Supporting Information

Multi-Tier Electronic Structure Analysis of Sita's Mo and W Complexes Capable of Thermal or Photochemical N_2 Splitting

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Note:

A repository with the TheoDORE descriptors and Ω-matrices as text for all complexes discussed in the main text is also available.

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Table S1. Computed Mayer bond orders of the four complexes **Mo**[therm], **Mo**[photo], **W**[therm] and **W**[photo] with different density functionals

		Mo[therm]	**Mo**[photo]	**W**[therm]	**W**[photo]
	B.O.(M1, M2)	0.22	0.23	0.19	0.20
	B.O.(N1, N2)	1.40	1.36	0.67	0.67
LC-BLYP	*B.O.*(M1, N1)	1.56	1.56	2.00	2.00
	B.O.(M2, N2)	1.56	1.56	2.00	2.00
	B.O.(M1, M2)	0.24	0.25	0.21	0.21
	B.O.(N1, N2)	1.45	1.42	0.71	0.72
CAM-B3LYP	*B.O.*(M1, N1)	1.46	1.47	1.93	1.92
	B.O.(M2, N2)	1.46	1.47	1.93	1.92
	B.O.(M1, M2)	0.28	0.29	0.24	0.25
	B.O.(N1, N2)	1.55	1.51	0.79	0.80
B3LYP	*B.O.*(M1, N1)	1.37	1.39	1.85	1.85
	B.O.(M2, N2)	1.37	1.38	1.85	1.85
	B.O.(M1, M2)	0.30	0.32	0.26	0.27
	B.O.(N1, N2)	1.61	1.58	0.84	0.86
BLYP	*B.O.*(M1, N1)	1.36	1.37	1.82	1.82
	B.O.(M2, N2)	1.36	1.37	1.82	1.82
	B.O.(M1, M2)	0.28	0.30	0.24	0.25
	B.O.(N1, N2)	1.58	1.53	0.84	0.84
PBE0	*B.O.*(M1, N1)	1.41	1.42	1.87	1.88
	B.O.(M2, N2)	1.41	1.43	1.87	1.88
	B.O.(M1, M2)	0.31	0.33	0.27	0.27
	B.O.(N1, N2)	1.66	1.62	0.91	0.92
PBE	*B.O.*(M1, N1)	1.39	1.40	1.83	1.84
	B.O.(M2, N2)	1.39	1.40	1.83	1.84
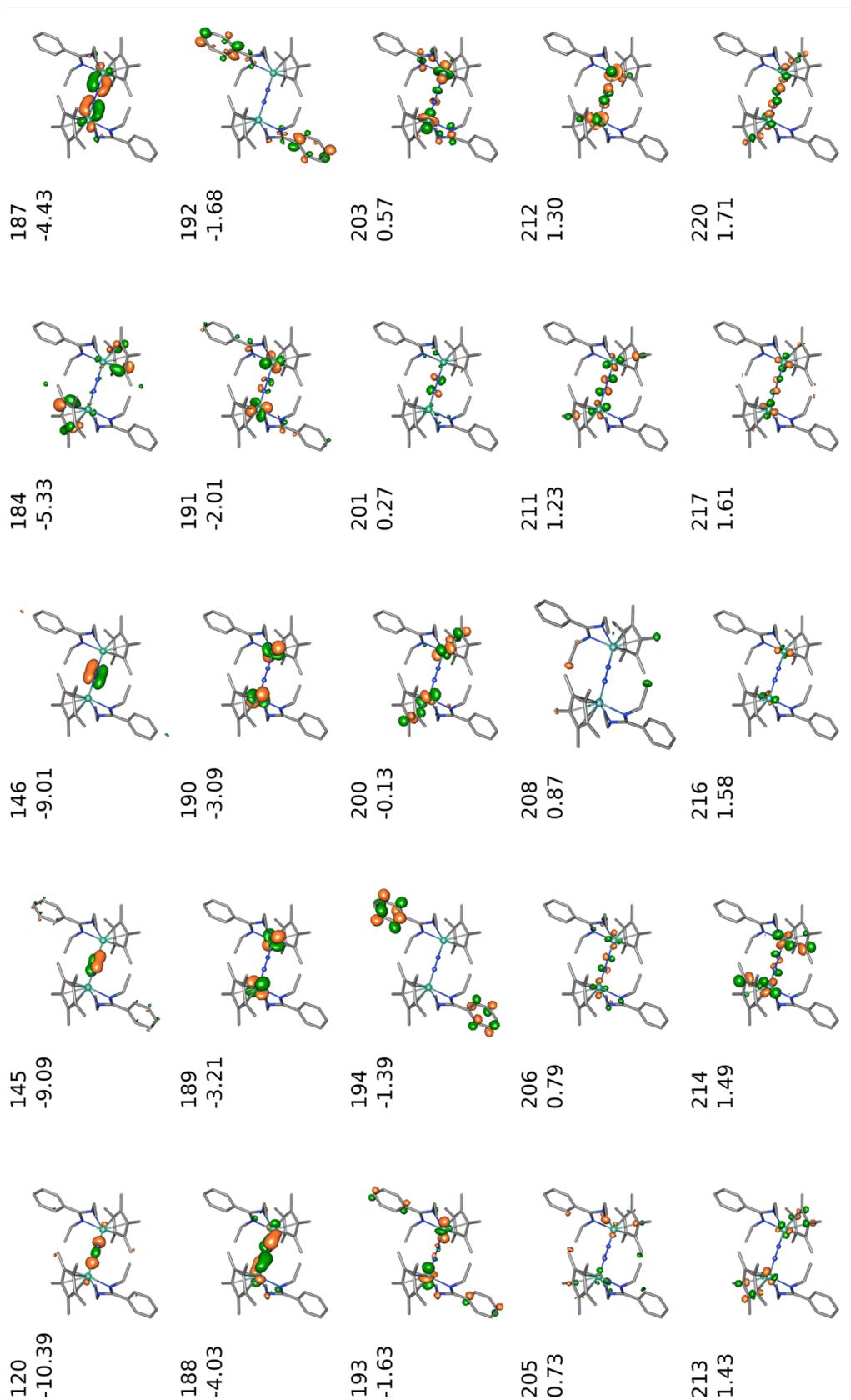
Figure S1. Selected molecular orbitals of **Mo^therm** plotted with a contour value of 0.065 (201, 203, 205, 214 plotted with a contour value of 0.055). The energies are given in eV.

