102612
H	-4.330223336555	2.958394913508	2.665654676840
H	-5.819322548262	3.457001827330	0.734326391921

<sup>Pd</sup>TS2\_t! 3-A (C1): E(UPBE1PBE-D3(BJ)/def2SVP) = -2049.12128300

Pd	0.518625530362	-0.562083437638	-0.025949427078
P	2.763829483096	0.148757658483	0.011284340512
P	-1.466067804092	-1.781541959624	-0.204672865759
N	1.360986865770	-2.322983915371	-0.700412652299
N	-0.290888354980	0.999211925902	0.688984486734
C	2.712436129155	-2.431663059830	-0.750350338199
H	3.123732576985	-3.403210178448	-1.064891037642
C	3.546264615551	-1.406525854796	-0.429267532922
H	4.628329393400	-1.533276737608	-0.488319220730
C	3.346292242988	1.361825841146	-1.313048048238
C	3.346014364328	0.583162931451	1.748273312529
C	0.548114716165	-3.363504834407	-1.006011672074
H	1.030913627807	-4.284251684658	-1.368493298343
C	-0.806192387468	-3.306853944098	-0.875546121150
H	-1.426500744761	-4.167790687676	-1.129215010850
C	-2.725255974152	-1.145601147787	-1.450295960858
C	-2.216323246994	-2.212099528730	1.470443213465
C	-0.555797853916	2.771099693290	-0.090609379382
H	0.092151669593	3.211793319787	0.704999796759

O	-0.128022508365	2.633556733016	-1.243079861127
C	-2.601118077049	-0.939669158975	2.228668634188
H	-1.762266305455	-0.228497196419	2.265281096676
H	-2.873101967479	-1.208382205065	3.263075768267
H	-3.457905815617	-0.418886152941	1.784529342575
C	-1.091435811360	-2.912790261441	2.239739300079
H	-0.206708660215	-2.263177219541	2.331512154289
H	-0.776894749918	-3.844473021411	1.748232989043
H	-1.444580082257	-3.154942641616	3.255455300209
C	-3.410854787489	-3.154648300686	1.337755471166
H	-3.151079610911	-4.067200077383	0.779518268715
H	-4.265599501642	-2.673828125365	0.841032847308
H	-3.746309155495	-3.465235473757	2.341549343278
C	-3.709702218323	-0.172805890747	-0.808758755587
H	-3.200921220672	0.618311609206	-0.242442217458
H	-4.423353642397	-0.681590379543	-0.145006482463
H	-4.293758551302	0.321553140081	-1.601479509819
C	-3.478821893374	-2.302162340507	-2.109642173014
H	-2.797352640576	-2.964579939571	-2.662193826975
H	-4.203946626220	-1.889978698831	-2.830888305774
H	-4.040789858729	-2.908908187162	-1.385154846848
C	-1.891832840379	-0.412392728714	-2.508458195802
H	-1.408361181027	0.488220431877	-2.099474335584
H	-2.550513168097	-0.103766946663	-3.337450055926
H	-1.108723020901	-1.065607180481	-2.925687229976
C	3.011729827910	-0.646092540091	2.599448486910
H	3.279178829594	-0.444395351317	3.649726875029
H	3.560406465662	-1.537943906042	2.263789081254
H	1.934994341306	-0.875731367080	2.560105123587
C	2.550641964201	1.776697007860	2.281400453344
H	2.807255309730	1.936963273014	3.341834771742
H	1.467282976090	1.594766292153	2.212108423875
H	2.771760097137	2.706211529599	1.741505479730
C	4.846452997210	0.859704110085	1.811630687166
H	5.119701315383	1.779102236503	1.274655590009
H	5.435782164527	0.026478336981	1.399222916266
H	5.150271635624	0.991069430280	2.863803600129
C	3.112007160734	2.815686867754	-0.911435834772
H	3.370430753992	3.459661576215	-1.768440703046
H	3.747554012132	3.125313856830	-0.069086598651
H	2.053125125136	2.999363602541	-0.683495635556
C	4.820010763025	1.139684995518	-1.659591662062
H	5.492160140810	1.318087682608	-0.808850093112
H	5.102915825701	1.845824436963	-2.457770262350
H	4.999106468893	0.123531985008	-2.038505987769
C	2.482584932626	1.026673931794	-2.535140194274

