Supplementary Material (ESI) for *Dalton Transactions*

Supporting information

Ring opening at N1-C2 bond of azetidin-2-ones by a molybdenum hydroxo-carbonyl complex: evidence from a computational study

Violeta Yeguas,[a] Natalia Díaz,[a] Pablo Campomanes,[b] and Ramón López*[a]

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

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

rlopez@uniovi.es

Index

Table 1S. Absolute electronic energies (in hartree), Gibbs energies of solvation, relative electronic energies in gas phase, relative Gibbs energies of solvation, and relative energies in dichloromethane solution (in kcal/mol) at the B3LYP/6-31+G(d,p) (LANL2DZ for Mo by f polarization functions with exponent 1.043) level of theory for the critical structures located along the reaction mechanisms found for the reaction between azetidin-2-one and $[Mo(OH)(\eta^3\text{-}C_3H_5)(CO)_2(N_2C_2H_4)]$.

Species	E	ΔG_{solv}	ΔE	$\Delta\Delta G_{solv}$	ΔE_{sol}
azetidin-2-one + **R**	-922.846521	-10.5	0.0	0.0	0.0
TSA	-922.785062	-3.3	38.6	7.2	45.8
TS1B	-922.802425	-4.5	27.7	6.0	33.7
M1B	-922.828852	-2.9	11.1	7.6	18.7
TS2B	-922.789233	-3.7	35.9	6.8	42.7
TS1C	-922.779190	-5.8	42.3	4.7	47.0
M1C	-922.829096	-2.8	10.9	7.7	18.6
TS2C	-922.823162	-4.4	14.7	6.1	20.8
M2C	-922.824596	-4.6	13.8	5.9	19.7
TS3C	-922.819948	-3.7	16.7	6.8	23.5
M3C	-922.828518	-4.3	11.3	6.2	17.5
TS4C	-922.790049	-4.4	35.4	6.1	41.5
P	-922.888967	-3.9	-26.6	6.6	-20.0
TS-RR'	-675.531779	-4.1	4.4	-0.1	4.3
azetidin-2-one + **R'**	-922.844690	-10.9	1.2	-0.4	0.8
TS'A	-922.782832	-3.9	40.0	6.7	46.6
TS1'B	-922.801075	-4.9	28.5	5.6	34.1
M1'B	-922.828959	-3.3	11.0	7.2	18.2
TS2'B	-922.794665	-5.0	32.5	5.5	38.0
TS1'C	-922.779116	-5.4	42.3	5.1	47.4
M1'C	-922.827506	-3.8	11.9	6.7	18.6
TS2'C	-922.819961	-4.3	16.7	6.2	22.9
M2'C	-922.820797	-4.5	16.1	6.0	22.1
TS3'C	-922.820290	-2.7	16.5	7.8	24.3
P'	-922.887322	-8.5	-25.6	2.0	-23.6
TS-PP'	-922.883099	-4.5	3.7	-0.5	3.1

Table 2S. Absolute electronic energies (in hartree), Gibbs energies of solvation, relative electronic energies in gas phase, relative Gibbs energies of solvation, and relative energies in dichloromethane solution (in kcal/mol) at the B3LYP/6-31+G(d,p) (LANL2DZ for Mo by f polarization function with exponent 1.043) level of theory for the critical structures located for the reaction of $[Mo(OH)(\eta^3\text{-}C_3H_5)(CO)_2(N_2C_2H_4)]$ toward *N*-sulfonate azetidin-2-one and 3-formylamine-*N*-sulfonate azetidin-2-one.

Species	E	ΔG_{solv}	ΔE	$\Delta\Delta G_{solv}$	ΔE_{sol}
N-sulfonate azetidin-2-one					
+ **R**	-1546.141580	-51.4	0.0	0.0	0.0
TS1B-s	-1546.091236	-44.8	31.6	6.6	38.2
M1B-s	-1546.114892	-42.7	16.7	8.7	25.4
TS2B1-s	-1546.099594	-40.7	26.3	10.7	37.0
M2B1-s	-1546.154523	-36.4	-8.1	15.0	6.9
TS3B1-s	-1546.123008	-36.1	11.7	15.3	27.0
M2B2-s	-1546.102493	-43.6	24.5	7.8	32.3
TS2B2-s	-1546.066770	-53.1	46.9	-1.7	45.2
P-s	-1546.193559	-37.0	-32.6	14.4	-18.2
TS1'B-s	-1546.114502	-39.6	17.0	11.8	28.8
M1'B-s	-1546.134222	-37.3	4.6	14.1	18.7
TS2'B1-s	-1546.124955	-39.9	10.4	11.5	21.9
M2'B1-s	-1546.161988	-35.6	-12.8	15.8	3.0
TS3'B1-s	-1546.130640	-33.8	6.8	17.6	24.4
TS2'B2-s	-1546.129598	-36.5	7.5	14.9	22.4
M2'B2-s	-1546.131733	-37.4	6.2	14.0	20.2
TS3'B2-s	-1546.115077	-39.4	16.6	12.0	28.6
P'-s	-1546.195853	-37.5	-34.1	13.9	-20.2
3-formylamine-*N*-sulfonate azetidin-2-one + **R'**	-1714.849798	-49.2	0.0	0.0	0.0
TS1'B-sf	-1714.829473	-35.9	12.8	13.3	26.1
M1'B-sf	-1714.847456	-35.1	1.5	14.1	15.6
TS2'B1-sf	-1714.834656	-37.2	9.5	12.0	21.5
M2'B1-sf	-1714.867853	-34.2	-11.3	15.0	3.7
TS3'B1-sf	-1714.839976	-31.5	6.2	17.7	23.9
TS2'B2-sf	-1714.842450	-34.2	4.6	15.0	19.6
M2'B2-sf	-1714.843562	-35.1	3.9	14.1	18.0
TS3'B2-sf	-1714.822038	-37.8	17.4	11.4	28.8
P'-sf	-1714.901213	-35.9	-32.3	13.3	-19.0

Table 3S. Imaginary vibrational frequencies corresponding to all the located transition states.

Species	ω_i (cm^{-1})	Species	ω_i (cm^{-1})
TSA	1400	**TS1B-s**	76
TS1B	106	**TS2B1-s**	289
TS2B	1027	**TS3B1-s**	1661
TS1C	1579	**TS2B2-s**	284
TS2C	311	**TS1'B-s**	102
TS3C	450	**TS2'B1-s**	269
TS4C	413	**TS3'B1-s**	1640
TS'A	839	**TS2'B2-s**	131
TS1'B	107	**TS3'B2-s**	178
TS2'B	412	**TS1'B-sf**	94
TS1'C	1556	**TS2'B1-sf**	687
TS2'C	287	**TS3'B1-sf**	1652
TS3'C	461	**TS2'B2-sf**	84
TS-RR'	99	**TS3'B2-sf**	219
TS-PP'	28		

Table 4S. Cartesian coordinates, in angstroms, corresponding to all the located structures.

$[Mo(OH)(\eta^3\text{-}C_3H_5)(CO)_2(N_2C_2H_4)]$ (**R**)

C	0.061743	-0.102850	-2.101039
Mo	0.058341	-0.086825	-0.096779
O	2.094772	-0.077144	-0.192003
O	0.104811	-0.100966	-3.261463
C	0.156694	-2.081298	-0.269147
O	0.255162	-3.234783	-0.359829
N	0.424883	2.048032	0.295236
C	0.972584	2.359937	1.435491
C	1.023511	1.301696	2.415350
N	0.515642	0.161426	2.042133
C	-2.080258	0.746424	-0.866510
C	-2.170053	0.340606	0.480373
C	-1.995073	-1.026563	0.775441
H	2.504152	-0.659843	-0.842525
H	0.574464	-0.572177	2.745920
H	1.449100	1.471025	3.403561
H	1.358482	3.353262	1.660762
H	0.411848	2.807276	-0.383240
H	-2.169812	1.078859	1.277528
H	-2.451226	0.078387	-1.638730
H	-2.101962	1.803874	-1.113459
H	-2.362705	-1.764429	0.067900
H	-1.950217	-1.353211	1.810304

[Mo(OH)(η^3-C_3H_5)(CO)$_2$($N_2C_2H_4$)] (**R'**)

C	-0.000256	0.001486	0.007713
Mo	0.005396	0.002908	2.042125
N	0.528114	0.003299	4.135472
C	1.468514	0.825269	4.555358
C	1.922434	1.761830	3.579840
N	1.333364	1.664206	2.405215
O	0.052964	0.003933	-1.147173
C	-2.255344	0.192896	2.941442
C	-1.760821	1.471315	2.627987
C	-1.484142	1.781501	1.284718
O	1.659298	-1.122781	1.731803
C	-0.885403	-1.821142	1.907438
O	-1.347628	-2.879712	1.858497
H	2.382656	-0.862397	2.319403
H	0.228820	-0.676014	4.832304
H	1.865915	0.804572	5.568046
H	2.688569	2.502481	3.799761
H	1.681602	2.321538	1.710043
H	-1.390879	2.117645	3.419966
H	-2.115823	1.354055	0.510748
H	-1.001226	2.720815	1.033720
H	-2.917608	-0.297439	2.233106
H	-2.372242	-0.103554	3.979211

TS-RR'

C	0.001006	-0.026445	0.034341
Mo	-0.013267	0.019689	2.055773
O	2.035768	0.058830	1.834951
O	0.048281	-0.024686	-1.123483
C	0.370553	-1.980422	1.946655
O	0.636289	-3.103628	1.900089
N	0.126861	2.136745	2.357253
C	0.650310	2.555156	3.494843
C	0.811995	1.552586	4.493862
N	0.418431	0.345767	4.147338
C	-2.217407	0.550114	1.289325
C	-2.279924	0.164004	2.645592
C	-1.928914	-1.160900	2.958780
H	2.371967	0.764333	1.269233
H	0.548299	-0.358413	4.870445
H	1.202328	1.786677	5.482328
H	0.903070	3.597313	3.678497
H	0.004287	2.871111	1.663226
H	-2.374035	0.911185	3.428173
H	-2.499829	-0.178036	0.533437
H	-2.373985	1.589760	1.017468
H	-2.179945	-1.947448	2.252461
H	-1.835220	-1.468994	3.995549

Azetidin-2-one

C	0.011894	-0.033857	-0.073855
C	-0.033922	0.073244	1.479318
C	1.545639	0.110456	0.074683
N	1.431866	0.198766	1.442122
H	2.131252	0.309935	2.165185
O	2.496709	0.139645	-0.675394
H	-0.461180	0.785811	-0.619218
H	-0.306313	-0.991591	-0.491655
H	-0.545217	0.958418	1.870451
H	-0.389494	-0.822816	1.997616

TSA

C	0.255610	-1.534915	1.274170
O	-0.082648	-2.344237	2.030570

Mo	0.819671	-0.122685	-0.046322
O	-1.251324	-0.070006	-0.576542
C	-2.399328	0.382943	0.334247
N	-3.066201	-1.237438	0.052288
C	-4.186133	-0.570679	-0.650079
C	-3.581879	0.849409	-0.565580
N	1.015258	1.612052	-1.390854
C	0.691782	2.787689	-0.926148
C	0.286061	2.818653	0.454700
N	0.333184	1.673170	1.074253
C	3.104784	-0.426534	-0.717894
C	3.019526	0.293181	0.489616
C	2.497632	-0.394687	1.611103
C	0.894343	-1.625897	-1.378440
O	0.903916	-2.472168	-2.172380
O	-2.126876	0.845087	1.448888
H	1.253810	1.604000	-2.380775
H	0.696919	3.688875	-1.538215
H	-0.094289	3.726773	0.918263
H	-0.109566	1.666640	1.991517
H	3.168187	1.368815	0.512693
H	2.743330	-1.446409	1.732652
H	2.305707	0.147160	2.532244
H	3.339296	-1.486454	-0.679501
H	3.386466	0.081162	-1.635357
H	-1.893715	-1.049923	-0.556955
H	-3.305183	-1.868478	0.813444
H	-4.205067	1.574175	-0.035135
H	-3.250971	1.274147	-1.517160
H	-5.126761	-0.652723	-0.095602
H	-4.349134	-0.953564	-1.664424