3

168
-5.27

173
-2.96

180
-0.08

189
1.08

196
1.61

167
-5.33

172
-4.14

177
-0.57

186
0.93

195
1.60

142
-8.62

171
-4.39

176
-1.54

183
0.66

194
1.53

141
-8.63

170
-4.62

175
-1.98

182
0.58

193
1.49

106
-10.37

169
-4.69

174
-2.87

181
0.35

192
1.30
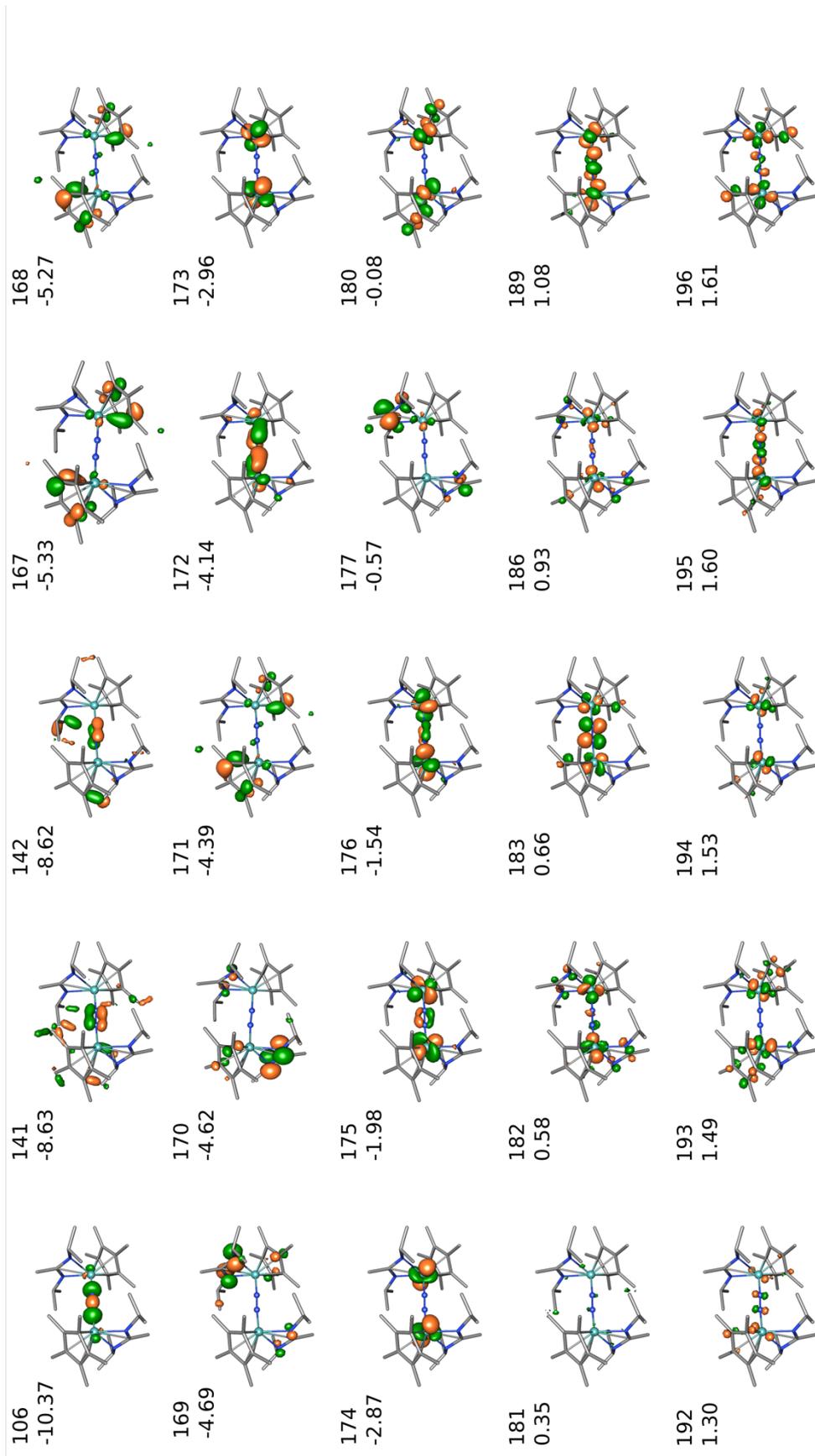
Figure S2. Selected molecular orbitals of **Mo^photo** plotted with a contour value of 0.065 (181, 182, 186, 196 plotted with a contour value of 0.055). The energies are given in eV.