H	2.837572335379	1.614385514372	-3.398134895072
H	1.430568520206	1.286964909843	-2.350917375235
H	2.555771050751	-0.040141893583	-2.799588581968
C	-2.025567892141	2.947596940204	0.167249584541
C	-4.766345402764	3.309431138225	0.569911037419
C	-2.563024682733	2.865766334043	1.454951257232
C	-2.863497296915	3.227279129908	-0.913910698831
C	-4.230003701666	3.412282071563	-0.712993135081
C	-3.929648902540	3.036651403524	1.655180962414
H	-1.900960981700	2.638469999894	2.294814709221
H	-2.413873807332	3.288045114258	-1.907591522687
H	-4.882102069322	3.633725760381	-1.561767729959
H	-4.348854705517	2.956748886653	2.661343645819
H	-5.838976126368	3.446358204364	0.728329023051

**PdTS3\_bs ! 1-A (C1): E(UPBE1PBE/def2SVP) = -2049.12505205**

Pd	0.505122303034	-0.558843340700	0.054801928937
P	2.735161673582	0.180328617450	0.037298852660
P	-1.461159424001	-1.827037673548	-0.062759592168
N	1.393209522296	-2.390834305470	-0.278301997342
N	-0.317348012215	1.093609252214	0.608593931050
C	2.745580541333	-2.484172304276	-0.260944699062
H	3.175761899369	-3.489904081976	-0.383432005397
C	3.558515170560	-1.405795671476	-0.099740661786
H	4.643459978566	-1.521089838012	-0.097268778528
C	3.297525069645	1.138265691927	-1.490031748013
C	3.281478597595	0.944331350390	1.669403502918
C	0.613203522419	-3.492464603354	-0.401965304665
H	1.129284440876	-4.453248651884	-0.550689109954
C	-0.744734155112	-3.444926942730	-0.342454803676
H	-1.340127431269	-4.353551636730	-0.442504121650
C	-2.602162407735	-1.518015723552	-1.529301940911
C	-2.358279976574	-1.912157568865	1.592233171115
C	-0.629006183270	2.116442239589	-0.339535870577
H	0.150434274918	2.887473071267	-0.060692286870
O	-0.424193165484	1.790774540699	-1.613008118373
C	-2.819194798886	-0.518850400558	2.019738602724
H	-1.989145405439	0.202213792214	1.972682708616
H	-3.183251230263	-0.564058675590	3.059727776124
H	-3.635896714256	-0.128714582952	1.399911411608
C	-1.299690384448	-2.401113572038	2.586884437704
H	-0.434780212614	-1.719599527933	2.614349003274
H	-0.931915614334	-3.406082793931	2.334402955624
H	-1.741257445924	-2.432993840204	3.596366017135
C	-3.530376354746	-2.891002555975	1.564976261921
H	-3.225293682127	-3.892315579879	1.224098169375

H	-4.348674789075	-2.536676467156	0.922060041731
H	-3.937931939353	-2.998163657783	2.584182039006
C	-3.580285261813	-0.380985951030	-1.251455333361
H	-3.074659116792	0.521272315997	-0.882055572674
H	-4.358812687409	-0.668523105736	-0.530159117525
H	-4.087868002431	-0.106988179317	-2.190784650575
C	-3.361508728261	-2.789394013378	-1.916231811514
H	-2.674368890573	-3.596075714295	-2.208612279095
H	-4.001584082904	-2.566490840166	-2.785927035040
H	-4.013296606131	-3.160378998596	-1.113353435583
C	-1.666955052999	-1.122748895119	-2.677408999676
H	-1.194025298114	-0.147805362455	-2.486218863763
H	-2.252559779535	-1.050678020446	-3.609109562360
H	-0.877073873639	-1.875244453173	-2.831068774897
C	2.960620729043	-0.119225771202	2.725058950017
H	3.196643007533	0.280203653117	3.725042185595
H	3.542409233355	-1.039136290932	2.569356706722
H	1.892054472453	-0.386003648107	2.707697265237
C	2.452080747259	2.193519249282	1.972030899981
H	2.704051122035	2.556647040947	2.982303697184
H	1.374840098234	1.965964698067	1.945856498632
H	2.651774404943	3.012836143951	1.268737194863
C	4.773993065429	1.265948463041	1.697078638558
H	5.030038300891	2.093562819318	1.020136256451
H	5.390364805487	0.393713687589	1.430876939469
H	5.061102909137	1.575641170172	2.715982413308
C	2.942841288549	2.620032075919	-1.404100149118
H	3.185933207782	3.098942648699	-2.366939321235
H	3.513956388084	3.144844455612	-0.624733282812
H	1.867124941927	2.763608494804	-1.235644477179
C	4.796547300618	0.967550038704	-1.741607588258
H	5.416912112364	1.395060362673	-0.942410938757
H	5.058591021633	1.487875341013	-2.677861368199
H	5.067295460176	-0.090608644004	-1.865939882158
C	2.514569282984	0.498210981505	-2.642629433233
H	2.846935782023	0.944946456621	-3.594550938168
H	1.436434903422	0.681577324276	-2.527149706943
H	2.693882772624	-0.586767364168	-2.696506206756
C	-1.984291273062	2.765348791916	-0.034294731700
C	-4.463193198639	3.971908591211	0.436518062470
C	-2.423782991422	2.980748891448	1.274221495429
C	-2.781991657639	3.171402949263	-1.103553060269
C	-4.020185740425	3.768461147315	-0.869439984999
C	-3.659109168760	3.580841618435	1.508052415541
H	-1.793498105187	2.662544555254	2.107514336815
H	-2.412681616270	2.994452014880	-2.115941950178