TS1B

Mo	-0.769412	-0.134374	0.015997
C	-2.935760	-0.543536	0.863228
C	-2.984760	0.112169	-0.395000
C	-2.529526	-0.601824	-1.519316
N	-1.073894	1.698515	1.256573
C	-0.930078	2.865932	0.704802
C	-0.540315	2.843171	-0.688841
N	-0.470785	1.658558	-1.215903
C	-0.714153	-1.589443	1.376209
O	-0.653142	-2.404434	2.204471
C	-0.178544	-1.586782	-1.250968
O	0.144182	-2.427460	-1.977568
O	1.606632	0.148767	-1.156525
C	2.310460	0.141714	-0.055356
N	3.182460	-1.027275	0.269522
C	4.409065	-0.191366	0.141333
C	3.544169	1.092302	0.107383
O	1.326390	0.279690	1.094139
H	-3.158333	-1.606683	0.897875
H	-3.202907	0.004607	1.761899
H	-3.206963	1.173387	-0.462007
H	-2.694384	-1.674578	-1.565451
H	-2.440274	-0.101857	-2.478669
H	-1.269451	1.726980	2.255682
H	-1.028574	3.802790	1.252495
H	-0.241418	3.751512	-1.209972
H	-0.031473	1.609989	-2.133318
H	3.090836	-1.777824	-0.411750
H	5.095502	-0.297795	0.987946
H	4.963283	-0.359250	-0.789845
H	3.549358	1.671711	1.034213
H	3.693822	1.750255	-0.750858
H	1.635970	-0.364634	1.751571

M1B

C	0.149351	-0.325552	-0.177040
C	0.055284	0.115094	1.157317
C	1.255261	0.282048	1.880651
Mo	0.944129	-2.034994	1.334569
N	-1.132038	-2.741261	1.158740
C	-1.755688	-3.058139	2.260027
C	-1.104667	-2.657381	3.480614
N	0.038098	-2.042980	3.335345
C	1.614622	-2.426087	-0.534791
O	1.952682	-2.630948	-1.621548
C	2.884132	-1.723602	1.748233
O	3.999800	-1.538040	2.006387
H	-0.751915	-0.578540	-0.727463
H	0.985917	0.013923	-0.781239
H	-0.903075	0.126146	1.668619
H	2.130631	0.654542	1.355941
H	1.216046	0.516646	2.940447
H	-1.608721	-3.037270	0.308798
H	-2.717319	-3.569333	2.275671
H	-1.564626	-2.838969	4.451035
H	0.471672	-1.758324	4.211850
O	1.207967	-4.023884	1.794185
C	2.250873	-4.893803	1.690046
O	3.103419	-4.517804	0.624375
H	3.985180	-4.840865	0.856117
N	3.025092	-5.133518	2.942227
C	2.285395	-6.397692	3.199177
C	1.784232	-6.386974	1.735744
H	2.918760	-4.399015	3.638680
H	1.468251	-6.299053	3.925682
H	2.932195	-7.228874	3.499447
H	0.714589	-6.530622	1.575140
H	2.359436	-7.031841	1.066518

TS2B

C	0.804514	-1.540242	1.491784
O	0.743697	-2.323196	2.343125
Mo	0.850711	-0.136779	0.045712
O	-1.115505	0.296254	0.760985
C	-2.202381	0.448661	0.102422
C	-3.473146	0.865735	0.865973
C	-4.381355	-0.313477	0.452971
N	-3.464523	-0.998958	-0.468708
N	0.464565	1.623347	-1.174209
C	0.548943	2.796966	-0.615329
C	1.092301	2.809711	0.719529
N	1.382968	1.638987	1.218270
C	2.343902	-0.706158	-1.703420
C	3.045843	-0.076870	-0.651338
C	3.102086	-0.762092	0.579541
C	0.000093	-1.565007	-1.097749
O	-0.471510	-2.394307	-1.751504
O	-2.155041	0.765482	-1.219959
H	-0.051242	1.605372	-2.052421
H	0.194324	3.708138	-1.093866
H	1.226408	3.739634	1.270223
H	1.726114	1.667589	2.176876
H	3.352429	0.962181	-0.728574
H	3.171675	-1.846168	0.570396
H	3.524774	-0.274738	1.453115
H	2.408049	-1.786955	-1.795389
H	2.167515	-0.169562	-2.630546
H	-2.882232	-0.021813	-1.428120

H	-3.500542	-2.015451	-0.413749
H	-3.272730	0.904459	1.940117
H	-3.809235	1.853449	0.529020
H	-4.630478	-0.920900	1.333529
H	-5.334055	-0.002048	-0.005986

TS1C

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.156935
Mo	0.045640	0.000000	-2.018842
C	-1.144892	-1.911746	-1.245377
C	-1.426751	-1.677878	-2.611153
C	-2.127257	-0.499641	-2.929825
O	1.626720	1.392849	-1.739922
C	3.066588	1.296074	-1.330691
N	3.495254	-0.023939	-0.805905
C	4.713773	0.000519	-1.665744
C	4.131885	1.193259	-2.461579
C	-1.098856	1.656028	-1.891821
O	-1.720663	2.632101	-1.842396
N	0.540126	0.028340	-4.160179
C	1.482945	-0.766092	-4.593528
C	2.105959	-1.582774	-3.587925
N	1.619975	-1.445555	-2.382347
O	3.040676	2.342110	-0.494262
H	3.662444	0.016637	0.198424
H	1.807206	2.249010	-0.955666
H	0.146742	0.639342	-4.873662
H	1.805714	-0.792578	-5.633315
H	2.957526	-2.221160	-3.815124
H	2.161675	-1.894534	-1.645532
H	-2.270604	-0.214743	-3.967558
H	-2.879881	-0.135440	-2.236074
H	-0.960682	-2.277497	-3.387929
H	-0.514443	-2.748966	-0.961855
H	-1.886805	-1.617334	-0.507569
H	4.760875	2.081131	-2.540283
H	3.722846	0.931311	-3.439798
H	4.875982	-0.932159	-2.220663
H	5.631228	0.249170	-1.120903

M1C

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.006268
O	2.107677	0.000000	2.030750
C	2.947150	0.352477	1.035442
O	3.049059	-0.662836	0.023849
O	-0.033801	0.017290	-1.159869
C	0.170673	-1.992516	1.813190
O	0.324004	-3.137422	1.704458
N	0.350969	0.244863	4.157432
C	0.836993	1.388509	4.552825
C	0.902632	2.423768	3.549894
N	0.422098	2.115435	2.380921
C	-2.041071	-1.026606	2.757944
C	-2.217596	0.357647	2.552262
C	-2.085404	0.833834	1.228812
C	4.348882	0.883066	1.480492
C	4.131532	2.035099	0.473543
N	2.696655	1.648329	0.333662
H	2.395147	1.508863	-0.629504

H	2.986258	-1.512155	0.483511
H	0.333816	-0.473495	4.879197
H	1.175242	1.570006	5.572254
H	1.348749	3.392475	3.771750
H	0.586541	2.812062	1.656158
H	-2.015937	-1.425399	3.767885
H	-2.383553	-1.716422	1.991743
H	-2.256264	1.046755	3.390581
H	-2.094726	1.902915	1.039264
H	-2.454690	0.214233	0.416390
H	5.183495	0.208695	1.279902
H	4.353980	1.196191	2.526897
H	4.272862	3.054088	0.851066
H	4.712031	1.913659	-0.448579

TS2C

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.161190
Mo	0.029730	0.000000	-2.002232
C	1.090669	-1.996335	-1.213415
C	0.662602	-2.171542	-2.547215
C	-0.724231	-2.152638	-2.795888
O	-0.158209	2.054551	-1.999655
C	-0.571504	2.917782	-1.049922
N	0.431060	3.246001	0.008483
C	0.121491	4.694440	-0.100258
C	-0.603865	4.427150	-1.440687
C	-1.982515	-0.099134	-1.839107
O	-3.136666	-0.167751	-1.783425
N	0.235132	0.419415	-4.150137
C	1.322404	1.028245	-4.534795
C	2.373277	1.116523	-3.550167
N	2.114542	0.572411	-2.395727
O	-1.806947	2.459255	-0.461302
H	0.225197	2.820505	0.909799
H	-2.460209	3.168190	-0.466866
H	-0.492070	0.375161	-4.861784
H	1.455945	1.433930	-5.536841
H	3.320963	1.600953	-3.781997
H	2.859111	0.671147	-1.708093
H	-1.090654	-2.167071	-3.818257
H	-1.394271	-2.575835	-2.052848
H	1.373407	-2.119106	-3.366936
H	2.150270	-1.895957	-0.997404
H	0.494006	-2.430259	-0.415982
H	-1.590610	4.879713	-1.583936
H	0.013723	4.614588	-2.320940
H	1.010036	5.333669	-0.139669
H	-0.552212	5.076639	0.679675

M2C

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.162225
Mo	0.018850	0.000000	-1.999154
C	0.135034	-2.264280	-1.233544
C	-0.336413	-2.227799	-2.563894
C	-1.585338	-1.618601	-2.797277
O	0.736270	1.937504	-1.977729
C	0.739107	2.884056	-1.021461
N	1.753934	2.736743	0.064776
C	2.145512	4.163247	-0.042102

C	1.399274	4.249867	-1.396231
C	-1.845951	0.761542	-1.813189
O	-2.921388	1.181253	-1.739536
N	0.364204	0.325969	-4.146315
C	1.603737	0.418056	-4.539800
C	2.599848	0.026633	-3.571816
N	2.143707	-0.372446	-2.419239
O	-0.599683	3.020566	-0.512923
H	1.408231	2.406369	0.963222
H	-0.617181	3.699927	0.174696
H	-0.318070	0.615123	-4.844984
H	1.889774	0.749136	-5.537333
H	3.661273	0.057612	-3.814661
H	2.865211	-0.620327	-1.744736
H	-1.930454	-1.464960	-3.815582
H	-2.366364	-1.724618	-2.049684
H	0.323125	-2.474707	-3.390899
H	1.138140	-2.626500	-1.028285
H	-0.583759	-2.411564	-0.432373
H	0.708961	5.084552	-1.540536
H	2.052505	4.150033	-2.265258
H	3.229120	4.322728	-0.063557
H	1.715575	4.820284	0.729374

TS3C

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.163564
Mo	0.040220	0.000000	-1.995434
C	-2.223823	0.023212	-2.842618
C	-1.801183	-1.297230	-2.593662
C	-1.530573	-1.659131	-1.256130
O	1.929403	0.802317	-1.922567
C	2.564645	1.592602	-1.014372
O	1.712872	2.709751	-0.729727
C	4.040313	1.958937	-1.412541
C	4.507574	1.271149	-0.097388
N	3.111862	0.970187	0.181436
C	-0.730928	1.864034	-1.807095
O	-1.214098	2.912321	-1.736292
N	1.225695	-1.800392	-2.431192
C	1.839490	-1.849177	-3.579645
C	1.465036	-0.834145	-4.534247
N	0.547013	0.002610	-4.139615
H	2.657751	0.566344	0.987359
H	2.034710	3.118311	0.084790
H	5.152137	0.391742	-0.242788
H	4.998526	1.942995	0.622813
H	4.361027	1.467685	-2.332748
H	4.228299	3.033606	-1.470404
H	1.510200	-2.523967	-1.773578
H	2.575317	-2.612114	-3.830813
H	1.917504	-0.800684	-5.524581
H	0.305032	0.713123	-4.827967
H	-1.102812	-2.633532	-1.038483
H	-2.150798	-1.239497	-0.469083
H	-1.500976	-1.945517	-3.411945
H	-2.860258	0.514901	-2.112317
H	-2.328526	0.373382	-3.865367

