

Supporting Information for:

The Alkene Epoxidation Catalysts [Ru(pdc)(tpy)] and [Ru(pdc)(pybox)] Revisited: Revealing a Unique Ru^{IV}=O Structure from a Dimethyl Sulfoxide Coordinating Complex

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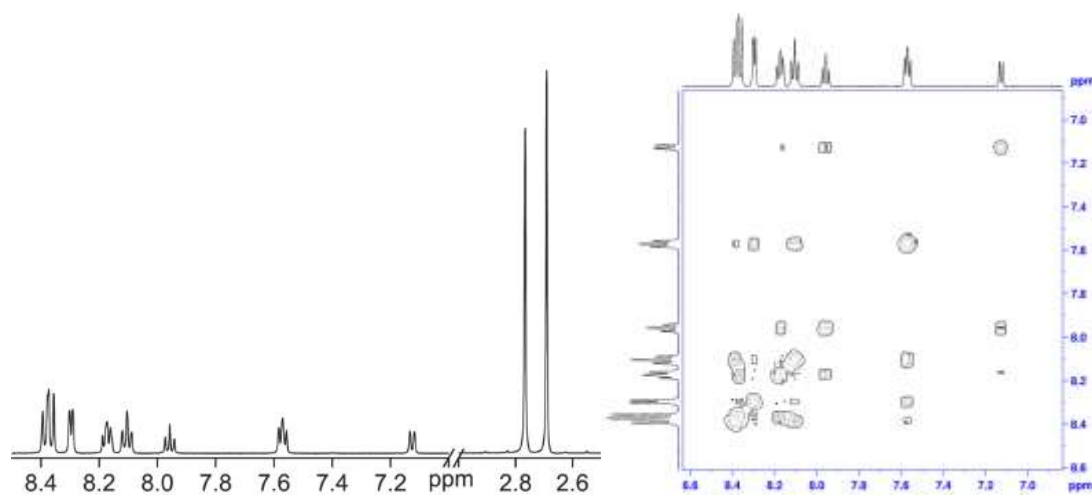


Figure S1. The ^1H NMR (left) and aromatic region of the COSY (right) spectra of complex **1**- $\text{dms}\text{-}d_6$ (500 MHz, D_2O).

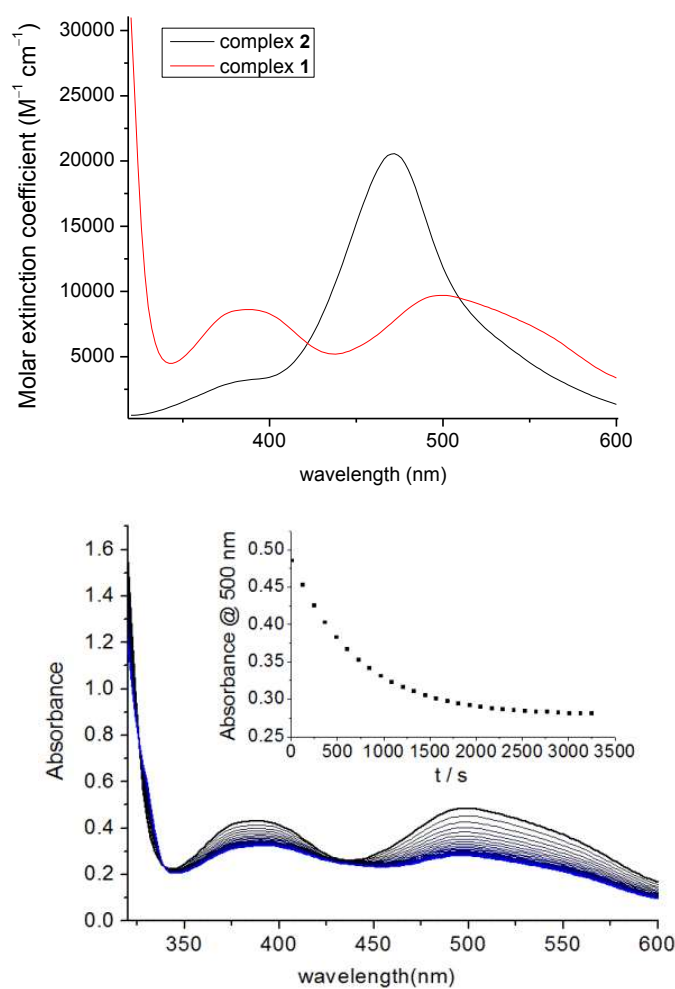


Figure S2. (Upper) Electronic absorption spectra of complexes **1** and **2** in methanol. (Lower) Uv-vis spectral changes of complex **1** versus time upon addition of $\text{dms}\text{-}d_6$. Conditions: solvent = methanol, $[\mathbf{1}] = 0.05 \text{ mM}$, and $[\text{dms}\text{-}d_6] = 0.01 \text{ M}$.