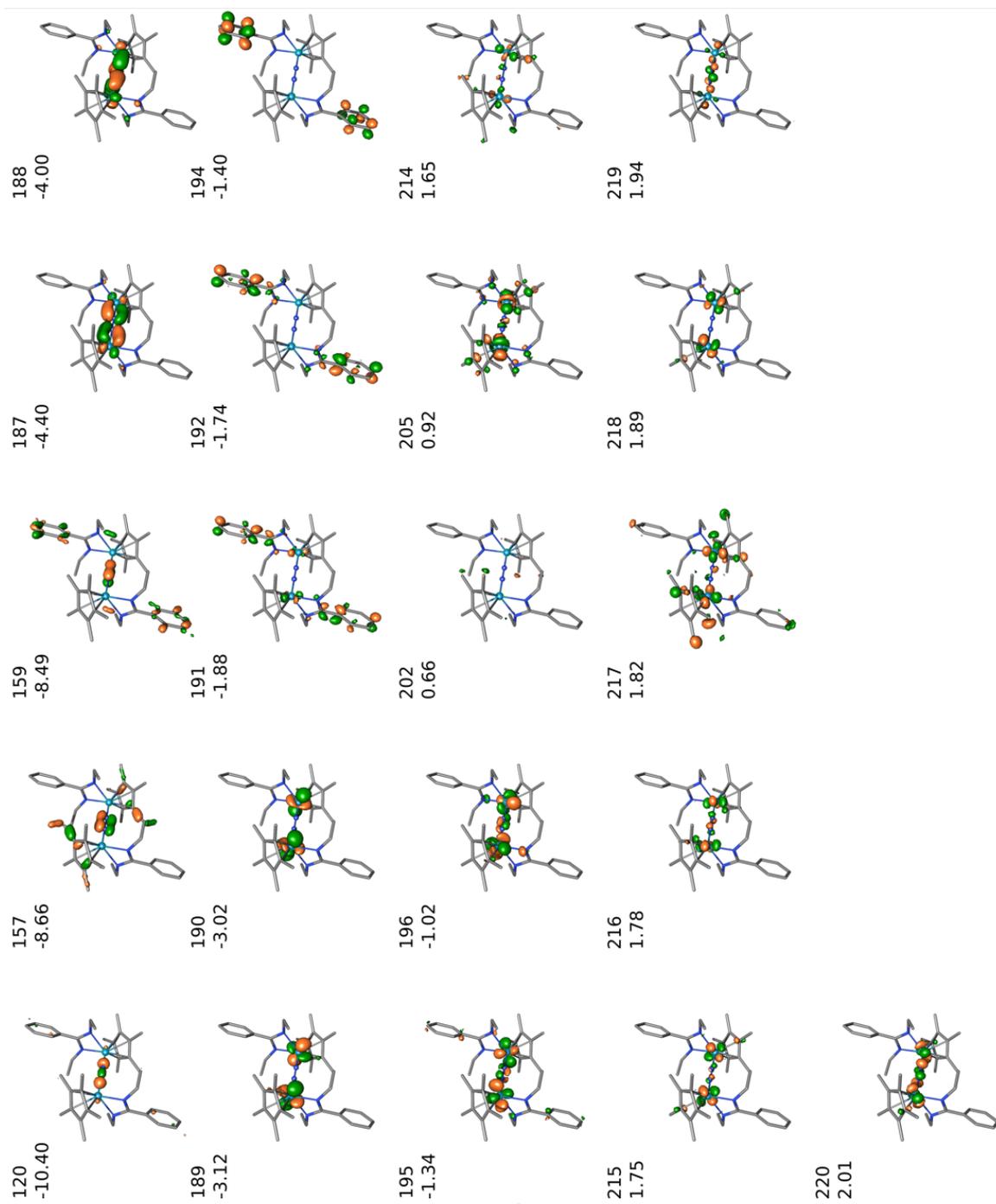
Figure S3. Selected molecular orbitals of **W^therm** plotted with a contour value of 0.065 (202, 205, 214, 217 plotted with a contour value of 0.055). The energies are given in eV.
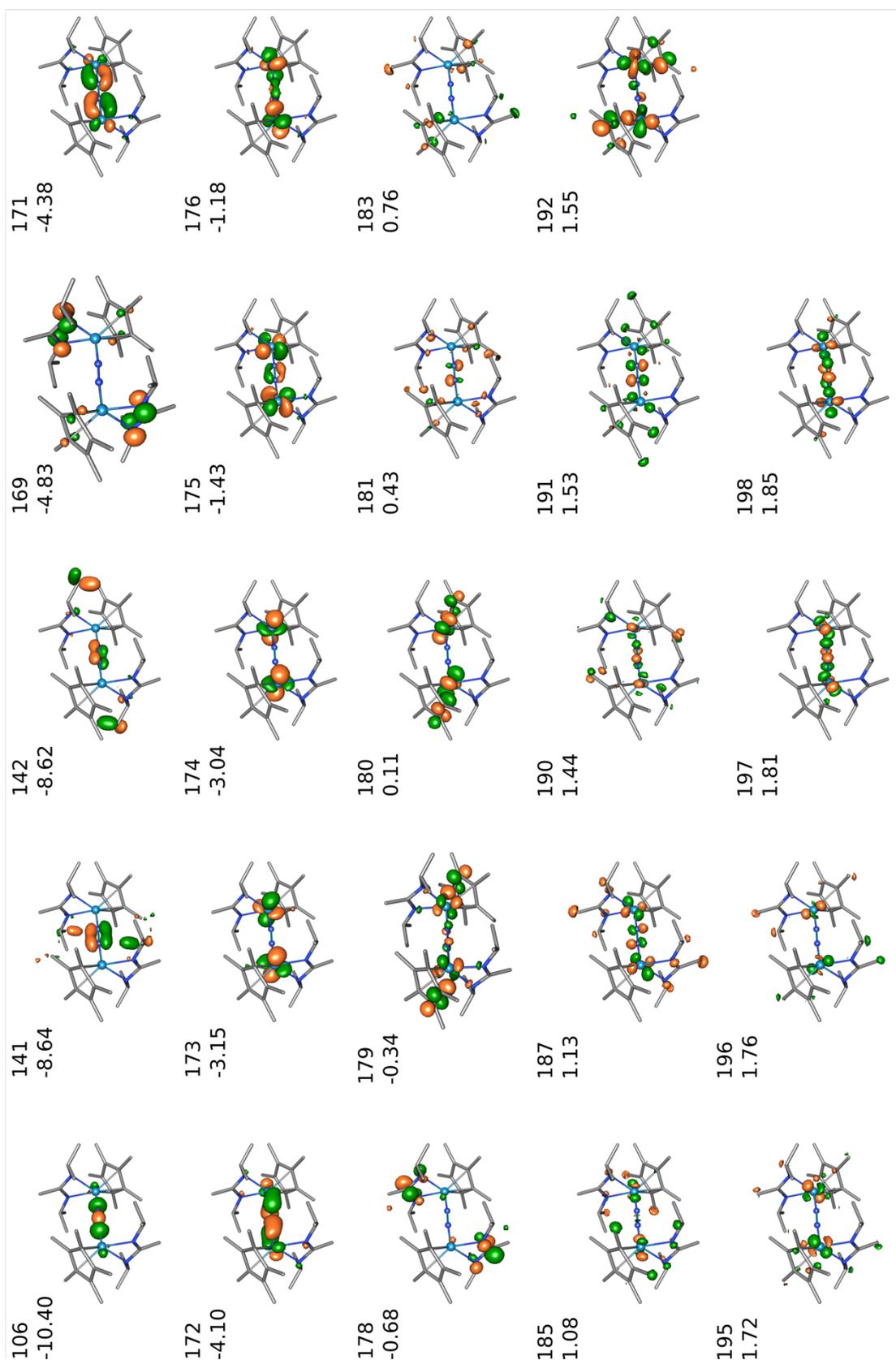
Figure S4. Selected molecular orbitals of **W**^{photo} plotted with a contour value of 0.065 (181, 183, 185, 187, 190, 191, 192, 195, 196 plotted with a contour value of 0.050). The energies are given in eV.

