

Electronic Supplementary Information

Reactivity of a Rhenium Hydroxo-Carbonyl
Complex toward Carbon Disulfide: Insights
from Theory

Violeta Yeguas,^a Pablo Campomanes,^b and Ramón López*^a

^aDepartamento de Química Física y Analítica, Universidad de Oviedo, C/Julián Clavería, 8, 33006 Oviedo, Spain.

^bLaboratory of Computational Chemistry and Biochemistry, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.

rlopez@uniovi.es

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Table 1S. Electronic energy, enthalpy, entropy, Gibbs energy in gas-phase, and Gibbs energy of solvation of the most chemically significant structures located for the reaction $[\text{Re}(\text{OH})(\text{CO})_3(\text{bipy})] + \text{CS}_2 \rightarrow [\text{Re}(\text{SH})(\text{CO})_3(\text{bipy})] + \text{OCS}$ at the B3LYP/6-31+G(d,p) (LANL2DZ + *f* for Re) level of theory.

Species	E (h)	H (h)	S (cal/K mol)	G (h)	ΔG_{solv} (kcal/mol)
Reactants	-1824.991913	-1824.761636	199.801	-1824.856567	-1.7
TS1	-1824.964370	-1824.733403	164.804	-1824.811707	-0.1
M1	-1824.972496	-1824.739568	163.845	-1824.817416	-2.2
TS2-A	-1824.964109	-1824.732078	162.885	-1824.809470	-3.1
M2-A	-1825.003957	-1824.770408	162.925	-1824.847819	-2.4
TS3-A1	-1824.996636	-1824.763971	158.587	-1824.839321	-0.9
M3-A1	-1825.004132	-1824.770496	161.626	-1824.847290	-1.7
TS4-A1a	-1824.972463	-1824.739893	160.737	-1824.816265	-2.5
M4-A1a	-1824.997783	-1824.765240	157.607	-1824.840124	-1.2
TS5-A1a	-1824.954019	-1824.726531	162.357	-1824.803672	0.2
TS4-A1b	-1824.960882	-1824.733333	161.819	-1824.810219	-1.7
M4-A1b	-1825.005662	-1824.774960	165.288	-1824.853494	-2.5
TS5-A1b	-1824.963905	-1824.734709	162.357	-1824.812040	-3.7
TS3-A2	-1824.965325	-1824.737754	162.084	-1824.814765	-0.8
M3-A2	-1825.014351	-1824.783680	165.107	-1824.862128	-0.7
TS4-A2	-1825.003288	-1824.773963	163.540	-1824.851666	-0.8
M4-A2	-1825.013852	-1824.783144	164.464	-1824.861286	-0.5
TS5-A2	-1824.972547	-1824.745600	163.367	-1824.823221	0.8
TS2-B	-1824.951350	-1824.724005	162.795	-1824.801354	-1.1
M2-B	-1825.001235	-1824.770585	163.149	-1824.848102	-0.7
TS3-B1	-1824.983220	-1824.753610	161.489	-1824.830338	-0.8
TS3-B2	-1824.988634	-1824.759270	162.731	-1824.836589	-0.2
M3-B2	-1825.002221	-1824.771448	163.684	-1824.849220	0.1
TS4-B2a	-1824.983167	-1824.753457	161.358	-1824.830124	-0.4
TS4-B2b	-1824.966378	-1824.739281	162.520	-1824.816500	-0.4
M4-B2b	-1824.995793	-1824.764996	169.454	-1824.845509	0.3
TS5-B2b	-1824.960299	-1824.731180	163.425	-1824.808828	-2.8
TS4-B2c	-1824.995161	-1824.765393	160.623	-1824.841710	1.0
Products	-1825.020761	-1824.790598	197.793	-1824.884577	-1.2

Table 2S. Electronic energy (in hartree) of the most chemically significant structures located for the reaction $[\text{Re}(\text{OH})(\text{CO})_3(\text{bipy})] + \text{CS}_2 \rightarrow [\text{Re}(\text{SH})(\text{CO})_3(\text{bipy})] + \text{OCS}$ at the levels of theory DFT/6-31+G(d,p)(LANL2DZ+f for Re)//B3LYP/6-31+G(d,p)(LANL2DZ+f for Re) (DFT = B3PW91, M05, TPSS, TPSSh).

Species	B3PW91	M05	TPSS	TPSSh
Reactants	-1824.548149	-1824.287547	-1825.164336	-1825.014673
TS1	-1824.528309	-1824.265828	-1825.147088	-1824.997670
M1	-1824.539176	-1824.276842	-1825.151627	-1825.005278
TS2-A	-1824.531653	-1824.269964	-1825.144165	-1824.997148
M2-A	-1824.574220	-1824.307817	-1825.183568	-1825.038178
TS3-A1	-1824.566997	-1824.300914	-1825.175984	-1825.030814
M3-A1	-1824.574946	-1824.308191	-1825.184103	-1825.038942
TS4-A1a	-1824.542112	-1824.279187	-1825.153140	-1825.006814
M4-A1a	-1824.568155	-1824.301890	-1825.177190	-1825.031965
TS5-A1a	-1824.525946	-1824.261055	-1825.139983	-1824.991582
TS4-A1b	-1824.533378	-1824.266628	-1825.146694	-1824.998766
M4-A1b	-1824.575467	-1824.310827	-1825.187304	-1825.040977
TS5-A1b	-1824.532076	-1824.270868	-1825.146760	-1824.998740
TS3-A2	-1824.537598	-1824.271000	-1825.150536	-1825.002872
M3-A2	-1824.583821	-1824.319038	-1825.194798	-1825.048984
TS4-A2	-1824.572626	-1824.306820	-1825.184069	-1825.037888
M4-A2	-1824.583354	-1824.318388	-1825.194367	-1825.048589
TS5-A2	-1824.544520	-1824.280076	-1825.158212	-1825.009840
TS2-B	-1824.520278	-1824.256611	-1825.135082	-1824.987014
M2-B	-1824.567861	-1824.305313	-1825.180154	-1825.034165
TS3-B1	-1824.550802	-1824.290246	-1825.164114	-1825.017099
TS3-B2	-1824.554920	-1824.292010	-1825.167523	-1825.021270
M3-B2	-1824.568873	-1824.306562	-1825.181007	-1825.035165
TS4-B2a	-1824.550783	-1824.290252	-1825.163992	-1825.017087
TS4-B2b	-1824.535644	-1824.273079	-1825.149437	-1825.001622
M4-B2b	-1824.561731	-1824.300792	-1825.173855	-1825.027976
TS5-B2b	-1824.526683	-1824.268187	-1825.141233	-1824.993382
TS4-B2c	-1824.561050	-1824.300275	-1825.172537	-1825.026826
Products	-1824.582576	-1824.320220	-1825.195871	-1825.048424

Table 3S. Electronic energy, Gibbs energy in gas phase, Gibbs energy of solvation, and relative electronic energy, Gibbs energy in gas phase, Gibbs energy of solvation, and Gibbs energy in solution at the B3LYP/6-31+G(d,p) (LANL2DZ + *f* for Re) theory level of the most chemically significant structures located for the reaction $[\text{Re}(\text{OCH}_3)(\text{CO})_3(\text{bipy})] + \text{CS}_2 \rightarrow [\text{Re}(\text{SCH}_3)(\text{CO})_3(\text{bipy})] + \text{OCS}$. Relative Gibbs energy in solution obtained from single-point TPSS, and TPSSh energy calculations on the gas-phase optimized geometries at the above-mentioned theory level are also included.

Species	E (h)	G (h)	ΔG_{solv} (kcal/mol)	ΔE (kcal/mol)	ΔG (kcal/mol)	$\Delta\Delta G_{\text{solv}}$ (kcal/mol)	$\Delta G_{\text{sol}}^{\text{B3LYP}}$ (kcal/mol)	$\Delta G_{\text{sol}}^{\text{TPSS}}$ (kcal/mol)	$\Delta G_{\text{sol}}^{\text{TPSSh}}$ (kcal/mol)
Reactants	-1864.284801	-1864.123712	0.1	0.0	0.0	0.0	0.0	0.0	0.0
TS1-OCH₃	-1864.259391	-1864.080557	1.7	15.9	27.1	1.6	28.7	26.1	25.7
M1-OCH₃	-1864.265514	-1864.083230	-0.4	12.1	25.4	-0.5	24.9	24.1	22.1
TS2-A-OCH₃	-1864.261989	-1864.079390	-1.9	14.3	27.8	-2.0	25.8	23.7	22.3
M2-A-OCH₃	-1864.304400	-1864.122454	-1.0	-12.3	0.8	-1.1	-0.3	-1.4	-3.9
TS3-A1-OCH₃	-1864.298979	-1864.115416	0.3	-8.9	5.2	0.2	5.4	4.6	2.0
M3-A1-OCH₃	-1864.304709	-1864.122431	-0.9	-12.5	0.8	-1.0	-0.2	-1.3	-4.0
TS4-A1a-OCH₃	-1864.274015	-1864.092059	-1.6	6.8	19.9	-1.7	18.2	16.4	14.5
M4-A1a-OCH₃	-1864.299193	-1864.117458	0.6	-9.0	3.9	0.5	4.4	3.2	0.7
TS5-A1a-OCH₃	-1864.217595	-1864.039421	1.0	42.2	52.9	0.9	53.8	47.5	48.7
TS4-A1b-OCH₃	-1864.228401	-1864.050446	-1.0	35.4	46.0	-1.1	44.9	38.9	39.8
M4-A1b-OCH₃	-1864.324050	-1864.145274	-1.8	-24.6	-13.5	-1.9	-15.4	-15.9	-18.3
TS5-A1b-OCH₃	-1864.284517	-1864.104754	-2.6	0.2	11.9	-2.7	9.2	7.7	6.4
TS3-A2-OCH₃	-1864.231816	-1864.053629	-0.3	33.2	44.0	-0.4	43.6	38.0	38.8
M3-A2-OCH₃	-1864.332452	-1864.153084	-0.4	-29.9	-18.4	-0.5	-18.9	-18.6	-21.3
TS4-A2-OCH₃	-1864.319376	-1864.138672	-0.1	-21.7	-9.4	-0.2	-9.6	-9.4	-11.9
M4-A2-OCH₃	-1864.329595	-1864.149456	-0.6	-28.1	-16.2	-0.7	-16.9	-16.7	-19.4
TS5-A2-OCH₃	-1864.228967	-1864.051702	1.4	35.0	45.2	1.3	46.5	41.1	42.2
TS2-B-OCH₃	-1864.207225	-1864.028518	-1.5	48.7	59.7	-1.6	58.1	52.0	53.2
Products	-1864.325134	-1864.164770	-0.4	-25.3	-25.8	-0.5	-26.3	-25.8	-27.3

Table 4S. Electronic energy (in hartree) of the most chemically significant structures located for the reaction $[\text{Re}(\text{OCH}_3)(\text{CO})_3(\text{bipy})] + \text{CS}_2 \rightarrow [\text{Re}(\text{SCH}_3)(\text{CO})_3(\text{bipy})] + \text{OCS}$ at the levels of theory DFT/6-31+G(d,p)(LANL2DZ+f for Re)//B3LYP/6-31+G(d,p)(LANL2DZ+f for Re) (DFT = TPSS, TPSSh).

Species	TPSS	TPSSh
Reactants	-1864.473625	-1864.320122
TS1-OCH₃	-1864.452279	-1864.299387
M1-OCH₃	-1864.455648	-1864.305378
TS2-A-OCH₃	-1864.454136	-1864.302879
M2-A-OCH₃	-1864.494906	-1864.345414
TS3-A1-OCH₃	-1864.489047	-1864.339785
M3-A1-OCH₃	-1864.495291	-1864.346111
TS4-A1a-OCH₃	-1864.465616	-1864.315203
M4-A1a-OCH₃	-1864.489990	-1864.340406
TS5-A1a-OCH₃	-1864.416510	-1864.261061
TS4-A1b-OCH₃	-1864.426792	-1864.271885
M4-A1b-OCH₃	-1864.513552	-1864.363913
TS5-A1b-OCH₃	-1864.475681	-1864.324291
TS3-A2-OCH₃	-1864.429601	-1864.274797
M3-A2-OCH₃	-1864.520721	-1864.371582
TS4-A2-OCH₃	-1864.507831	-1864.358348
M4-A2-OCH₃	-1864.518137	-1864.368955
TS5-A2-OCH₃	-1864.426300	-1864.271042
TS2-B-OCH₃	-1864.405826	-1864.250393
Products	-1864.513156	-1864.362084

Table 5S. Imaginary vibrational frequencies corresponding to all the located transition states.