Kinetic studies on the following reactions:

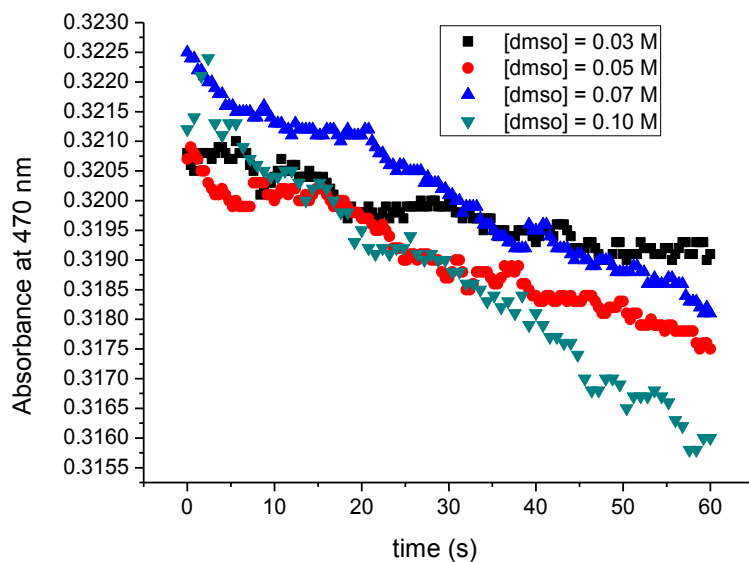
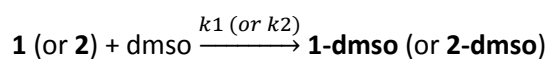


Figure S3. Absorbance change at 470 nm for complex **1** upon mixing with methanolic dmsO solutions. Initial reaction conditions: **[1]** = 5×10^{-5} M for all cases; [dmsO] = 0.03 M, 0.05 M, 0.07 M and 0.1 M, respectively.

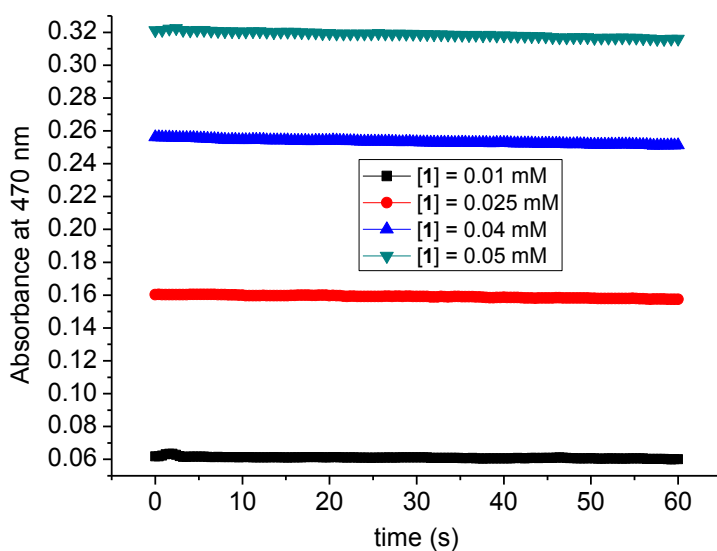


Figure S4. Absorbance change at 470 nm for complex **1** upon mixing with methanolic dmsO solutions. Initial reaction conditions: [dmsO] = 0.1 M for all cases; **[1]** = 1×10^{-5} M, 2.5×10^{-5} M, 4×10^{-5} M and 5×10^{-5} M, respectively.

