

Electronic Supplementary Information

**Revisiting the Catalytic Mechanism of Mo-Cu Carbon Monoxide Dehydrogenase Using
QM/MM and DFT Calculations**

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1. QM/MM results

Table S1. ONIOM energy data

	E1 ^a [hartree]	E _{disp} ^b [hartree]	ZPE ^b [hartree]	G _{corr} ^b [hartree]	E2 ^c [hartree]	Δ(E2+E _{disp} +ZPE) [kcal/mol]	Δ(E2+E _{disp} +G _{corr}) [kcal/mol]
Int1A ^d	-4242.434323	-0.232352	18.983989	17.898412	-5687.003849	3.1	2.1
Int1B	-4242.418828	-0.234356	18.985450	17.900064	-5686.979003	18.3	17.5
Int1A	-4242.441216	-0.229973	18.988007	17.903960	-5687.015153	0.0	0.0
TS1A	-4242.434619	-0.231451	18.987348	17.904278	-5687.003642	5.9	6.5
Int2A	-4242.448097	-0.232935	18.989278	17.907395	-5687.013398	0.0	1.4
TS2A	-4242.440786	-0.231046	18.988905	17.908478	-5687.009393	3.5	5.8
Int3A	-4242.452768	-0.229705	18.991194	17.910601	-5687.022600	-2.5	-0.3
TS3A	-4242.448438	-0.228392	18.990187	17.911563	-5687.021309	-1.5	1.9
Int4A	-4242.464099	-0.224995	18.991112	17.909934	-5687.036449	-8.3	-6.5
TS4A	-4242.434329	-0.230658	18.988758	17.906299	-5687.006575	5.4	6.4
Int5A	-4242.464432	-0.224734	18.990723	17.905247	-5687.048003	-15.6	-16.5
Int6A	-4242.486655	-0.236075	18.990798	17.909650	-5687.044636	-20.6	-18.8
Int1'	-4303.446977	-0.263144	19.091715	18.006792	-5748.002612	0.0	0.0
TS1'	-4303.434936	-0.260442	19.089395	18.001200	-5747.996505	4.1	2.0
Int2'	-4303.459247	-0.259585	19.093526	18.010206	-5748.014555	-4.1	-3.1
TS2'	-4303.451429	-0.257097	19.090755	18.006491	-5748.012861	-3.2	-2.8
Int2'	-4303.503985	-0.255582	19.092560	18.007463	-5748.069815	-36.9	-37.0

^a ONIOM(B3LYP/B1:MM)-ME energy.

^b Obtained from ONIOM(B3LYP/B1:MM)-ME frequency calculations.

^c ONIOM(B3LYP/B2:MM)-EE//ONIOM(B3LYP/B1:MM)-ME energy.

^d **Int1A** in Figure 1.

Table S2. ONIOM energy data for **Int4A** and **TS4A** obtained after removing all the water molecules

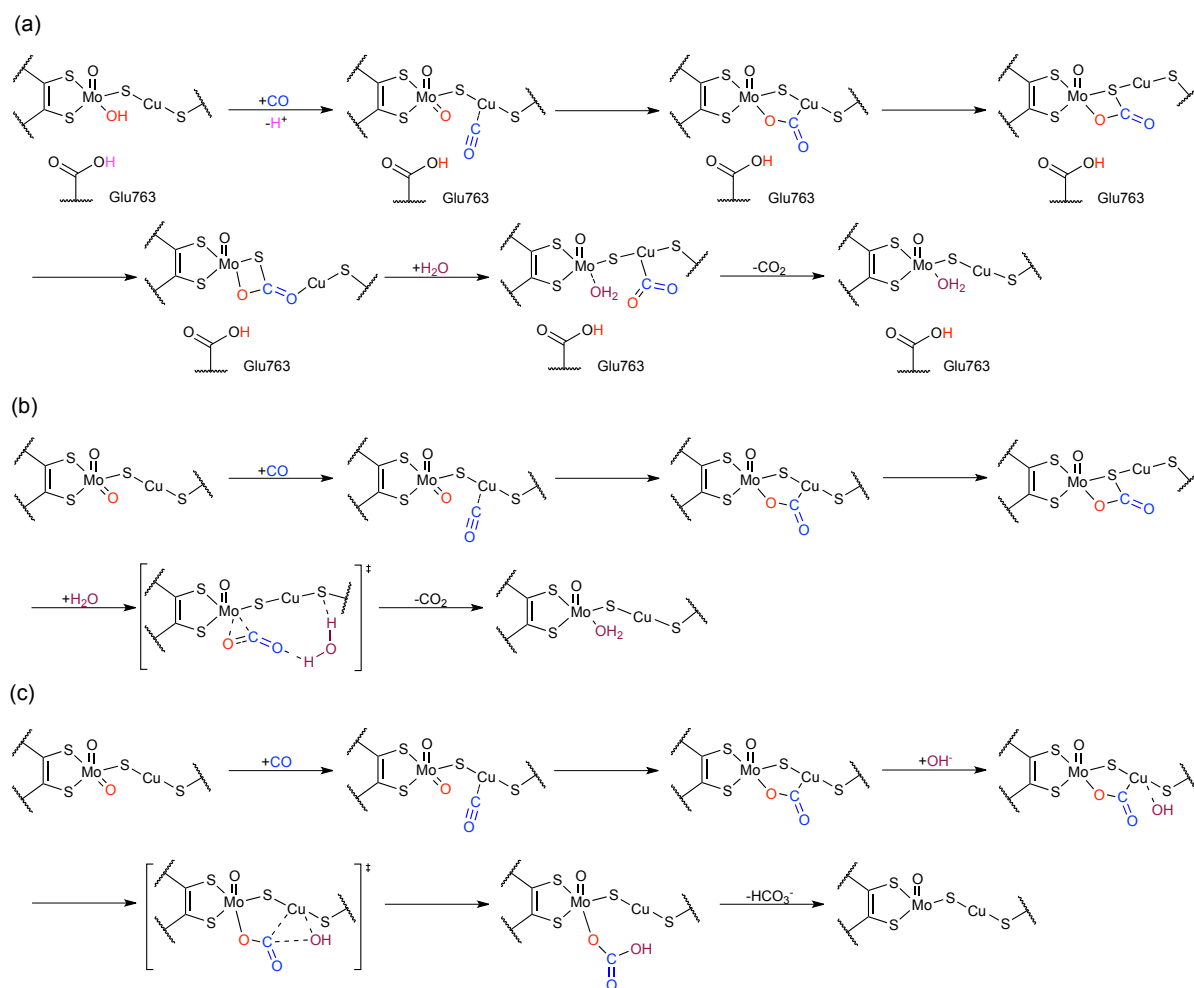
	E1 ^a [hartree]	E _{disp} ^b [hartree]	ZPE ^b [hartree]	G _{corr} ^b [hartree]	E2 ^c [hartree]	Δ(E2+E _{disp} +ZPE) [kcal/mol]	Δ(E2+E _{disp} +G _{corr}) [kcal/mol]
Int4A	-4143.896324	-0.22928746	17.691975	16.669494	-5588.382931	0.0	0.0
TS4A	-4143.934298	-0.22419654	17.697215	16.680120	-5588.420457	17.1	13.7

^a ONIOM(B3LYP/B1:MM)-ME energy.

^b Obtained from ONIOM(B3LYP/B1:MM)-ME frequency calculations.

^c ONIOM(B3LYP/B2:MM)-EE//ONIOM(B3LYP/B1:MM)-ME energy.