Species	ω_i (cm⁻¹)
TS1	309
TS2-A	143
TS3-A1	47
TS4-A1a	150
TS5-A1a	1590
TS4-A1b	1688
TS5-A1b	165
TS3-A2	1695
TS4-A2	319
TS5-A2	1213
TS2-B	1564
TS3-B1	157
TS3-B2	340
TS4-B2a	158
TS4-B2b	1330
TS5-B2b	195
TS4-B2c	32
TS1-OCH₃	284
TS2-A-OCH₃	93
TS3-A1-OCH₃	26
TS4-A1a-OCH₃	143
TS5-A1a-OCH₃	586
TS4-A1b-OCH₃	606
TS5-A1b-OCH₃	129
TS3-A2-OCH₃	602
TS4-A2-OCH₃	71
TS5-A2-OCH₃	549
TS2-B-OCH₃	580

Table 6S. Cartesian coordinates, in angstroms, corresponding to all the located structures.

CS ₂			
S	0.000000	0.000000	-0.293051
C	0.000000	0.000000	1.270000
S	0.000000	0.000000	2.833051

[Re(OH)(CO) ₃ (bipy)]			
C	-0.024620	0.111630	-0.037442
O	-0.048644	0.169373	1.126860
Re	0.093095	0.016576	-1.946429
C	-1.721920	0.613601	-2.074012
O	-2.818992	0.988820	-2.197225
C	-0.499807	-1.821793	-1.905308
O	-0.846351	-2.937712	-1.891516
N	2.236326	-0.507712	-2.099550
C	2.805812	-0.369167	-3.322256
C	1.874614	-0.094949	-4.439353
N	0.562415	-0.013843	-4.107600
O	0.964465	1.890574	-2.210300
H	0.566108	2.607222	-1.705365
C	-0.347301	0.189790	-5.076000
C	3.014325	-0.801110	-1.043389
C	-0.001954	0.326171	-6.416673
H	-1.380514	0.248116	-4.754821
H	-0.775951	0.491838	-7.157860
C	1.345977	0.252678	-6.768567
C	2.290609	0.035995	-5.770090
H	1.658046	0.359838	-7.802720
H	3.340559	-0.027796	-6.027169
C	4.391625	-0.967731	-1.146132
H	2.507701	-0.898571	-0.090544
H	4.973184	-1.201329	-0.261206
C	4.989465	-0.819219	-2.397798
C	4.187130	-0.521392	-3.494975
H	6.061856	-0.935070	-2.519853
H	4.635141	-0.406840	-4.474118

[Re(SH)(CO) ₃ (bipy)]			
C	2.933926	-2.085879	-0.103654
C	1.818501	-1.256212	-0.275351
N	1.181912	-0.707013	0.792176
C	1.628557	-0.987673	2.031797
C	2.728710	-1.803281	2.268928
C	3.397007	-2.361950	1.178404
C	1.247948	-0.924523	-1.596517
C	1.768145	-1.407397	-2.804090
C	1.158830	-1.060145	-4.005126
C	0.032745	-0.236181	-3.973609
C	-0.433838	0.210544	-2.742947
N	0.158464	-0.112668	-1.576925
Re	-0.592065	0.538335	0.390846
C	-1.124203	0.846014	2.210384
O	-1.419330	0.996589	3.325799
C	-2.170316	1.452403	-0.210884
O	-3.122528	1.983779	-0.616933
C	0.427196	2.174195	0.360233
O	1.038589	3.167727	0.344838

S	-1.792342	-1.697673	0.349914
H	-2.962720	-1.376992	0.934688
H	1.075819	-0.541176	2.848873
H	3.044225	-1.994558	3.288565
H	4.259270	-3.005109	1.322795
H	3.433266	-2.517610	-0.962095
H	-1.309155	0.844032	-2.672178
H	-0.483985	0.056228	-4.880959
H	1.552593	-1.430333	-4.946354
H	2.637298	-2.053320	-2.807208

COS

S	-0.001063	0.000000	0.016567
C	0.003027	0.000000	1.588511
O	0.019329	0.000000	2.754735

TS1

C	1.119578	-2.173229	-3.524340
C	0.640608	-1.747492	-2.279465
N	-0.125612	-0.630495	-2.173193
C	-0.437022	0.059533	-3.286981
C	0.003519	-0.313632	-4.552019
C	0.804311	-1.449902	-4.670554
Re	-0.637620	0.012351	-0.130227
C	-2.409451	-0.717797	-0.215097
O	-3.480894	-1.170502	-0.290811
C	0.890024	-2.481711	-1.019552
N	0.324368	-1.951562	0.095237
C	0.465492	-2.592398	1.269667
C	1.166844	-3.787496	1.393695
C	1.765282	-4.331389	0.259003
C	1.623194	-3.671913	-0.959122
C	-0.911753	0.417744	1.739439
O	-1.122601	0.631822	2.859844
O	1.424074	0.628008	-0.220661
C	-1.328544	1.749736	-0.569039
O	-1.740152	2.792686	-0.881468
C	2.812035	0.924457	1.031454
S	3.786150	1.998757	0.314188
S	2.535454	0.002820	2.326071
H	1.606421	1.377248	-0.805570
H	0.004028	-2.122972	2.128709
H	1.250922	-4.261158	2.365214
H	2.333903	-5.254035	0.317498
H	2.079312	-4.083912	-1.850396
H	-1.055579	0.937945	-3.145641
H	-0.274734	0.280368	-5.415384
H	1.175240	-1.770964	-5.638723
H	1.734614	-3.060944	-3.600703

M1

C	-1.095324	0.368926	1.752910
O	-1.400437	0.545577	2.854714
Re	-0.706822	0.017470	-0.117386
N	-0.051350	-0.537786	-2.142376
C	0.736256	-1.642090	-2.253559
C	0.993447	-2.379020	-0.998406
N	0.404609	-1.869344	0.115187
O	1.338365	0.959531	-0.115419
C	2.540128	0.616269	0.646009

S	2.251520	0.247036	2.243023
C	-1.529485	1.698165	-0.562108
O	-2.020416	2.703717	-0.877092
C	-2.389920	-0.849114	-0.284169
O	-3.412303	-1.393783	-0.404752
S	3.918274	0.706147	-0.306826
H	1.690893	1.236869	-0.983493
C	-0.356474	0.163542	-3.254328
C	1.238518	-2.042351	-3.497698
C	1.772239	-3.539368	-0.937470
C	0.576293	-2.499636	1.292759
C	1.939127	-4.190599	0.281595
H	2.252862	-3.927874	-1.826151
H	2.546076	-5.088247	0.342282
C	1.323307	-3.667070	1.416197
H	0.105010	-2.042641	2.151922
H	1.429956	-4.132847	2.389093
C	0.928606	-1.308653	-4.637874
H	1.871235	-2.917129	-3.575910
H	1.318947	-1.609934	-5.604641
C	0.109856	-0.184891	-4.515886
H	-0.994639	1.027475	-3.112046
H	-0.163967	0.417086	-5.375013

TS2-A

C	0.480911	0.727697	1.026240
O	0.611805	0.715296	-0.134255
Re	0.294285	0.758818	2.894321
N	2.126479	1.964870	3.170404
C	1.981472	3.311682	3.266521
C	0.607404	3.819743	3.085309
N	-0.348598	2.872916	2.892452
C	-1.446413	-0.042459	2.732349
O	-2.520111	-0.473688	2.623926
C	1.071921	-1.010685	2.996813
O	1.562221	-2.060133	2.992970
O	-0.613313	1.326908	5.248694
C	0.234122	1.041494	6.329726
S	-0.183624	1.689282	7.809604
S	1.527872	0.071050	5.831220
C	-1.624821	3.265789	2.698802
C	0.282642	5.182899	3.089276
C	3.082507	4.142465	3.512376
C	3.358107	1.431779	3.293294
H	-1.353264	1.859553	5.597271
C	-2.011318	4.599946	2.697834
H	-2.348155	2.474538	2.540783
H	-3.053138	4.857069	2.542183
C	-1.036212	5.579457	2.898997
H	1.053300	5.928433	3.239033
H	-1.297644	6.632722	2.904523
C	4.350441	3.585098	3.635077
H	2.951526	5.212488	3.612642
H	5.210428	4.218574	3.827289
C	4.493035	2.202318	3.511467
H	3.419529	0.353568	3.223811
H	5.459463	1.719066	3.599409

M2-A

O	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.164531
Re	0.001445	0.000000	3.089830
N	-1.349988	-1.729870	3.209734
C	-0.943555	-3.012580	3.142971
H	0.117111	-3.168968	2.996086
C	-1.818471	-4.086087	3.264621
H	-1.435476	-5.098726	3.204499
C	-3.173273	-3.827006	3.471969
H	-3.885903	-4.638383	3.580108
C	-3.600474	-2.504555	3.537746
H	-4.648813	-2.284571	3.695047
C	-2.670644	-1.467103	3.400823
C	-3.042680	-0.037967	3.424484
C	-4.355398	0.412555	3.610043
H	-5.159704	-0.294505	3.769257
C	-4.626264	1.776898	3.598492
H	-5.639839	2.135058	3.747539
C	-3.573761	2.669851	3.394522
H	-3.731438	3.742455	3.377593
C	-2.292601	2.160956	3.217212
H	-1.446229	2.818964	3.062537
N	-2.022550	0.840343	3.231015
C	0.975301	1.660271	3.110460
O	1.525134	2.684298	3.123836
C	1.684417	-0.946550	3.103411
O	2.686341	-1.531061	3.082398
S	-0.217722	0.119889	5.638440
C	0.311857	-1.326169	6.428379
S	0.208424	-1.598360	8.069166
O	0.843916	-2.274111	5.609982
H	1.138511	-2.994877	6.195175

TS3-A1

O	-0.021820	-0.040478	0.017670
C	-0.037375	-0.064808	1.182706
Re	-0.067126	-0.099913	3.099653
N	-1.477066	-1.779973	3.185313
C	-1.114261	-3.074579	3.127453
H	-0.058624	-3.271282	2.991623
C	-2.028991	-4.118275	3.230437
H	-1.678370	-5.142815	3.179451
C	-3.374058	-3.812478	3.420276
H	-4.116743	-4.598248	3.514604
C	-3.755032	-2.474850	3.493042
H	-4.796472	-2.219302	3.642570
C	-2.788283	-1.471749	3.372400
C	-3.109069	-0.030467	3.407684
C	-4.406402	0.465685	3.587169
H	-5.236523	-0.213916	3.732401
C	-4.628533	1.838697	3.587365
H	-5.630389	2.230646	3.731108
C	-3.543876	2.696854	3.401665
H	-3.663730	3.774426	3.394110
C	-2.280296	2.144381	3.230031
H	-1.409228	2.772843	3.089726
N	-2.058022	0.814695	3.232266
C	0.976204	1.518807	3.174475
O	1.569497	2.515953	3.223542
C	1.568521	-1.118881	3.129854
O	2.535982	-1.761171	3.144412

S	-0.327727	-0.030040	5.667055
C	0.606601	-1.397200	6.261676
S	0.106403	-2.982607	6.388524
O	1.831126	-1.033639	6.688091
H	2.271355	-1.836229	7.023555

M3-A1

O	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.164560
Re	0.005201	0.000000	3.087051
N	1.042051	1.937557	3.177114
C	0.417371	3.128155	3.102153
H	-0.656646	3.097112	2.983311
C	1.099468	4.339153	3.177637
H	0.545223	5.268601	3.112875
C	2.480992	4.320868	3.354441
H	3.045858	5.244867	3.426909
C	3.132384	3.092490	3.435296
H	4.206500	3.059558	3.567614
C	2.391538	1.909622	3.338909
C	3.004412	0.565640	3.371177
C	4.377763	0.349815	3.537959
H	5.050135	1.187276	3.674823
C	4.879504	-0.947692	3.535576
H	5.942130	-1.123752	3.668926
C	3.993543	-2.011237	3.361184
H	4.333311	-3.040854	3.352736
C	2.641044	-1.732350	3.202551
H	1.917803	-2.527912	3.071165
N	2.148544	-0.477827	3.206071
C	-0.660720	-1.804473	3.105266
O	-1.019560	-2.910509	3.114853
C	-1.827555	0.623799	3.089641
O	-2.925923	0.988767	3.036729
S	0.250763	-0.124735	5.630719
C	-0.467929	1.193782	6.493233
S	-1.299649	2.538473	5.943532
O	-0.281450	1.027836	7.826172
H	-0.707111	1.787209	8.261409