H	-4.643304698114	4.076708451014	-1.713002553389
H	-3.999616556564	3.741408189627	2.534221253127
H	-5.434054579343	4.438463190810	0.621093216972

**PdTS4\_bs ! 1-A (C1): E(UPBE1PBE/def2SVP) = -2049.12135195**

Pd	0.061108034650	-0.777985557953	0.065119419384
P	2.395613559763	-0.952288275915	0.048899249364
P	-2.260242599306	-1.188016909110	0.109179599205
N	0.160747823848	-2.820175113978	0.239370110761
N	-0.079741231274	1.149488138037	0.166289086800
C	1.373467181420	-3.418206695918	0.302125110696
H	1.382950596530	-4.511360952645	0.429941094231
C	2.543860874967	-2.728067166276	0.221684996005
H	3.501524615857	-3.246887664412	0.279495139707
C	3.289904456769	-0.533660961409	-1.568155314873
C	3.209557813343	-0.196989440100	1.569481419095
C	-0.985220692591	-3.532747158297	0.395515227325
H	-0.876216307297	-4.618446117734	0.538940664095
C	-2.217259525640	-2.961356950134	0.382091975112
H	-3.113001776661	-3.572081215060	0.503962560970
C	-3.224731136395	-0.972257459169	-1.498798043083
C	-3.103699559308	-0.428083312625	1.610759467307
C	0.183564528535	2.085137565319	-0.896203827902
H	1.233184871492	1.994215594329	-1.261770982794
O	-0.745080683766	1.552672870380	-1.714538669457
C	-3.052046808425	1.099559870866	1.541222735181
H	-2.030351109560	1.456198362902	1.338061057569
H	-3.377758491741	1.511348630089	2.511003301882
H	-3.717114918143	1.506987459321	0.769739091370
C	-2.262336563257	-0.891066638587	2.805230175483
H	-1.222891802396	-0.538441764394	2.716689584847
H	-2.245538346487	-1.987118346263	2.896394061006
H	-2.687002575944	-0.469738178620	3.731092538770
C	-4.541760402403	-0.917359059348	1.771072559230
H	-4.605343045331	-2.016027100301	1.799152722261
H	-5.193952807714	-0.549988733388	0.965745318382
H	-4.950779488543	-0.537430338668	2.722372383035
C	-3.737708429874	0.454928079701	-1.674936359046
H	-2.925584444335	1.185638025830	-1.555523583502
H	-4.557179392711	0.686355103777	-0.979034017382
H	-4.138014660168	0.560353250969	-2.697115663559
C	-4.385481176783	-1.965292912620	-1.585481590442
H	-4.032641028452	-3.006086593685	-1.560267305898
H	-4.907303613414	-1.813788171410	-2.545055901714
H	-5.124216485036	-1.828862675788	-0.783301354397
C	-2.203680366046	-1.291834135559	-2.597182216828