171
-4.38

176
-1.18

183
0.76

192
1.55

169
-4.83

175
-1.43

181
0.43

191
1.53

198
1.85

142
-8.62

174
-3.04

180
0.11

190
1.44

197
1.81

141
-8.64

173
-3.15

179
-0.34

187
1.13

196
1.76

106
-10.40

172
-4.10

178
-0.68

185
1.08

195
1.72
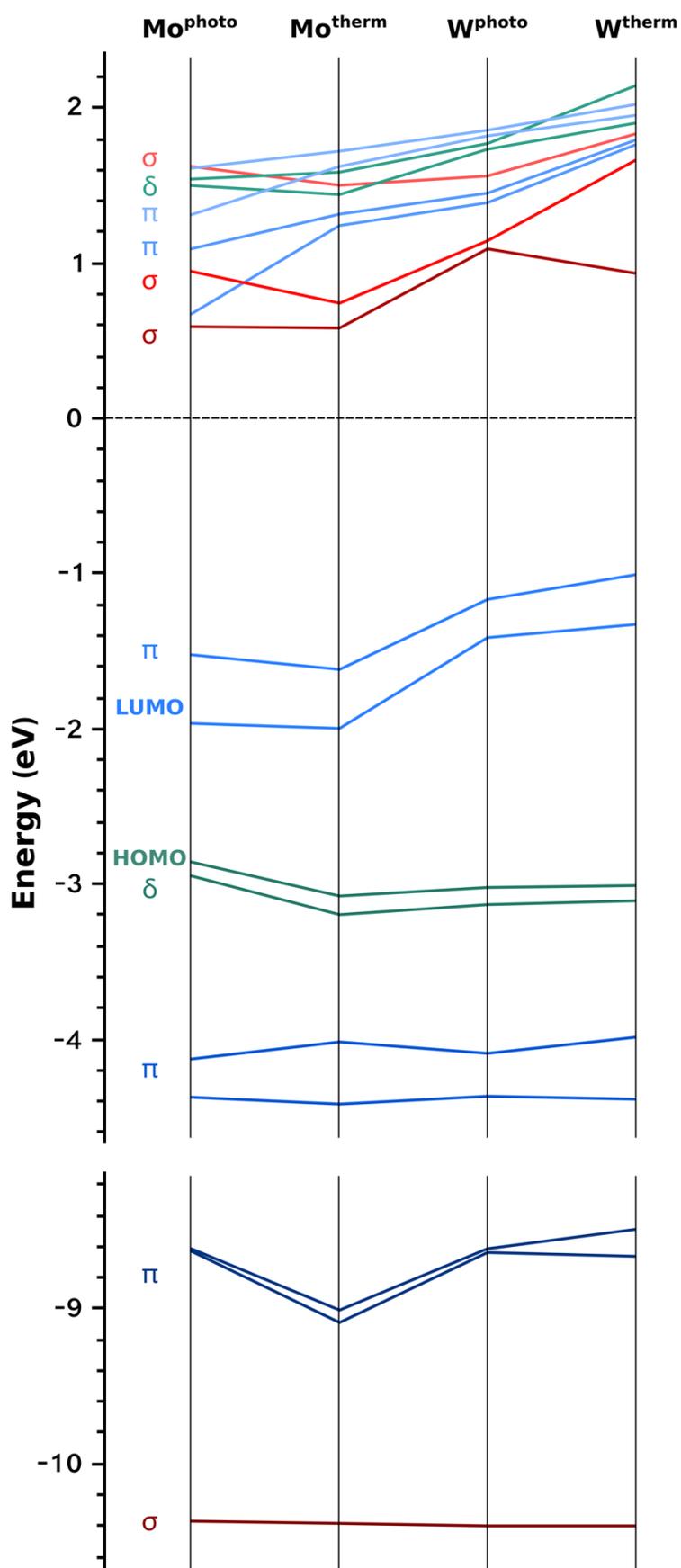
Figure S5. Molecular orbital energy diagrams in eV from a LC-BLYP calculation for the four complexes **Mo**^{photo}, **Mo**^{therm}, **W**^{photo} and **W**^{therm}, from left to right.