TS4-A1a

C	-2.462480	-0.493340	-0.155775
O	-3.611527	-0.354533	-0.322936
Re	-0.614347	-0.699396	0.108839
N	-0.164453	0.708777	-1.553001
C	0.009561	2.018105	-1.244403
C	-0.172128	2.366920	0.179677
N	-0.471255	1.330879	1.002676
C	-0.961592	-1.706973	1.712151
O	-1.209936	-2.276927	2.692487
C	-0.660040	-2.347364	-0.889292
O	-0.728662	-3.316081	-1.524139
S	2.295696	-1.350342	-1.018485
C	2.913348	-1.052961	0.525199
O	4.250284	-1.182301	0.680155
S	1.980045	-0.607744	1.880311
C	-0.063451	3.674258	0.671759
C	0.329442	2.958832	-2.232159
H	4.463789	-1.002181	1.610624
C	-0.273229	3.920536	2.024155

H	0.180458	4.492521	0.005967
H	-0.191616	4.929276	2.416316
C	-0.590713	2.849726	2.861165
C	-0.675524	1.576823	2.311263
H	-0.764617	2.988243	3.922380
H	-0.905218	0.716343	2.927347
C	0.456982	2.550865	-3.555434
H	0.480028	3.998934	-1.971608
H	0.707395	3.270114	-4.328713
C	0.258183	1.204926	-3.866060
C	-0.044486	0.321393	-2.837659
H	0.345380	0.835775	-4.881756
H	-0.186006	-0.734286	-3.032476

M4-A1a

C	-1.724393	0.724998	-1.859899
O	-2.144582	1.233553	-2.818529
Re	-1.032562	-0.122358	-0.278854
N	0.959223	-0.152164	-1.199903
C	1.798610	0.871009	-0.898652
C	1.272313	1.869990	0.052864
N	-0.015528	1.687642	0.447595
S	-0.301637	-1.144133	1.960022
C	1.270185	-1.903123	2.130619
O	1.441625	-2.403898	3.380743
C	-2.724658	0.145887	0.603896
O	-3.736645	0.354000	1.136325
C	-1.640539	-1.849257	-0.886627
O	-1.971720	-2.896747	-1.259773
S	2.517854	-2.094500	1.053189
C	-0.564438	2.562344	1.312971
C	3.070428	0.955846	-1.473964
H	0.630125	-2.253466	3.896780
C	0.129849	3.653488	1.822304
H	-1.590491	2.369279	1.601027
H	-0.362005	4.325739	2.516444
C	1.454102	3.846418	1.428025
C	2.027310	2.945224	0.536509
H	2.033399	4.680595	1.810832
H	3.057757	3.071421	0.229464
C	3.488052	-0.024182	-2.368973
H	3.730671	1.777895	-1.227963
H	4.473847	0.030570	-2.819593
C	2.621494	-1.073666	-2.667892
C	1.373784	-1.103479	-2.056302
H	2.902433	-1.868465	-3.349594
H	0.679058	-1.911210	-2.247956

TS5-A1a

C	-0.075688	0.247067	2.631872
Re	0.161197	0.392965	0.729735
C	1.941597	-0.327780	0.879005
O	2.999333	-0.801329	0.959099
O	-0.217577	0.156104	3.782514
N	-0.903963	-1.499522	0.370391
C	-2.252768	-1.430202	0.213915
C	-2.835150	-0.072979	0.262322
N	-1.949123	0.942677	0.432615
S	0.518478	0.614102	-1.810176
C	-0.753920	-0.446968	-2.737041

S	-2.304120	-0.043825	-3.147333
C	0.872927	2.171930	0.938659
O	1.263072	3.259046	1.059329
O	-0.056914	-1.496557	-2.970614
C	-2.403270	2.211406	0.435262
C	-3.014102	-2.586218	0.010313
H	0.933795	-0.809416	-2.318797
C	-3.748478	2.528222	0.294294
H	-1.656427	2.986430	0.555363
H	-4.057603	3.567388	0.297233
C	-4.669075	1.489562	0.152562
C	-4.205535	0.179415	0.137138
H	-5.729000	1.696051	0.044565
H	-4.902595	-0.638172	0.006485
C	-2.386171	-3.825692	-0.044631
H	-4.085700	-2.518382	-0.125509
H	-2.967921	-4.726206	-0.212673
C	-1.000749	-3.886055	0.103461
C	-0.300814	-2.703481	0.306549
H	-0.462281	-4.825669	0.054044
H	0.775991	-2.705902	0.421163

TS4-A1b

C	-0.588458	3.656697	0.721746
C	-0.473729	2.350243	0.231527
N	-1.072473	1.309728	0.870107
C	-1.780994	1.551325	1.990842
C	-1.929012	2.824539	2.528577
C	-1.322900	3.899528	1.878024
C	0.302813	2.001141	-0.975973
N	0.292501	0.686246	-1.325331
C	1.009336	0.290075	-2.394284
C	1.766479	1.170932	-3.160400
C	1.775403	2.520563	-2.816565
C	1.036174	2.937355	-1.712157
Re	-0.934759	-0.661352	-0.094055
C	-0.784578	-2.273854	-1.150094
O	-0.664290	-3.249137	-1.764788
S	-2.992817	0.252451	-1.321011
C	-2.941136	0.133448	-3.037626
O	-3.876094	0.629198	-3.763234
C	0.582594	-1.200475	0.957708
O	1.501764	-1.524826	1.593970
C	-2.117854	-1.609464	1.092126
O	-2.833676	-2.145175	1.834583
S	-1.779158	-0.600652	-4.130698
H	-3.087000	0.116427	-4.743471
H	-2.241967	0.690052	2.458781
H	-2.513226	2.960547	3.431785
H	-0.115305	4.480197	0.201962
H	-1.421372	4.910034	2.261503
H	1.036064	3.981837	-1.427188
H	2.347098	3.239486	-3.394688
H	0.966219	-0.763385	-2.635982
H	2.320113	0.795799	-4.013600

M4-A1b

C	-1.724393	0.724997	-1.859899
O	-2.144582	1.233552	-2.818529
Re	-1.032562	-0.122358	-0.278854
N	0.959223	-0.152164	-1.199903

C	1.798610	0.871009	-0.898652
C	1.272312	1.869990	0.052864
N	-0.015529	1.687642	0.447595
S	-0.301637	-1.144133	1.960022
C	1.270185	-1.903123	2.130619
O	1.441626	-2.403898	3.380743
C	-2.724658	0.145886	0.603896
O	-3.736645	0.353999	1.136325
C	-1.640539	-1.849258	-0.886627
O	-1.971719	-2.896748	-1.259773
S	2.517854	-2.094500	1.053189
C	-0.564439	2.562344	1.312971
C	3.070428	0.955847	-1.473964
H	0.630126	-2.253466	3.896780
C	0.129848	3.653488	1.822304
H	-1.590492	2.369278	1.601027
H	-0.362006	4.325739	2.516444
C	1.454101	3.846418	1.428025
C	2.027309	2.945224	0.536509
H	2.033398	4.680595	1.810832
H	3.057756	3.071422	0.229464
C	3.488052	-0.024181	-2.368973
H	3.730670	1.777896	-1.227963
H	4.473847	0.030571	-2.819593
C	2.621494	-1.073665	-2.667892
C	1.373784	-1.103479	-2.056302
H	2.902433	-1.868464	-3.349594
H	0.679058	-1.911210	-2.247956

TS5-A1b

C	3.442716	-1.086486	1.154752
C	2.314119	-0.500324	0.566993
N	1.251544	-1.256506	0.185697
C	1.293764	-2.589044	0.388863
C	2.379971	-3.229011	0.971617
C	3.479477	-2.461358	1.359080
C	2.184092	0.951635	0.330839
N	1.018943	1.348446	-0.238515
C	0.814371	2.661661	-0.457343
C	1.753957	3.633070	-0.134008
C	2.964790	3.232197	0.431817
C	3.179153	1.878207	0.666878
Re	-0.462341	-0.226821	-0.758286
C	-1.781297	0.876085	-1.646275
O	-2.581679	1.556665	-2.132271
C	-1.333661	0.043281	0.884351
O	-1.864303	0.209381	1.911295
C	-1.578250	-1.756984	-1.079656
O	-2.236835	-2.703741	-1.225943
S	0.926490	-1.745166	-3.054635
C	0.668127	-0.270428	-4.283494
S	0.865372	1.204148	-3.425471
O	0.434957	-0.534507	-5.433807
H	0.175331	-2.665839	-3.702171
H	0.424361	-3.148046	0.065789
H	2.358476	-4.304198	1.109597
H	4.286013	-0.474945	1.449635
H	4.350170	-2.924370	1.812328
H	4.112463	1.548206	1.105393
H	3.729228	3.959693	0.685263
H	-0.126145	2.928187	-0.922718

H	1.537232	4.675940	-0.336215
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TS3-A2

C	-1.449914	-1.366192	1.741651
Re	-0.293862	-0.935585	0.264815
C	-0.871283	-2.515138	-0.669223
O	-1.254578	-3.444717	-1.253393
O	-2.148132	-1.626457	2.636150
N	-1.731334	0.469757	-0.621173
C	-1.582289	1.784955	-0.309291
C	-0.514614	2.096713	0.663196
N	0.209328	1.033749	1.104398
S	1.106305	-0.255014	-1.769491
C	2.669356	0.209224	-1.228558
S	3.972874	0.817499	-2.212670
C	1.135926	-1.969357	1.057925
O	1.977531	-2.588977	1.558341
O	3.090327	0.167924	-0.006311
C	1.192723	1.239784	2.001320
C	-0.254850	3.390590	1.128538
C	-2.411270	2.758260	-0.880688
C	-2.694942	0.110699	-1.492978
H	4.191396	0.635606	-0.599790
C	1.494438	2.500038	2.506891
H	1.756125	0.366894	2.301240
H	2.298783	2.608248	3.225731
C	0.758917	3.596471	2.060057
H	-0.835576	4.230860	0.769503
H	0.969804	4.596067	2.426589
C	-3.402101	2.381093	-1.781281
H	-2.280988	3.803467	-0.630182
H	-4.045553	3.129700	-2.232318
C	-3.548948	1.028916	-2.092400
H	-2.770814	-0.947771	-1.710182
H	-4.304466	0.682969	-2.788944

M3-A2

C	-0.309096	-0.083907	-2.597915
Re	0.098767	-0.163461	-0.719134
C	0.950765	-1.871159	-0.955511
O	1.506355	-2.882086	-1.104625
O	-0.559293	-0.035252	-3.734484
N	1.890381	1.088509	-0.921588
C	1.744692	2.418970	-0.681667
C	0.368490	2.872932	-0.394227
N	-0.581885	1.900975	-0.378515
S	0.780070	-0.171412	1.745250
C	-0.647008	0.270094	2.678105
S	-0.283067	0.319179	4.468937
C	-1.569440	-1.079977	-0.375747
O	-2.578369	-1.621262	-0.195638
O	-1.761574	0.527215	2.259617
C	-1.861671	2.241531	-0.133375
C	3.117284	0.607190	-1.205446
H	-1.542131	0.664811	4.807509
C	-2.257168	3.555441	0.094428
H	-2.574898	1.429440	-0.102468
H	-3.301218	3.771943	0.290466
C	-1.290456	4.559691	0.080310
C	0.034822	4.212897	-0.166138

H	-1.560070	5.595579	0.260268
H	0.799118	4.979655	-0.179450
C	4.248067	1.412992	-1.263913
H	3.180849	-0.458902	-1.386238
H	5.210586	0.969999	-1.494157
C	4.109573	2.779187	-1.016337
C	2.846126	3.282912	-0.725428
H	4.969087	3.441142	-1.047672
H	2.720298	4.340036	-0.528298