2. Summary of previously reported DFT studies

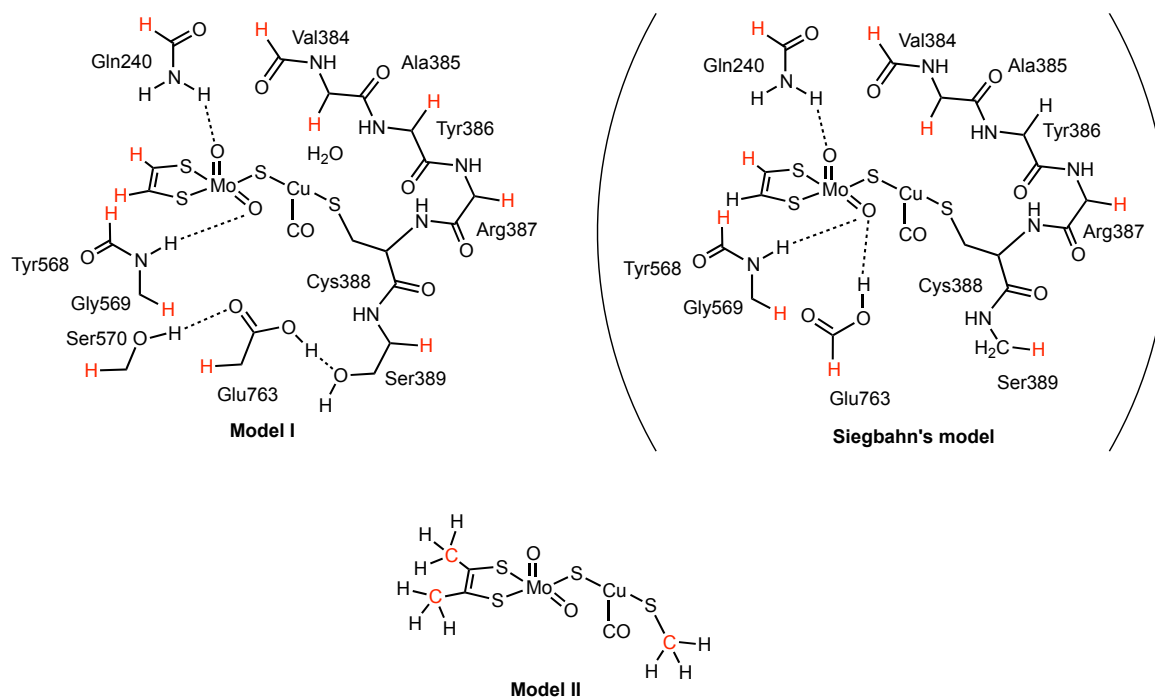


Scheme S1. Reaction mechanisms proposed based on DFT studies (a) by Siegbahn et al,(b) by Hofmann et al, and (c) by Stein et al.

Calculation methods:

- Siegbahn et al: B3LYP/LACV3P*//B3LYP/LACVP
- Hofmann et al: B3LYP/SDD//B3LYP/LANL2DZ
- Stein et al: PBE/TZP

3. DFT Results



Scheme S2. Models I and II. Red-colored atoms are fixed ones (at the positions in the crystal structure) when geometric constraints are imposed. Model I is based on our QM/MM model, and Model II was used previously by Hofmann et al. Siegbahn's model is also shown for comparison.

Notes:

These active-site models were built based on the published crystal structure (PDB code 1N5W) of MoCu-CODH, and the hydrogen atoms were attached to saturate the dangling bonds. However, for models I, to avoid arbitrariness in the positions of fixed hydrogen atoms, such hydrogen atoms were placed according to how ONIOM places H-link atoms at QM-MM boundaries. Model I is slightly larger than Siegbahn's model. Model II was examined both with and without constraints.

Table S3. DFT energy data obtained using model I

	E1 ^a [hartree]	E _{disp} [hartree]	ZPE ^b [hartree]	G _{corr} ^b [hartree]	E2 ^c [hartree]	$\Delta(E2+E_{\text{disp}}+ZPE)$ [kcal/mol]	$\Delta(E2+E_{\text{disp}}+G_{\text{corr}})$ [kcal/mol]
Int1A	-4194.670982	-0.220074	0.554400	0.453717	-5639.285032	0.0	0.0
TS1A	-4194.659169	-0.221854	0.554186	0.456296	-5639.268416	9.2	10.9
Int2A	-4194.675727	-0.224990	0.556445	0.460127	-5639.279034	2.0	4.7
TS2A	-4194.668750	-0.219755	0.555739	0.459081	-5639.275697	6.9	9.4
Int3A	-4194.689164	-0.217302	0.557363	0.460775	-5639.297926	-4.5	-1.9
TS3A	-4194.684670	-0.217334	0.556905	0.461373	-5639.291686	-0.9	2.3
Int4A	-4194.699097	-0.214680	0.557980	0.462042	-5639.303606	-6.0	-3.0
TS4A	-4194.665978	-0.218402	0.555758	0.456287	-5639.273625	9.1	9.8
Int5A	-4194.678165	-0.210994	0.555714	0.453294	-5639.290254	3.2	2.2
Int6A	-4194.688588	-0.223104	0.557439	0.458359	-5639.292422	-4.6	-3.6

^a B3LYP/B1 energy.

^b Obtained from B3LYP/B1 frequency calculations.

^c B3LYP(SCRF)/B2//B3LYP/B1 energy.

Table S4. DFT energy data obtained using model II

without any constraint	E1 ^a [hartree]	E _{disp} [hartree]	ZPE ^b [hartree]	G _{corr} ^b [hartree]	E2 ^c [hartree]	Δ(E2+E _{disp} +ZPE) [kcal/mol]	Δ(E2+E _{disp} +G _{corr}) [kcal/mol]
Int1A	-2318.330800	-0.071605	0.144823	0.084923	-3762.103487	0.0	0.0
TS1A	-2318.322234	-0.071683	0.144622	0.088745	-3762.088418	9.3	11.8
Int2A	-2318.342204	-0.071905	0.146953	0.092111	-3762.103303	1.3	4.4
TS2A	-2318.340929	-0.072165	0.146634	0.092943	-3762.103270	0.9	4.8
Int3A	-2318.365943	-0.069807	0.148218	0.092915	-3762.128660	-12.5	-9.7
TS3A	-2318.354867	-0.068513	0.147619	0.093687	-3762.115501	-3.8	-0.1
Int4A	-2318.369712	-0.066315	0.148502	0.093041	-3762.125471	-8.2	-5.4
TS4A	-2318.334945	-0.069205	0.146323	0.089223	-3762.099885	4.7	6.5
Int5A	-2318.346811	-0.065790	0.146747	0.084515	-3762.116237	-3.1	-4.6
Int7A	-2394.768289	-0.077597	0.173174	0.114982	-3838.578018	-3.0	9.5
Int8A	-2394.774265	-0.076562	0.172302	0.110644	-3838.584759	-7.2	3.2
with constraints							
Int1A	-2318.327975	-0.071013	0.135501	0.075460	-3762.101310	0.0	0.0
TS1A	-2318.321194	-0.071207	0.135222	0.078911	-3762.087258	8.5	10.9
Int2A	-2318.341956	-0.071755	0.137655	0.082371	-3762.103599	-0.6	2.4
TS2A	-2318.335097	-0.071322	0.137134	0.082988	-3762.097139	3.4	7.1
Int3A	-2318.364576	-0.069387	0.138777	0.082061	-3762.127199	-13.2	-11.1
TS3A	-2318.352167	-0.068424	0.138232	0.083373	-3762.112975	-4.0	-0.7
Int4A	-2318.367971	-0.066882	0.139298	0.084156	-3762.124173	-9.4	-6.3
TS4A	-2318.333601	-0.068334	0.136871	0.078801	-3762.098332	4.4	5.6
Int5A	-2318.345274	-0.064718	0.137363	0.075440	-3762.114404	-3.1	-4.3
Int7A	-2394.766981	-0.077314	0.163452	0.103670	-3838.577045	-4.2	7.4
Int8A	-2394.771616	-0.073238	0.162291	0.098869	-3838.583471	-6.4	2.9
H₂O	-76.407024	-0.000574	0.021140	0.002820	-76.467903		

^a B3LYP/B1 energy.^b Obtained from B3LYP/B1 frequency calculations.^c B3LYP(SCRF)/B2//B3LYP/B1 energy.