M3C

C	0.000000	0.000000	0.000000

O	0.000000	0.000000	1.160076
Mo	0.036215	0.000000	-2.007587
C	1.062049	-2.021185	-1.216584
C	0.656328	-2.180806	-2.558586
C	-0.723773	-2.138706	-2.836254
O	-0.117876	2.052224	-1.968949
C	-0.709245	2.945897	-1.128155
N	0.194020	3.607390	-0.142571
C	0.297992	4.819175	-0.998247
C	-0.931479	4.339327	-1.805122
C	-1.978275	-0.107561	-1.842174
O	-3.130200	-0.196194	-1.792252
N	0.227522	0.433305	-4.155974
C	1.332040	0.997790	-4.560437
C	2.403102	1.028663	-3.598083
N	2.130892	0.504843	-2.433594
O	-1.824764	2.356772	-0.485907
H	1.059509	3.099650	0.027640
H	-1.919696	2.811212	0.362653
H	-0.516663	0.425850	-4.851233
H	1.463372	1.402245	-5.563163
H	3.378408	1.441175	-3.852780
H	2.908021	0.526961	-1.775675
H	-1.068084	-2.139038	-3.866157
H	-1.415076	-2.561051	-2.112465
H	1.383206	-2.130572	-3.364273
H	2.119207	-1.941528	-0.980314
H	0.443174	-2.448348	-0.432440
H	-1.869856	4.812178	-1.504402
H	-0.841031	4.332358	-2.892474
H	1.211239	4.861573	-1.606053
H	0.195155	5.756817	-0.441814

TS4C

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.004733
N	2.187142	0.000000	2.417639
C	2.561194	-0.376640	3.609072
C	1.509302	-0.592580	4.575215
N	0.290305	-0.363930	4.178609
O	-0.003858	0.033920	-1.158307
C	0.436039	2.182795	1.217842
C	0.010543	2.207443	2.566867
C	-1.319434	1.802856	2.814728
O	0.434340	-2.102742	2.071388
C	1.024189	-2.862644	1.252329
O	0.593587	-2.865075	-0.029839
C	-1.929710	-0.469899	1.788806
O	-3.042321	-0.778314	1.667934
C	1.761502	-4.078633	1.832417
C	3.121608	-3.393229	2.020344
N	3.034659	-2.485565	0.902830
H	3.773772	-1.778501	0.888276
H	1.363966	-3.128444	-0.562901
H	-0.421082	-0.549319	4.882787
H	1.750372	-0.919134	5.586760
H	3.604295	-0.520821	3.885506
H	2.945410	0.118681	1.751360
H	-1.666368	1.684569	3.837093
H	-2.087424	2.055457	2.089264
H	0.715987	2.353471	3.379059

H	1.479443	2.369579	0.980893
H	-0.270971	2.465961	0.442984
H	1.815085	-4.888569	1.099902
H	1.266272	-4.435690	2.740410
H	3.129018	-2.886561	3.017095
H	3.984014	-4.082811	2.019888

[Mo(OCOCH2CH2NH2)((3-C3H5)(CO)2(N2C2H4)] (**P**)

C	-1.864010	-0.063348	-0.902540
O	-2.941386	-0.235040	-1.285057
Mo	0.023332	0.229389	-0.242249
C	-1.233988	2.202833	0.139387
C	0.148093	2.492157	0.186456
C	0.876539	2.332666	-1.009718
N	-0.283032	-0.101041	1.877893
C	0.754708	-0.325075	2.638061
C	2.030890	-0.169570	1.995074
N	1.985304	0.133922	0.723963
C	0.551370	0.039231	-2.181063
O	0.875758	-0.113003	-3.282324
O	0.179379	-1.899551	-0.288274
C	-0.588979	-2.726896	0.355551
C	-0.222581	-4.196974	0.142246
C	-1.047566	-5.181406	0.971420
N	-2.445524	-5.196238	0.528705
O	-1.540798	-2.392650	1.080378
H	-1.181004	-0.350816	2.288426
H	0.671249	-0.654667	3.672035
H	2.964394	-0.319552	2.535388
H	2.898349	0.192897	0.276703
H	0.846451	-4.308059	0.361999
H	-0.346752	-4.416237	-0.925156
H	-0.928526	-4.934867	2.040513
H	-0.634614	-6.186539	0.822750
H	-2.872178	-4.299097	0.749346
H	-2.971123	-5.918227	1.013393
H	-1.814824	2.193815	1.056435
H	-1.786423	2.463507	-0.759474
H	0.656567	2.631737	1.136049
H	1.958344	2.424990	-1.003408
H	0.392400	2.576936	-1.951069

TS'A

C	-0.486331	0.607383	-2.228325
O	-0.350457	0.643451	-3.378181
Mo	-0.638483	0.524858	-0.221304
O	1.091323	-0.790538	-0.453230
C	1.348417	-1.973610	0.435430
O	0.526641	-2.226760	1.314116
N	-0.228537	0.300352	1.897860
C	0.668261	1.062666	2.458553
C	1.240120	2.067192	1.602095
N	0.818526	2.053100	0.364374
C	-2.869529	0.863445	0.512981
C	-2.210564	2.098557	0.327103
C	-1.839896	2.425338	-0.996088
C	-1.701646	-1.161045	-0.545616
O	-2.302917	-2.129047	-0.740037
C	2.219307	-3.005078	-0.313460
C	3.576984	-2.338785	-0.002625
N	3.066315	-1.134203	0.683033
H	-0.501256	-0.520512	2.436855
H	1.020845	0.912106	3.477174

H	2.004513	2.755677	1.958259
H	1.280232	2.732075	-0.238465
H	-1.845336	2.673367	1.173213
H	-2.497829	2.128357	-1.808199
H	-1.235021	3.306725	-1.187022
H	-3.564437	0.526093	-0.251259
H	-3.067902	0.500812	1.516724
H	2.073133	-0.441181	-0.152940
H	3.509124	-0.943913	1.579797
H	2.090870	-3.990417	0.142830
H	1.954074	-3.064572	-1.373969
H	4.186206	-2.971590	0.654381
H	4.179656	-2.111258	-0.893574

TS1'B

C	2.626021	-0.406929	-1.466318
C	2.982364	0.303614	-0.306289
C	2.934054	-0.383896	0.933281
Mo	0.769178	-0.117312	0.010600
O	-1.373056	-0.005441	1.096228
C	-2.309374	-0.078608	-0.090120
C	-3.450195	-1.117081	0.171578
C	-4.425468	0.085308	0.177103
N	-3.283657	1.045576	0.066609
N	0.364416	1.621411	-1.216122
C	0.371598	2.823523	-0.706780
C	0.737033	2.881408	0.683086
N	0.908051	1.716492	1.253371
C	0.369009	-1.634536	-1.267293
O	0.156518	-2.502052	-2.000693
C	0.749208	-1.567886	1.407692
O	0.713199	-2.367750	2.245675
O	-1.566765	-0.134994	-1.167954
H	2.866440	-1.464353	-1.530968
H	2.535906	0.111594	-2.415379
H	3.121260	1.380796	-0.338551
H	3.222342	-1.431903	0.950821
H	3.131731	0.156976	1.853957
H	-0.062761	1.533850	-2.136258
H	0.041485	3.706405	-1.251087
H	0.806418	3.825668	1.221260
H	1.109687	1.763696	2.250744
H	-3.304443	1.618339	-0.773884
H	-5.008505	0.227628	1.092736
H	-5.105312	0.109239	-0.681850
H	-3.366408	-1.664317	1.113031
H	-3.573175	-1.813175	-0.660199
H	-1.586482	0.834713	1.531755

M1'B

C	2.598065	-0.340582	-1.557413
Mo	0.790440	-0.138009	0.014450
O	-1.207970	-0.474465	0.471823
C	-2.386777	0.168579	0.320338
C	-3.588436	-0.636930	0.913947
C	-3.943188	-1.003180	-0.545501
N	-3.029841	0.071525	-1.028232
C	2.973605	0.501287	-0.488104
C	3.093225	-0.074174	0.789441
N	0.245366	1.484482	-1.341711
C	0.091546	2.691095	-0.862260
C	0.355696	2.828679	0.542772
N	0.726827	1.734189	1.146582
C	0.474389	-1.753380	-1.148508
O	0.244992	-2.667901	-1.822762
C	1.017374	-1.474693	1.516210
O	1.110979	-2.223412	2.393858

O	-2.275943	1.533605	0.732567
H	2.403022	0.086657	-2.536577
H	2.958373	-1.365960	-1.560816
H	2.979048	1.580954	-0.610109
H	3.451809	-1.096408	0.871783
H	3.266155	0.556370	1.655983
H	0.028175	1.406463	-2.333711
H	-0.233105	3.533741	-1.469579
H	0.221081	3.777443	1.058225
H	0.853770	1.836790	2.151673
H	-3.048372	1.976992	0.354517
H	-2.381893	-0.211112	-1.760936
H	-3.620040	-2.015343	-0.816531
H	-4.983405	-0.861931	-0.857130
H	-3.294090	-1.453416	1.574586
H	-4.331775	-0.001705	1.403993

TS2'B

C	0.804514	-1.540242	1.491784
O	0.743697	-2.323196	2.343125
Mo	0.850711	-0.136779	0.045712
O	-1.115505	0.296254	0.760985
C	-2.202381	0.448661	0.102422
C	-3.473146	0.865735	0.865973
C	-4.381355	-0.313477	0.452971
N	-3.464523	-0.998958	-0.468708
N	0.464565	1.623347	-1.174209
C	0.548943	2.796966	-0.615329
C	1.092301	2.809711	0.719529
N	1.382968	1.638987	1.218270
C	2.343902	-0.706158	-1.703420
C	3.045843	-0.076870	-0.651338
C	3.102086	-0.762092	0.579541
C	0.000093	-1.565007	-1.097749
O	-0.471510	-2.394307	-1.751504
O	-2.155041	0.765482	-1.219959
H	-0.051242	1.605372	-2.052421
H	0.194324	3.708138	-1.093866
H	1.226408	3.739634	1.270223
H	1.726114	1.667589	2.176876
H	3.352429	0.962181	-0.728574
H	3.171675	-1.846168	0.570396
H	3.524774	-0.274738	1.453115
H	2.408049	-1.786955	-1.795389
H	2.167515	-0.169562	-2.630546
H	-2.882232	-0.021813	-1.428120
H	-3.500542	-2.015451	-0.413749
H	-3.272730	0.904459	1.940117
H	-3.809235	1.853449	0.529020
H	-4.630478	-0.920900	1.333529
H	-5.334055	-0.002048	-0.005986

TS1'C

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.159397
Mo	0.011445	0.000000	-2.009912
N	-1.690902	-1.294329	-2.379253
C	-2.232136	-1.293674	-3.565190
C	-1.515819	-0.548825	-4.567717
N	-0.438785	0.063000	-4.147419
O	-1.529514	1.487145	-1.901284
C	-2.763302	1.601743	-1.066319
O	-3.561692	2.020919	-2.065862
N	-3.144991	0.362836	-0.335359
C	-3.221549	1.116191	0.957075

C	-2.620139	2.369321	0.275657
C	1.214968	1.612062	-1.828180
O	1.867685	2.562935	-1.732786
C	1.017970	-2.018997	-1.234118
C	1.414517	-1.746901	-2.560004
C	2.195761	-0.590147	-2.773259
H	-4.051187	0.042281	-0.672114
H	-4.245857	1.257116	1.319124
H	-2.618214	0.662374	1.748672
H	-3.228510	3.274731	0.309464
H	-1.591207	2.600670	0.559651
H	-2.381937	1.811108	-2.632411
H	-2.257623	-1.702850	-1.636856
H	-3.181567	-1.777632	-3.786811
H	-1.871902	-0.485733	-5.594386
H	0.028058	0.618688	-4.862433
H	2.433114	-0.278048	-3.785991
H	2.921575	-0.305381	-2.016607
H	0.974651	-2.286495	-3.393604
H	0.314160	-2.820955	-1.034211
H	1.708360	-1.790028	-0.427270