TS4-A2

C	-0.282610	-0.123954	-2.593748
Re	0.057065	-0.124945	-0.697339
C	0.860023	-1.867907	-0.819737
O	1.386599	-2.902279	-0.898130
O	-0.490443	-0.125697	-3.739415
N	1.895515	1.059112	-0.890822
C	1.785814	2.403793	-0.719446
C	0.416475	2.913828	-0.503106
N	-0.565715	1.973709	-0.478640
S	0.653595	-0.042673	1.788572
C	-0.759867	0.523705	2.650486
S	-0.457754	0.701807	4.506887
C	-1.649790	-0.968973	-0.365398
O	-2.681448	-1.466428	-0.184647
O	-1.842305	0.822909	2.195268
C	-1.841707	2.366248	-0.298294
C	3.115306	0.526476	-1.106822
H	-0.834303	-0.566214	4.766877
C	-2.201049	3.700830	-0.143076
H	-2.583268	1.580210	-0.261036
H	-3.243543	3.958740	0.005028
C	-1.201291	4.672145	-0.164295
C	0.119547	4.272589	-0.346512
H	-1.442310	5.722962	-0.038785
H	0.908973	5.013355	-0.364932
C	4.273253	1.292755	-1.162387
H	3.150133	-0.548540	-1.234866
H	5.227997	0.809273	-1.336713
C	4.171550	2.673090	-0.984712
C	2.916179	3.229565	-0.763693
H	5.053020	3.305479	-1.016208
H	2.818530	4.298416	-0.621491

M4-A2

C	-1.478909	-1.421137	1.686543
O	-2.208857	-1.712416	2.546072
Re	-0.269447	-0.942356	0.268194
C	1.158462	-1.927845	1.123910
O	1.999783	-2.518361	1.659060
C	-0.744024	-2.533617	-0.701009
O	-1.064055	-3.471920	-1.309691
N	-1.711118	0.416380	-0.676877
C	-1.620385	1.734515	-0.355460
C	-0.606824	2.079273	0.662500
N	0.127946	1.039209	1.138591
S	1.217356	-0.215132	-1.680786
C	2.756389	0.310712	-0.991716
O	3.066450	0.332096	0.185318
S	4.001001	0.892059	-2.193265

C	1.062682	1.275494	2.078960
C	-2.627033	0.028147	-1.586967
H	3.277953	0.667626	-3.307675
C	1.303280	2.544792	2.594523
H	1.639973	0.421492	2.404984
H	2.072447	2.677770	3.346816
C	0.556597	3.618196	2.111735
C	-0.407629	3.381023	1.136234
H	0.721522	4.624272	2.484193
H	-0.996323	4.203159	0.749187
C	-3.488061	0.918587	-2.217011
H	-2.658285	-1.031539	-1.809233
H	-4.204002	0.549381	-2.942846
C	-3.400532	2.273961	-1.896657
C	-2.459660	2.681059	-0.956702
H	-4.052184	3.001624	-2.369758
H	-2.376752	3.728813	-0.696800

TS5-A2

C	-1.837891	0.458034	1.811981
O	-2.290124	0.834461	2.815383
Re	-1.091908	-0.163294	0.151345
N	0.875766	-0.481739	1.091371
C	1.740742	0.567255	1.092835
C	1.283867	1.772735	0.372242
N	0.038606	1.700694	-0.166265
S	-0.122498	-0.938007	-2.092539
C	1.778563	-0.856954	-1.971587
O	2.412973	0.168108	-1.911344
C	-1.819905	-1.920465	0.457087
O	-2.219953	-2.992621	0.655760
C	-2.703922	0.334772	-0.778126
O	-3.659177	0.674219	-1.345321
S	2.254813	-2.543557	-1.971094
C	1.243969	-1.631584	1.690562
C	-0.430678	2.750214	-0.869655
H	0.517248	-2.388117	-1.998984
C	2.464271	-1.785561	2.337538
H	0.531196	-2.445148	1.643733
H	2.709972	-2.735812	2.797778
C	3.348232	-0.707726	2.362661
C	2.981986	0.476394	1.730968
H	4.311851	-0.789269	2.855088
H	3.663089	1.317720	1.726197
C	0.302316	3.914909	-1.060715
H	-1.424098	2.640340	-1.286812
H	-0.123132	4.727311	-1.639113
C	1.577695	4.001760	-0.501803
C	2.069311	2.920395	0.220613
H	2.183394	4.892667	-0.633053
H	3.064836	2.961328	0.643264

TS2-B

C	-1.056426	0.405453	1.757692
O	-1.323476	0.623547	2.863312
Re	-0.716111	-0.009622	-0.104566
C	-1.467948	1.695527	-0.580599
O	-1.916501	2.714797	-0.914179
C	-2.447008	-0.806693	-0.213328
O	-3.494933	-1.310360	-0.288566

N	-0.118690	-0.641826	-2.124192
C	0.652651	-1.757905	-2.213144
C	0.898131	-2.474628	-0.942686
N	0.323496	-1.930498	0.161248
O	1.329841	0.769236	-0.189712
C	2.398005	0.796196	0.681230
S	2.360180	0.225569	2.231585
S	3.630835	1.550475	-0.296783
H	2.131769	1.335624	-0.973443
C	-0.409620	0.044850	-3.246501
C	1.651539	-3.650448	-0.858727
C	0.052104	-0.334309	-4.501869
H	-1.029491	0.924267	-3.120253
H	-0.210644	0.256932	-5.371896
C	0.854027	-1.471384	-4.602497
C	1.152458	-2.188509	-3.447860
H	1.240938	-1.796346	-5.563016
H	1.772824	-3.073594	-3.509218
C	1.804171	-4.281958	0.373077
H	2.116874	-4.071230	-1.741057
H	2.387778	-5.193766	0.450364
C	1.200320	-3.722854	1.497167
C	0.480110	-2.541188	1.350557
H	1.295453	-4.172915	2.478734
H	0.018128	-2.057664	2.200738

M2-B

C	-0.986657	0.261604	1.833915
O	-0.750942	-0.023139	0.735691
Re	-1.493125	0.653802	3.661983
C	-0.472723	-0.871224	4.232087
O	0.131405	-1.784539	4.624142
C	-3.031020	-0.455617	3.435707
O	-3.983357	-1.115731	3.306243
N	-2.108345	1.360345	5.653545
C	-2.744412	2.559392	5.712010
C	-3.037702	3.197231	4.409900
N	-2.616800	2.517167	3.312726
O	0.132983	2.000741	4.170611
C	0.781870	2.848940	3.470469
S	0.595491	3.234638	1.845680
S	2.060829	3.743998	4.377254
H	1.899520	3.089566	5.549376
C	-2.857681	3.028739	2.091233
C	-3.542919	4.225021	1.902005
H	-2.479424	2.459922	1.252603
H	-3.711207	4.591588	0.895812
C	-3.975203	4.933022	3.021651
C	-3.717705	4.414462	4.288017
H	-4.502262	5.875821	2.914600
H	-4.044650	4.953716	5.168062
C	-3.098502	3.125712	6.942537
C	-2.797053	2.454808	8.123921
H	-3.600937	4.084020	6.981286
H	-3.065429	2.887900	9.082299
C	-2.147468	1.222426	8.052253
C	-1.821071	0.714430	6.799508
H	-1.891167	0.660389	8.943389
H	-1.312302	-0.236199	6.696120

TS3-B1

C	0.515298	-1.483706	1.390695
O	0.506602	-0.753907	0.488657
Re	0.618026	-2.702523	2.880889
C	-0.513074	-1.518090	3.894066
O	-1.175638	-0.824963	4.548365
C	2.136763	-1.792541	3.509840
O	3.090342	-1.236650	3.895714
N	0.815559	-4.322230	4.372798
C	1.563841	-5.404468	4.039575
C	2.168359	-5.370090	2.691949
N	1.895012	-4.262867	1.956928
O	-1.678211	-3.962236	3.206960
C	-2.021644	-4.359196	2.077124
S	-1.115775	-4.086016	0.654535
S	-3.562834	-5.287146	1.895594
H	-3.903311	-5.213811	3.200204
C	1.731431	-6.470798	4.932306
C	2.971890	-6.397772	2.181000
C	1.118198	-6.426187	6.179951
H	2.331337	-7.328448	4.655237
H	1.240866	-7.246704	6.879794
C	0.343015	-5.313252	6.509198
C	0.216017	-4.289052	5.578598
H	-0.161356	-5.234036	7.465766
H	-0.386178	-3.414138	5.788001
C	3.509058	-6.280942	0.903839
H	3.175969	-7.281198	2.772976
H	4.132558	-7.070928	0.497480
C	3.230091	-5.133789	0.159216
C	2.418086	-4.156191	0.719994
H	3.623590	-4.994471	-0.841438
H	2.161519	-3.259594	0.169691

TS3-B2

C	-1.024600	0.333588	1.622005
O	-0.878195	0.025688	0.514068
Re	-1.375282	0.768932	3.475309
C	-0.255409	-0.704923	3.993994
O	0.413492	-1.586100	4.352193
C	-2.889755	-0.394680	3.423475
O	-3.827648	-1.086569	3.400229
N	-1.826892	1.525436	5.493002
C	-2.488478	2.709132	5.572303
C	-2.915311	3.296078	4.282871
N	-2.579508	2.588575	3.173389
O	0.233805	2.185095	3.798677
C	0.804133	3.034043	3.044614
S	0.511820	3.359828	1.432229
S	2.096713	4.026093	3.971393
H	3.101399	3.186937	3.649877
C	-2.742444	3.309426	6.810956
C	-3.628710	4.496073	4.183527
C	-2.310831	2.689140	7.979773
H	-3.266191	4.255415	6.865184
H	-2.499410	3.149290	8.944501
C	-1.633337	1.473769	7.886993
C	-1.411790	0.929851	6.626356
H	-1.274398	0.952669	8.767437
H	-0.884515	-0.008681	6.507024
C	-4.006549	4.969073	2.929511

H	-3.887821	5.058211	5.071847
H	-4.559220	5.899018	2.840791
C	-3.660523	4.233067	1.797902
C	-2.938616	3.054972	1.962746
H	-3.923609	4.564276	0.799794
H	-2.625427	2.464478	1.112170

M3-B2

C	2.195422	-1.019616	-0.860668
O	3.257852	-1.131424	-1.310303
Re	0.374562	-0.919128	-0.210135
N	-0.272088	0.886431	-1.294528
C	-1.499879	1.380161	-0.989998
C	-2.283358	0.594933	-0.010908
N	-1.690484	-0.537148	0.449589
O	0.674389	0.472873	1.421328
C	1.480076	1.448632	1.588873
S	2.664736	2.015205	0.539897
C	0.738733	-2.424595	0.928448
O	0.913889	-3.333809	1.631765
C	-0.150564	-2.104100	-1.613005
O	-0.488655	-2.812199	-2.475525
S	1.180484	2.217481	3.203794
H	2.125297	3.168646	3.091742
C	-3.560713	0.965913	0.425246
C	-1.974468	2.552391	-1.589485
C	-4.235629	0.166988	1.343502
H	-4.024121	1.872991	0.058202
H	-5.224652	0.448987	1.690420
C	-3.618980	-0.994752	1.807419
C	-2.348181	-1.307025	1.336511
H	-4.102093	-1.649338	2.524168
H	-1.828881	-2.195478	1.674359
C	-1.179186	3.220078	-2.517169
H	-2.952459	2.942844	-1.337899
H	-1.537214	4.129902	-2.988545
C	0.078311	2.703694	-2.823884
C	0.497758	1.542057	-2.182852
H	0.738055	3.192064	-3.531970
H	1.475953	1.119612	-2.369701

TS4-B2a

C	2.055633	-0.807615	-1.446217
O	2.933342	-0.834366	-2.201359
Re	0.511179	-0.810692	-0.264668
N	-0.727257	0.599928	-1.339105
C	-1.907633	0.898593	-0.827051
C	-2.264583	0.160784	0.375962
N	-1.328854	-0.645647	0.845056
C	1.439723	-1.902565	1.033814
O	1.942643	-2.552573	1.850823
C	-0.092369	-2.364640	-1.145186
O	-0.467241	-3.315144	-1.709142
O	0.811884	0.794176	1.858533
C	1.411001	1.789153	1.425804
S	1.881774	1.942328	-0.219520
S	1.778129	3.089495	2.625197
H	2.388967	3.934931	1.774227
C	-3.538588	0.314324	1.014346
C	-2.763698	1.901214	-1.387493

C	-3.814757	-0.382483	2.137661
H	-4.281503	0.986601	0.594795
H	-4.778786	-0.275720	2.629600
C	-2.826929	-1.266417	2.668416
C	-1.630022	-1.393446	2.052259
H	-3.033355	-1.840672	3.568447
H	-0.882506	-2.072304	2.456976
C	-2.384464	2.549638	-2.509651
H	-3.712093	2.137501	-0.913929
H	-3.023606	3.312022	-2.949034
C	-1.133242	2.219301	-3.114312
C	-0.340824	1.273827	-2.560266
H	-0.812638	2.727333	-4.020642
H	0.610938	1.028336	-3.022153