Table S2. All transitions discussed in the main text with their excitation energies (eV) and oscillator strengths. The contributions C (%) and the character of the donor and acceptor orbitals are listed.

| **Mo^{photo}**				**Mo^{therm}**			
S_n E (eV), f_{osc}	C (%)	Don. Orbital	Acc. Orbital	S_n E (eV), f_{osc}	C (%)	Don. Orbital	Acc. Orbital
S_{14} 4.64, 0.100	10	168 $L_{Cp\bullet}$	175 π*-π-π*	S_{15} 4.55, 0.075	11	187 π-π*-π	191 π*-π-π*
	28	171 π-π*-π	175 π*-π-π*		18	188 π-π*-π	192 core/L_{Am}
	32	172 π-π*-π	176 π*-π-π*	S_{16} 4.58, 0.132	16	187 π-π*-π	194 Mo-L_{Am}
S_{17} 4.88, 0.001	21	168 $L_{Cp\bullet}$	175 π*-π-π*		15	188 π-π*-π	192 core/L_{AM}
	36	170 $L_{Cp\bullet}L_{Am}$	176 π*-π-π*		10	189 δ/δ*	193 π*-π-π*
					14	190 δ/δ*	208 $L_{Cp\bullet}L_{Am}$
S_{18} 4.88, 0.000	14	167 core/L_{Cp*}	175 π*-π-π*	S_{18} 4.76, 0.024	27	188 π-π*-π	194 Mo-L_{Am}
	10	169 $L_{Cp\bullet}L_{Am}$	176 π*-π-π*		20	188 π-π*-π	200 core/L_{Am}
	17	170 $L_{Cp\bullet}L_{Am}$	176 π*-π-π*				
S_{19} 4.89, 0.006	20	169 $L_{Cp\bullet}L_{Am}$	176 π*-π-π*	S_{26} 5.08, 0.058	20	184 Mo-$L_{Cp\bullet}$	191 π*-π-π*
	12	174 δ/δ*	186 σ*-σ-σ*		10	187 π-π*-π	194 Mo-L_{Am}
S_{20} 4.93, 0.043	12	167 core/L_{Cp*}	175 π*-π-π*	S_{29} 5.24, 0.126	15	188 π-π*-π	200 core/L_{Am}
	38	168 $L_{Cp\bullet}$	175 π*-π-π*		26	188 π-π*-π	201 Mo-L_{Cp*}
	18	170 $L_{Cp\bullet}L_{Am}$	176 π*-π-π*		11	188 π-π*-π	206 $L_{Cp\bullet}L_{Am}$
S_{21} 4.93, 0.033	39	167 core/L_{Cp*}	175 π*-π-π*				
	32	169 $L_{Cp\bullet}L_{Am}$	176 π*-π-π*				
S_{22} 4.94, 0.001	67	172 π-π*-π	177 core/L_{Cp*}/L_{Am}				
S_{25} 5.15, 0.036	44	171 π-π*-π	177 core/L_{Cp*}/L_{Am}				
S_{29} 5.30, 0.075	45	172 π-π*-π	180 Mo-L_{Cp*}				
	20	172 π-π*-π	181 $L_{Cp\bullet}L_{Am}$				
S_{43} 5.86, 0.009	24	168 $L_{Cp\bullet}$	176 π*-π-π*				
S_{44} 4.86, 0.004	numerous low contributors						