M1'C

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.009231
O	2.062895	0.000000	1.908989
C	3.003210	-0.955632	1.664385
C	3.010936	-1.822786	0.362634
C	3.299683	-3.027962	1.289326
N	2.921211	-2.195758	2.463183
O	0.025294	0.024319	-1.159727
C	-0.040043	-2.009377	1.832961
O	-0.130486	-3.157816	1.707938
N	0.428544	0.232568	4.155255
C	0.940913	1.366168	4.541579
C	0.942544	2.420608	3.557278
N	0.424048	2.115473	2.399340
C	-2.075275	-0.828291	2.880091
C	-2.198468	0.537912	2.552689
C	-2.090245	0.893548	1.192756
O	4.282802	-0.332263	1.858627
H	3.566188	-2.213539	3.250636
H	4.083683	0.611525	1.929803
H	0.456125	-0.504821	4.857220
H	1.334279	1.532828	5.543613
H	1.337342	3.408294	3.791428
H	0.445779	2.874262	1.720219
H	-2.042314	-1.133123	3.921767
H	-2.481301	-1.565506	2.193101
H	-2.175749	1.298374	3.327835
H	-2.063558	1.941232	0.908054
H	-2.490722	0.216503	0.443440
H	3.786495	-1.552698	-0.355586
H	2.041620	-1.875230	-0.135630
H	2.665337	-3.911417	1.161627
H	4.353916	-3.331498	1.277321

TS2'C

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.162077
Mo	0.045195	0.000000	-2.000852

C	-1.282097	-1.863639	-1.221585
C	-1.537957	-1.594806	-2.581621
C	-2.141388	-0.358162	-2.898138
O	1.812551	1.045445	-1.914878
C	2.184931	2.308264	-1.630657
O	3.612956	2.357323	-1.844619
C	-1.021324	1.692171	-1.819999
O	-1.680519	2.637682	-1.688920
N	0.568125	0.028282	-4.152913
C	1.635835	-0.625623	-4.499029
C	2.184772	-1.520446	-3.501460
N	1.538040	-1.586082	-2.375655
C	1.769468	3.051173	-0.313402
C	1.452877	4.267216	-1.216510
N	1.494145	3.376094	-2.403425
H	2.034465	3.714539	-3.197008
H	4.033638	2.789515	-1.092245
H	0.207632	0.657791	-4.867802
H	2.098628	-0.538307	-5.481566
H	3.076953	-2.108566	-3.712862
H	1.953808	-2.216071	-1.691938
H	-2.258722	-0.066982	-3.937914
H	-2.885401	0.046166	-2.217498
H	-1.112501	-2.221305	-3.360132
H	-0.714177	-2.746422	-0.942619
H	-1.988353	-1.507750	-0.476829
H	2.546895	3.171193	0.448140
H	0.885345	2.615994	0.153519
H	0.482014	4.750373	-1.066592
H	2.240622	5.033126	-1.194414

M2'C

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.160062
Mo	0.104029	0.000000	-2.005638
N	-1.234214	-1.687519	-2.536726
C	-1.776389	-1.647510	-3.716096
C	-1.226954	-0.673249	-4.636849
N	-0.235631	0.038547	-4.190382
O	-1.683732	0.998946	-2.144553
C	-2.497845	1.666316	-1.307884
O	-3.596711	2.093861	-2.137750
N	-2.953608	0.926230	-0.100125
C	-2.845554	2.137369	0.749139
C	-1.999784	2.813642	-0.358081
C	1.035112	1.752262	-1.750335
O	1.563041	2.779012	-1.618599
C	1.439806	-1.792688	-1.157183
C	1.838984	-1.468445	-2.472012
C	2.414605	-0.198448	-2.681625
H	-3.867761	0.485433	-0.180455
H	-3.798840	2.652701	0.941991
H	-2.347517	1.956860	1.707374
H	-2.274380	3.828080	-0.658710
H	-0.927107	2.775059	-0.165876
H	-1.642729	-2.376360	-1.907506
H	-2.583796	-2.310204	-4.026292
H	-1.625615	-0.575730	-5.645877
H	0.121510	0.720819	-4.856892
H	2.626961	0.138248	-3.692179
H	3.049590	0.221388	-1.906576

H	1.538712	-2.086665	-3.312979
H	0.897845	-2.715421	-0.971113
H	2.043757	-1.435831	-0.327610
H	-4.164884	2.678813	-1.617898

TS3'C

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.162984
Mo	0.036093	0.000000	-1.995587
N	-2.027286	-0.623948	-2.456038
C	-2.497454	-0.278248	-3.616723
C	-1.525834	0.198477	-4.576678
N	-0.292574	0.246234	-4.162837
O	-0.903647	1.834501	-2.046574
C	-1.246188	2.683244	-1.044915
O	-2.327684	2.050183	-0.325377
C	-1.523236	4.155160	-1.516833
C	-0.394845	4.617518	-0.550309
N	-0.221453	3.223838	-0.169118
C	1.756580	1.016769	-1.752531
O	2.742727	1.613126	-1.625123
C	0.197958	-2.260473	-1.229292
C	0.711694	-2.155194	-2.539864
C	1.877955	-1.384840	-2.723790
H	0.338060	2.792949	0.551653
H	-2.417015	2.516234	0.517152
H	-1.319033	4.302551	-2.578761
H	-2.523477	4.518165	-1.268648
H	-0.726194	5.288310	0.256383
H	-0.756869	-2.750553	-1.063545
H	0.898192	-2.313972	-0.400417
H	0.123752	-2.484233	-3.391750
H	2.241243	-1.184330	-3.727588
H	2.635753	-1.389121	-1.945452
H	-2.734852	-0.911412	-1.782439
H	-3.553931	-0.339828	-3.875203
H	-1.828178	0.479815	-5.584813
H	0.367611	0.591927	-4.857158
H	0.475479	5.072391	-1.044477

[Mo(OCOCH2CH2NH2)((3-C3H5)(CO)2(N2C2H4)] (**P'**)

C	-1.383226	-1.025845	1.689923
O	-1.620255	-1.660136	2.632150
Mo	-0.900059	0.071323	0.079391
C	-1.229404	-1.632785	-0.941041
O	-1.417848	-2.619735	-1.515409
O	1.062722	-0.694510	0.437904
C	1.932098	-0.995847	-0.480052
C	3.299997	-1.404692	0.071555
C	3.912160	-0.380002	1.030362
N	4.153076	0.904023	0.346141
C	-2.930423	0.929535	0.998271
C	-2.748495	1.370360	-0.329570
C	-2.767319	0.382573	-1.340817
N	-0.061703	1.873132	1.033653
C	0.752368	2.605520	0.328375
C	0.903166	2.221533	-1.054827
N	0.171424	1.218010	-1.441055
O	1.719857	-0.987355	-1.700888

H	-0.120946	2.141026	2.014443
H	1.309898	3.443347	0.744099
H	1.626353	2.714215	-1.701228
H	0.384732	0.865387	-2.372554
H	3.966359	-1.589606	-0.777637
H	3.177059	-2.353524	0.608243
H	4.828477	-0.812053	1.465867
H	3.209497	-0.198124	1.849578
H	4.769853	0.767302	-0.452293
H	4.622547	1.555669	0.970156
H	-2.806112	1.627207	1.821323
H	-3.612444	0.105347	1.187093
H	-2.417505	2.382463	-0.543586
H	-2.512852	0.653024	-2.361213
H	-3.455584	-0.452206	-1.239260

TS-PP'

Mo	0.985256	0.014712	0.068947
N	0.358694	1.602009	-1.316670
C	0.491920	2.844412	-0.948550
C	1.122414	3.045659	0.331900
N	1.456768	1.957759	0.961313
C	0.193006	-1.612760	-0.820937
O	-0.294781	-2.530947	-1.330486
C	1.265017	-1.211666	1.639790
O	1.392232	-1.897054	2.564659
O	-0.991579	0.085213	0.872805
C	-1.793424	1.053571	1.226079
O	-1.481381	2.244481	1.346137
C	-3.219047	0.565544	1.498039
C	-4.171431	1.643006	2.016117
N	-4.399633	2.679077	0.999486
H	-0.138342	1.480909	-2.197670
H	0.121896	3.681627	-1.537498
H	1.247864	4.040670	0.752910
H	1.834389	2.120146	1.893245
H	-3.153173	-0.265929	2.210253
H	-3.607823	0.142651	0.563266
H	-3.774292	2.045104	2.963030
H	-5.135516	1.171881	2.242146
H	-3.535920	3.203420	0.879245
H	-5.117234	3.329794	1.307154
C	3.325910	-0.300162	0.403871
C	3.073132	0.223773	-0.884036
C	2.372139	-0.599830	-1.786742
H	2.048663	-0.202466	-2.744006
H	2.546207	-1.671837	-1.759906
H	3.245398	1.273527	-1.103645
H	3.768702	0.334949	1.165499
H	3.544400	-1.360292	0.500571

N-sulfonate azetidin-2-one

C	0.000000	0.000000	0.000000

C	0.000000	0.000000	1.552374
C	1.543449	0.000000	1.432918
O	2.450929	-0.054616	2.240858
N	1.470098	0.077234	0.059677
S	2.580996	-0.171772	-1.319680
O	1.744836	0.383852	-2.412706
O	2.762522	-1.641293	-1.369452
O	3.778638	0.608625	-0.958304
H	-0.455656	0.864092	-0.491713
H	-0.363584	-0.923700	-0.463093
H	-0.403085	-0.898744	2.028380
H	-0.413692	0.893382	2.029244

TS1B-s

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.368995
C	1.899967	0.000000	3.115638
O	2.988803	0.056591	3.494293
C	0.099073	1.319764	0.517582
C	1.269131	1.666813	1.215459
O	-1.035204	-1.417741	3.948862
C	-0.387235	-0.963621	5.202096
O	0.385001	0.057481	4.893672
N	-2.163165	0.078641	1.936636
C	-2.874138	1.071699	2.406192
C	-2.149215	1.970991	3.255850
N	-0.869808	1.710036	3.352475
C	0.503695	-1.836490	1.659022
O	0.747950	-2.860156	1.180698
C	-1.448465	-0.830452	6.342643
C	-1.007591	-2.222124	6.841934
N	0.195201	-2.142414	5.975159
S	0.702395	-3.601142	5.193100
O	1.962742	-3.260481	4.503375
O	0.776504	-4.599634	6.281988
O	-0.431587	-3.894108	4.212461
H	0.901729	-0.463997	-0.393224
H	-0.919349	-0.318628	-0.482667
H	-0.766735	1.977219	0.528526
H	2.216803	1.230363	0.911096
H	1.334997	2.620050	1.730514
H	-2.696839	-0.628140	1.435496
H	-3.947916	1.167657	2.246163
H	-2.652429	2.726848	3.857293
H	-0.374492	2.175046	4.110598
H	-1.701708	-3.021564	6.552625
H	-0.761194	-2.323266	7.903730
H	-2.483268	-0.733099	6.002221
H	-1.186547	-0.014283	7.021339
H	-0.912767	-2.426620	3.893588

M1B-s

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.152073
Mo	0.306372	0.000000	-2.035377
C	-1.645586	-0.584545	-2.295553
O	-2.684716	-1.018145	-2.542993
N	0.784632	0.511098	-4.074775
C	1.801074	1.324631	-4.278772
C	2.612221	1.580182	-3.138149
N	2.235671	0.966172	-2.032802

C	0.250931	-2.213700	-2.983695
C	1.518245	-1.991526	-2.407100
C	1.590787	-1.806945	-1.015857
O	-0.328467	1.919619	-1.964728
C	-1.502780	2.560125	-1.697354
O	-2.497501	2.124265	-2.588063
N	-1.930550	2.589804	-0.234840
S	-3.356800	1.761242	0.325521
O	-2.973488	0.330966	0.353181
C	-1.326427	4.109737	-1.625642
C	-2.006992	4.074725	-0.241397
O	-3.635161	2.394016	1.635032
O	-4.409914	2.067055	-0.717915
H	-1.464912	4.529426	0.594707
H	-3.035398	4.453672	-0.250814
H	-0.273191	4.400807	-1.612025
H	-1.863704	4.646750	-2.411559
H	2.810512	1.179948	-1.220553
H	3.486864	2.227107	-3.187822
H	2.018921	1.767547	-5.249568
H	0.189512	0.370371	-4.888124
H	-3.363610	2.105952	-2.103778
H	-0.476663	-2.796424	-2.425076
H	0.147146	-2.247230	-4.064259
H	2.367033	-1.736433	-3.036307
H	0.898397	-2.349610	-0.378211
H	2.526535	-1.507616	-0.553124