TS4-B2b

C	-1.332551	-2.069487	0.741903
Re	0.176974	-1.015433	0.152032
C	1.226728	-1.820722	1.530583
O	1.872498	-2.287748	2.380499
O	-2.202249	-2.720456	1.146767
N	-0.214180	0.813657	1.310444
C	0.573130	1.888721	1.043370
C	1.661461	1.662834	0.066205
N	1.756005	0.403631	-0.434149
O	-0.793571	0.106916	-1.421221
C	-1.930998	0.622440	-1.591125
S	-2.336250	1.695334	-2.910402
C	0.647570	-2.441125	-1.053437
O	0.967897	-3.277941	-1.792579
S	-3.359540	0.412411	-0.578438
H	-3.644431	1.413968	-1.856453
C	2.729142	0.121158	-1.319607
C	-1.216089	0.938899	2.200647
C	-1.475654	2.127951	2.875448
H	-1.823867	0.058652	2.364045
H	-2.298318	2.174751	3.579802
C	-0.677615	3.237200	2.605164
C	0.356370	3.115037	1.679873
H	-0.855804	4.185453	3.102197
H	0.983633	3.968936	1.457610
C	3.654282	1.067513	-1.747748
H	2.755866	-0.895277	-1.693030
H	4.417159	0.786725	-2.465144
C	3.564755	2.363923	-1.242295
C	2.559414	2.661508	-0.326738
H	4.263049	3.133274	-1.556014
H	2.473226	3.664773	0.070784

M4-B2b

C	-2.444591	0.328665	0.737736
Re	-0.851027	-0.584784	0.154949
C	-1.174279	-1.897588	1.505635
O	-1.349934	-2.693397	2.338451
O	-3.395473	0.853064	1.149230
N	0.612286	0.555995	1.336538
C	1.921660	0.342461	1.042771
C	2.200594	-0.755805	0.090642
N	1.116417	-1.423502	-0.379674
O	-0.117423	0.788076	-1.329333

C	-0.086403	2.028584	-1.624308
S	1.236742	2.824103	-2.282284
C	-1.920063	-1.586482	-1.095735
O	-2.530704	-2.209261	-1.862507
S	-1.649802	2.897954	-1.277391
H	-1.234094	4.106090	-1.695649
C	1.294184	-2.451278	-1.228170
C	0.284349	1.525330	2.210819
C	2.552187	-2.864757	-1.654339
H	0.394867	-2.945374	-1.575806
H	2.639908	-3.696720	-2.344020
C	3.672268	-2.179315	-1.186011
C	3.493092	-1.118411	-0.303008
H	4.670752	-2.462355	-1.503588
H	4.353167	-0.574344	0.065613
C	1.234847	2.325863	2.835560
H	-0.773381	1.660003	2.401352
H	0.915991	3.097141	3.527537
C	2.580572	2.119611	2.536413
C	2.924723	1.117140	1.634315
H	3.352124	2.731534	2.992578
H	3.965190	0.950517	1.386918

TS5-B2b

C	1.209675	-0.374316	-2.252541
O	1.734292	-0.201386	-3.274524
Re	0.268722	-0.641977	-0.596630
C	1.586301	-1.962823	-0.091133
O	2.345298	-2.774050	0.234339
C	-0.764299	-1.977542	-1.417073
O	-1.418987	-2.797374	-1.930016
N	-1.322804	0.868812	-0.875332
C	-2.231794	1.018697	0.123202
C	-2.024544	0.162959	1.310685
N	-0.968911	-0.685853	1.240940
O	1.537513	0.285622	1.637453
C	2.347195	1.187505	1.377975
S	1.688802	2.099030	-0.238389
S	3.742437	1.732083	2.089684
H	2.862647	2.234943	-0.884503
C	-0.691809	-1.473477	2.296128
C	-1.445244	1.620235	-1.987761
C	-2.469737	2.541827	-2.164765
H	-0.690070	1.471122	-2.749320
H	-2.519834	3.118527	-3.081494
C	-3.408942	2.702087	-1.145192
C	-3.285980	1.933530	0.007647
H	-4.222420	3.413684	-1.244309
H	-4.004529	2.045026	0.809750
C	-1.459107	-1.470295	3.456061
H	0.180040	-2.107705	2.205341
H	-1.188538	-2.122977	4.278343
C	-2.553487	-0.610201	3.533034
C	-2.836103	0.216650	2.449478
H	-3.173074	-0.575358	4.423472
H	-3.673871	0.900932	2.497455

TS4-B2c

O	-0.261926	0.009244	0.125507
C	-0.149270	0.031907	1.285878
Re	0.070684	0.061678	3.179440

N	1.677751	1.558388	3.156658
C	1.470921	2.888202	3.131359
H	0.442476	3.209345	3.018590
C	2.503405	3.812178	3.248628
H	2.280927	4.873052	3.224752
C	3.806075	3.338764	3.404882
H	4.639315	4.026592	3.508320
C	4.025510	1.964840	3.427820
H	5.030977	1.582636	3.550064
C	2.943554	1.086060	3.300385
C	3.090564	-0.385823	3.291771
C	4.324759	-1.032215	3.403928
H	5.235443	-0.460556	3.528948
C	4.380354	-2.422651	3.364570
H	5.332990	-2.933922	3.458741
C	3.196381	-3.139861	3.211980
H	3.185266	-4.223545	3.185373
C	2.000128	-2.436667	3.114640
H	1.055154	-2.955793	3.011926
N	1.941490	-1.093951	3.147408
C	-1.150139	-1.422250	3.334129
O	-1.854315	-2.341700	3.411794
C	-1.419180	1.271415	3.337654
O	-2.291687	2.033345	3.426894
O	0.580821	0.168228	5.280567
C	0.574641	-0.618288	6.288363
S	1.839015	-1.604989	6.787804
S	-0.991951	-0.525576	7.198374
H	-0.677438	-1.426629	8.146864

[Re(OCH₃)(CO)₃(bipy)]

C	0.060969	0.124096	-2.019518
Re	0.018825	0.101298	-0.066614
O	-2.053741	0.038888	-0.149569
C	-2.880786	1.081876	-0.586309
O	0.072822	0.084985	-3.176136
C	0.137012	2.027963	0.079868
O	0.211958	3.176994	0.231150
C	1.964665	0.039938	-0.056442
O	3.128405	0.021900	-0.072405
N	-0.331868	-1.998009	0.158473
C	-0.747613	-2.398279	1.325399
C	-0.654343	-1.416226	2.379147
N	-0.212228	-0.246900	2.002808
C	-0.042048	0.717824	3.058245
C	-1.203321	-3.751047	1.580056
C	-0.387664	-2.982800	-0.890657
H	-3.931556	0.775303	-0.471063
H	-2.738441	2.013093	-0.009359
H	-2.727629	1.329973	-1.651343
C	-0.616800	-4.263702	-0.592310
H	-0.242946	-2.682677	-1.927433
H	-0.658995	-5.008450	-1.385714
C	-1.208827	-4.650394	0.593462
H	-1.541082	-4.033396	2.576107
H	-1.551080	-5.666369	0.784718
C	-0.221748	0.354339	4.330177
H	0.233237	1.743902	2.818865
H	-0.093050	1.083912	5.128351
C	-0.588289	-1.011881	4.648910
C	-0.746060	-1.906260	3.670433

H	-0.734876	-1.308386	5.686464
H	-1.021345	-2.932338	3.909812

TS1-OCH₃

C	-1.368928	0.889587	2.067346
Re	-0.961974	0.479588	0.223094
C	-2.616691	-0.470809	0.085159
O	-3.617501	-1.059629	-0.022119
O	-1.655601	1.099206	3.171527
N	-0.301158	-0.159355	-1.781703
C	0.455086	-1.286160	-1.850305
C	0.675850	-1.994432	-0.571640
N	0.154923	-1.397486	0.532097
O	0.984370	1.448406	0.283356
C	1.400481	2.424903	-0.655105
C	-1.873439	2.091741	-0.281898
O	-2.435530	3.051136	-0.627383
C	2.463900	0.722537	1.209746
S	3.541622	0.188907	0.124608
S	2.117121	0.912891	2.773441
C	-0.568076	0.518898	-2.914429
C	0.318814	-1.986320	1.731403
H	2.084787	3.133232	-0.170806
H	1.921467	1.976453	-1.512958
H	0.533192	2.987154	-1.020468
C	-0.094098	0.123067	-4.160033
H	-1.181148	1.405378	-2.806181
H	-0.337926	0.709352	-5.038959
C	0.695347	-1.024329	-4.238851
C	0.968152	-1.733661	-3.073518
H	1.093474	-1.362091	-5.190381
H	1.584227	-2.622746	-3.116657
C	0.989967	-3.194378	1.890273
H	-0.095339	-1.460654	2.582050
H	1.098027	-3.620097	2.881374
C	1.517024	-3.819880	0.761833
C	1.355306	-3.213166	-0.480354
H	2.049726	-4.761798	0.844857
H	1.763244	-3.682719	-1.366280

M1-OCH₃

C	-1.321477	0.818192	2.153500
Re	-0.931873	0.470513	0.282864
C	-2.598363	-0.425081	0.126904
O	-3.612923	-0.985989	0.014080
O	-1.629809	0.991167	3.255260
N	-0.302747	-0.101582	-1.747215
C	0.430592	-1.240269	-1.869635
C	0.670722	-1.990907	-0.619981
N	0.160541	-1.432787	0.509646
O	1.112544	1.488374	0.334978
C	1.474589	2.489923	-0.645510
C	-1.801569	2.124487	-0.156395
O	-2.333706	3.111928	-0.468232
C	2.245716	0.792636	0.985679
S	3.452894	0.253365	-0.037696
S	2.036770	0.682966	2.636577
C	0.891496	-1.666120	-3.121586
C	0.338880	-2.061103	1.687130
H	2.264113	3.117110	-0.226560

H	1.830051	2.027556	-1.568458
H	0.579307	3.087931	-0.819389
C	1.010544	-3.274743	1.795471
H	-0.062996	-1.565293	2.560394
H	1.131289	-3.732898	2.770324
C	1.525877	-3.859198	0.640812
C	1.350600	-3.211483	-0.578658
H	2.063178	-4.801074	0.686115
H	1.756233	-3.646536	-1.482853
C	0.597813	-0.920226	-4.257368
H	1.484253	-2.567628	-3.207133
H	0.956994	-1.240927	-5.230047
C	-0.163085	0.242397	-4.123060
C	-0.591145	0.612505	-2.854416
H	-0.422018	0.856606	-4.978225
H	-1.185097	1.506019	-2.704085

TS2-A-OCH₃

C	1.317951	-1.770410	-1.490946
Re	0.940445	-0.427061	-0.232255
C	2.431565	0.614597	-0.904141
O	3.333571	1.173683	-1.367941
O	1.541574	-2.600929	-2.280617
N	-0.687567	0.420770	-1.481609
C	-1.957495	0.038797	-1.191743
C	-2.085468	-1.027513	-0.180343
N	-0.923633	-1.432043	0.400565
C	2.131063	-1.274071	1.010299
O	2.811720	-1.826104	1.776403
O	0.196925	0.877515	1.826072
C	-0.134837	0.287685	3.102139
C	-0.094567	2.248021	1.621218
S	0.697056	2.810222	0.232789
S	-1.089939	3.063387	2.679771
C	-0.961369	-2.452062	1.283767
C	-0.489148	1.341104	-2.445704
H	0.364942	-0.680927	3.118377
H	0.239464	0.920415	3.908317
H	-1.216482	0.176104	3.209202
C	-2.137178	-3.095490	1.646791
H	-0.008754	-2.755743	1.700596
H	-2.104830	-3.908146	2.363915
C	-3.336591	-2.674028	1.068468
C	-3.305257	-1.636433	0.143783
H	-4.276915	-3.151503	1.324580
H	-4.221594	-1.309279	-0.330997
C	-1.530990	1.921927	-3.157698
H	0.539253	1.619384	-2.634193
H	-1.311219	2.654605	-3.925787
C	-2.841663	1.565646	-2.836905
C	-3.055114	0.615485	-1.844772
H	-3.683496	2.021828	-3.347835
H	-4.064969	0.331175	-1.577292