H	-1.403178860107	-0.538607615591	-2.613804299444
H	-2.712380838188	-1.288314897801	-3.575777495374
H	-1.756617071422	-2.288244514485	-2.451916898120
C	2.491361895447	-0.839504451776	2.760968332222
H	2.888638400996	-0.411849176942	3.695967017649
H	2.635430054046	-1.929163458184	2.786029573510
H	1.408717912904	-0.640356359828	2.727646245808
C	2.960029587060	1.311361825207	1.612730979294
H	3.317464552947	1.709091281400	2.576881232655
H	1.885357862611	1.540685864208	1.533242268134
H	3.489813100085	1.852757290351	0.818635675300
C	4.702212301176	-0.514328984722	1.637142861685
H	5.268481752717	-0.035677849620	0.825463630204
H	4.889836881738	-1.598274161703	1.599273734652
H	5.114464078380	-0.141092631683	2.589538952320
C	3.820033794017	0.897581861520	-1.620362261628
H	4.202891180925	1.096041401703	-2.634871212911
H	4.650653904430	1.061093944575	-0.919332517208
H	3.041335798379	1.644107622326	-1.415544059100
C	4.450054923177	-1.502264089394	-1.810222332494
H	5.211342570739	-1.454335400387	-1.017737043522
H	4.942868764456	-1.238826410767	-2.760861365727
H	4.098625111159	-2.540068565818	-1.890254130134
C	2.226398866676	-0.736390430449	-2.654351748117
H	2.686579061538	-0.608522756459	-3.648385182504
H	1.396259203089	-0.019322472983	-2.559633141898
H	1.799625370381	-1.750652876088	-2.606885304826
C	-0.056536540495	3.515135483157	-0.458092183756
C	-0.516188592024	6.123734896307	0.445640376396
C	1.006466899300	4.312418420236	-0.030612497023
C	-1.351668866379	4.036857764784	-0.442200597593
C	-1.581025055514	5.334167958829	0.008729925907
C	0.779988445161	5.610887212703	0.423820551051
H	2.024303977996	3.911498299899	-0.054256256683
H	-2.171317990903	3.408087892066	-0.795559967296
H	-2.597348793950	5.736419175986	0.017428391450
H	1.618781167934	6.227404066806	0.756808760260
H	-0.696678732952	7.142456490470	0.797695321249

**PhCHO\_s ! 1-A' (CS): E(RPBE1PBE-D3(BJ)/def2SVP) = -344.934123145**

O	1.434084702321	2.475527421502	0.000000000000
C	0.318366459465	2.020172377784	0.000000000000
H	-0.579688016574	2.691936900609	0.000000000000
C	0.000000000000	0.575656170632	0.000000000000
C	1.035101876884	-0.368041810438	0.000000000000
C	-1.332541106353	0.152292734895	0.000000000000

C	0.734693551968	-1.724455750344	-0.000000000000
C	-1.632977244241	-1.207448729841	-0.000000000000
C	-0.598842825239	-2.143444210210	0.000000000000
H	2.065969964745	-0.006287333102	0.000000000000
H	-2.134413909408	0.896851043010	0.000000000000
H	1.538971023276	-2.463882910621	-0.000000000000
H	-2.673338500266	-1.540318769148	-0.000000000000
H	-0.832982455241	-3.210902997637	-0.000000000000

**PhCO\_d ! 2-A' (CS): E(UPBE1PBE-D3(BJ)/def2SVP) = -344.283193896**

O	-1.376133900742	2.580558869433	-0.000000000000
C	-0.315299655157	2.055474420011	-0.000000000000
C	-0.000000000000	0.613385418537	-0.000000000000
C	-1.036314450830	-0.333346570599	-0.000000000000
C	1.334968317672	0.196724183374	0.000000000000
C	-0.730277436943	-1.688579878331	0.000000000000
C	1.636449212882	-1.162390348103	0.000000000000
C	0.604935724632	-2.101304579399	0.000000000000
H	-2.071174719542	0.016986773111	-0.000000000000
H	2.125600386010	0.950710255072	-0.000000000000
H	-1.531808477107	-2.431101421617	0.000000000000
H	2.677500627054	-1.492775755169	0.000000000000
H	0.842183115980	-3.168066679801	0.000000000000