4. NPA charges for CO₂ and *n*-butylisocyanate

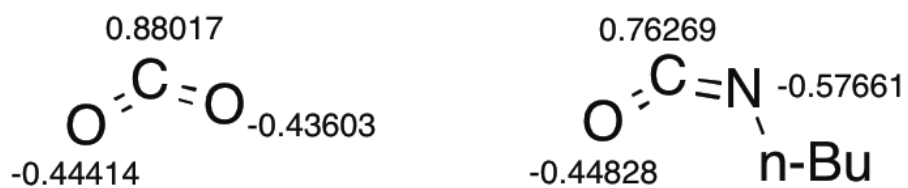
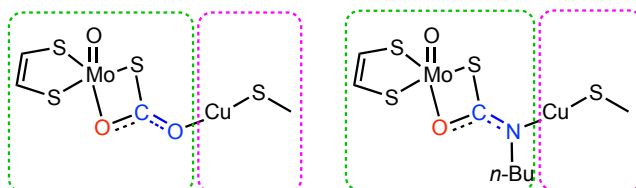


Figure S1. NPA charges (B3LYP/6-31G*) for CO₂ and *n*-butylisocyanate. Geometries were taken from the QM/MM-optimized **Int4A** and **Int3'**.

5. Heterolytic bond dissociation energies (BDEs) of the Cu–O and Cu–N coordination bonds in **Int4A** and **Int3'**



Scheme S3. Models used for calculating BDE.

Table S5. Heterolytic BDE

		ZPE (a.u.)	B3LYP- D3/B2(SCRF)//B3LYP/ B1 (a.u.)	BDE (kcal/mol)
Cu–O	Int4A	0.092753	-3683.520503	39.0
	[LMo(O)SCO] ²⁻	0.052531	-1604.705007	
	[Me–S–Cu] ⁰	0.038911	-2078.752054	
Cu–N	Int3'	0.218694	-3820.956670	53.6
	[LMo(O)SCN] ²⁻	0.177819	-1742.117275	
	[Me–S–Cu] ⁰	0.038911	-2078.752054	

Notes:

Initial geometries were taken from the QM/MM-optimized **Int4A** and **Int3'**. Geometry optimization and single-point energy calculations were performed using the same methods as used in our DFT calculations. All atoms were allowed to move during the geometry optimizations.

6. XYZ coordinates of optimized geometries

QM atoms in ONIOM-optimized geometries

====Int1A in Figure 1====

h 98.986243 151.169552 147.345846
C 98.839681 150.132260 146.913017
O 98.843471 149.948537 145.702226
N 98.591548 149.181423 147.838641
H 98.586761 148.185941 147.589415
H 98.787862 149.331475 148.833239
h 103.441305 140.653699 144.267307
C 103.046659 141.599652 143.790517
O 103.803978 142.482514 143.393917
N 101.693650 141.587329 143.708213
H 101.213223 140.833034 144.211948
C 100.831410 142.600608 143.113264
H 100.595266 143.387334 143.845427
h 101.303801 143.098752 142.229048
C 99.512553 141.956527 142.646755
O 99.411528 140.773604 142.358297
N 98.509388 142.861524 142.466391
H 98.618747 143.769401 142.913188
C 97.221544 142.640134 141.811417
H 96.816362 143.650857 141.697510
h 97.353610 142.207653 140.788574
C 96.209015 141.815885 142.641651
O 95.678001 140.802718 142.202213
N 95.938565 142.340226 143.865096
H 96.562881 143.044275 144.255916
C 95.054398 141.695454 144.828164
H 95.139486 142.289532 145.740898
h 93.984553 141.716491 144.505632
C 95.461503 140.243588 145.197221
O 94.691349 139.294610 145.079940
N 96.734786 140.127576 145.676267
H 97.300509 140.966163 145.771950
C 97.333297 138.842079 145.979042
H 96.671985 138.104072 145.517705
C 98.731628 138.697576 145.340105
H 98.664713 139.027865 144.300741
H 99.006316 137.641999 145.372108
S 100.136489 139.555226 146.180641
C 97.409636 138.412093 147.465543
O 97.714444 137.239532 147.692389
N 97.231209 139.373654 148.407197
H 96.856288 140.273207 148.129697
C 97.289121 139.204533 149.861842
H 97.148739 140.204170 150.276654
C 96.153863 138.342636 150.404649
H 96.228393 137.331682 150.018049
H 96.182425 138.323241 151.505063
O 94.922625 138.935029 149.944655
H 94.180800 138.553438 150.501940
h 98.282749 138.881040 150.257444
h 98.407371 145.691305 151.623889
C 98.019952 144.792249 152.197514
O 97.743101 144.877696 153.391921
N 97.884430 143.697698 151.434940
H 98.126463 143.742035 150.442536

C 97.421168 142.432146 151.958051
H 97.381532 141.740450 151.119606
H 98.131552 142.024818 152.686237
h 96.413618 142.450444 152.424138
h 93.610944 143.452088 152.873789
C 92.823418 142.685771 152.690746
H 93.171109 141.757273 153.155536
H 91.908332 142.996507 153.209115
O 92.497484 142.501547 151.327919
H 93.303123 142.085690 150.952176
h 92.815715 141.088375 148.042134
C 93.289494 142.092275 148.161543
H 93.288529 142.629052 147.215300
H 92.754941 142.657684 148.922967
C 94.679785 141.800364 148.632197
O 95.639927 141.674596 147.906136
O 94.687469 141.543553 149.965025
h 93.513576 145.540917 148.999731
C 94.394560 145.448697 148.352593
S 95.868341 144.846717 149.077274
C 94.398100 145.858752 147.061430
S 95.794289 145.774380 146.018984
h 93.519729 146.336057 146.713877
O 102.877097 145.111230 147.676528
H 102.758459 144.874931 146.726657
H 102.268600 144.509322 148.130531
Cu 99.577252 141.674153 146.789668
S 98.461212 143.513158 145.734577
Mo 97.735188 144.895664 147.458116
O 98.515307 144.076344 148.806469
O 98.539739 146.421266 147.347725
C 100.384100 142.438724 148.353367
O 101.215887 142.815270 149.049574
H 95.091990 140.660650 150.176802

====Int1B====

h 99.089328 151.037228 147.320357
C 99.043544 149.992456 146.884221
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H 98.813437 149.215637 148.799240
h 103.398294 140.589535 144.036036
C 103.009860 141.493276 143.476371
O 103.773076 142.242540 142.872450
N 101.658487 141.590493 143.562191
H 101.192982 140.903168 144.167828
C 100.778635 142.594790 142.973673
H 100.559520 143.382702 143.709516
h 101.224695 143.097870 142.080414
C 99.448576 141.950426 142.532740
O 99.347427 140.771963 142.231203
N 98.435841 142.852455 142.392661
H 98.565140 143.760024 142.834195
C 97.141990 142.647917 141.743851
H 96.739852 143.661574 141.654109