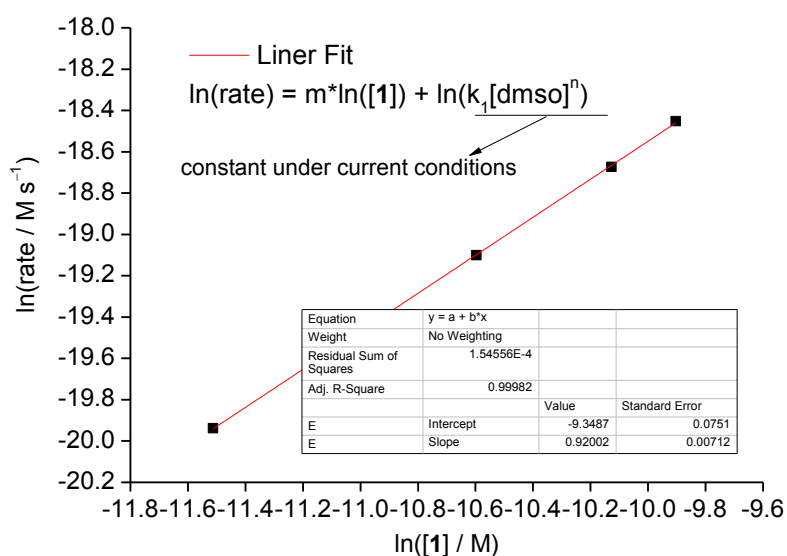


Figure S5. Plot of $\ln(\text{rate})$ versus $\ln([1])$, showing that the ligand exchange reaction is first order in **1**. Initial reaction conditions: $[\text{dms}] = 0.1 \text{ M}$ for all cases; $[1] = 1 \times 10^{-5} \text{ M}$, $2.5 \times 10^{-5} \text{ M}$, $4 \times 10^{-5} \text{ M}$ and $5 \times 10^{-5} \text{ M}$, respectively.

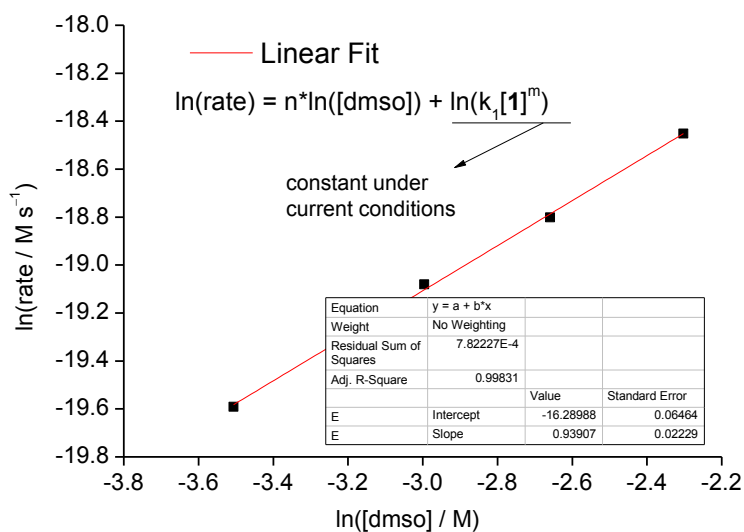


Figure S6. Plot of $\ln(\text{rate})$ versus $\ln([\text{dms}])$, showing that the ligand exchange reaction is first order in dms . Initial reaction conditions: $[1] = 5 \times 10^{-5} \text{ M}$ for all cases; $[\text{dms}] = 0.03 \text{ M}$, 0.05 M , 0.07 M and 0.1 M , respectively.