M2-A-OCH₃

C	-0.611076	-0.701360	-2.590253
Re	-0.141222	-0.756370	-0.723686
C	0.605785	-2.517925	-0.938431
O	1.095323	-3.563531	-1.072820
O	-0.894060	-0.673864	-3.719917

N	1.709177	0.390638	-1.010474
C	1.657745	1.721355	-0.734753
C	0.324481	2.251233	-0.385106
N	-0.686818	1.341878	-0.372644
S	0.721364	-0.694214	1.685696
C	-0.527523	-0.428605	2.872706
S	-0.193318	-0.218732	4.490576
C	-1.843391	-1.563215	-0.310844
O	-2.886841	-2.024698	-0.093172
O	-1.776530	-0.414978	2.355602
C	-2.903478	-0.316412	3.243143
C	0.084053	3.601515	-0.103760
C	2.890457	-0.158676	-1.356712
H	-3.777324	-0.394720	2.594153
H	-2.888470	-1.132039	3.970096
H	-2.890436	0.637136	3.777871
C	4.066344	0.576899	-1.444626
H	2.879165	-1.222162	-1.561763
H	4.989231	0.080753	-1.723456
C	4.024425	1.942563	-1.161297
C	2.807997	2.516836	-0.807027
H	4.922302	2.549979	-1.212799
H	2.757389	3.574651	-0.581868
C	-1.207231	4.025794	0.191891
H	0.897190	4.316345	-0.111427
H	-1.402636	5.069566	0.415893
C	-2.239085	3.086589	0.194735
C	-1.935756	1.760260	-0.089362
H	-3.262546	3.366486	0.418255
H	-2.703070	0.996780	-0.086413

TS3-A1-OCH₃

C	0.433994	-0.283712	-2.634571
O	0.404963	-0.196513	-3.796619
Re	0.485074	-0.427422	-0.721171
C	-0.359922	-2.155772	-0.802510
O	-0.899381	-3.184078	-0.848086
S	0.641610	-0.402809	1.849705
C	-0.593076	-1.539958	2.416118
S	-2.211528	-1.197808	2.621143
N	-1.323605	0.785818	-0.446368
C	-1.141936	2.097108	-0.136653
C	0.258992	2.563336	-0.123604
N	1.197288	1.628546	-0.432707
C	2.203203	-1.295513	-0.799676
O	3.257476	-1.781710	-0.840279
O	-0.044566	-2.723771	2.719238
C	-0.866042	-3.784560	3.241775
C	-2.575903	0.295895	-0.494718
C	2.495795	1.989729	-0.462793
H	-0.177030	-4.613781	3.405001
H	-1.640758	-4.054558	2.519938
H	-1.337594	-3.474037	4.177699
C	-3.701375	1.080535	-0.262435
H	-2.669586	-0.756282	-0.729412
H	-4.686263	0.630353	-0.313224
C	-3.525203	2.424558	0.056501
C	-2.231321	2.935406	0.121221
H	-4.377109	3.066603	0.256463
H	-2.075953	3.977450	0.370980
C	2.924160	3.283443	-0.190760

H	3.202018	1.206458	-0.709893
H	3.982311	3.517077	-0.227178
C	1.969709	4.249550	0.130747
C	0.628221	3.884105	0.161024
H	2.263882	5.269936	0.355116
H	-0.125291	4.620403	0.410276

M3-A1-OCH₃

C	0.407063	0.552344	-2.664745
Re	0.506659	0.568645	-0.744727
S	0.393382	0.713950	1.805163
C	1.209243	-0.575969	2.652428
O	1.118677	-0.326965	3.975721
C	1.708914	-1.234860	4.918122
O	0.344721	0.543113	-3.828085
N	-0.532912	-1.363487	-0.579525
C	-1.868217	-1.326045	-0.329257
C	-2.471183	0.021651	-0.272943
N	-1.622630	1.058693	-0.503442
C	1.176021	2.370336	-0.779760
O	1.536456	3.476054	-0.800555
C	2.336939	-0.055621	-0.832286
O	3.433077	-0.415961	-0.940471
S	1.987860	-1.921512	2.037640
C	0.080162	-2.557885	-0.682520
C	-2.109027	2.315588	-0.490071
H	1.265652	-2.230071	4.825020
H	2.787626	-1.307877	4.756953
H	1.490259	-0.800595	5.894683
C	-0.601017	-3.764287	-0.548835
H	1.144023	-2.532983	-0.873418
H	-0.057031	-4.697582	-0.640261
C	-1.967729	-3.736433	-0.280187
C	-2.606721	-2.503918	-0.170626
H	-2.530771	-4.656541	-0.159458
H	-3.669430	-2.463685	0.032591
C	-3.447542	2.603040	-0.249670
H	-1.392434	3.106338	-0.675741
H	-3.782493	3.634282	-0.248480
C	-4.325595	1.546116	-0.008057
C	-3.830537	0.246262	-0.022898
H	-5.376978	1.729307	0.189516
H	-4.497043	-0.586239	0.163982

TS4-A1a-OCH₃

C	-0.905811	2.669409	-0.459720
N	-1.032411	1.339993	-0.282433
C	-2.204321	0.851169	0.194568
C	-3.266052	1.705055	0.521004
C	-3.126387	3.076791	0.340467
C	-1.923519	3.568862	-0.167996
Re	0.599521	-0.108875	-0.712140
C	1.975746	1.129195	-1.248181
O	2.768079	1.894816	-1.611754
C	-2.274633	-0.618481	0.328248
N	-1.151768	-1.292865	-0.024688
C	-1.150352	-2.638006	0.047483
C	-2.251301	-3.371205	0.471978
C	-3.407699	-2.685606	0.847094
C	-3.416999	-1.297072	0.772772
C	0.050745	-0.266365	-2.501586

O	-0.301318	-0.363591	-3.612495
C	1.849068	-1.549861	-0.974042
O	2.562829	-2.446282	-1.159930
S	1.458514	1.683381	1.780427
C	1.590250	0.270348	2.696326
S	1.292610	-1.302775	2.111265
O	1.960638	0.415994	3.988510
C	2.037327	-0.858264	4.563301
H	-4.305888	-0.747670	1.056249
H	-4.286919	-3.221679	1.190031
H	-2.192659	-4.453184	0.510588
H	-0.228757	-3.129297	-0.238946
H	-4.191825	1.304416	0.914461
H	-3.940967	3.748249	0.592637
H	-1.763966	4.629283	-0.327886
H	0.050076	3.011259	-0.836360
H	2.334680	-0.768373	5.607055
H	1.063784	-1.342592	4.503628
H	2.773169	-1.455017	4.026326

M4-A1a-OCH₃

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.399561
N	1.164991	0.000000	2.097545
C	2.329892	-0.055465	1.424803
C	2.396804	-0.088075	0.037032
C	1.206108	-0.047946	-0.689354
C	-1.235522	0.002418	2.210561
N	-1.058506	0.004321	3.557057
C	-2.139235	-0.046751	4.358349
C	-3.439204	-0.076659	3.867802
C	-3.631944	-0.038450	2.486354
C	-2.519604	0.004966	1.653876
Re	1.010523	0.127758	4.285309
C	2.896573	0.173349	4.675695
O	4.042106	0.200657	4.868734
C	0.618631	0.177752	6.170932
O	0.340177	0.207858	7.298679
C	0.967839	2.045948	4.214684
O	0.941177	3.208917	4.170741
S	1.193935	-2.428705	4.572130
C	0.443509	-3.514117	3.432339
O	0.607655	-4.829889	3.686245
C	1.350285	-5.314465	4.818974
S	-0.454687	-3.162881	2.063197
H	3.229870	-0.070874	2.027245
H	3.362656	-0.138453	-0.452949
H	1.215486	-0.062242	-1.774600
H	-0.933754	0.011594	-0.547359
H	-2.650364	0.015041	0.579432
H	-4.631414	-0.050743	2.063320
H	-4.273063	-0.123522	4.559156
H	-1.944514	-0.060795	5.423723
H	1.294816	-6.400796	4.737892
H	2.390685	-4.981163	4.775913
H	0.898046	-4.978079	5.755829

TS5-A1a-OCH₃

C	3.164990	-1.766590	-0.409213
C	1.978180	-1.144180	-0.002876
N	0.788080	-1.475362	-0.566075

C	0.765496	-2.382213	-1.562521
C	1.909595	-3.020183	-2.023768
C	3.133447	-2.711419	-1.426735
C	1.923514	-0.112957	1.053900
N	0.695127	0.409087	1.306084
C	0.579698	1.392763	2.220314
C	1.660373	1.877002	2.945918
C	2.917675	1.311691	2.728021
C	3.046595	0.308704	1.775563
Re	-1.003363	-0.456394	0.213496
C	-2.389661	0.640351	0.968680
O	-3.198167	1.333366	1.438251
C	-1.264533	-1.774832	1.589588
O	-1.422898	-2.571269	2.422559
S	-0.686749	1.223608	-1.694472
C	0.724580	2.349780	-1.497335
O	0.327592	3.545371	-1.410851
C	-2.310104	-1.334352	-0.897686
O	-3.069357	-1.886067	-1.583200
S	2.340373	1.844387	-1.531882
C	-1.762287	3.560028	-1.508925
H	-0.204926	-2.595856	-1.993396
H	1.834154	-3.741128	-2.829997
H	4.049725	-3.190613	-1.756530
H	4.108475	-1.494017	0.045664
H	4.018176	-0.124688	1.576614
H	3.785893	1.655382	3.281041
H	1.510278	2.675198	3.664030
H	-0.416026	1.791377	2.370403
H	-1.680883	3.889458	-2.536341
H	-2.589336	2.899756	-1.291010
H	-1.566476	4.307964	-0.752678

TS4-A1b-OCH₃

C	5.244535	0.751715	-1.616712
O	3.354875	0.386652	-2.429217
C	2.648404	0.085594	-1.427250
S	3.427178	0.080033	0.105616
S	0.954965	-0.283683	-1.741512
Re	-0.495282	-0.920033	0.272613
N	0.026898	1.026488	1.142883
C	-0.610355	2.119110	0.642947
C	-1.631312	1.847404	-0.389139
N	-1.831306	0.536614	-0.689272
C	-1.746438	-1.312403	1.679448
O	-2.506446	-1.548713	2.530480
C	0.833313	-2.025191	1.139200
O	1.599524	-2.699935	1.689155
C	-1.070996	-2.475085	-0.703810
O	-1.450182	-3.388950	-1.314629
C	0.947040	1.194148	2.111951
C	-2.762222	0.211731	-1.607971
H	5.465656	0.377683	-2.607217
H	5.075754	1.817147	-1.534479
H	5.823035	0.299604	-0.823818
C	1.269635	2.443603	2.633281
H	1.430964	0.296155	2.470814
H	2.018996	2.519110	3.413123
C	0.627760	3.569362	2.122565
C	-0.321450	3.403088	1.116792
H	0.857504	4.561180	2.498900

H	-0.833404	4.266432	0.710772
C	-3.533740	1.161598	-2.267176
H	-2.879001	-0.845037	-1.814846
H	-4.266383	0.842522	-3.000033
C	-3.334063	2.509751	-1.968391
C	-2.375990	2.851686	-1.019625
H	-3.911867	3.282204	-2.465814
H	-2.205447	3.893077	-0.777313

M4-A1b-OCH₃

C	0.944531	2.964838	-2.174431
C	0.939086	1.633015	-1.773889
N	-0.057511	1.094976	-1.044697
C	-1.107309	1.881139	-0.684066
C	-1.156665	3.231156	-1.049967
C	-0.121534	3.781459	-1.800145
Re	-0.092325	-0.991275	-0.350147
S	0.531292	-0.089354	1.972365
C	1.984487	0.911446	2.137615
S	3.216319	0.836976	0.805393
C	-2.182328	1.209610	0.074808
N	-2.009370	-0.120861	0.290905
C	-2.957893	-0.802784	0.961060
C	-4.115630	-0.204263	1.445085
C	-4.301736	1.161393	1.230640
C	-3.326467	1.870829	0.537035
C	-0.821663	-1.619458	-2.015070
O	-1.265633	-1.999003	-3.022818
C	-0.326033	-2.730814	0.441275
O	-0.507600	-3.768929	0.930607
C	1.662959	-1.552019	-0.924572
O	2.696280	-1.902590	-1.320462
O	2.181721	1.600909	3.119921
C	4.447591	2.011294	1.468642
H	-2.768693	-1.858312	1.113448
H	-4.843771	-0.801524	1.982399
H	-3.452701	2.932432	0.366083
H	-5.188372	1.667459	1.598970
H	-1.995455	3.848951	-0.755212
H	-0.150548	4.827638	-2.087641
H	1.753169	0.968716	-2.031966
H	1.775673	3.344081	-2.758325
H	5.264954	2.043694	0.744167
H	4.010882	3.004569	1.586058
H	4.819130	1.663041	2.433328