TS2B1-s

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.049703
O	2.021532	0.000000	1.793143
C	2.881155	-1.037272	1.676139
C	4.372362	-0.582062	1.804352
C	4.734945	-1.097161	0.402179
N	3.315330	-1.277931	-0.002361
S	2.939012	-2.736925	-0.706463
O	3.123685	-3.793623	0.494589
O	-0.008093	0.124873	-1.146852
C	0.061431	-2.079529	1.996842
O	-0.146913	-3.214858	2.025182
N	0.470217	0.275214	4.125449
C	0.923577	1.456449	4.505528
C	0.858461	2.471659	3.517460
N	0.351057	2.090560	2.355787
C	-2.035339	-0.869460	2.968333
C	-2.238821	0.480396	2.617615
C	-2.151003	0.829327	1.258790
O	2.529768	-2.166210	2.253418
O	1.519100	-2.692630	-1.089043
O	3.928104	-3.088066	-1.741699
H	5.257761	-0.386558	-0.248966
H	5.307258	-2.031674	0.424750
H	4.444486	0.504323	1.908170
H	4.881476	-1.075661	2.637793
H	0.361847	2.815129	1.641222
H	1.205298	3.486383	3.704939
H	1.324856	1.642607	5.500558
H	0.589953	-0.464870	4.813297
H	2.849728	-3.231411	1.364188
H	-2.392748	-1.639926	2.290287

H	-1.982655	-1.155129	4.014602
H	-2.214722	1.253585	3.381398
H	-2.494785	0.117479	0.512950
H	-2.165309	1.873131	0.960045

M2B1-s

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.167535
Mo	0.021313	0.000000	-1.981644
N	0.334847	0.339148	-4.184618
C	0.330607	1.548397	-4.632877
C	-0.029709	2.599033	-3.671329
N	-0.357345	2.199809	-2.485987
C	0.750215	-1.820961	-1.705396
O	1.186147	-2.886462	-1.524359
C	-1.529960	-1.575481	-2.774834
C	-2.133951	-0.305732	-2.578201
C	-2.235868	0.149419	-1.244922
O	1.991144	0.741369	-1.851088
C	2.894718	1.140873	-2.691508
C	3.577390	2.453786	-2.297279
C	3.830601	3.356907	-3.509236
N	2.567960	3.575109	-4.236535
S	2.711814	3.560518	-5.817932
O	3.097525	1.962533	-6.234921
O	3.219061	0.537141	-3.729393
O	3.827440	4.351514	-6.380282
O	1.375478	3.773935	-6.426761
H	3.247409	1.462636	-5.398388
H	-1.333918	-1.918346	-3.787340
H	-1.722627	-2.365823	-2.053479
H	-2.440103	-0.565816	-0.452770
H	-2.570202	1.164731	-1.049700
H	-2.350891	0.350398	-3.415504
H	-0.569967	2.958597	-1.841063
H	-0.007557	3.636074	-3.993033
H	0.598648	1.831605	-5.647591
H	0.673548	-0.342105	-4.861570
H	2.947848	2.959980	-1.559472
H	4.531540	2.215628	-1.805341
H	4.242979	4.316288	-3.157537
H	4.611323	2.899213	-4.131567

TS3B1-s

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	1.983227
O	2.112640	0.000000	1.904566
C	2.963363	0.480367	2.762681
O	2.713018	1.363783	3.598262
O	0.010544	0.009613	-1.167042
N	0.451303	-0.180635	4.173042
C	0.959158	-1.291400	4.590169
C	0.982185	-2.401027	3.633131
N	0.481076	-2.158835	2.467896
C	0.030012	1.971694	1.721657
O	0.041580	3.121482	1.542590
C	-2.020819	0.896139	2.761187
C	-2.125456	-0.506757	2.565861
C	-2.040579	-0.966230	1.232712
C	4.349198	-0.162977	2.709559
C	4.731645	-0.798542	4.063466

N	3.858400	-1.892540	4.499778
S	4.326865	-3.482945	4.162143
O	3.390173	-4.229607	3.282415
O	4.014872	-3.810885	5.703536
O	5.758530	-3.620978	3.816863
H	3.871648	-2.610868	5.682902
H	-1.970184	1.289352	3.773234
H	-2.480500	1.561503	2.034478
H	-2.480578	-0.370140	0.437806
H	-1.978763	-2.032624	1.034141
H	-2.095954	-1.197375	3.403097
H	0.586982	-2.938554	1.820361
H	1.452381	-3.347669	3.889961
H	1.396094	-1.421447	5.576390
H	0.560083	0.601345	4.815621
H	4.383976	-0.908687	1.910777
H	5.081386	0.623762	2.481168
H	5.782004	-1.121996	4.017418
H	4.656377	-0.018571	4.830365

M2B2-s

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.155509
Mo	0.213543	0.000000	-2.030408
C	2.367125	-0.114443	-1.011249
C	2.521053	0.350582	-2.337092
C	1.966111	1.597574	-2.661255
O	-1.713302	-0.647705	-2.195847
C	-2.659480	-1.194717	-1.396751
O	-2.051559	-1.832894	-0.269926
C	-3.666565	-2.088624	-2.196975
C	-4.738950	-1.008491	-1.925015
N	-3.835417	-0.387605	-0.936419
S	-3.840008	1.343110	-0.727943
O	-5.120136	1.583969	-0.014243
O	-2.607936	1.556205	0.081461
O	-3.794175	1.943584	-2.090807
C	-0.533680	1.931245	-1.965743
O	-0.826724	3.042298	-2.015883
N	0.143933	-0.308370	-4.167141
C	0.123235	-1.557561	-4.589825
C	0.422989	-2.539900	-3.604475
N	0.662673	-2.073544	-2.394900
H	-2.583972	-1.545026	0.486619
H	-3.381456	-2.234395	-3.241403
H	-3.853362	-3.047994	-1.706557
H	-4.926860	-0.359964	-2.790295
H	-5.692067	-1.338082	-1.496360
H	0.830841	-2.788801	-1.691265
H	0.463420	-3.600954	-3.847184
H	-0.089262	-1.829168	-5.622997
H	-0.108597	0.377658	-4.874874
H	1.950262	2.378958	-1.906815
H	1.930531	1.931497	-3.693688
H	2.695280	-1.115946	-0.748837
H	2.410039	0.615084	-0.206356
H	2.844034	-0.327813	-3.121929

TS2B2-s

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.037586

N	2.144249	0.000000	2.428114
C	2.540565	-0.459948	3.603976
C	1.507603	-0.739059	4.539467
N	0.276290	-0.484860	4.130225
O	0.086087	0.045957	-1.150436
C	0.483301	2.200635	1.269916
C	0.090005	2.218470	2.624491
C	-1.231721	1.815144	2.915575
C	-1.997665	-0.400001	1.888615
O	-3.138555	-0.551997	1.898687
O	0.393763	-2.107753	1.805055
C	-0.194248	-3.153737	2.158841
O	-1.120063	-3.104369	3.147534
C	0.369930	-4.506783	1.732349
C	-0.513771	-4.827557	0.513946
N	-1.753919	-4.179391	0.914746
S	-2.694095	-3.564038	-0.345510
O	-2.630679	-4.551265	-1.469708
O	-4.045648	-3.379948	0.248361
O	-2.023676	-2.257089	-0.699005
H	-0.452724	-0.774523	4.777458
H	1.726169	-1.147217	5.525164
H	3.589450	-0.620643	3.849848
H	2.898866	0.155859	1.764280
H	0.827823	2.316248	3.415532
H	-0.244346	2.472434	0.510115
H	1.522548	2.374996	1.006683
H	-2.024389	2.085195	2.223137
H	-1.539378	1.684956	3.948812
H	-1.820026	-3.689556	2.737946
H	1.440714	-4.424858	1.514630
H	0.217811	-5.225070	2.544819
H	-0.074569	-4.368764	-0.384162
H	-0.614480	-5.907518	0.312136

P-s

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	2.002817
O	2.106386	0.000000	2.052339
C	2.960300	-0.216162	1.082971
C	4.241513	0.613539	1.214900
C	4.261358	1.724941	0.146417
N	3.048321	2.558514	0.195789
S	3.110373	4.050900	1.070029
O	3.662528	3.667388	2.398762
O	-0.051131	0.012666	-1.159674
C	0.045573	-1.976772	1.744877
O	0.068346	-3.132514	1.604806
N	0.497925	2.143987	2.406274
C	1.061829	2.389622	3.539759
C	1.011734	1.324665	4.535029
N	0.441662	0.217295	4.178179
C	-2.039582	0.942099	1.243245
C	-2.143214	0.506743	2.582998
C	-2.030978	-0.889411	2.808807
O	2.782379	-0.960550	0.116646
O	3.949177	5.009637	0.306299
O	1.655189	4.426240	1.108041
H	5.174318	2.326281	0.258223
H	4.289666	1.255359	-0.842554
H	4.299236	1.063513	2.207627

H	5.109766	-0.037985	1.053597
H	0.664017	2.919985	1.740203
H	1.599730	3.317067	3.729843
H	1.445743	1.473614	5.524895
H	0.444618	-0.506808	4.894368
H	2.707403	2.783421	-0.734825
H	-2.474333	-1.573009	2.088982
H	-1.990831	-1.262949	3.829382
H	-2.119513	1.214878	3.406083
H	-2.467165	0.325121	0.457584
H	-1.975884	2.003769	1.023769

TS1'B-s

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	1.991808
C	1.961089	0.000000	1.729160
O	3.119071	-0.005494	1.580677
O	0.008793	0.013496	-1.162841
C	0.919694	1.966469	2.847077
C	-0.468048	2.115506	2.564119
C	-0.851812	2.077898	1.207139
O	0.560344	-2.244585	2.218051
C	-0.488350	-3.014083	1.459521
O	-1.294441	-2.171659	0.910423
N	-2.167699	-0.368590	2.453151
C	-2.522038	-0.711863	3.642936
C	-1.455796	-0.698146	4.644302
N	-0.278348	-0.384985	4.217938
C	0.208326	-4.140853	0.631528
C	-0.087936	-5.133912	1.771637
N	-1.032840	-4.161708	2.382497
S	-1.086870	-4.111208	4.092139
O	-1.222245	-5.516986	4.527019
O	-2.245256	-3.228596	4.438342
O	0.222414	-3.472777	4.531537
H	0.614520	-2.607394	3.147277
H	1.242331	1.898248	3.882801
H	1.639712	2.435671	2.180559
H	-0.193753	2.505394	0.455250
H	-1.906247	2.059308	0.946166
H	-1.208056	2.104167	3.359028
H	-2.854685	-0.554974	1.726217
H	-3.503139	-1.102830	3.897582
H	-1.658916	-1.013657	5.664172
H	0.450846	-0.496079	4.919890
H	-0.355256	-4.336342	-0.283918
H	1.260772	-3.956724	0.402536
H	-0.570892	-6.078468	1.501909
H	0.789197	-5.345216	2.396434

M1'B-s

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	1.982580
C	1.968365	0.000000	1.725700
O	3.119593	0.004421	1.548541
O	0.004060	-0.005544	-1.168056
C	0.888152	2.036961	2.736919
C	-0.518108	2.128128	2.545023
C	-0.973778	2.038868	1.209792
O	0.084316	-2.084644	1.859510
C	0.548995	-3.093014	2.600485

O	1.383994	-2.650658	3.669721
N	-2.179477	-0.418022	2.469246
C	-2.465694	-0.788000	3.670115
C	-1.361607	-0.773982	4.636356
N	-0.220170	-0.385168	4.182834
C	1.219685	-4.272310	1.827321
C	0.398493	-5.254578	2.686044
N	-0.497243	-4.137426	3.076888
S	-1.226961	-4.173320	4.625481
O	-1.601405	-5.586636	4.843515
O	-2.389778	-3.229445	4.541759
O	-0.188887	-3.653281	5.599026
H	1.018008	-3.019380	4.508622
H	1.284142	1.999750	3.748830
H	1.545919	2.506667	2.008846
H	-0.378937	2.483304	0.415916
H	-2.040091	1.977342	1.007794
H	-1.207976	2.116362	3.383736
H	-2.955476	-0.497061	1.814850
H	-3.450275	-1.124957	3.982684
H	-1.516783	-1.143685	5.645571
H	0.550250	-0.492592	4.839506
H	0.922943	-4.264117	0.776035
H	2.306917	-4.314158	1.926575
H	-0.128423	-6.063507	2.170729
H	0.970624	-5.674991	3.523286