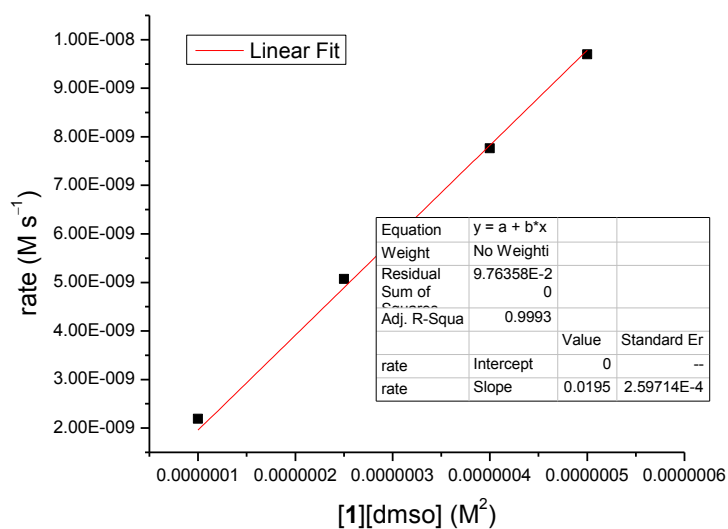


Figure S7. Plot of rate versus $[1][\text{dmso}]$. By applying the linear fit according to $\text{rate} = k_1[1][\text{dmso}]$, the second order rate constant k_1 is obtained as $1.95 \times 10^{-2} \text{ M}^{-1} \text{ s}^{-1}$.

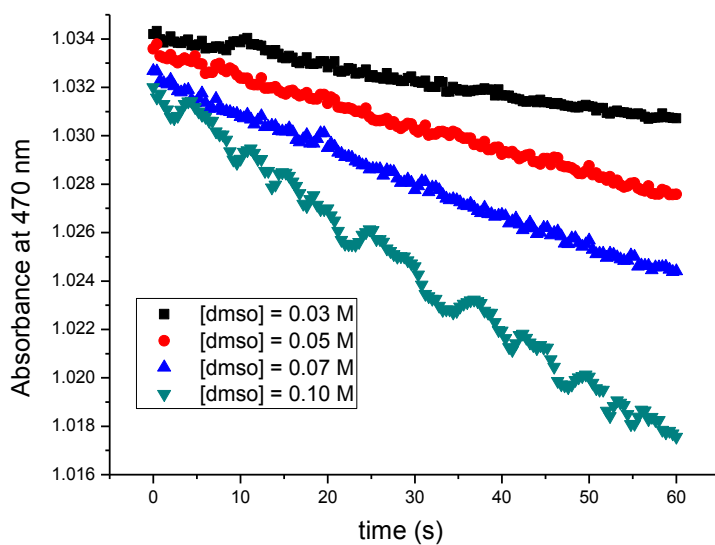


Figure S8. Absorbance change at 470 nm for complex **2** upon mixing with methanolic dmso solutions. Initial reaction conditions: $[2] = 5 \times 10^{-5} \text{ M}$ for all cases; $[\text{dmso}] = 0.03 \text{ M}$, 0.05 M , 0.07 M and 0.1 M , respectively.

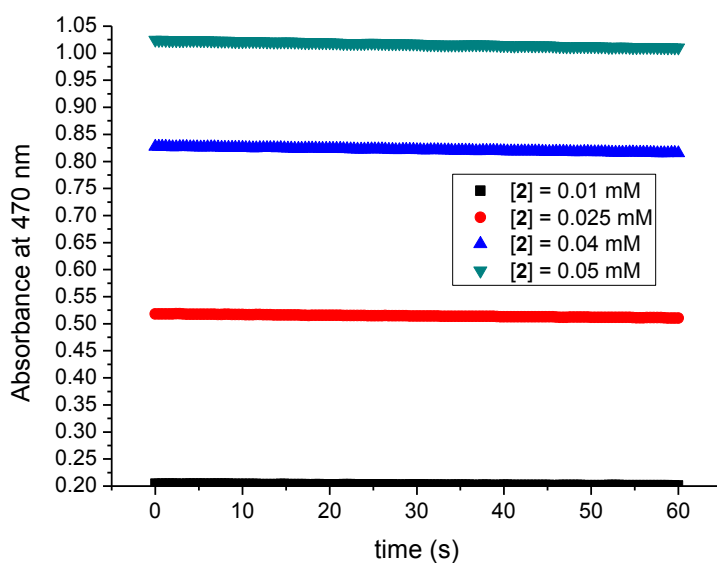


Figure S9. Absorbance change at 470 nm for complex **2** upon mixing with methanolic dmso solutions. Initial reaction conditions: [dmso] = 0.1 M for all cases; [**2**] = 1×10^{-5} M, 2.5×10^{-5} M, 4×10^{-5} M and 5×10^{-5} M, respectively.