TS5-A1b-OCH₃

C	3.499090	-1.052627	1.122246
C	2.387143	-0.451531	0.517545
N	1.331789	-1.196820	0.096156
C	1.373479	-2.534977	0.258408
C	2.448691	-3.190791	0.843546
C	3.532790	-2.432400	1.289292
C	2.280915	1.001510	0.278469
N	1.140281	1.410561	-0.330444
C	0.987297	2.717322	-0.618659
C	1.945795	3.673230	-0.305415
C	3.111347	3.265600	0.344783
C	3.279015	1.916334	0.637160
Re	-0.389105	-0.135404	-0.794085
C	-1.802473	1.021318	-1.435534

O	-2.619757	1.720659	-1.863477
C	0.282535	-0.298542	-2.542619
O	0.708422	-0.404932	-3.625128
C	-1.534562	-1.644026	-1.096428
O	-2.190273	-2.587505	-1.280988
S	-1.340772	-0.970856	1.993848
C	-2.254238	0.666320	2.290634
S	-1.352029	1.948118	1.582384
O	-3.286432	0.647092	2.920351
C	-2.655726	-2.201160	2.317814
H	0.508891	-3.084060	-0.093746
H	2.426928	-4.269810	0.947907
H	4.330882	-0.447887	1.460590
H	4.389293	-2.906609	1.757764
H	4.177417	1.581386	1.140216
H	3.876520	3.984554	0.619512
H	0.056972	2.994993	-1.097863
H	1.768124	4.712564	-0.557713
H	-2.250827	-3.018025	2.918675
H	-3.430468	-1.671743	2.882048
H	-3.072772	-2.588462	1.385759

TS3-A2-OCH₃

C	0.441983	1.095306	-4.861148
O	0.231165	0.863768	-2.795640
C	1.394589	0.523567	-2.425260
S	1.813306	0.331052	-0.726784
Re	-0.251818	0.773186	0.711351
C	0.759363	2.019281	1.772209
O	1.387415	2.737924	2.436996
S	2.577890	0.258643	-3.633978
N	0.428960	-1.067773	1.694330
C	0.059235	-2.245012	1.122811
C	-0.847686	-2.136353	-0.037658
N	-1.180956	-0.871378	-0.408489
C	-1.771119	0.978962	1.876602
O	-2.691478	1.104594	2.580114
C	-0.861758	2.249800	-0.375532
O	-1.258155	3.134736	-1.012281
C	-2.021842	-0.695458	-1.445811
C	1.242739	-1.091577	2.768764
H	-0.623809	0.958905	-4.736370
H	0.795769	2.117151	-4.829369
H	0.892991	0.458464	-5.608954
C	-2.573278	-1.757891	-2.153600
H	-2.240384	0.329781	-1.712288
H	-3.245986	-1.558297	-2.980263
C	-2.234551	-3.059160	-1.783915
C	-1.363386	-3.247341	-0.715243
H	-2.639849	-3.913697	-2.316405
H	-1.089444	-4.250392	-0.413466
C	1.724362	-2.271461	3.323335
H	1.511368	-0.127916	3.184017
H	2.379344	-2.229790	4.186442
C	1.352437	-3.484587	2.742679
C	0.511103	-3.467432	1.635197
H	1.711828	-4.427305	3.142705
H	0.214606	-4.398991	1.169847

M3-A2-OCH₃

C	-0.335767	-0.082009	-2.561132
Re	0.082733	-0.142613	-0.683985
S	0.788269	-0.133108	1.772721
C	-0.624974	0.330391	2.724107
S	-0.256288	0.342794	4.498808
C	-1.887347	0.850014	5.143957
O	-0.591278	-0.046161	-3.697334
C	-1.606730	-1.008502	-0.316674
O	-2.629630	-1.518978	-0.123971
C	0.888848	-1.875565	-0.897234
O	1.417400	-2.902946	-1.031955
N	1.903130	1.062343	-0.921277
C	1.791554	2.400008	-0.705285
C	0.429517	2.891515	-0.412989
N	-0.542294	1.942280	-0.367553
O	-1.735344	0.619606	2.305733
C	-1.810300	2.316286	-0.110669
C	2.913022	3.235993	-0.774544
H	-1.799118	0.847187	6.233169
H	-2.149455	1.851251	4.797187
H	-2.657915	0.143111	4.832351
C	-2.173192	3.643062	0.095634
H	-2.540211	1.520763	-0.053247
H	-3.209572	3.886901	0.300273
C	-1.184683	4.624994	0.047518
C	0.129123	4.243234	-0.208169
H	-1.428903	5.670357	0.208032
H	0.910174	4.992043	-0.247508
C	4.161705	2.696117	-1.064357
H	2.814140	4.299535	-0.597487
H	5.036565	3.336429	-1.115158
C	4.265494	1.322101	-1.284573
C	3.115836	0.545487	-1.202324
H	5.215549	0.851282	-1.511326
H	3.151157	-0.525406	-1.360794

TS4-A2-OCH₃

C	-0.381848	-0.764486	-2.661702
O	-0.546821	-0.773331	-3.814486
Re	-0.114879	-0.756293	-0.753400
C	-1.849889	-1.561102	-0.478819
O	-2.897386	-2.036110	-0.329819
C	0.654565	-2.516404	-0.829569
O	1.161375	-3.562773	-0.877055
N	1.755464	0.386598	-0.878932
C	1.667395	1.734234	-0.719048
C	0.301704	2.274601	-0.562773
N	-0.700837	1.356065	-0.573336
S	0.382194	-0.663467	1.752135
C	-1.051001	-0.057954	2.566107
O	-2.102284	0.276028	2.056700
S	-0.830406	0.072646	4.417291
C	-1.337059	-1.637672	4.849498
C	-1.974064	1.777229	-0.446683
C	2.971577	-0.173114	-1.039589
H	-1.265536	-1.713163	5.937340
H	-2.368330	-1.827081	4.543674
H	-0.663834	-2.366142	4.392375
C	-2.310104	3.120281	-0.314385
H	-2.733614	1.007897	-0.434327
H	-3.351850	3.401403	-0.209601

C	-1.289565	4.069783	-0.301311
C	0.028483	3.640677	-0.427260
H	-1.512654	5.126390	-0.192307
H	0.833979	4.364127	-0.418726
C	4.146981	0.568020	-1.050545
H	2.988327	-1.249471	-1.159540
H	5.097690	0.063373	-1.181654
C	4.067391	1.951447	-0.885327
C	2.816067	2.535561	-0.720064
H	4.962641	2.565002	-0.883435
H	2.735273	3.607047	-0.587603

M4-A2-OCH₃

C	-0.559931	-0.553222	-2.686618
Re	-0.180665	-0.723457	-0.808161
S	0.460847	-0.871722	1.664549
C	-0.984560	-0.444932	2.588657
S	-0.869532	-0.461700	4.396828
C	0.822922	-1.026900	4.793226
O	-0.791920	-0.452354	-3.823772
C	-1.866378	-1.631622	-0.529539
O	-2.883760	-2.168360	-0.390241
C	0.652833	-2.428727	-1.109764
O	1.198846	-3.439468	-1.295001
N	1.628187	0.513194	-0.933230
C	1.495089	1.834661	-0.641622
C	0.122282	2.292251	-0.344990
N	-0.839656	1.332492	-0.381361
O	-2.070309	-0.126556	2.127456
C	-2.117399	1.677925	-0.132655
C	2.852091	0.030007	-1.227636
H	0.869188	-1.058916	5.885511
H	1.009150	-2.024394	4.392249
H	1.574515	-0.330569	4.417822
C	-2.498481	2.985378	0.151091
H	-2.841001	0.874948	-0.143909
H	-3.541347	3.205567	0.349011
C	-1.519580	3.976711	0.191714
C	-0.196447	3.624771	-0.059082
H	-1.778033	5.006521	0.417224
H	0.577339	4.381600	-0.030931
C	3.991665	0.825013	-1.248209
H	2.905565	-1.028638	-1.450759
H	4.950616	0.381098	-1.491339
C	3.865977	2.182284	-0.949059
C	2.606252	2.687568	-0.645390
H	4.732294	2.836119	-0.951529
H	2.490003	3.737807	-0.409435

TS5-A2-OCH₃

C	1.402185	3.409190	-0.144067
C	0.837265	2.173611	0.189703
N	-0.293823	1.734971	-0.419527
C	-0.858070	2.495083	-1.377488
C	-0.341873	3.727198	-1.760170
C	0.810107	4.194580	-1.126685
C	1.424277	1.258032	1.188456
N	0.779191	0.074062	1.353674
C	1.290768	-0.834351	2.207239
C	2.444707	-0.605788	2.946916

C	3.098536	0.618016	2.803342
C	2.581111	1.555512	1.916339
Re	-1.085419	-0.221385	0.220320
C	-2.632199	-0.272596	-0.925291
O	-3.555512	-0.266835	-1.631445
C	-2.126297	0.583494	1.627445
O	-2.756391	1.073384	2.474179
S	0.262096	-1.230393	-1.697875
C	2.063203	-0.834820	-1.570841
S	3.034771	-2.214282	-1.977527
C	-1.516322	-1.977592	0.874856
O	-1.737612	-3.041189	1.292081
O	2.441403	0.289986	-1.277454
H	0.748927	-1.768238	2.292664
H	2.815246	-1.375498	3.614532
H	4.001836	0.835653	3.364151
H	3.085934	2.502863	1.778141
H	-1.748145	2.092356	-1.844976
H	-0.835783	4.297476	-2.538907
H	1.246057	5.150459	-1.399167
H	2.309019	3.745561	0.341673
C	0.872531	-3.678901	-1.966888
H	0.959278	-3.750297	-3.042808
H	1.578522	-4.263142	-1.394784
H	-0.136600	-3.718554	-1.583208

TS2-B-OCH₃

C	0.046909	-0.309176	3.280242
O	0.799778	0.146121	1.444575
C	1.744130	1.077986	1.658921
S	1.666077	1.690251	3.253796
Re	0.206017	-0.938069	-0.380763
N	-0.050393	1.069315	-1.260548
C	-1.144097	1.774484	-0.877276
C	-2.113763	1.040069	-0.037575
N	-1.787534	-0.246667	0.256199
C	2.013578	-1.317664	-0.981983
O	3.052145	-1.605037	-1.404324
C	0.206181	-2.627123	0.529980
O	0.157061	-3.652865	1.080345
C	-0.472650	-1.799792	-1.943133
O	-0.897024	-2.313386	-2.899085
S	2.846122	1.518801	0.458741
C	-2.665104	-1.000902	0.948598
C	0.845410	1.645465	-2.083903
H	-0.640250	0.412675	3.700329
H	0.797777	-0.693006	3.957213
H	-0.412854	-1.062699	2.655068
C	-3.885093	-0.514499	1.402189
H	-2.365868	-2.025063	1.138586
H	-4.551562	-1.166375	1.955923
C	-4.215385	0.814772	1.132094
C	-3.323978	1.592913	0.401348
H	-5.154270	1.236300	1.476844
H	-3.569957	2.621576	0.170401
C	0.689071	2.940001	-2.571913
H	1.703934	1.045655	-2.351435
H	1.436961	3.353676	-3.238632
C	-0.413013	3.683259	-2.156377
C	-1.339565	3.094679	-1.299214
H	-0.553540	4.705545	-2.492914