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 C 96.130467 141.809375 142.564476
 O 95.632739 140.776941 142.133430
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 H 96.441264 143.060727 144.165042
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 O 94.625668 139.276775 144.953210
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 H 98.597622 139.102535 144.181162
 H 98.991219 137.721308 145.240890
 S 100.028149 139.669861 146.079012
 C 97.350411 138.382756 147.334173
 O 97.735004 137.233482 147.546542
 N 97.088287 139.330958 148.266248
 H 96.649093 140.175561 147.937638
 C 97.125307 139.236535 149.732564
 H 96.930935 140.249874 150.081274
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 H 96.266897 137.311120 150.249760
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 O 94.799385 138.614283 149.590961
 H 94.065261 138.367277 150.228151
 h 98.127681 138.956867 150.154002
 h 98.378609 145.669398 151.548420
 C 98.023772 144.775282 152.146031
 O 97.794425 144.879610 153.349213
 N 97.887216 143.656459 151.416904
 H 98.021983 143.665045 150.406645
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 C 92.876735 142.682650 152.629957
 H 93.180100 141.766318 153.146385
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 C 94.869848 141.938725 148.754658
 O 95.038628 141.782112 149.946345
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 S 95.707824 145.110965 149.012571
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 S 95.774828 145.764245 145.916946
 h 93.496042 146.497763 146.466746
 O 102.878117 145.342188 146.967820
 H 103.099003 144.905726 146.115582

H 102.529215 144.622238 147.514965
 Cu 99.540951 141.809299 146.614320
 S 98.334505 143.646008 145.552562
 Mo 97.575144 144.823523 147.404378
 O 98.028317 143.622113 148.644852
 O 98.588797 146.208760 147.576401
 C 100.442164 142.713534 148.031007
 O 101.229393 143.253523 148.668304
 H 96.706319 142.338403 148.433872
 =====

====Int1A====

h 98.923438 150.841282 147.261381
 C 98.831031 150.090786 146.942410
 O 98.817783 149.916084 145.729546
 N 98.639136 149.126713 147.865088
 H 98.612885 148.130877 147.619463
 H 98.806061 149.286049 148.862977
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 C 103.021838 141.428521 143.636404
 O 103.794977 142.203135 143.079321
 N 101.673553 141.527135 143.738250
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 H 96.804486 143.626015 141.687150
 h 97.301838 142.296113 141.074321
 C 96.188043 141.802552 142.647539
 O 95.654474 140.786919 142.216962
 N 95.916918 142.339578 143.865650
 H 96.544407 143.044075 144.250120
 C 95.040730 141.702055 144.841566
 H 95.132941 142.304095 145.748572
 h 94.264847 141.715395 144.613011
 C 95.451003 140.252244 145.217320
 O 94.685847 139.300121 145.092444
 N 96.720604 140.141479 145.706802
 H 97.279848 140.982626 145.818225
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Optimized geometries in DFT calculations
using Model I

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C	93.220650	142.007430	148.976000	C	98.803299	139.138485	145.423993
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H	92.283385	142.185367	149.510730	H	99.208454	138.126423	145.496127
C	94.251615	141.399104	149.881833	S	100.036555	140.245484	146.254491
O	93.694454	140.489502	150.733732	C	97.486336	138.605483	147.494446
O	95.446047	141.595823	149.835922	O	97.916309	137.474616	147.717282
H	93.211367	146.090982	148.920492	N	97.071882	139.445167	148.483598
C	94.080951	145.961025	148.261186	H	96.834156	140.396423	148.228612
S	95.573883	145.587265	149.112747	C	97.453141	139.212583	149.873813
C	94.042348	145.995888	146.912816	H	97.280002	140.148258	150.405669
S	95.454494	145.670240	145.920291	C	96.643826	138.089819	150.522237
H	93.145028	146.187599	146.328051	H	96.889214	137.133564	150.048803
Cu	99.730562	142.645198	146.750342	H	96.874544	138.029250	151.591081
S	98.272251	144.141368	145.680744	O	95.230352	138.324036	150.431890
Mo	97.454940	145.458669	147.488953	H	95.058486	138.474433	149.483459
O	98.233033	144.631169	148.819345	H	98.515081	138.959904	149.933647
O	98.146265	147.040487	147.366580	H	98.013633	146.288202	151.182990
C	100.894781	143.578519	147.932042	C	97.862843	145.592925	152.027125
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				H	96.460253	143.067662	152.496411
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H	99.292331	151.213029	146.938833	H	93.710501	142.431393	153.965399
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H	96.467623	143.796604	141.501210	Mo	97.415905	145.450058	147.414339
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O	95.169245	141.234950	142.089846				

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O 103.208440 143.146119 143.986266
N 101.423423 141.822116 143.405096
H 100.974502 140.929355 143.619079
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H 98.328968 144.151233 142.754053
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Cu 99.399834 141.596889 146.376875
S 98.746866 143.951447 146.309832
Mo 97.327386 145.722421 147.475279
O 98.466733 144.458336 148.826795
O 98.030999 147.282095 147.392228
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====TS4A====

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C 102.622109 142.043937 143.978095
O 103.078329 143.158731 144.225127
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 H 96.811130 138.262172 145.531083
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 H 98.777339 139.342446 144.494699
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 C 97.453653 139.228772 149.901757
 H 97.313897 140.183022 150.411547
 C 96.650437 138.141295 150.614192
 H 96.872810 137.164567 150.173013
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 H 98.515081 138.959904 149.933653
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 H 97.378552 144.275408 150.518463
 C 97.533807 143.150826 152.301992
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 C 94.089772 145.980066 148.256302
 S 95.686454 145.760453 149.052042
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 S 95.460481 145.803471 145.868164
 H 93.144980 146.187621 146.328040
 Cu 99.170445 142.327275 146.253422
 S 98.557128 144.374730 145.762620
 Mo 97.334023 145.890413 147.295336
 O 98.980935 144.978536 148.628650
 O 97.935725 147.491203 147.188747
 C 99.989475 144.559607 148.121450
 O 101.115187 144.255400 148.019145
 H 94.465934 139.951957 150.994199
 O 101.500575 145.707219 144.251599
 H 102.071886 144.922636 144.348097
 H 100.734738 145.512793 144.821236
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====Int5A====

H 1.867877 7.935759 -0.156112
 C 0.806899 8.032563 -0.469659
 O 0.341974 9.111151 -0.827797
 N 0.135097 6.865845 -0.404922
 H -0.838976 6.860375 -0.678683
 H 0.528319 5.967691 -0.109500
 H 5.728017 -2.156423 -2.816769
 C 5.218424 -1.216719 -3.129047
 O 5.744518 -0.113422 -2.984686
 N 4.019270 -1.446317 -3.706302
 H 3.574155 -2.344448 -3.530320
 C 3.122986 -0.369827 -4.095914
 H 2.973006 0.354000 -3.284710
 H 3.555702 0.217327 -4.922424
 C 1.800912 -0.959561 -4.576014
 O 1.661456 -2.140790 -4.878880
 N 0.783627 -0.053425 -4.698505
 H 0.925535 0.891906 -4.365689
 C -0.471975 -0.423723 -5.336325
 H -0.990520 0.508461 -5.591741
 H -0.247983 -0.946231 -6.292746
 C -1.466087 -1.258075 -4.458575
 O -2.191727 -2.101377 -4.966392
 N -1.521163 -0.902397 -3.133030
 H -0.951007 -0.124220 -2.819349
 C -2.454531 -1.430035 -2.130655
 H -2.497732 -0.669486 -1.341757
 H -3.485831 -1.573581 -2.488631
 C -2.069712 -2.768078 -1.464461
 O -2.937431 -3.514642 -1.012836
 N -0.736922 -3.012679 -1.358340
 H -0.105145 -2.342057 -1.785661
 C -0.163983 -4.322979 -1.076108
 H -0.819208 -5.078507 -1.529062
 C 1.220618 -4.421608 -1.744194
 H 1.098241 -4.228639 -2.815898
 H 1.570145 -5.448039 -1.612240
 S 2.549461 -3.323161 -1.058919
 C -0.042294 -4.749295 0.401450