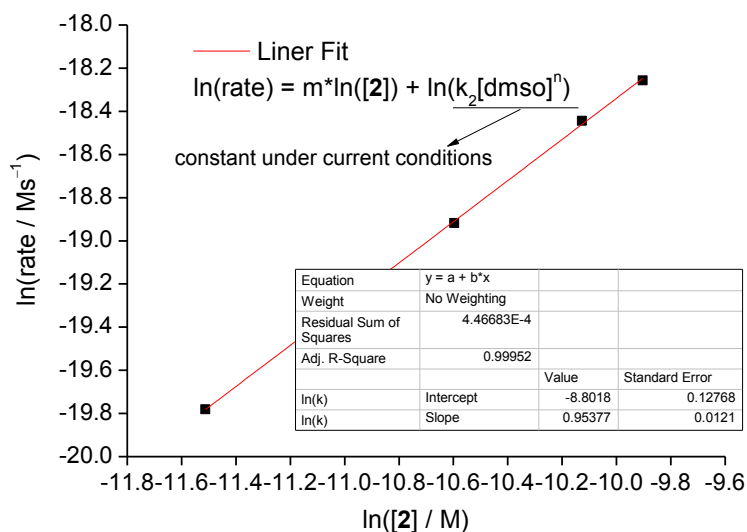


Figure S10. Plot of $\ln(\text{rate})$ versus $\ln([\mathbf{2}])$, showing that the ligand exchange reaction is first order in **2**. Initial reaction conditions: [dmso] = 0.1 M for all cases; [**2**] = 1×10^{-5} M, 2.5×10^{-5} M, 4×10^{-5} M and 5×10^{-5} M, respectively.

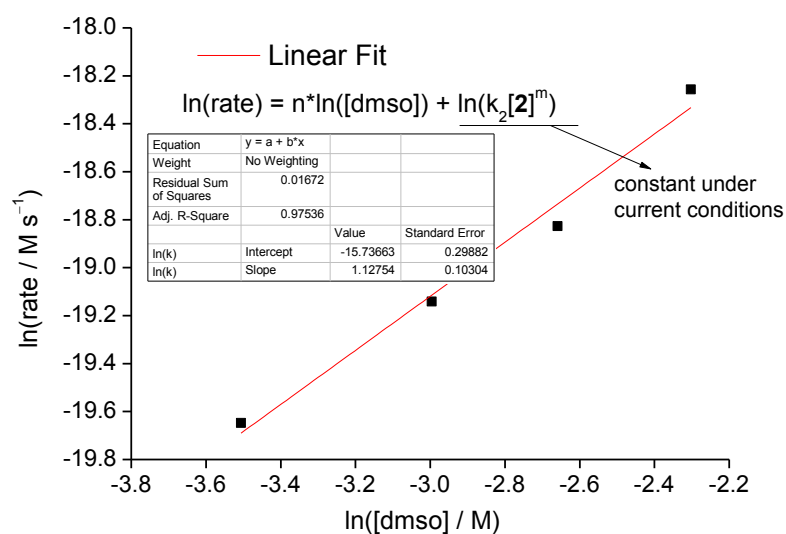


Figure S11. Plot of $\ln(\text{rate})$ versus $\ln([\text{dmso}])$, showing that the ligand exchange reaction is first order in dmso. Initial reaction conditions: $[\mathbf{2}] = 5 \times 10^{-5} \text{ M}$ for all cases; $[\text{dmso}] = 0.03 \text{ M}$, 0.05 M , 0.07 M and 0.1 M , respectively.