**Pd1\_s\_h-truncated ! 1-A' (CS): E(RPBE1PBE-D3(BJ)/def2SVP) = -1076.20860483**

Pd	-0.007770476241	-0.694938916237	-0.000000000000
N	0.002359056128	-2.472003349646	-0.000000000000
P	-0.000361426740	-0.346233529856	2.301847923000
N	-0.002005497538	1.441739956804	0.000000000000
P	-0.000361426740	-0.346233529856	-2.301847923000
C	0.011176129336	1.439372668151	2.381171215000
H	0.025484770025	1.992439624841	3.321941752000
C	0.011176129336	1.439372668151	-2.381171215000
H	0.025484770025	1.992439624841	-3.321941752000
C	0.011176129336	2.093800719446	1.181959802000
H	0.022349328854	3.195322468367	1.157437419000
C	0.011176129336	2.093800719446	-1.181959802000
H	0.022349328854	3.195322468367	-1.157437419000
H	-1.188568318792	-0.780758388523	2.935017229332
H	1.189525567460	-0.823024134026	-2.900720494883
H	1.189525567460	-0.823024134026	2.900720494883
H	-1.188568318792	-0.780758388523	-2.935017229332

**Pd1\_t\_h-truncated ! 3-A" (CS): E(UPBE1PBE-D3(BJ)/def2SVP) = -1076.26355547**

Pd	-0.021903113550	-0.660391521088	0.000000000000
N	-0.158279311424	-2.546864116839	0.000000000000

P	0.025023451718	-0.365992546774	2.311192937996
N	0.039534819573	1.428990692317	-0.000000000000
P	0.025023451718	-0.365992546774	-2.311192937996
C	0.025023451718	1.426736904450	2.387181402007
H	0.032633568541	1.988711611776	3.323038887011
C	0.025023451718	1.426736904450	-2.387181402007
H	0.032633568541	1.988711611776	-3.323038887011
C	0.037369521954	2.078405549935	1.187735676011
H	0.045420016987	3.179936346739	1.161248302018
C	0.037369521954	2.078405549935	-1.187735676011
H	0.045420016987	3.179936346739	-1.161248302018
H	-1.140228899744	-0.796900550509	2.989444039392
H	1.231843029542	-0.811151961846	-2.903507388306
H	1.231843029542	-0.811151961846	2.903507388306
H	-1.140228899744	-0.796900550509	-2.989444039392

**Pd<sub>2</sub>\_d\_h-truncated ! 2-A (C1): E(UPBE1PBE-D3(BJ)/def2SVP) = -1076.90242126**

Pd	-0.000004147155	-0.628470525173	-0.000683354084
N	0.000022211851	-2.554862973592	-0.258937226064
P	-2.300238571910	-0.339542003969	0.058218509461
N	0.000002859022	1.445928088212	0.001568957753
P	2.300230139141	-0.339533981657	0.058201163393
C	-2.386100249267	1.449506149859	-0.026554013015
H	-3.322240829519	2.010699367435	-0.046400354630
C	2.386105555198	1.449517400815	-0.026520233140
H	3.322246810163	2.010709156670	-0.046346437208
C	-1.185705755625	2.098344883014	-0.035168581924
H	-1.153033474102	3.198640021847	-0.075128630865
C	1.185708528587	2.098353844175	-0.035155531764
H	1.153025573137	3.198648792411	-0.075111701763
H	-2.975038596784	-0.834450314272	-1.083172207636
H	2.896876740929	-0.721829965908	1.285422390985
H	-2.896871566627	-0.721772732823	1.285466975154
H	2.975015247247	-0.834421367885	-1.083207932904
H	0.000113386777	-3.022228484639	0.665585131153

**Pd<sub>3</sub>\_bs\_h-truncated ! 1-A (C1): E(UPBE1PBE/def2SVP) = -1190.56669138**

Pd	0.238470869667	-0.102158431927	-0.170422927270
P	0.589037725316	2.221178762966	-0.145410275304
P	-0.691795626575	-2.255883655635	-0.164239690924
N	-1.703178975589	0.453667292694	0.208319537490
N	2.018894917963	-0.630835446574	-0.762374277728
C	-2.028022484939	1.770500187237	0.213531162961
H	-3.089582402869	2.017613904039	0.365841465118
C	-1.111155194300	2.758582053933	0.037819966085
H	-1.411463808790	3.807226676738	0.057175240040