O	0.306335	-5.901052	0.659524	C	102.741569	141.946535	143.632571
N	-0.346936	-3.836811	1.363848	O	103.469546	142.782117	143.108736
H	-0.511133	-2.879804	1.073497	N	101.390957	141.869317	143.515295
C	0.033469	-4.044224	2.759942	H	100.932703	141.184329	144.118729
H	-0.121397	-3.090723	3.264838	C	100.517960	142.907598	142.979239
C	-0.796447	-5.132519	3.441571	H	100.246345	143.619761	143.768940
H	-0.564303	-6.108014	3.003564	H	100.980146	143.494656	142.172562
H	-0.568383	-5.156689	4.512454	C	99.252455	142.312699	142.351144
O	-2.205764	-4.882476	3.339925	O	99.225590	141.231646	141.772727
H	-2.375116	-4.746372	2.388881	N	98.186672	143.170970	142.399058
H	1.090735	-4.317217	2.838696	H	98.195936	143.878081	143.132794
H	0.589254	3.010649	4.087861	C	96.929140	142.835723	141.756517
C	0.590183	2.222765	4.859177	H	96.422126	143.776150	141.502263
O	0.775843	2.444218	6.051475	H	97.176495	142.331028	140.802173
N	0.381808	0.993395	4.315341	C	95.899258	142.017383	142.606144
H	0.047896	0.969236	3.355536	O	95.080276	141.283705	142.063818
C	0.103219	-0.156769	5.152204	N	95.920707	142.281976	143.950424
H	0.396063	-1.070823	4.631197	H	96.620540	142.929140	144.325918
H	0.674207	-0.056195	6.077636	C	94.980461	141.779499	144.951806
H	-0.964421	-0.209724	5.401463	H	94.985250	142.528915	145.753769
H	-3.860621	0.388336	5.593180	H	93.938481	141.703738	144.606425
C	-4.315169	-0.337038	6.287175	C	95.332959	140.418107	145.596078
H	-3.498243	-0.876576	6.794921	O	94.461499	139.645677	145.992409
H	-4.862138	0.230767	7.048138	N	96.668458	140.191477	145.762997
O	-5.243469	-1.205985	5.666630	H	97.300281	140.896504	145.391114
H	-4.755029	-1.759799	5.031066	C	97.268927	138.893075	146.040642
H	-4.385010	-2.027212	1.103812	H	96.651299	138.123908	145.559260
C	-4.204851	-1.243033	1.854048	C	98.682995	138.832149	145.421626
H	-3.848506	-0.331107	1.371445	H	98.600365	139.032504	144.348185
H	-5.136479	-1.062363	2.397374	H	99.048972	137.811771	145.555456
C	-3.153297	-1.820902	2.754160	S	99.971498	139.946255	146.169492
O	-3.693285	-2.688982	3.658988	C	97.367257	138.458211	147.517892
O	-1.957984	-1.645145	2.659337	O	97.728275	137.314434	147.791017
H	-4.212802	2.814047	1.825498	N	97.045857	139.377796	148.469896
C	-3.341704	2.686178	1.162527	H	96.863024	140.320690	148.150878
S	-1.762936	2.445608	1.990307	C	97.455345	139.216367	149.862818
C	-3.387521	2.722512	-0.178132	H	97.311068	140.185408	150.342737
S	-1.909340	2.522210	-1.181788	C	96.642001	138.152875	150.594424
H	-4.279683	2.910020	-0.766932	H	96.834027	137.167091	150.160430
Cu	1.777478	-1.332973	-0.514279	H	96.912270	138.137444	151.655378
S	1.417523	0.756898	0.021778	O	95.234498	138.437295	150.549436
Mo	-0.071552	2.505668	0.302837	H	95.003555	138.458304	149.602306
O	3.664725	1.360921	3.003676	H	98.515123	138.959976	149.933639
O	0.626129	4.081486	0.308147	H	98.013574	146.288213	151.183050
C	3.232773	0.275432	3.044066	C	97.847043	145.609727	152.038235
O	2.851792	-0.829038	3.122589	O	97.605251	145.998649	153.176018
H	-2.995465	-3.361183	3.882610	N	97.960328	144.308473	151.664807
O	3.715884	2.107150	-2.218149	H	98.032678	144.115457	150.669754
H	4.466765	1.486634	-2.254636	C	97.546818	143.234559	152.545472
H	3.191013	1.833020	-1.440434	H	98.061494	142.310075	152.266572
====				H	97.806922	143.503180	153.571933
====Int6A====				H	96.460161	143.067544	152.496276
H	99.292328	151.213010	146.938832	H	93.563853	143.665734	152.688170
C	98.295133	151.032094	146.479038	C	92.812068	143.038190	153.191570
O	97.689324	151.937261	145.916026	H	93.325851	142.448199	153.969648
N	97.860444	149.760495	146.612807	H	92.104252	143.706523	153.693461
H	96.962992	149.509280	146.216965	O	92.062858	142.230357	152.302193
H	98.355878	149.003470	147.078194	H	92.683292	141.643886	151.834894
H	103.152515	141.120839	144.278218	H	93.039476	141.250044	148.198884
				C	93.348405	142.111724	148.812723

H	93.679167	142.943609	148.190619
H	92.500091	142.408844	149.436702
C	94.460996	141.590858	149.669075
O	93.982469	140.771397	150.635999
O	95.656064	141.773591	149.508469
H	93.211364	146.090944	148.920488
C	94.063829	145.928275	148.262793
S	95.547584	145.494738	149.134280
C	94.042054	146.012840	146.921015
S	95.501483	145.730948	145.935118
H	93.145116	146.187601	146.328084
Cu	99.183512	142.012374	146.186645
S	98.339383	143.970782	145.764783
Mo	97.289101	145.425542	147.471325
O	100.290066	141.095354	149.861460
O	98.203453	146.871057	147.618800
C	101.214319	141.265236	149.161979
O	102.170576	141.445967	148.515172
H	94.662255	140.084626	150.876890
O	97.844026	143.610020	148.715494
H	98.344668	143.055575	148.056032
H	97.007050	143.130105	148.911510

Geometries obtained by DFT calculations on model II without any constraints

====Int1A====

Mo	-0.486936	1.530176	-0.064401
O	-0.082116	1.994882	1.564211
O	-1.008732	2.913445	-0.958714
S	1.637006	1.069464	-0.988794
S	-1.043640	-0.623802	-1.320266
S	-2.714766	0.837940	0.971696
C	-3.445496	-0.446870	-0.009076
C	-2.728601	-1.078800	-0.966895
C	-3.225272	-2.227699	-1.816221
H	-2.559720	-3.097069	-1.715825
H	-3.225245	-1.960140	-2.883125
H	-4.239524	-2.550561	-1.553052
C	-4.873824	-0.762016	0.376707
H	-5.289805	-1.607468	-0.183078
H	-5.528941	0.105565	0.208056
H	-4.946275	-1.001722	1.447819
Cu	2.662224	-0.555342	0.257511
S	4.907812	-0.874268	0.063550
C	5.418200	0.376165	-1.194876
H	5.053651	1.372120	-0.926378
H	5.016914	0.127157	-2.183087
H	6.514479	0.407288	-1.262081
C	1.684405	-1.637648	1.406486
O	1.111356	-2.339519	2.117039

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====TS1A====

Mo	-0.501874	-0.680639	0.691951
O	0.496303	-1.598378	-0.525023
O	-0.924393	-1.739997	1.981982
S	1.201659	0.633359	1.448541
S	-1.984406	1.347005	0.973764
S	-2.289730	-1.092022	-1.067649

C	-3.646784	0.005047	-0.741927
C	-3.515826	1.041326	0.119222
C	-4.582450	2.068781	0.426091
H	-4.209245	3.084290	0.228603
H	-4.863160	2.043639	1.489345
H	-5.496301	1.928275	-0.162755
C	-4.889724	-0.317031	-1.541940
H	-5.693416	0.414639	-1.399744
H	-5.286872	-1.306658	-1.272087
H	-4.659955	-0.358029	-2.616632
Cu	2.926064	0.321547	-0.158046
S	4.616335	1.623402	-0.852569
C	4.204774	3.288702	-0.160441
H	4.149661	3.264370	0.933137
H	3.243636	3.650773	-0.539534
H	4.983492	4.007312	-0.451082
C	2.369650	-1.546344	-0.532423
O	2.821948	-2.599104	-0.745377