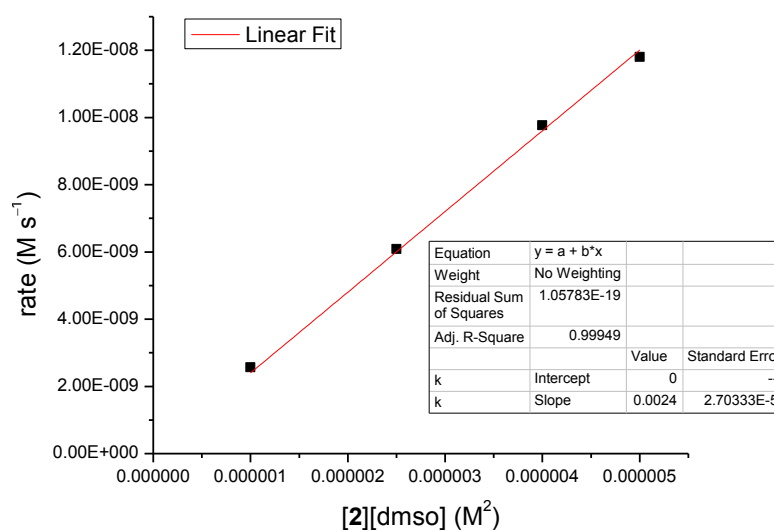


Figure S12. Plot of rate versus $[\mathbf{2}][\text{dmso}]$. By applying the linear fit according to $\text{rate} = k_2[\mathbf{2}][\text{dmso}]$, the second order rate constant k_2 is obtained as $2.4 \times 10^{-3} \text{ M}^{-1} \text{ s}^{-1}$.

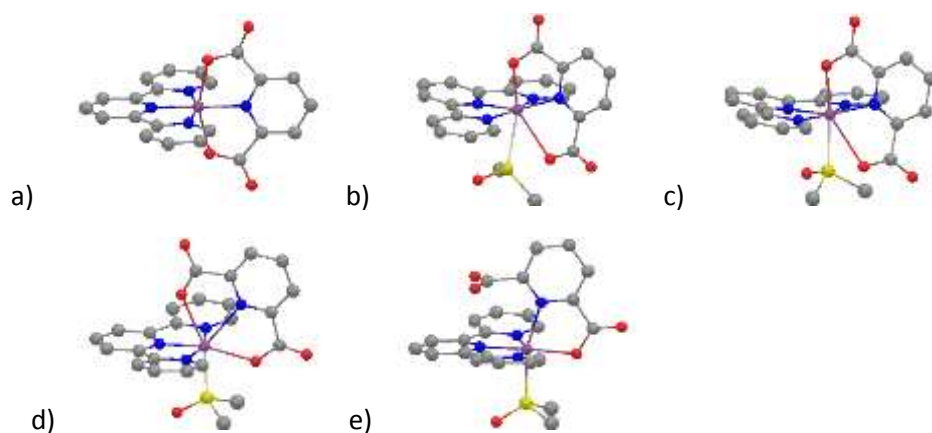


Figure S13. Optimized geometries of **Figure S13a**. a) **1**; b) **ts-cis-1-dmsso**; c) **cis-1-dmsso**; d) **ts-1-dmsso**; e) **1-dmsso**. The hydrogen atoms are omitted for clarity. (Purple = Ru; Red = O; Blue = N; Yellow = S; Grey = C).

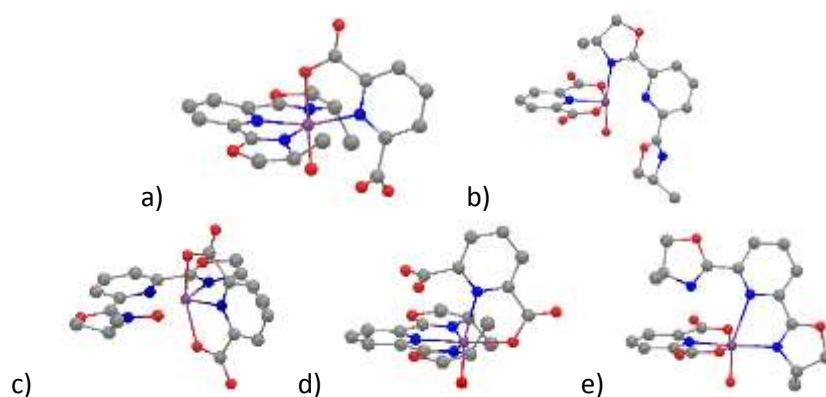


Figure S14. Optimized geometries a) **2a-oxo**, b) **2b-oxo**, c) **2-oxo-N**, d) **trans-2a-oxo** and e) **trans-2b-oxo**. The hydrogen atoms are omitted for clarity. (Purple = Ru; Red = O; Blue = N; Grey = C).