H	-2.202834	3.657975	-0.968376
[Re(SCH ₃)(CO) ₃ (bipy)]			
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.400953
N	1.163603	0.000000	2.102440
C	2.329896	0.015853	1.428217
C	2.397545	0.016685	0.040206
C	1.207583	0.006720	-0.689442
C	-1.232450	0.002791	2.213911
C	-2.520304	0.006297	1.662463
C	-3.629377	0.018079	2.501185
C	-3.427004	0.029559	3.882274
C	-2.124432	0.025307	4.366452
N	-1.045612	0.004471	3.559712
Re	1.029485	0.062609	4.302151
C	0.641600	0.251214	6.172089
O	0.360022	0.378578	7.294905
C	1.138695	-1.859015	4.472280
O	1.212414	-3.017691	4.586962
C	2.901686	0.247297	4.680558
O	4.045148	0.372117	4.862788
S	0.774537	2.543640	3.913444
C	1.665544	3.446528	5.245657
H	1.540309	4.516633	5.057682
H	1.253031	3.216721	6.231662
H	2.734206	3.216076	5.241532
H	3.228595	0.029534	2.032129
H	3.365064	0.029199	-0.449274
H	-0.933986	-0.000281	-0.547966
H	1.218979	0.008578	-1.774742
H	-1.922964	0.040239	5.430280
H	-4.257753	0.045930	4.579000
H	-4.631537	0.022672	2.084458
H	-2.656401	0.004943	0.588187

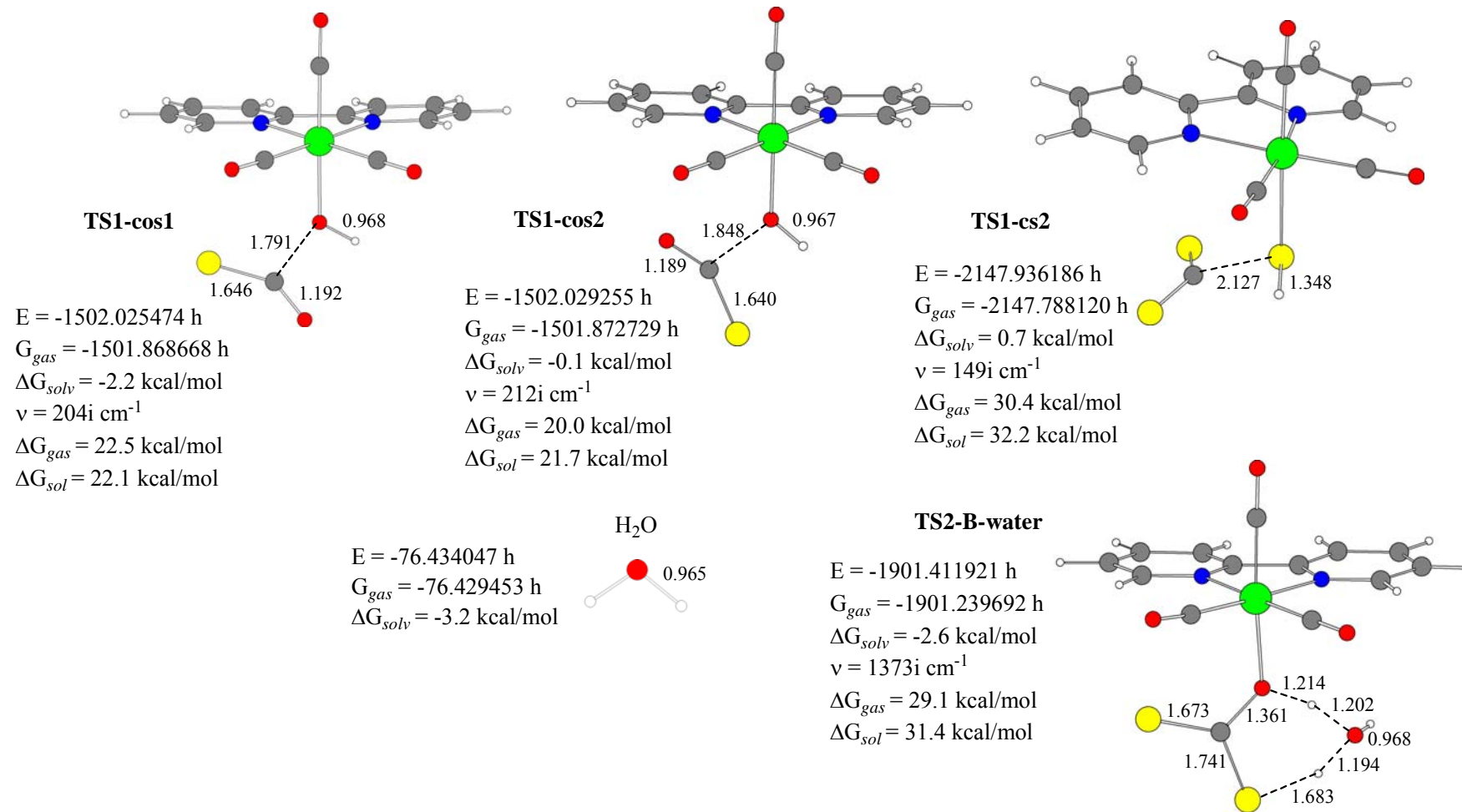


Figure 1S. B3LYP/6-31+G(d,p) (LANL2DZ + *f* for Re) optimized structures of the transition states analogous to **TS1** for the reaction of [Re(OH)(CO)₃(bipy)] toward COS (**TS1-cos1** and **TS1-cos2**) and CS₂ (**TS1-cs2**), of a water molecule, and of the transition state analogous to **TS2-B** with an additional water molecule (**TS2-B-water**), which assists the hydrogen migration. Most significant distances (in angstroms) and energy data are also displayed.

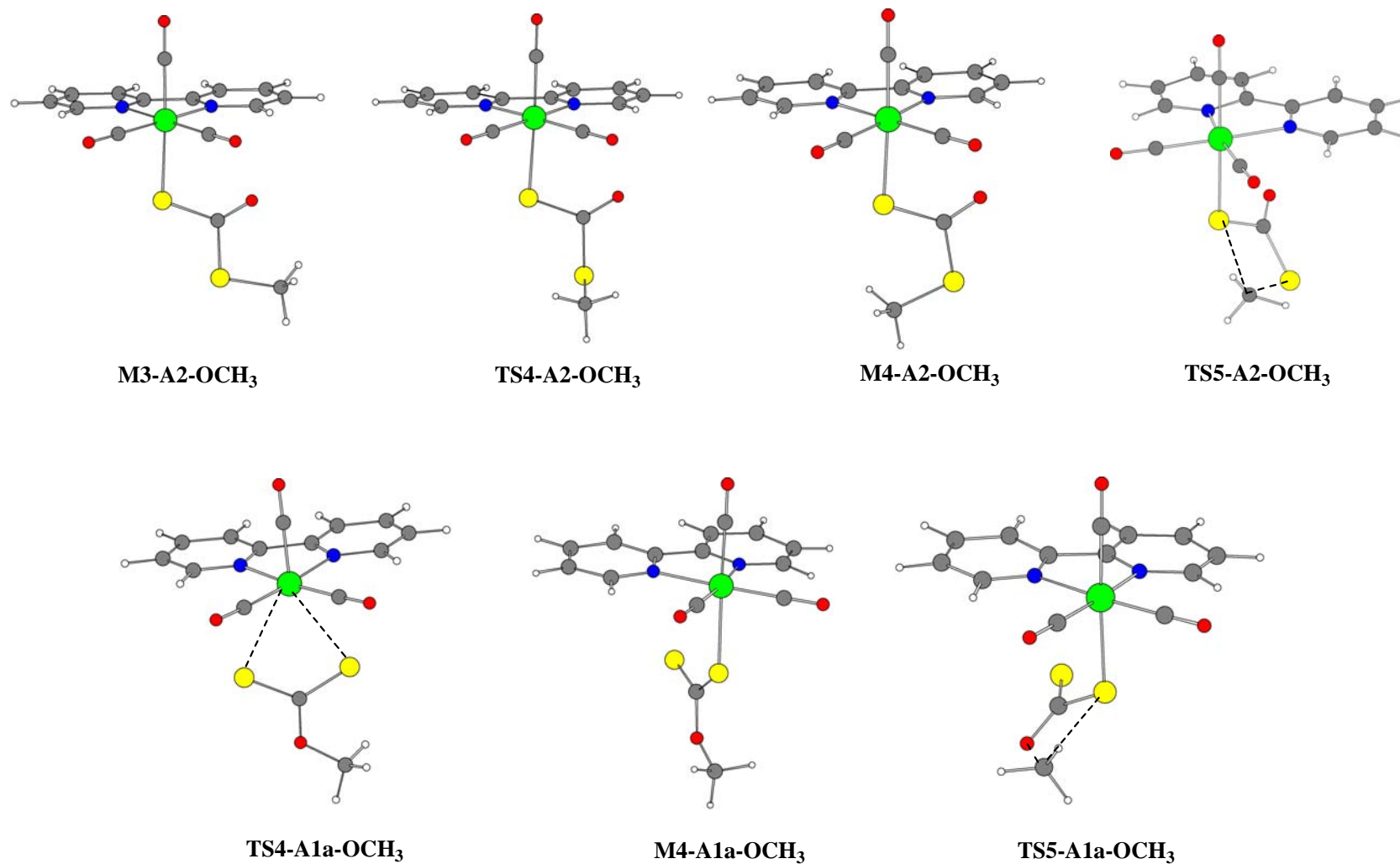


Figure 1S. B3LYP/6-31+G(d,p) (LANL2DZ + *f* for Re) optimized structures of the species, which are not shown in Figure 3, for the reaction of [Re(OCH₃)(CO)₃(bipy)] toward CS₂.

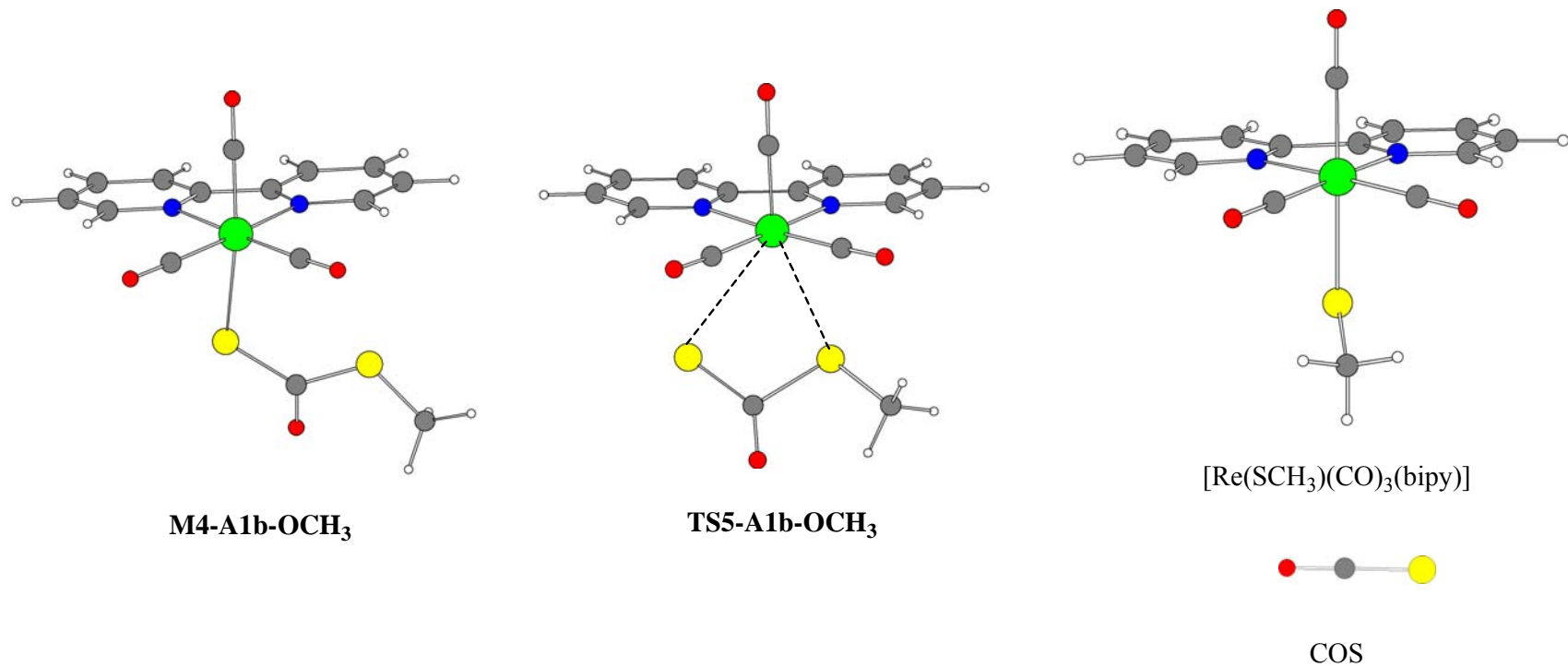


Figure 1S. (Cont.)