W^{photo}				W^{therm}			
S_n E (eV), f_{osc}	C (%)	Don. Orbital	Acc. Orbital	S_n E (eV), f_{osc}	C (%)	Don. Orbital	Acc. Orbital
S$_{12}$ 4.84, 0.039	13	173 δ/δ*	180 W-L$_{Cp^*}$	**S$_{16}$** 4.69, 0.171	31	187 π-π*-π	191 W-L$_{Am}$
	16	174 δ/δ*	183 W-L$_{Cp^*}$		11	188 π-π*-π	196 π*-π-π*
	19	174 δ/δ*	187 σ*-σ-σ*				
S$_{15}$ 4.94, 0.021	47	169 L$_{Am}$L$_{Cp^*}$	175 π*-π-π*	**S$_{22}$** 5.10, 0.105	18	188 π-π*-π	196 π*-π-π*
	15	172 π-π*-π	178 W-L$_{Am}$		18	189 δ/δ*	192 L$_{Am}$
					11	190 δ/δ*	191 W-L$_{Am}$
S$_{16}$ 4.95, 0.115	18	171 π-π*-π	176 π*-π-π*	**S$_{42}$** 5.66, 0.034	17	189 δ/δ*	194 L$_{Cp^*}$
	28	172 π-π*-π	175 π*-π-π*		11	190 δ/δ*	202 W-L$_{Cp^*}$
S$_{20}$ 5.27, 0.034	51	171 π-π*-π	178 W-L$_{Am}$	**S$_{44}$** 5.73, 0.043	22	188 π-π*-π	195 π*-π-π*
					11	190 δ/δ*	202 W-L$_{Cp^*}$
S$_{32}$ 5.77, 0.047	14	171 π-π*-π	181 L$_{Am}$				
	32	172 π-π*-π	181 L$_{Am}$				
S$_{33}$ 5.77, 0.030	18	171 π-π*-π	181 L$_{Am}$				
	24	172 π-π*-π	181 L$_{Am}$				
	10	173 δ/δ*	179 W-L$_{Cp^*}$L$_{Am}$				
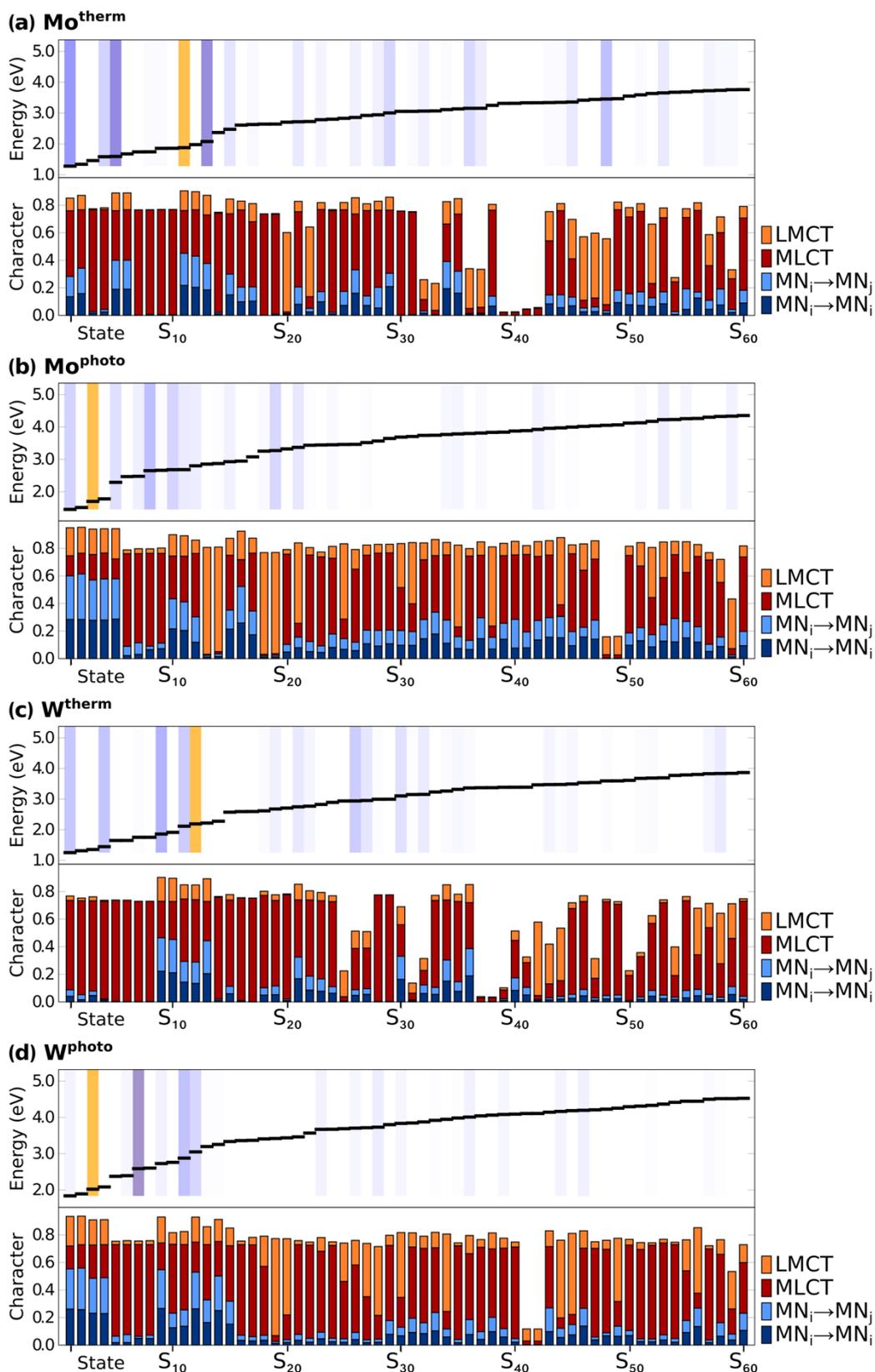
Figure S6. Character of states S_1-S_{60} from a BLYP-calculation for (a) **Mo**[therm], (b) **Mo**[photo], (c) **W**[therm], (b) **W**[photo] based on the fragmentation scheme M-N/N-M. Each upper panel shows the oscillator strength as coloured bars (yellow: most intense, shades of blue: less intense) and the energy in eV as a step function.
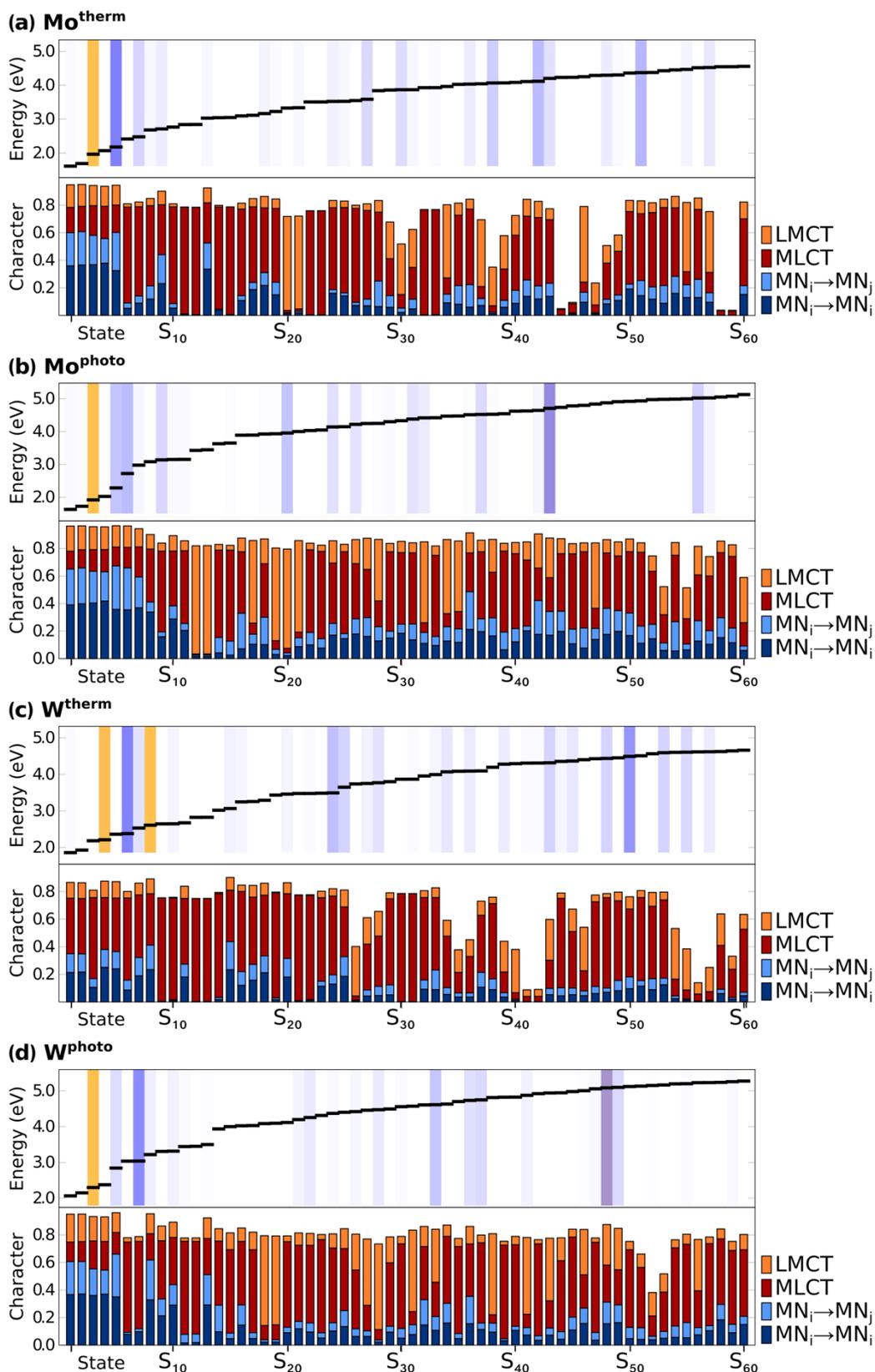
Figure S7. Character of states S_1-S_{60} from a BLYP-calculation for (a) **Mo^therm**, (b) **Mo^photo**, (c) **W^therm**, (b) **W^photo** based on the fragmentation scheme M-N/N-M. Each upper panel shows the oscillator strength as coloured bars (yellow: most intense, shades of blue: less intense) and the energy in eV as a step function.