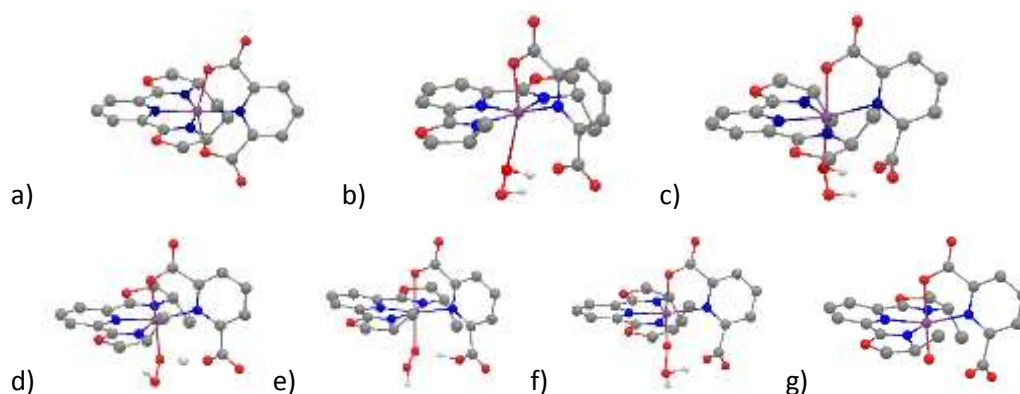


Figure S15. Optimized geometries of **Figure 7**. a) **2'**; b) **ts-2a-HOOH-COO**; c) **2a-HOOH-COO**; d) **ts-2a-OOH-COOH**; e) **2a-OOH-COOH**; f) **ts-2a-oxo**; g) **2a-oxo**. The hydrogen atoms except the HO type are omitted for clarity. (Purple = Ru; Red = O; Blue = N; Grey = C; White = H).

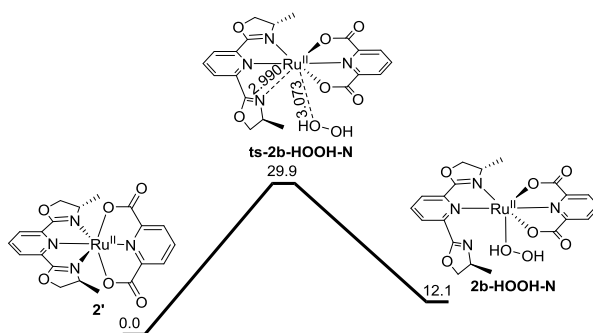


Figure S16. Reaction diagram of formation of **2b-oxo** via H_2O_2 with complex **2'**. The relative Gibbs free energies are given in kcal/mol, and the bond lengths are given in Å.

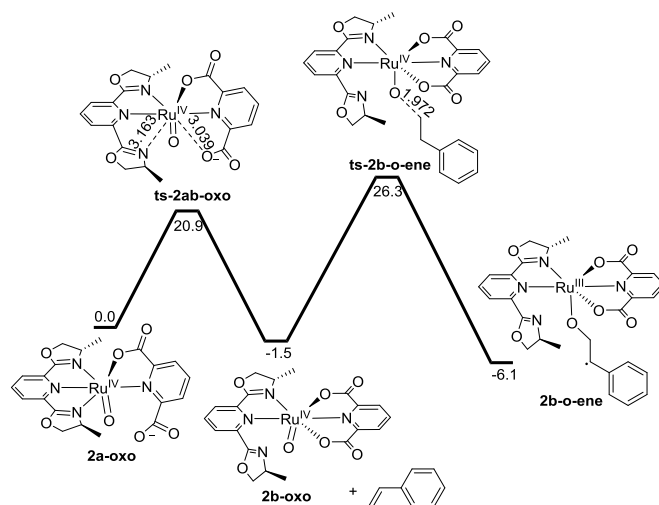


Figure S17. Reaction diagram of epoxidation of styrene using **2b-oxo**. The relative Gibbs free energies are given in kcal/mol, and the bond lengths are given in Å. The activation energy is calculated to 27.8 kcal/mol via **ts-2b-o-ene** when catalyst **2b-oxo** reacting with **styrene**, which implies that it is much slower than the reaction via **ts-trans-2a-o-ene**.