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====Int2A====

Mo	-0.622143	-0.180076	0.751042
O	0.567407	-1.622518	-0.054144
O	-0.773092	-0.572347	2.407693
S	1.184120	1.187044	0.469878
S	-2.139515	1.711841	0.374787
S	-2.369429	-1.343321	-0.559479
C	-3.787087	-0.257819	-0.593555
C	-3.692970	1.028251	-0.187216
C	-4.818496	2.037206	-0.194446
H	-4.530626	2.934448	-0.761247
H	-5.050989	2.377098	0.825705
H	-5.743454	1.646419	-0.634409
C	-5.037124	-0.922120	-1.123803
H	-5.882804	-0.231120	-1.219899
H	-5.353458	-1.748447	-0.470189
H	-4.851033	-1.364346	-2.113300
Cu	3.033878	0.000801	-0.177356
S	5.142045	0.812399	-0.404072
C	4.850033	2.619254	-0.664783
H	4.184829	3.025966	0.103343
H	4.398226	2.816019	-1.643704
H	5.807614	3.155099	-0.616127
C	1.853701	-1.590478	-0.340115
O	2.514213	-2.528095	-0.756122

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====TS2A====

Mo	0.720917	-0.187044	0.473659
O	-0.557691	1.519581	0.429959
O	0.426113	-0.958246	1.965450
S	-0.889656	-0.762423	-1.205089
S	2.410177	-1.499491	-0.661372
S	2.550991	1.397816	0.688718
C	4.048483	0.507797	0.254728
C	3.988071	-0.718786	-0.307315
C	5.175841	-1.551777	-0.728866
H	5.091882	-1.837584	-1.787558
H	5.221362	-2.491659	-0.158464
H	6.134364	-1.035099	-0.597036

C	5.312123	1.271547	0.574049
H	6.222060	0.755708	0.244048
H	5.403451	1.449817	1.656023
H	5.298135	2.263417	0.098535
Cu	-2.833386	-0.086735	-0.399199
S	-4.956408	-0.016837	0.265169
C	-5.048028	-1.396301	1.494130
H	-4.350202	-1.240240	2.323174
H	-4.821642	-2.364521	1.033989
H	-6.065006	-1.442701	1.906111
C	-1.441515	1.569062	-0.492944
O	-1.890421	2.447268	-1.186651

====Int3A====

Mo	0.903593	-1.434632	-0.860775
O	-0.162639	-2.862955	0.342477
O	1.740424	-2.193474	-2.139525
S	-1.558001	-1.541181	-1.366751
S	1.145595	0.937537	-1.074030
S	2.417692	-1.145176	0.982330
C	3.055138	0.534277	0.861375
C	2.516838	1.415644	-0.006702
C	2.942887	2.852886	-0.186613
H	2.085696	3.529454	-0.057328
H	3.322898	3.028079	-1.204459
H	3.723724	3.163567	0.518740
C	4.192963	0.815337	1.813404
H	4.528796	1.859153	1.784627
H	5.062077	0.178396	1.589649
H	3.900805	0.585936	2.848675
C	-1.419295	-2.831857	0.010040
O	-2.349263	-3.473284	0.453607
Cu	-3.095378	-0.079176	-0.729708
S	-4.704406	1.335664	-0.260016
C	-3.906741	2.522953	0.914442
H	-3.017186	2.984754	0.475780
H	-4.625338	3.316781	1.156943
H	-3.613660	2.029405	1.846849

====TS3A====

Mo	-1.070042	-0.840180	0.832066
O	0.193101	-2.105656	-0.397050
O	-1.513550	-1.633718	2.273840
S	1.396462	-0.236565	0.928750
S	-1.917137	1.397984	0.901365
S	-2.822775	-1.163194	-0.769307
C	-3.879156	0.292225	-0.673988
C	-3.496307	1.375918	0.032063
C	-4.275818	2.660995	0.172187
H	-3.666360	3.520213	-0.144018
H	-4.547564	2.845949	1.222356
H	-5.200607	2.672071	-0.417893
C	-5.163289	0.153661	-1.455757
H	-5.768189	1.068743	-1.455300
H	-5.786232	-0.658777	-1.052175
H	-4.954792	-0.109179	-2.503262
C	1.381417	-1.617248	-0.260696

O	2.413406	-1.926044	-0.875222
Cu	3.484044	0.049587	-0.236469
S	5.424981	0.940025	-0.747335
C	5.425789	2.570984	0.125285
H	4.609488	3.213728	-0.221004
H	6.375480	3.085008	-0.077017
H	5.328443	2.449622	1.209683

====Int4A====

Mo	-1.218136	-0.462976	0.875136
O	0.309000	-1.621558	-0.175385
O	-1.489574	-1.135203	2.419274
S	1.012950	0.662655	0.741938
S	-2.497866	1.557333	0.698765
S	-2.857862	-1.302548	-0.669850
C	-4.176208	-0.076973	-0.740283
C	-4.026303	1.130500	-0.157463
C	-5.045494	2.244187	-0.158802
H	-4.609131	3.168906	-0.564321
H	-5.373043	2.481847	0.864679
H	-5.940379	2.010561	-0.749044
C	-5.393383	-0.547245	-1.499792
H	-6.169796	0.222758	-1.589351
H	-5.847617	-1.424215	-1.014334
H	-5.119275	-0.866241	-2.516345
C	1.359966	-0.885114	-0.082223
O	2.478744	-1.238871	-0.561237
Cu	4.157190	-0.359767	-0.524628
S	6.173602	0.435630	-0.598918
C	5.996104	2.146893	0.081822
H	5.322474	2.755599	-0.529124
H	6.984392	2.624287	0.086706
H	5.613880	2.134887	1.107022

====TS4A====

Mo	1.216146	0.979672	1.819314
O	2.131945	1.354102	3.218056
S	2.371992	1.737199	-0.117063
S	1.978313	-1.149502	1.158613
C	3.141963	-0.898778	-0.205432
C	3.298811	0.318695	-0.756553
C	4.212234	0.666848	-1.904693
C	3.842411	-2.164768	-0.631231
S	-1.158615	0.733974	1.985536
Cu	-2.314654	-0.292971	0.425385
S	-3.616772	-1.331511	-1.021651
C	-2.494317	-1.663374	-2.454723
C	-1.178580	3.246472	1.966110
O	-0.077848	3.444103	2.399159
O	-2.235374	3.594449	1.550335
H	-3.046388	-2.227810	-3.218396
H	-1.623342	-2.253897	-2.153615
H	3.647026	1.138609	-2.721955
H	3.111121	-2.949338	-0.874007
H	-2.135835	-0.733424	-2.908701
H	4.486874	-2.025315	-1.508111
H	4.732378	-0.206005	-2.318456
H	4.465897	-2.564194	0.182946

H 4.976083 1.396458 -1.595864
=====

=====Int5A=====

Mo 0.957694 -0.035955 1.296292
O 1.784544 0.626842 2.649539
S 1.837952 0.942639 -0.680881
S 2.145732 -1.955659 0.561920
C 3.114946 -1.480691 -0.896416
C 2.984959 -0.250683 -1.423390
C 3.710879 0.284143 -2.631420
C 4.014234 -2.578598 -1.404997
S -1.350924 -0.197065 1.513277
Cu -2.570660 -1.028535 -0.111694
S -3.971392 -1.861994 -1.602972
C -3.014979 -1.797164 -3.185588
C -1.292398 3.179590 0.591124
O -1.023486 3.536825 1.674382
O -1.595941 2.938956 -0.512658
H -3.629765 -2.217241 -3.993199
H -2.090402 -2.379478 -3.119460
H 2.997107 0.631558 -3.392967
H 3.434095 -3.486970 -1.625062
H -2.752123 -0.768568 -3.453909
H 4.558224 -2.300805 -2.316971
H 4.366488 -0.459393 -3.102584
H 4.758264 -2.864335 -0.645725
H 4.329165 1.155852 -2.367733
=====