H	1.256057363804	2.784059579519	0.968590408138
H	1.042463128068	2.706818954092	-1.395580891615
C	-2.655849284478	-0.503291402299	0.335668405508
H	-3.682234514071	-0.156827811718	0.529925911090
C	-2.388304301174	-1.831448923455	0.224636172947
H	-3.182556845054	-2.571349158114	0.332317568696
H	-0.281391113342	-3.163574413884	0.840600889152
H	-0.711219421630	-2.824499276425	-1.461514129533
C	3.150563791834	-0.695286305135	0.119681525734
H	3.858325181003	0.107816057742	-0.222772426024
O	2.634539218690	-0.446162730475	1.341327917617
H	3.683590439307	-1.672277994023	0.029356554101

**Pd3\_bs\_h-truncated ! 3-A (C1): E(UPBE1PBE-D3(BJ)/def2SVP) = -1190.57279322**

Pd	0.223748531664	-0.098428015643	-0.179946257655
P	0.555729276971	2.225513953687	-0.145526745247
P	-0.671913311430	-2.262956249763	-0.159663113816
N	-1.715339775761	0.432669288614	0.203426432023
N	2.024121347724	-0.612539118153	-0.727043664523
C	-2.054141511217	1.746912090091	0.221885612139
H	-3.117141093503	1.980237391960	0.384255341806
C	-1.149058663914	2.745505347764	0.048886484531
H	-1.460048726166	3.790803117217	0.077253066767
H	1.224614698762	2.778903383080	0.971574912181
H	0.998605730232	2.726639704378	-1.393205246990
C	-2.654357367617	-0.536233040970	0.347279210522
H	-3.682244858812	-0.200886576703	0.551875516615
C	-2.370952184460	-1.861337134302	0.241678618758
H	-3.154053269617	-2.611242660767	0.361121543011
H	-0.228669084310	-3.147214552727	0.851816600708
H	-0.694983895323	-2.846383384090	-1.450141025375
C	3.206414982871	-0.659382222896	0.108564191427
H	3.885986379166	0.142704583369	-0.292672477284
O	2.739192157848	-0.405092110351	1.332432322510
H	3.735822379431	-1.637202393532	-0.010405150228

**Pd4\_s\_h-truncated ! 1-A (C1): E(RPBE1PBE-D3(BJ)/def2SVP) = -1190.71623035**

Pd	0.195802543009	-0.089994694262	-0.175364946171
N	2.066947973723	-0.614047486271	-0.708901297356
P	-0.579682813812	-2.266557964064	-0.004605734105
N	-1.746752502270	0.379928362804	0.164606557524
P	0.489179119738	2.240877624448	-0.093959117772
C	-2.330211105919	-1.937082909007	0.180140821032
H	-3.092313302931	-2.711319967169	0.281523520866
C	-1.237867038193	2.710708218535	0.064784180832
H	-1.582429076004	3.745661625103	0.092081643010

C	-2.660965563695	-0.618289375999	0.256239572833
H	-3.709046247403	-0.314405784258	0.397877202174
C	-2.121434176619	1.687042741591	0.189367160281
H	-3.195793341753	1.888042279710	0.315385668029
H	-0.445549250166	-3.074577828058	-1.159637414861
H	1.109078149808	2.756631056208	1.068078237516
H	-0.154609073822	-2.903105239989	1.186201694874
H	0.951624091057	2.831991368574	-1.294293327670
O	3.134744574348	-0.231922387591	1.251181533477
C	3.150817356935	-0.569642083832	0.059802224059
H	2.219247199321	-0.967685085871	-1.645635031201
H	4.129067554571	-0.868477976676	-0.397714733933

**Pd<sub>5</sub>\_s\_h-truncated ! 1-A (C1): E(RPBE1PBE-D3(BJ)/def2SVP) = -1190.60319313**

Pd	0.222543055828	-0.104371065257	-0.080338352403
N	2.087287078130	-0.691892028302	-0.472645024674
P	-0.712794808152	-2.259826417829	-0.072641206651
N	-1.744517171510	0.464435993424	0.120203334280
P	0.584361979641	2.211934579831	-0.107564638048
C	-2.444963897260	-1.814341991894	0.032964880437
H	-3.254975471981	-2.545158955401	0.039426286344
C	-1.105973986250	2.762759668831	0.135981958369
H	-1.395814808485	3.812967259766	0.190851720832
C	-2.712044186619	-0.482404199745	0.124119639589
H	-3.752155575053	-0.130215138153	0.204187104403
C	-2.048143549601	1.783846221957	0.194600830029
H	-3.112857950949	2.042984575414	0.301452679649
H	-0.533970190325	-2.941912593792	-1.301219775953
H	1.324515793309	2.804671779822	0.942614689192
H	-0.489721935912	-3.086408825026	1.057806188072
H	0.961288700911	2.687978828895	-1.387207980991
O	3.180648833177	0.131024831000	0.084640977680
C	2.948685628254	-1.157324015438	0.552279064522
H	2.570532094192	-1.210948243203	1.587041615554
H	3.702731140988	-1.925732622651	0.313985127557