TS2'B1-s

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.166710
Mo	0.019456	0.000000	-1.985500
N	0.220212	0.374275	-4.191744
C	-0.192796	1.491271	-4.685589
C	-0.787611	2.431334	-3.725338
N	-0.853891	2.028762	-2.501099
C	1.134060	-1.619370	-1.717890
O	1.794129	-2.563346	-1.544281
C	-1.146165	-1.883143	-2.773093
C	-2.013831	-0.779045	-2.567646
C	-2.199239	-0.366315	-1.227583
O	1.810932	1.128908	-1.769325
C	2.777516	1.452314	-2.548069
C	3.988206	2.147114	-1.907324
C	4.097170	3.334833	-2.865199
N	2.677650	3.375637	-3.282190
S	2.456178	3.592966	-4.899978
O	2.885042	2.264132	-5.575403
O	2.990009	0.704181	-3.642560
O	3.250580	4.729651	-5.428342
O	0.965345	3.766376	-5.078208
H	3.042157	1.309485	-4.506343
H	-0.883494	-2.171822	-3.787430
H	-1.153506	-2.698135	-2.053297
H	-2.236168	-1.117099	-0.442501
H	-2.751968	0.545981	-1.019251
H	-2.385875	-0.188179	-3.398959
H	-1.205336	2.732207	-1.854470
H	-1.107347	3.412941	-4.060244
H	-0.063740	1.782692	-5.722112
H	0.732469	-0.207094	-4.851877
H	3.708764	2.456994	-0.896690

H	4.860429	1.482443	-1.856404
H	4.427736	4.270296	-2.391856
H	4.793733	3.115724	-3.686378

M2'B1-s

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.167535
Mo	0.021313	0.000000	-1.981644
N	0.334847	0.339148	-4.184618
C	0.330607	1.548397	-4.632877
C	-0.029709	2.599033	-3.671329
N	-0.357345	2.199809	-2.485987
C	0.750215	-1.820961	-1.705396
O	1.186147	-2.886462	-1.524359
C	-1.529960	-1.575481	-2.774834
C	-2.133951	-0.305732	-2.578201
C	-2.235868	0.149419	-1.244922
O	1.991144	0.741369	-1.851088
C	2.894718	1.140873	-2.691508
C	3.577390	2.453786	-2.297279
C	3.830601	3.356907	-3.509236
N	2.567960	3.575109	-4.236535
S	2.711814	3.560518	-5.817932
O	3.097525	1.962533	-6.234921
O	3.219061	0.537141	-3.729393
O	3.827440	4.351514	-6.380282
O	1.375478	3.773935	-6.426761
H	3.247409	1.462636	-5.398388
H	-1.333918	-1.918346	-3.787340
H	-1.722627	-2.365823	-2.053479
H	-2.440103	-0.565816	-0.452770
H	-2.570202	1.164731	-1.049700
H	-2.350891	0.350398	-3.415504
H	-0.569967	2.958597	-1.841063
H	-0.007557	3.636074	-3.993033
H	0.598648	1.831605	-5.647591
H	0.673548	-0.342105	-4.861570
H	2.947848	2.959980	-1.559472
H	4.531540	2.215628	-1.805341
H	4.242979	4.316288	-3.157537
H	4.611323	2.899213	-4.131567

TS3'B1-s

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	1.983227
O	2.112640	0.000000	1.904566
C	2.963363	0.480367	2.762681
O	2.713018	1.363783	3.598262
O	0.010544	0.009613	-1.167042
N	0.451303	-0.180635	4.173042
C	0.959158	-1.291400	4.590169
C	0.982185	-2.401027	3.633131
N	0.481076	-2.158835	2.467896
C	0.030012	1.971694	1.721657
O	0.041580	3.121482	1.542590
C	-2.020819	0.896139	2.761187
C	-2.125456	-0.506757	2.565861
C	-2.040579	-0.966230	1.232712
C	4.349198	-0.162977	2.709559
C	4.731645	-0.798542	4.063466
N	3.858400	-1.892540	4.499778

S	4.326865	-3.482945	4.162143
O	3.390173	-4.229607	3.282415
O	4.014872	-3.810885	5.703536
O	5.758530	-3.620978	3.816863
H	3.871648	-2.610868	5.682902
H	-1.970184	1.289352	3.773234
H	-2.480500	1.561503	2.034478
H	-2.480578	-0.370140	0.437806
H	-1.978763	-2.032624	1.034141
H	-2.095954	-1.197375	3.403097
H	0.586982	-2.938554	1.820361
H	1.452381	-3.347669	3.889961
H	1.396094	-1.421447	5.576390
H	0.560083	0.601345	4.815621
H	4.383976	-0.908687	1.910777
H	5.081386	0.623762	2.481168
H	5.782004	-1.121996	4.017418
H	4.656377	-0.018571	4.830365

TS2'B2-s

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	1.975967
C	1.955668	0.000000	1.676913
O	3.100425	0.052452	1.464315
O	0.016263	-0.005552	-1.169393
C	0.878181	2.026798	2.786876
C	-0.512940	2.136268	2.537657
C	-0.921677	2.052493	1.183554
O	-0.122507	-2.039045	2.013885
C	0.651753	-3.144063	2.131915
O	1.945054	-2.856785	2.651483
N	-2.189960	-0.432207	2.522242
C	-2.375316	-1.000250	3.663818
C	-1.256858	-0.974068	4.617217
N	-0.169325	-0.416189	4.215923
C	0.699998	-4.123642	0.909255
C	-0.035089	-5.188046	1.780639
N	-0.009408	-4.231570	2.878473
S	-0.518297	-4.264976	4.475061
O	-0.562997	-5.699809	4.836190
O	-1.864765	-3.595912	4.572667
O	0.535290	-3.435628	5.158249
H	1.847258	-2.948376	3.618726
H	1.233247	1.974025	3.812895
H	1.575302	2.477596	2.084631
H	-0.298986	2.504348	0.415442
H	-1.981953	2.006593	0.946959
H	-1.235162	2.114542	3.348175
H	-2.986121	-0.505769	1.891414
H	-3.298830	-1.498398	3.952517
H	-1.373697	-1.441006	5.590135
H	0.588561	-0.489445	4.892993
H	0.127084	-3.756849	0.055193
H	1.714797	-4.396824	0.612452
H	-1.043158	-5.455172	1.431805
H	0.529096	-6.108730	1.978069

M2'B2-s

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.169914
Mo	0.029635	0.000000	-1.969864

C	0.868750	-2.065700	-2.781913
C	-0.527603	-2.121469	-2.558647
C	-0.972616	-2.023184	-1.216653
N	-0.087411	0.434420	-4.241013
C	-1.146377	1.042684	-4.638951
C	-2.296164	1.059843	-3.717935
N	-2.159528	0.463982	-2.585863
C	1.972756	-0.074668	-1.628831
O	3.115585	-0.170990	-1.411593
O	-0.060963	2.023678	-2.070584
C	0.612885	3.142715	-1.708834
O	2.013046	2.980200	-1.714595
C	0.073727	3.867402	-0.440844
C	-0.671604	4.832960	-1.400208
N	0.183416	4.348708	-2.499471
S	-0.331784	4.279198	-4.129386
O	0.767618	3.508060	-4.781252
O	-0.467097	5.698259	-4.529669
O	-1.661678	3.558041	-4.208503
H	-2.978411	0.530843	-1.984321
H	-3.206744	1.567259	-4.030745
H	-1.230072	1.549192	-5.596102
H	0.690343	0.523763	-4.892716
H	0.868927	4.348432	0.133012
H	-0.547124	3.240629	0.202291
H	-0.574119	5.907481	-1.211900
H	-1.731965	4.574891	-1.528279
H	2.260013	2.918391	-2.651400
H	-2.037841	-1.944480	-1.013562
H	-0.389565	-2.493750	-0.429156
H	-1.228412	-2.060768	-3.385946
H	1.244346	-2.019020	-3.800680
H	1.539733	-2.532050	-2.065277

TS3'B2-s

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	1.981130
N	0.459859	0.000000	4.185975
C	1.247809	-0.912192	4.651900
C	1.748297	-1.894100	3.682211
N	1.320383	-1.786172	2.468121
O	0.009776	0.013679	-1.168214
C	-0.866738	1.762531	1.703339
O	-1.394918	2.781610	1.504276
O	1.951982	0.913543	1.856168
C	2.512839	1.902797	2.395021
O	1.724044	2.845096	2.983774
C	-1.423769	-1.708224	1.185001
C	-1.680743	-1.376772	2.537823
C	-2.202580	-0.080878	2.778411
C	3.921763	2.291415	1.925270
C	4.750745	1.661797	3.054382
N	3.746129	1.743722	4.113419
S	3.881213	0.643838	5.337100
O	5.241040	0.718708	5.942306
O	3.682173	-0.765873	4.727205
O	2.748522	0.955341	6.266955
H	1.736457	-2.451493	1.820058
H	2.448575	-2.656693	4.011560
H	1.550533	-0.955822	5.691428
H	0.240030	0.714955	4.877864

H	4.008687	3.382858	1.908391
H	4.118347	1.897253	0.922571
H	5.687994	2.196188	3.275860
H	5.007111	0.623963	2.790172
H	2.266430	3.101588	3.761795
H	-0.909906	-2.636747	0.950807
H	-2.100068	-1.348613	0.414081
H	-1.346824	-2.013507	3.351079
H	-2.300822	0.271528	3.801359
H	-2.917788	0.339219	2.075710

P'-s

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.167124
Mo	0.028876	0.000000	-1.983919
C	-1.740878	-1.297697	-2.813237
C	-2.141503	0.046666	-2.601909
C	-2.175009	0.487783	-1.257915
N	0.482251	0.289542	-4.158801
C	0.642188	1.489268	-4.608357
C	0.319140	2.567823	-3.667059
N	-0.021472	2.202141	-2.475191
C	0.447756	-1.929033	-1.718741
O	0.677574	-3.053506	-1.529956
O	2.130408	0.401489	-1.833667
C	3.050767	-0.107276	-2.593268
C	4.445437	0.495410	-2.404092
C	4.581531	1.833433	-3.156592
N	4.386878	1.647565	-4.601330
S	3.668556	2.956295	-5.471342
O	3.039152	2.252909	-6.628994
O	2.862283	-0.975371	-3.463690
O	4.764392	3.895145	-5.789500
O	2.636304	3.566462	-4.552409
H	-0.194803	2.979229	-1.840210
H	0.408751	3.601984	-3.984940
H	1.067142	1.723644	-5.585146
H	0.830285	-0.442828	-4.775894
H	5.182925	-0.222639	-2.776040
H	4.625267	0.678426	-1.339560
H	5.584152	2.243299	-2.980268
H	3.851354	2.545817	-2.752449
H	3.837323	0.817284	-4.811350
H	-2.355094	1.537593	-1.041792
H	-2.495390	-0.203356	-0.482848
H	-2.251596	0.740336	-3.429865
H	-1.582898	-1.653355	-3.827720
H	-2.060105	-2.057582	-2.104184

3-formylamine-N-sulfonate azetidin-2-one

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.557377
N	1.262907	0.000000	2.264219
C	1.846910	-1.105484	2.785693
O	1.433888	-2.254682	2.673940
N	-0.726138	1.284853	0.066753
S	-0.991370	2.412904	-1.310402
O	-1.146455	1.428050	-2.405717
C	-0.620219	1.419076	1.424415
O	-0.845857	2.296982	2.236568
O	0.263803	3.196485	-1.350732

O	-2.202001	3.156045	-0.921540
H	-0.562034	-0.797902	-0.490753
H	0.997629	0.091848	-0.441130
H	1.672949	0.899768	2.481981
H	2.772809	-0.865306	3.344630
H	-0.664392	-0.748873	1.994506