=====Int7A=====

Mo 0.898628 0.411458 0.034145
O 0.917927 1.048374 1.616175
S 2.923864 1.184507 -1.100727
S 2.340330 -1.601418 0.376184
C 4.002082 -1.049353 0.055148
C 4.255137 0.113677 -0.588836
C 5.618148 0.640940 -0.973928
C 5.055197 -2.040310 0.500812
S -0.618371 -1.448056 -0.403660
Cu -2.799313 -1.192102 -0.442376
S -5.013005 -1.350689 -0.479221
C -5.537627 0.061067 -1.558314
C -0.828427 1.487135 -0.604345
O 0.188525 2.004902 -1.178444
O -2.013346 1.748438 -0.564762
O -4.311845 1.508181 1.275803
H -6.624171 0.012233 -1.708436
H -5.050233 0.019764 -2.538023
H 5.665265 0.849524 -2.052905
H 4.841000 -3.036890 0.090466
H -5.290698 1.010384 -1.074899
H 6.068809 -1.760111 0.191705
H 6.425640 -0.059718 -0.734433
H 5.055084 -2.146917 1.594778
H 5.838129 1.590376 -0.463897
H -3.491087 1.606079 0.757013
H -4.553995 0.581827 1.077881
=====

=====Int8A=====

C 5.636155 -1.840362 1.124932
S 5.486494 -0.338989 0.054320
Cu 3.346133 -0.321065 -0.541802
S 1.293119 -0.445515 -1.286039
Mo -0.526677 0.728736 -0.114766
O 1.115374 0.760333 1.502241
O -0.708769 2.412677 -0.344611
C -4.583439 -1.111713 1.713329
C -3.483839 -0.709587 0.762261
S -1.998140 -0.107986 1.596948
C -3.536988 -0.747222 -0.585081
S -2.126551 -0.276785 -1.600078
C -4.722620 -1.214814 -1.396342
H 6.665061 -1.913715 1.502420
H 5.412770 -2.758589 0.569526
H 0.983366 -0.055063 2.017962
H -4.230547 -1.879454 2.418921
H -4.423150 -2.014619 -2.088625
H 4.961067 -1.789747 1.986202
H -5.547951 -1.594512 -0.781171
H -5.467926 -1.511720 1.202345
H -5.117161 -0.398517 -2.019818
H -4.910619 -0.258218 2.326935
H 1.898955 0.543564 0.924954
C 0.503555 -2.846615 1.339827
O -0.015168 -3.599463 0.614340
O 1.042320 -2.184576 2.146746
=====

Geometries obtained by DFT calculations on
model II with constraints

=====Int1A=====

H 0.756486 -4.415652 -1.519628
C 1.578996 -4.830463 -2.107928
S 3.057634 -3.724551 -2.021153
Cu 2.161468 -1.671127 -1.705761
S -0.122169 -1.328855 -1.806719
Mo -0.503030 -0.013724 0.108695
O -0.205159 -1.153965 1.393280
O 0.748371 1.175878 0.175336
H -3.798426 3.279055 2.457934
C -4.347580 2.595016 1.793180
C -3.408767 1.861643 0.868957
S -2.255152 0.815603 1.716212
C -3.438289 1.921517 -0.481690
S -2.304272 0.982042 -1.472122
C -4.430106 2.742663 -1.274593
H -5.174943 3.248048 -0.650413
H -5.100387 3.186414 1.261451
H -3.917880 3.511114 -1.872216
H 1.834714 -5.824234 -1.716930
H 1.233727 -4.946923 -3.142544
H -4.881697 1.892496 2.451261
H -4.969550 2.106469 -1.991467
C 3.126894 -0.082613 -1.605090
O 3.653300 0.933060 -1.738427
=====

====TS1A====

H	97.731050	138.931097	145.237416
C	98.814892	138.777133	145.275196
S	99.516349	139.299281	146.902914
Cu	98.982609	141.467766	147.160207
S	98.124290	143.290845	145.929428
Mo	97.269075	144.732034	147.479039
O	97.951445	143.865247	148.925751
O	98.111018	146.226769	147.333638
H	93.222592	147.036398	149.812275
C	92.888338	146.202584	149.176283
C	93.993296	145.732560	148.263038
S	95.381944	145.043269	149.126329
C	93.952868	145.778844	146.911775
S	95.276878	145.114504	145.927599
C	92.805770	146.350284	146.108519
H	91.954200	146.653535	146.726594
H	91.993287	146.534469	148.639129
H	93.129117	147.229730	145.531842
H	99.014280	137.708131	145.118139
H	99.265057	139.333242	144.445001
H	92.584931	145.397407	149.861620
H	92.442521	145.617083	145.373377
C	99.321167	142.575810	148.790023
O	100.088310	142.676044	149.659962

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====Int2A====

H	0.748442	-5.217273	-1.506129
C	1.578992	-4.830459	-2.107921
S	2.895557	-4.083061	-1.047665
Cu	1.861375	-2.241215	-0.223383
S	0.643136	-0.677586	-1.356881
Mo	-0.130663	0.954228	0.043892
O	0.662274	-0.192708	1.527990
O	0.885965	2.323100	-0.076551
H	-3.968246	3.411885	2.425654
C	-4.347567	2.594999	1.793168
C	-3.270698	2.069799	0.876841
S	-1.897541	1.321012	1.735427
C	-3.309336	2.127910	-0.471914
S	-2.010531	1.414141	-1.470320
C	-4.430117	2.742676	-1.274588
H	-5.275645	3.068659	-0.659306
H	-5.226519	2.971155	1.258408
H	-4.076193	3.615907	-1.843377
H	2.001419	-5.666409	-2.681596
H	1.175872	-4.096345	-2.813196
H	-4.687653	1.807423	2.481702
H	-4.813772	2.027872	-2.017394
C	1.440910	-1.253048	1.457341
O	1.983466	-1.801990	2.401305

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====TS2A====

H	0.493896	-4.700446	-2.187328
C	1.579013	-4.830484	-2.107974
S	2.250256	-4.068092	-0.560935
Cu	1.733228	-1.903876	-0.705313
S	1.272254	0.118265	-1.437076

Mo	0.023056	1.514787	0.056252
O	1.013159	0.166023	1.364732
O	0.871070	2.992692	0.110411
H	-4.057509	3.445219	2.429367
C	-4.347663	2.595120	1.793204
C	-3.214725	2.194146	0.879388
S	-1.753866	1.595471	1.729803
C	-3.246480	2.275892	-0.466599
S	-1.831198	1.798145	-1.462176
C	-4.430041	2.742580	-1.274572
H	-5.326148	2.922107	-0.669896
H	-5.258276	2.879869	1.254688
H	-4.201361	3.673867	-1.815662
H	1.792862	-5.907592	-2.096130
H	2.040817	-4.402557	-3.005051
H	-4.606856	1.774529	2.478675
H	-4.691030	1.999784	-2.042863
C	2.069071	-0.373317	0.870420
O	3.188882	-0.541695	1.281568