**Pd<sub>TS1</sub>\_t\_h-truncated ! 3-A (C1): E(UPBE1PBE-D3(BJ)/def2SVP) = -1190.53380405**

Pd	-0.079901818588	-0.000030128567	-0.145784283080
N	-1.883302313897	-0.000087441035	-0.808168106115
P	0.233844208341	-2.321987443924	-0.155646592567
N	1.957245062356	0.000151411200	0.283907114752
P	0.233245860602	2.321970633964	-0.155356559562
C	1.993671151211	-2.384309427483	0.181451461842
H	2.556443403070	-3.316319127493	0.260485770517
C	1.993217311857	2.384603648092	0.180918420194
H	2.555832439711	3.316724923136	0.259711588258

C	2.613559533107	-1.182982326579	0.353381249766
H	3.696565793301	-1.144654273632	0.550587431702
C	2.613350103997	1.183419578047	0.352996301842
H	3.696396848685	1.145339656133	0.550029499352
H	-0.390461195985	-3.068455281497	0.873650636878
H	0.053658399343	2.882598644078	-1.442893071235
H	0.055129170232	-2.882202185419	-1.443491646040
H	-0.390658787138	3.067947951768	0.874548331409
H	-3.892353473162	-0.000576450898	1.907563351872
C	-3.995313768006	-0.000279660510	0.781832443031
H	-2.812327233420	-0.000089440666	-0.000148398173
O	-5.035949746994	-0.000229376573	0.193428561072

**Pd<sup>Pd</sup>TS2\_bs\_h-truncated ! 1-A (C1): E(UPBE1PBE/def2SVP) = -1190.53570490**

Pd	0.168773131406	-0.119462966083	-0.226659939927
P	0.539116502520	2.212306887989	-0.201354844677
P	-0.773916686704	-2.257572020608	-0.157309052317
N	-1.761615822182	0.458162413349	0.275728527577
N	1.851072790969	-0.697881860817	-0.802472165245
C	-2.070005171791	1.778465266241	0.303553019153
H	-3.117262781324	2.043758431453	0.516023325960
C	-1.149443330049	2.754122576150	0.079170241773
H	-1.436496147833	3.806028200538	0.117391420677
H	1.272672058202	2.776247422290	0.868779297282
H	0.922789844522	2.696811462783	-1.474797518791
C	-2.699643985972	-0.498167750797	0.476389462063
H	-3.712395943163	-0.158034680801	0.743221748268
C	-2.436339835214	-1.829058877646	0.353839484157
H	-3.219826427503	-2.569812189645	0.520504573550
H	-0.257112765979	-3.129074222502	0.829549615828
H	-0.880857078835	-2.851480305602	-1.438448790789
C	3.588622101131	-0.682813292503	0.218271972821
H	3.956819930870	0.022699287319	-0.564346077362
O	3.288645706198	-0.272072438680	1.341709137278
H	3.895604929391	-1.743541863697	0.054625382599

**Pd<sup>Pd</sup>TS2\_t\_h-truncated ! 3-A (C1): E(UPBE1PBE-D3(BJ)/def2SVP) = -1190.55206188**

Pd	0.163297708980	-0.111852851211	-0.220781678548
P	0.513322002018	2.217172652328	-0.193479554910
P	-0.741763341058	-2.264841837799	-0.161353538023
N	-1.768053292902	0.436548933066	0.263349029729
N	1.897627110178	-0.658537054682	-0.766056246871
C	-2.091849939166	1.753671798904	0.295954668164
H	-3.143106907619	2.004140253733	0.506023137961
C	-1.182499700535	2.741377121339	0.079642990233
H	-1.482752493475	3.789513214203	0.120582714082