Cartesian Coordinates of all Complexes in Å

Mo^therm

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Mo	4.333826199934	5.198417156440	4.833908225430
Mo	5.434629180140	0.704784189903	6.332966828169
N	4.737159807350	3.526849945590	5.393958204314
N	5.032232216455	2.376134967259	5.771512942044
C	3.584710185996	4.725692007186	2.428934156455
C	3.205084777690	4.063255755812	1.147594949271
C	2.259313797770	4.675446098217	0.296631894459
H	1.831019957873	5.649803233128	0.577409109360
C	1.878988817141	4.052471123477	-0.902680076535
H	1.144574934711	4.538954881205	-1.562811760990
C	2.435940992409	2.812041021882	-1.260970116515
H	2.134669801008	2.323090768996	-2.200070817212
C	3.379949812091	2.199053209362	-0.418534753070
H	3.818584833787	1.227603903434	-0.693428046140
C	3.765174974045	2.822653142433	0.778346177641
H	4.495705753821	2.342114161921	1.443016086184
N	2.731031922719	4.953795977077	3.441238062715
C	1.413175781113	4.356011956099	3.555945169095
H	0.893518960000	4.361169846745	2.572293035804
H	0.815882836622	5.001657942540	4.234658912649
C	1.463704799911	2.929198748101	4.114073176210
H	1.993221780705	2.256554138416	3.408643919240
C	0.443805083419	2.524962893477	4.280053853777
H	2.023621955306	2.913554151912	5.071248984201
N	4.814133929989	5.135133907587	2.759425986368
C	6.012256839704	4.970831780254	1.965991907003
H	6.562673146770	5.938455134672	1.958083882194
H	5.748900139840	4.746443163829	0.908505788869
C	6.925844846872	3.882949191760	2.539807902843
H	7.145822241750	4.100252124821	3.604534753275
H	7.878434804824	3.819132003062	1.974894785040
H	6.430920182846	2.890834985081	2.511801196939
C	3.420627138044	7.432976042502	5.098241257318
C	4.771502881632	7.582538995918	4.677364894922
C	5.642273040875	6.881930014510	5.599939919310
C	4.774338213333	6.319650082698	6.637478171866
C	3.380637213337	6.628871103911	6.304125080567
C	2.215923909238	7.961167963464	4.379022170417
H	1.332993785990	7.314747261530	4.547297889713
H	2.385671799640	8.016372263257	3.286115043943
H	1.953784846223	8.982556255558	4.731908252330
C	5.227204927963	8.294428977921	3.438979005039
H	4.480823172870	8.215366192680	2.624430753439
H	6.180709833378	7.875622227745	3.062742977014
H	5.395674855309	9.375351827237	3.636798160969
C	7.142449795142	6.950511915157	5.632093258136
H	7.505500842832	7.863199791825	6.159497234175
H	7.568511036225	6.967413836490	4.609168235311
H	7.572659785857	6.073459892792	6.153433921256
C	5.232724246670	5.636989206044	7.895103888167
H	6.173396074620	5.076650825559	7.733386791696
H	4.475471074174	4.905496911206	8.239433173964
H	5.404793108487	6.361122762057	8.721934872894
C	2.182923886813	6.412318015011	7.184616225874
H	2.020952256084	7.265351211222	7.884249933613
H	2.294496147169	5.497331921551	7.798320015211
H	1.257713030548	6.295649777747	6.585962766676
C	6.182995879094	1.178489904600	8.738293858369
C	6.562729239558	1.839948765596	10.020086041278
C	7.509833216969	1.227842033196	10.869502800301
H	7.939111855726	0.254389262203	10.587242870616
C	7.890383097929	1.849770824514	12.069373093160
H	8.626076001769	1.363434178062	12.728172838480
C	7.332152959604	3.089004985527	12.429778254605
H	7.633778170585	3.577266249634	13.369140898040
C	6.386564016657	3.701759960057	11.589000083481
H	5.946992880408	4.672320248207	11.865444056713
C	6.001280116028	3.079287174526	10.391553123936
H	5.269395171672	3.559709206867	9.728350094727
N	7.036869937953	0.949856757460	7.726191039464
C	8.354916054191	1.547132239102	7.611287079148
H	8.875456072133	1.540452963865	8.594453956901
H	8.951187157414	0.901984208452	6.931259917661
C	8.304828898396	2.974642902714	7.054993200377