TS1'B-sf

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.411271
C	1.267518	0.000000	2.057449
Mo	0.872012	-2.004504	0.924262
O	1.649561	-4.199628	1.263879
C	0.964030	-5.016435	0.250219
O	0.269007	-4.236899	-0.524037
N	0.067553	-2.557507	2.984393
C	-1.130403	-3.026942	3.074059
C	-1.885115	-3.106806	1.820455
N	-1.280568	-2.650246	0.780119
C	1.398244	-1.871744	-0.990567
O	1.703891	-1.786977	-2.109318
C	2.817535	-1.758602	1.200458
O	3.962640	-1.620019	1.371415
C	1.977193	-6.028724	-0.413555
C	1.370377	-7.155073	0.449377
N	0.281876	-6.246303	0.901862
S	-0.196696	-6.334814	2.543195
O	-0.280303	-7.774665	2.851568
N	1.720216	-6.068707	-1.835840
C	2.451667	-6.741579	-2.744115
O	3.397868	-7.493150	-2.505336
O	0.885760	-5.607599	3.326146
O	-1.493975	-5.593229	2.629213
H	0.771640	0.549324	-0.532428
H	-0.935704	-0.124992	-0.537656
H	-0.917411	-0.147477	1.973349
H	2.072551	0.587790	1.622912
H	1.309659	-0.094661	3.139318
H	-1.730806	-2.861525	-0.107571
H	-2.844199	-3.616801	1.793974
H	-1.557028	-3.413192	3.995717
H	0.593688	-2.613773	3.854554
H	2.042234	-7.484642	1.249661
H	0.996666	-8.025463	-0.096189
H	3.030852	-5.821324	-0.214981
H	1.512694	-4.623538	2.162644
H	1.003264	-5.405750	-2.129867
H	2.106011	-6.554703	-3.781272

M1'B-sf

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.165536
Mo	0.034226	0.000000	-1.994675
C	-0.820820	-1.793539	-1.744408
O	-1.391208	-2.788421	-1.563893
O	1.953200	-0.858741	-1.856512
C	2.523540	-2.008978	-2.282205
O	1.676976	-3.125017	-2.255432
C	-2.139078	0.052964	-2.894737
C	-1.685383	1.363421	-2.609805
C	-1.485717	1.676043	-1.243155

N	0.622655	-0.057707	-4.131217
C	1.560769	0.745811	-4.509515
C	1.895532	1.815998	-3.579362
N	1.283080	1.803308	-2.437331
N	3.319671	-1.869693	-3.588505
S	2.799947	-2.467575	-5.126955
O	3.044366	-1.369089	-6.102251
C	3.884967	-2.339596	-1.571362
N	4.276763	-1.252182	-0.700772
C	5.330651	-1.260731	0.137383
O	6.171999	-2.153182	0.242854
C	4.552852	-2.404138	-2.963929
O	1.313092	-2.675030	-4.893577
O	3.548444	-3.713419	-5.402765
H	1.553611	2.557025	-1.807717
H	2.637064	2.570172	-3.846448
H	2.125703	0.582693	-5.426556
H	0.531171	-0.889333	-4.733689
H	3.873968	-3.285722	-1.027558
H	4.791450	-3.424249	-3.281358
H	5.427082	-1.757945	-3.096766
H	1.301295	-3.213625	-3.160596
H	-1.027546	2.623275	-0.969524
H	-2.173543	1.268121	-0.506962
H	-1.340749	2.024466	-3.399163
H	-2.185752	-0.287381	-3.925068
H	-2.858036	-0.406920	-2.221279
H	3.593658	-0.498487	-0.669871
H	5.380213	-0.340400	0.755479

TS2'B1-sf

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.167193
Mo	0.033207	0.000000	-1.982695
C	-1.995407	0.981444	-1.241562
C	-2.074300	0.533890	-2.580777
C	-2.000285	-0.869268	-2.779967
O	2.154772	-0.128811	-1.757041
C	3.116999	-0.472103	-2.550657
C	4.499675	-0.732527	-1.880298
C	5.310119	0.239726	-2.749266
N	4.185820	1.109041	-3.167720
S	4.152277	1.482409	-4.765890
O	5.477115	1.878346	-5.289893
N	0.436929	0.208608	-4.177725
C	0.758752	1.362807	-4.653710
C	0.800325	2.463545	-3.682815
N	0.495892	2.161380	-2.465455
C	0.016063	-1.973218	-1.731930
O	0.015535	-3.124520	-1.566759
O	2.856746	-1.162026	-3.648305
N	4.433102	-0.375308	-0.470846
C	5.332201	-0.751687	0.459454
O	6.361359	-1.396545	0.258283
O	3.084809	2.529302	-4.926882
O	3.661301	0.177058	-5.487655
H	3.254466	-0.616366	-4.564506
H	-1.946485	-1.262432	-3.791646
H	-2.477932	-1.526499	-2.057550
H	-2.463137	0.390590	-0.458282
H	-1.922974	2.045846	-1.034923

H	-2.035633	1.228643	-3.414285
H	0.598413	2.934328	-1.810750
H	1.108751	3.454183	-4.002167
H	1.058633	1.533103	-5.682192
H	0.532190	-0.557388	-4.841579
H	4.800095	-1.781310	-1.968583
H	6.083252	0.781030	-2.192170
H	5.796390	-0.295915	-3.574409
H	3.579224	0.091076	-0.185618
H	5.048867	-0.410432	1.475829

M2'B1-sf

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	1.984366
O	2.127926	0.000000	1.872291
C	3.109464	0.236961	2.681169
O	3.068003	0.937665	3.703170
O	0.015838	0.002450	-1.166943
N	0.421394	-0.192011	4.170510
C	0.903542	-1.306415	4.603877
C	0.977992	-2.407704	3.634896
N	0.480232	-2.176212	2.464313
C	0.027890	1.965798	1.722578
O	0.052346	3.116638	1.549193
C	-2.018736	0.899657	2.770406
C	-2.120473	-0.500000	2.559416
C	-2.038110	-0.940870	1.218860
C	4.436054	-0.450230	2.298385
N	4.270866	-1.207933	1.060803
C	5.264550	-1.444738	0.179026
O	6.450516	-1.152628	0.324364
C	4.939373	-1.316190	3.478566
N	3.843686	-2.094143	4.080294
S	3.908771	-2.175089	5.661094
O	2.799017	-3.025716	6.157408
O	3.482334	-0.617994	6.226906
O	5.241451	-2.407722	6.253541
H	3.466452	-0.019915	5.449255
H	-1.965163	1.282312	3.786126
H	-2.476233	1.573357	2.050443
H	-2.480665	-0.333318	0.434422
H	-1.982100	-2.004977	1.006704
H	-2.094886	-1.200857	3.387958
H	0.570984	-2.959030	1.819090
H	1.434238	-3.344436	3.943797
H	1.275453	-1.462514	5.612218
H	0.467916	0.563595	4.851784
H	5.185545	0.327992	2.112450
H	5.727163	-1.975932	3.092269
H	5.426432	-0.636866	4.190165
H	3.312817	-1.361608	0.772577
H	4.899243	-1.957329	-0.733900

TS3'B1-sf

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.165529
Mo	0.023560	0.000000	-1.987200
C	-2.211854	-0.361101	-1.262138
C	-2.010683	-0.777530	-2.596936
C	-1.130589	-1.874621	-2.791587
O	1.788394	1.176235	-1.874137

C	2.782536	1.257579	-2.697794
C	3.651349	2.520863	-2.547179
N	3.345827	3.258122	-1.331491
C	4.280463	3.728931	-0.477946
O	5.498701	3.579763	-0.579086
N	0.331734	0.410338	-4.164342
C	0.112049	1.610538	-4.583336
C	-0.519122	2.530817	-3.636464
N	-0.789577	2.051709	-2.469182
C	1.151204	-1.617204	-1.715964
O	1.805611	-2.561543	-1.534822
O	3.054166	0.451362	-3.599470
C	3.489782	3.421103	-3.804884
N	2.117269	3.847400	-4.055101
S	1.523599	5.249112	-3.340258
O	2.542003	6.295118	-3.121104
O	0.609666	5.008102	-2.190107
O	0.686429	5.461744	-4.695557
H	1.411048	4.531782	-5.004015
H	-0.856666	-2.164359	-3.802692
H	-1.140907	-2.687405	-2.069682
H	-2.245387	-1.109987	-0.475567
H	-2.765150	0.551738	-1.060371
H	-2.368507	-0.184797	-3.433591
H	-1.133434	2.763908	-1.825769
H	-0.700320	3.566150	-3.914570
H	0.420356	1.967626	-5.563685
H	0.891485	-0.162850	-4.792465
H	4.698001	2.210748	-2.481781
H	4.173562	4.276144	-3.701345
H	3.806562	2.831351	-4.671667
H	2.369728	3.441431	-1.129758
H	3.830163	4.283438	0.366782

TS2'B2-sf

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.170154
Mo	0.040868	0.000000	-1.973620
C	-1.902527	-1.035429	-2.775548
C	-2.104974	0.354739	-2.570007
C	-2.068032	0.794860	-1.224151
O	2.141448	0.196646	-1.856524
C	3.217442	-0.459742	-2.349495
O	2.869177	-1.665537	-3.005757
C	4.383083	-0.580477	-1.282612
N	3.932951	-0.267451	0.049119
C	4.576976	-0.576800	1.192949
O	5.685221	-1.105075	1.284104
C	5.158164	0.512362	-2.080041
N	4.181711	0.336030	-3.149303
S	4.050907	1.006862	-4.680177
O	3.294087	-0.065458	-5.413756
O	3.240024	2.277160	-4.603107
O	5.441574	1.248090	-5.115261
N	0.325926	2.205359	-2.463855
C	0.752980	2.492057	-3.645290
C	0.801960	1.392064	-4.615699
N	0.453210	0.231048	-4.181478
C	0.185951	-1.965201	-1.708348
O	0.234402	-3.111201	-1.517846
H	5.130078	1.496748	-1.590696

H	6.186061	0.268138	-2.365952
H	4.881615	-1.549714	-1.305022
H	3.000837	0.139135	0.075085
H	3.990857	-0.295629	2.090396
H	3.067745	-1.513890	-3.949111
H	0.355102	2.987190	-1.811954
H	1.090876	3.481631	-3.944517
H	1.156637	1.573989	-5.624402
H	0.598239	-0.508994	-4.866691
H	-2.090241	1.859919	-1.007612
H	-2.488694	0.159447	-0.449088
H	-2.133236	1.055707	-3.398620
H	-1.810973	-1.416413	-3.789401
H	-2.324063	-1.737441	-2.060121

M2'B2-sf

C	0.000000	0.000000	0.000000
Mo	0.000000	0.000000	1.974770
O	2.085118	0.000000	2.015406
C	3.106428	0.889635	2.002775
N	4.208811	0.618138	2.981192
C	5.046255	-0.057310	1.977283
C	4.165387	0.593458	0.874463
N	3.645237	-0.249675	-0.171486
C	4.140321	-0.348476	-1.423382
O	5.162563	0.190498	-1.845412
O	0.001042	0.009334	-1.169730
C	-2.101284	0.728233	2.764900
C	-2.093148	-0.665589	2.518721
C	-1.960422	-1.069005	1.165872
N	0.387118	-0.121748	4.212951
C	0.952824	-1.188301	4.654587
C	1.073641	-2.309676	3.712737
N	0.565067	-2.155202	2.539850
C	-0.158478	1.954914	1.681828
O	-0.322366	3.091476	1.488721
O	2.689501	2.234880	2.067583
S	3.994227	0.068839	4.579064
O	3.474290	-1.350492	4.552689
O	2.978601	1.033673	5.103578
O	5.342127	0.147128	5.179187
H	0.705548	-2.952459	1.921819
H	1.591378	-3.212954	4.032184
H	1.348242	-1.287818	5.660004
H	0.432204	0.650214	4.876411
H	4.605699	1.495961	0.451617
H	6.100852	0.230661	2.012485
H	4.950878	-1.151823	1.984075
H	2.708312	2.468926	3.009497
H	-1.827352	-2.122914	0.934343
H	-2.454791	-0.488856	0.391020
H	-2.024109	-1.381869	3.331700
H	-2.083906	1.089490	3.789678
H	-2.592473	1.387116	2.053509
H	2.771104	-0.708405	0.066222
H	3.514246	-0.995815	-2.068835