H	1.235059450071	2.778281487181	0.886007838869
H	0.900471004282	2.716377772911	-1.460287827263
C	-2.694199016500	-0.532677512916	0.462572199106
H	-3.711724777861	-0.204228328840	0.725298179339
C	-2.412734475794	-1.859783366833	0.344478687863
H	-3.187315388674	-2.610117515826	0.509903946467
H	-0.220619871279	-3.136207990670	0.823590557087
H	-0.841042416794	-2.856860699502	-1.444241351383
C	3.598957103478	-0.652529722821	0.194657062744
H	4.012446357544	0.065952143130	-0.553576767377
O	3.277684301326	-0.265517938442	1.324747187345
H	3.918975555888	-1.708870945714	0.022292552014

**Pd<sup>d</sup>TS3\_bs\_h-truncated !** 1-A (C1): E(UPBE1PBE/def2SVP) = -1190.54988362

Pd	0.244140367905	-0.050770146749	-0.198992368710
P	0.268458867870	2.296759551130	-0.108052468171
P	-0.359937593994	-2.313347846827	-0.133927981647
N	-1.760043205770	0.223592476003	0.205756171120
N	2.050528723463	-0.310627670912	-0.818005897388
C	-2.261708082101	1.482481838983	0.243842317076
H	-3.346368726181	1.580422756111	0.403449378690
C	-1.488075546429	2.590895996868	0.093321982412
H	-1.928649456682	3.588125235657	0.136130468316
H	0.858936552776	2.881049354631	1.037419429997
H	0.651544373082	2.901757837963	-1.328717406078
C	-2.567021305697	-0.859413253729	0.320543900691
H	-3.634264324383	-0.666816086631	0.508859976034
C	-2.109656501507	-2.135178434936	0.206365523697
H	-2.789932372532	-2.982746621251	0.300995130761
H	0.156447675645	-3.092330869894	0.927469027231
H	-0.254153095128	-2.935090690919	-1.401645814534
C	3.148767539257	-0.324352547755	0.096297875749
H	3.636378901891	0.661919800707	-0.166897352072
O	2.816097159094	-0.269244144409	1.383167281880
H	3.895771922014	-1.115441607417	-0.175526899321

**Pd<sup>d</sup>TS4\_bs\_h-truncated !** 1-A (C1): E(UPBE1PBE/def2SVP) = -1190.56189490

Pd	-0.232795825233	-0.045900526710	-0.147400989480
P	0.283146105437	-2.328195240574	-0.073270422779
P	-0.179306885136	2.310881922082	-0.109306415191
N	1.783610492087	0.163612201188	0.170466206324
N	-2.080179557098	-0.189665417664	-0.705732136379
C	2.555563300116	-0.944635568011	0.260710021511
H	3.636464322880	-0.788135427288	0.396995659884
C	2.050836462691	-2.206294888657	0.182920818314
H	2.707080965478	-3.074311895924	0.257259168970

H	-0.202184960464	-3.070562577266	1.031054383568
H	0.100732598391	-2.984658182882	-1.315313677626
C	2.331460830335	1.406652160953	0.180249989080
H	3.423923949962	1.464121990150	0.300319114496
C	1.593829193041	2.539381438020	0.048300786541
H	2.073597808742	3.518966835125	0.068922934446
H	-0.728600045727	2.966378076523	1.017233319541
H	-0.556324320218	2.885554654418	-1.345970983206
C	-3.189767312516	-0.619584806256	0.105221191662
H	-3.030476850920	-1.654267500258	0.489496201964
O	-3.012441497329	0.353625851921	1.020092256416
H	-4.149213220190	-0.591706282885	-0.459191419974

**PhCHO\_s\_h-truncated ! 1-A' (CS): E(RPBE1PBE-D3(BJ)/def2SVP) = -114.284385739**

O	0.002563530275	-0.678358022055	-0.000000000000
C	0.002563530275	0.526704388718	0.000000000000
H	-0.958742339353	1.104337872204	0.000000000000
H	0.922852915500	1.162299971932	0.000000000000

**PhCO\_d\_h-truncated ! 2-A' (CS): E(UPBE1PBE-D3(BJ)/def2SVP) = -113.637114715**

O	0.058852143531	-0.599475300229	0.000000000000
C	0.058852143531	0.584198208839	-0.000000000000
H	-0.823930009435	1.290613148795	-0.000000000000