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====Int3A====

H	2.576697	-4.852875	-1.860497
C	1.513466	-5.092621	-1.965621
S	0.644998	-3.888199	-3.072124
Cu	0.944693	-1.973544	-2.033612
S	1.434105	-0.054871	-1.023606
Mo	0.008478	1.589014	0.239077
O	1.074051	0.216803	1.509634
O	0.797414	3.101119	0.226083
H	-4.228491	3.215866	2.567310
C	-4.413246	2.333029	1.935581
C	-3.244180	2.056027	1.027048
S	-1.729833	1.622170	1.894881
C	-3.282839	2.105582	-0.318975
S	-1.827863	1.702334	-1.300398
C	-4.495542	2.480385	-1.132183
H	-5.397810	2.626278	-0.527413
H	-5.351851	2.502516	1.396028
H	-4.319696	3.409676	-1.695805
H	1.429065	-6.096421	-2.402132
H	1.066940	-5.113948	-0.966549
H	-4.574556	1.492254	2.626693
H	-4.716891	1.706176	-1.881585
C	1.772841	-0.582075	0.760676
O	2.502920	-1.498329	1.082403

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====TS3A====

H	0.558531	-4.758116	-1.717027
C	1.579025	-4.830500	-2.107947
S	2.818191	-4.188981	-0.897447
Cu	2.293403	-2.082918	-0.557025
S	1.533626	0.219430	-0.877291
Mo	0.108384	2.066674	0.130473
O	1.309565	0.982424	1.586886
O	0.822937	3.603511	-0.047531
H	-4.245111	3.500316	2.412210
C	-4.347609	2.595051	1.793201
C	-3.162379	2.402786	0.888218

S	-1.623530	2.118685	1.772342
C	-3.203474	2.410784	-0.458654
S	-1.734951	2.005815	-1.421419
C	-4.430108	2.742664	-1.274595
H	-5.328287	2.894357	-0.665687
H	-5.298863	2.668787	1.253858
H	-4.267944	3.659576	-1.861484
H	1.791908	-5.888992	-2.311107
H	1.619191	-4.287376	-3.058884
H	-4.431355	1.753646	2.497002
H	-4.648080	1.947627	-2.003368
C	1.939078	0.092047	0.902464
O	2.670633	-0.820184	1.317247

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====Int4A====

H	0.471983	-5.446210	-1.381346
C	1.340685	-5.316175	-2.034476
S	2.903707	-5.124431	-1.058759
Cu	2.526514	-3.256187	-0.025872
S	1.065201	-0.282367	-1.061432
Mo	-0.126634	1.525301	0.178558
O	0.994056	0.153307	1.461432
O	0.678743	3.029715	0.134365
H	-4.442328	2.981903	2.522988
C	-4.585954	2.109383	1.866680
C	-3.400623	1.905363	0.961108
S	-1.869052	1.539697	1.831528
C	-3.437605	1.960019	-0.384629
S	-1.964959	1.628872	-1.364496
C	-4.668446	2.256988	-1.201126
H	-5.576747	2.367846	-0.597792
H	-5.527593	2.254988	1.325101
H	-4.542220	3.182776	-1.783647
H	1.431549	-6.207393	-2.668787
H	1.162292	-4.449876	-2.677579
H	-4.717252	1.244907	2.534883
H	-4.851055	1.458018	-1.935333
C	1.486624	-0.691945	0.628348
O	2.152758	-1.705780	1.000395

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====TS4A====

H	2.069724	-4.602261	-2.772696
C	1.513470	-5.092626	-1.965617
S	-0.115548	-4.270417	-1.656614
Cu	0.451531	-2.224680	-1.041525
S	1.226214	-0.246532	-0.479466
Mo	0.010288	1.689490	0.221227
O	2.190731	1.067198	1.969084
O	0.772139	3.221926	0.162600
H	-4.259448	3.225231	2.562541
C	-4.413237	2.333017	1.935579
C	-3.237582	2.097643	1.026556
S	-1.691830	1.722572	1.887126
C	-3.271930	2.166486	-0.315027
S	-1.785605	1.856858	-1.296415
C	-4.495555	2.480401	-1.132185
H	-5.412854	2.539724	-0.535531
H	-5.358012	2.466398	1.396559

H	-4.383183	3.437265	-1.665706
H	1.337241	-6.136034	-2.260117
H	2.142526	-5.094525	-1.068634
H	-4.542488	1.490177	2.630923
H	-4.651041	1.715053	-1.906798
C	2.383823	-0.091920	1.728457
O	2.821905	-1.167901	1.979866

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====Int5A====

H	1.604008	-4.737198	-2.842799
C	1.789193	-5.310649	-1.927655
S	0.575758	-4.883607	-0.596779
Cu	0.941072	-2.730940	-0.230232
S	1.560430	-0.647503	0.074995
Mo	0.279845	1.279918	0.268151
O	2.649173	0.408099	3.509395
O	1.183845	2.738730	0.337546
H	-3.938465	2.978682	2.627036
C	-4.137402	2.114854	1.973441
C	-2.970865	1.845608	1.062465
S	-1.436216	1.399689	1.914607
C	-3.005338	1.917897	-0.277804
S	-1.516445	1.588555	-1.254760
C	-4.219797	2.262335	-1.094243
H	-5.126705	2.391485	-0.492091
H	-5.071575	2.314712	1.435950
H	-4.065568	3.191163	-1.665823
H	1.693979	-6.377793	-2.169983
H	2.822266	-5.125887	-1.611733
H	-4.315587	1.260715	2.644260
H	-4.424268	1.477992	-1.838714
C	1.822345	-0.420930	3.554663
O	1.030685	-1.267228	3.714694

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====Int7A====

H	2.403720	-4.719606	-2.482998
C	1.513466	-5.092620	-1.965611
S	-0.031366	-4.327708	-2.635572
Cu	0.279970	-2.184202	-2.233691
S	0.550668	-0.023950	-2.051822
Mo	-0.110192	0.866268	0.175138
O	0.472707	-0.374133	1.787685
O	0.784735	2.302632	0.329638
H	-4.065496	3.137167	2.601128
C	-4.413226	2.333003	1.935601
C	-3.310066	1.870572	1.016842
S	-1.924110	1.118637	1.836490
C	-3.334947	1.954736	-0.329225
S	-1.998788	1.332449	-1.333221
C	-4.495562	2.480410	-1.132213
H	-5.368928	2.730974	-0.520821
H	-5.287136	2.707482	1.393977
H	-4.215322	3.381485	-1.697846
H	1.466156	-6.181540	-2.103783
H	1.630441	-4.886899	-0.896823
H	-4.749474	1.514847	2.589837
H	-4.812918	1.736801	-1.876761
C	1.298363	-0.597149	0.833295

O	2.294838	-1.281325	0.718115
O	3.862314	-0.562470	-1.632645
H	3.493119	-0.922658	-0.803228
H	3.024218	-0.273737	-2.048092

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====Int8A====

H	0.728054	-5.043185	-1.921359
C	1.789190	-5.310645	-1.927660
S	2.699961	-4.466087	-0.556807
Cu	2.023179	-2.350841	-0.770752
S	1.264685	-0.398330	-1.348031
Mo	0.271736	1.226583	0.220712
O	4.864200	-4.448343	-3.046884
O	1.154818	2.686655	0.276934
H	-3.887671	2.945746	2.651378
C	-4.137414	2.114869	1.973444
C	-2.980845	1.801612	1.058152
S	-1.469301	1.288608	1.898519
C	-3.001084	1.906264	-0.285176
S	-1.556901	1.551739	-1.293051
C	-4.219782	2.262317	-1.094240
H	-5.129909	2.370442	-0.492858
H	-5.050879	2.391568	1.435407
H	-4.071968	3.202559	-1.647740
H	1.874228	-6.398491	-1.805370
H	2.214586	-5.039126	-2.899206
H	-4.377930	1.256274	2.619780
H	-4.411759	1.489687	-1.852906
C	5.266826	-4.079705	-2.004358
O	5.901591	-3.702239	-1.090720
O	1.311019	-0.215424	1.629278
H	1.708759	-0.823878	0.935669
H	0.602223	-0.724063	2.060554

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