TS3'B2-sf

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.168124
Mo	0.039263	0.000000	-1.979646

C	-1.984092	-0.824776	-2.816463
C	-2.038364	0.573545	-2.587018
C	-1.967868	0.991218	-1.235886
N	0.514641	0.199076	-4.172107
C	0.888925	1.352247	-4.620821
C	0.918001	2.447660	-3.644754
N	0.548622	2.162564	-2.438031
C	-0.038554	-1.965961	-1.710477
O	-0.094994	-3.112810	-1.520127
O	2.212308	-0.101711	-1.811881
C	3.098386	-0.749616	-2.414864
C	4.566825	-0.589498	-1.949942
C	5.096221	0.397483	-3.003611
N	4.266064	0.008037	-4.134568
S	3.974545	1.181544	-5.251194
O	3.118502	0.524807	-6.289333
O	2.761471	-1.813702	-3.169004
N	4.638878	-0.146156	-0.568429
C	5.372994	-0.739728	0.404085
O	6.138734	-1.687643	0.261158
O	5.252606	1.761939	-5.748465
O	3.166890	2.301901	-4.542080
H	0.621334	2.942250	-1.788136
H	1.226248	3.438708	-3.963729
H	1.198947	1.514477	-5.647699
H	0.611826	-0.543586	-4.862550
H	5.070182	-1.556256	-2.010556
H	6.180840	0.307689	-3.168992
H	4.890544	1.422028	-2.651312
H	3.390342	-1.698728	-3.929977
H	-1.878133	2.050194	-1.009056
H	-2.459393	0.396299	-0.470691
H	-1.970253	1.284010	-3.404873
H	-1.909184	-1.193982	-3.835486
H	-2.482997	-1.494114	-2.120494
H	3.992994	0.584673	-0.297917
H	5.218544	-0.257542	1.389792

P'-sf

C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.167405
Mo	0.041138	0.000000	-1.982243
C	-2.030486	-0.699870	-2.830397
C	-2.007848	0.700189	-2.603891
C	-1.916186	1.113530	-1.253645
N	0.563843	0.163615	-4.157374
C	1.058263	1.270390	-4.599181
C	1.073490	2.385782	-3.644071
N	0.655315	2.122917	-2.450114
C	-0.142857	-1.965435	-1.731455
O	-0.253681	-3.109689	-1.555631
O	2.175538	-0.276863	-1.816796
C	2.924999	-0.981651	-2.603852
C	4.435912	-0.867325	-2.325461
C	5.053175	0.306035	-3.132621
N	4.773672	0.206515	-4.569124
S	4.380823	1.678252	-5.381228
O	3.575214	1.196673	-6.541047
O	2.542944	-1.673728	-3.557500
N	4.660864	-0.659215	-0.898823
C	5.662589	-1.216190	-0.180488

O	6.567893	-1.920215	-0.619244
O	5.663657	2.337526	-5.694560
O	3.546228	2.491883	-4.414293
H	0.718229	2.911538	-1.809009
H	1.445372	3.356751	-3.956117
H	1.519953	1.380671	-5.580321
H	0.680744	-0.628790	-4.787024
H	4.910179	-1.807114	-2.615799
H	6.135140	0.293927	-2.957637
H	4.649504	1.241862	-2.726461
H	4.033395	-0.459010	-4.782705
H	-1.773980	2.166128	-1.023519
H	-2.438532	0.542498	-0.490546
H	-1.901934	1.405128	-3.422759
H	-1.977448	-1.075983	-3.848354
H	-2.570521	-1.335824	-2.133363
H	3.927216	-0.154258	-0.415698
H	5.588398	-0.963643	0.896342

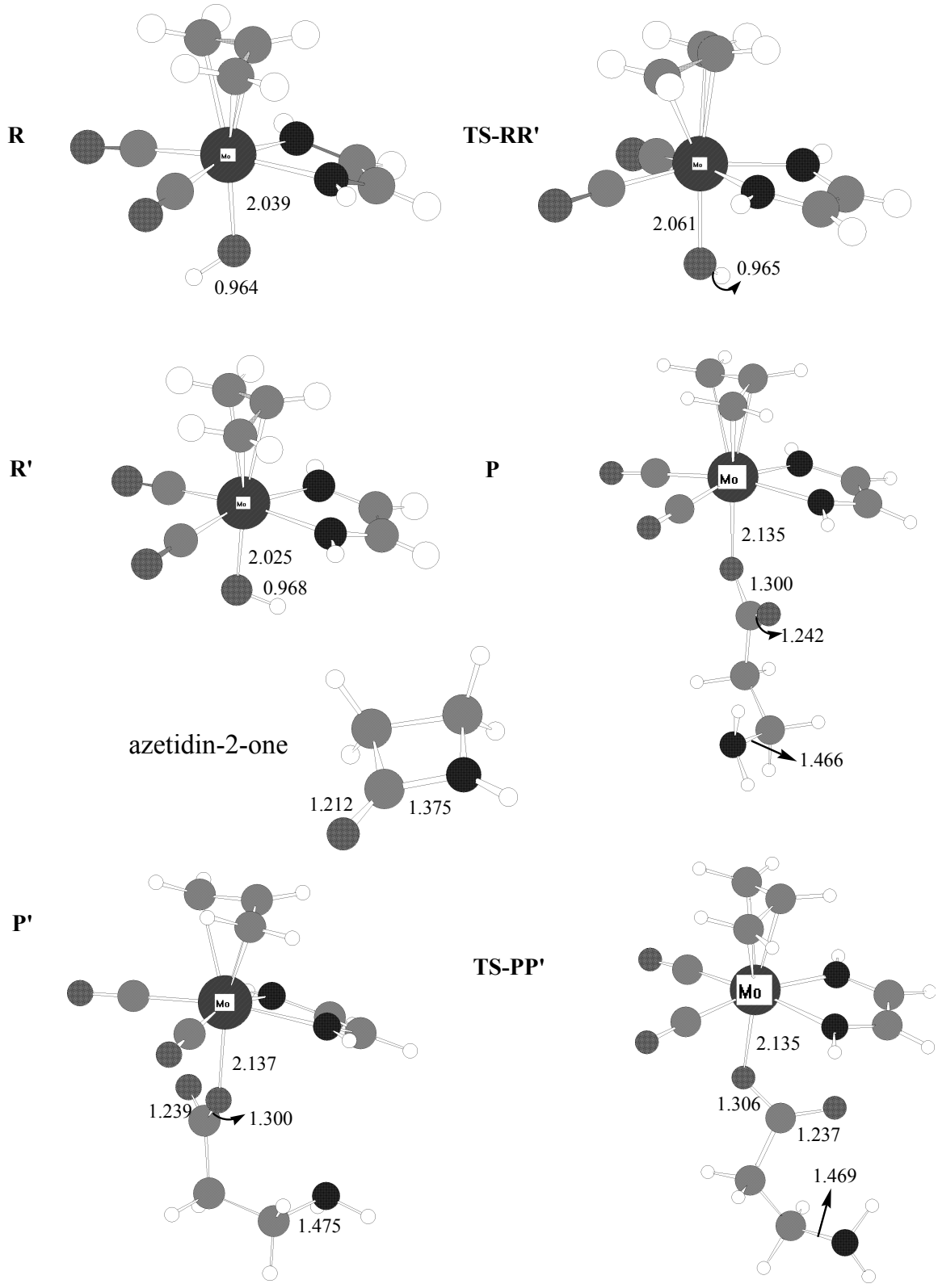

Figure 1S. B3LYP/6-31+G(d,p) (LANL2DZ for Mo augmented by f polarization functions with exponent 1.043) optimized geometries of azetidin-2-one, the **R** and **R'** conformers of [Mo(OH)(η^3-C_3H_5)$(CO)_2$($N_2C_2H_4$)], and the TS for their interconversion (**TS-RR'**) and the products **P** and **P'**, and the TS for their interconversion (**TS-PP'**). Only the most relevant distances are given in angstroms.

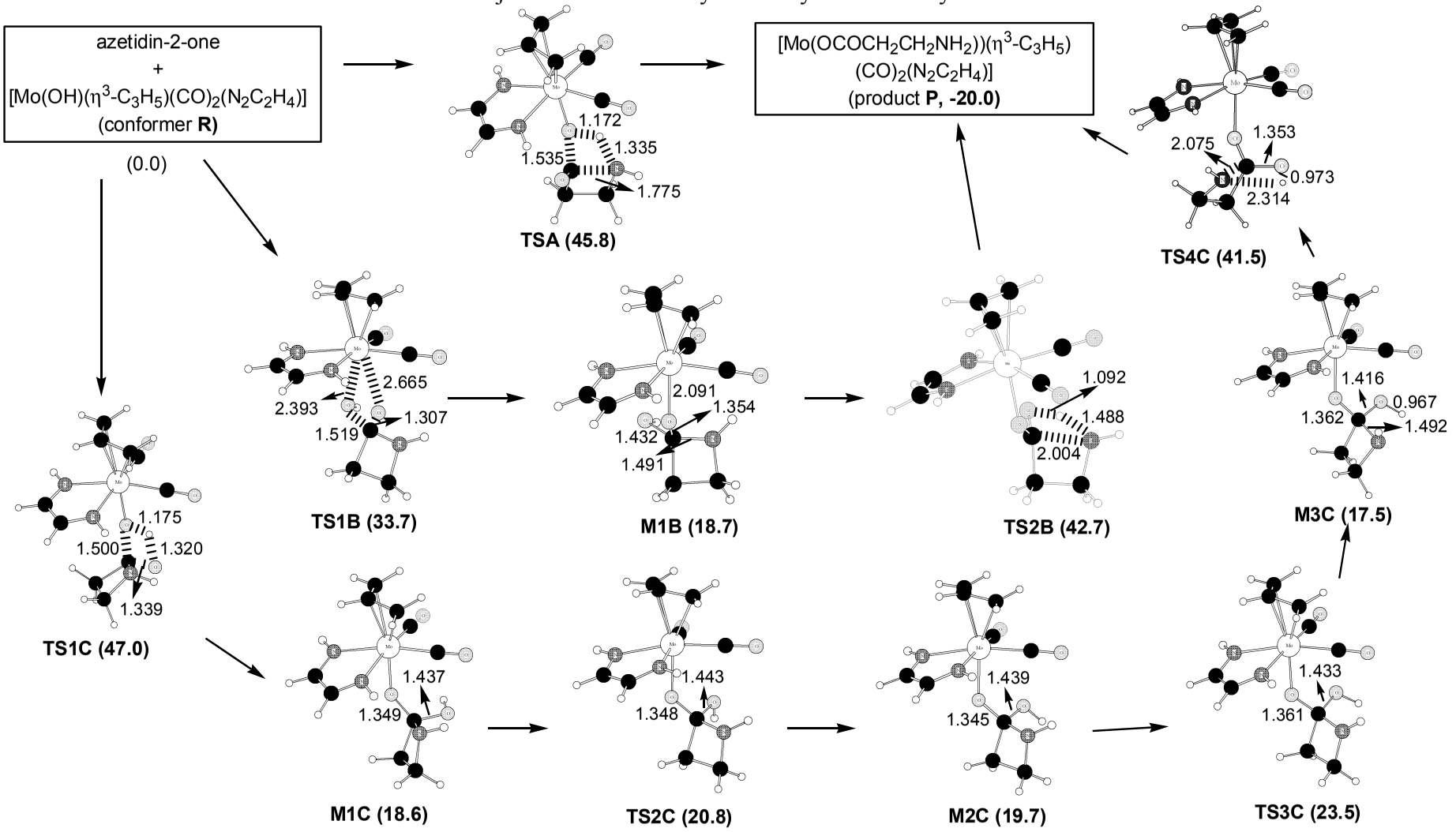

Figure 2S. Schematic view of the optimized structures involved in the reaction mechanisms found for the reaction between azetidin-2-one and the conformer **R** of $[Mo(OH)(\eta^3\text{-}C_3H_5)(CO)_2(N_2C_2H_4)]$. Relative energies in solution in kcal mol^{-1} and the most relevant distances in angstroms are also displayed.

Supplementary Material (ESI) for *Dalton Transactions*