H	7.776562892619	3.646720763565	7.761851765096
H	9.324825983502	3.378398264397	6.888542084236
H	7.744012141678	2.991870797232	6.098386257928
N	4.953485879209	0.770028040464	8.407106160374
C	3.754950211240	0.933578206927	9.199981957741
H	3.204640797978	-0.034143045283	9.206718913298
H	4.017654964733	1.157087859941	10.257827916405
C	2.841756970299	2.021998968683	8.626523156544
H	2.623164961460	1.806115818181	7.561214211138
H	1.888454739771	2.084901209917	9.190345110859
H	3.336437154437	3.014184085114	8.656475118015
C	6.346408988649	-1.530711869066	6.071713078693
C	4.995240080864	-1.678844985556	6.492138052896
C	4.125380106490	-0.978742955951	5.568325812100
C	4.994125104400	-0.418328903120	4.530486986866
C	6.387478964121	-0.728071163923	4.864878853105
C	7.550533826722	-2.058830234391	6.791975173952
H	8.433762935115	-1.412820174002	6.623707921492
H	7.380217070776	-2.113144987228	7.884830970232
H	7.812504082194	-3.080567254292	6.439977051462
C	4.538253192173	-2.388823050158	7.731121913070
H	5.285213867176	-2.311087970634	8.545255818884
H	3.586044771018	-1.967258228160	8.107586016490
H	4.366999792497	-3.469446914328	7.533993862627
C	2.625183243487	-1.046425255276	5.535644883556
H	2.261805164258	-1.959459213864	5.009050019531
H	2.198717181809	-1.062086255960	6.558425970169
H	2.195724155289	-0.169688093373	5.013141088843
C	4.536640789095	0.262789951031	3.271691788845
H	3.597472882887	0.825865236247	3.432777047681
H	5.295645009108	0.991383942076	2.925070107205
H	4.362093790221	-0.462800959126	2.446654185815
C	7.585724113780	-0.513634254842	3.984596203634
H	7.747438035188	-1.367837991128	3.286329889906
H	7.475048808861	0.400494042297	3.369449877116
H	8.510747112122	-0.396699841422	4.583484088354

Mo^photo

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Mo	6.942863187200	5.574366899574	14.733402180142
Mo	10.495910052502	4.367795145902	17.813648223844
N	9.158652156239	4.788103171934	16.676245228388
N	8.284763026291	5.106192145485	15.846359832580
N	5.416760981150	4.178476164123	15.306564112902
N	5.475102772853	6.231217155909	16.139190117682
N	12.029633998469	5.699391903955	17.154113980502
N	11.964627219316	3.595018029629	16.456421824090
C	5.102588977596	4.958534759342	16.357901191403
C	4.512403941914	4.459483041950	17.653837753000
H	4.056773863689	3.461049929741	17.531161766428
H	3.737623889753	5.155364882994	18.028698978533
H	5.298251207060	4.383986911367	18.432060103165
C	5.396418878521	2.715474111598	15.380662157193
H	4.474647145197	2.401760904714	15.923480008140
C	5.328080928586	2.127321116551	13.971407050318
H	6.206099757785	2.466139021300	13.387155149951
H	4.413298039189	2.457909256724	13.443592961911
H	5.333537804377	1.019402819056	14.006742861120
C	6.617840933333	2.178220030247	16.149965029000
H	6.661129219833	2.587183025237	17.173016191836
H	7.549516218872	2.493655179894	15.633947026477
H	6.595450914750	1.070981196338	16.210587241294
C	5.478733987135	7.248078865815	17.194088029892
H	4.912378861329	6.856552790356	18.067437928223
C	4.772189224524	8.523390744132	16.721457074188
H	3.738883860783	8.307508122808	16.385167049158
H	5.320577195195	8.973825889304	15.870985095862
H	4.727982815497	9.273202096976	17.537602911903
C	6.913190102140	7.542855994016	17.657080022005
H	7.511786939373	7.933040075971	16.810803890086
H	7.420870054576	6.622942202013	18.005869213657
H	6.917246774931	8.289300192024	18.478305961310
C	8.076935011873	6.337115048624	13.048968024483
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