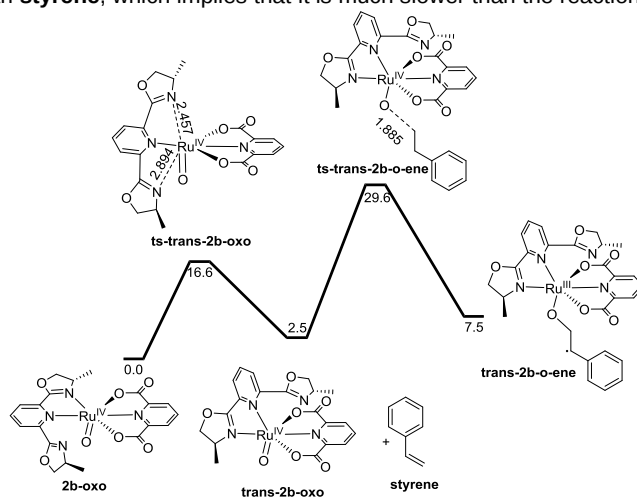


Figure S18. Reaction diagram of epoxidation of styrene using **trans-2b-oxo**. The relative Gibbs free energies are given in kcal/mol, and the bond lengths are given in Å. The free energy barrier of the transition from **2b-oxo** by overcoming **ts-trans-2b-oxo** is calculated to be 16.6 kcal/mol. However, the free energy barrier of the reaction between **trans-2b-oxo** and **styrene** reached 29.6 kcal/mol, which indicates that this pathway would be quite slow.

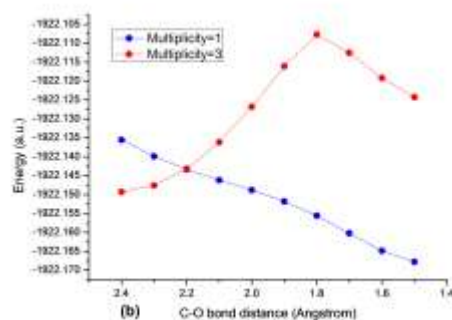


Figure S19. Reaction diagram of minimum energy crossing point of two spin surfaces between **trans-2a-o-ene** (triplet) and **trans-2a-epo-ene** (singlet)

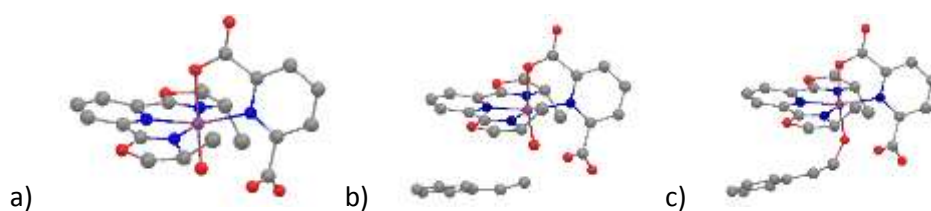


Figure S16. Optimized geometries of **Figure 8**. a) **2a-oxo**; b) **ts-2a-o-ene**; c) **2a-o-ene**. The hydrogen atoms except the HO type are omitted for clarity. (Purple = Ru; Red = O; Blue = N; Grey = C; White = H).

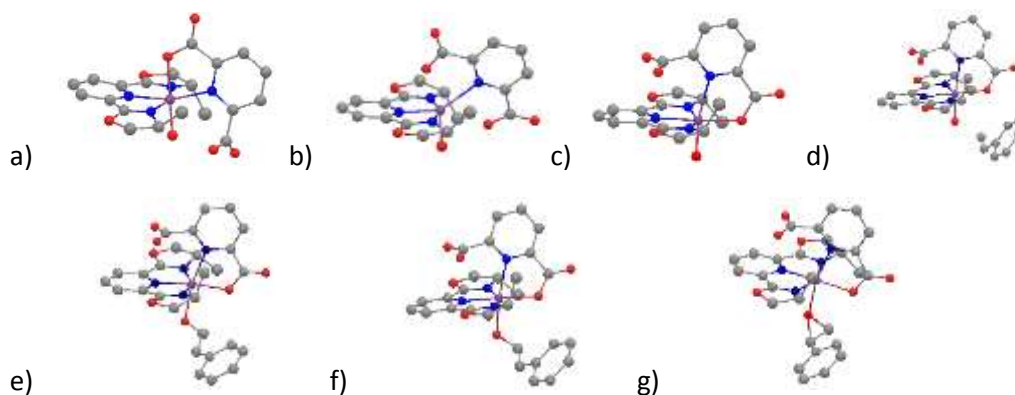


Figure S17. Optimized geometries of **Figure 9**. a) **2a-oxo**; b) **ts-trans-2a-oxo**; c) **trans-2a-oxo**; d) **ts-trans-2a-o-ene**; e) **trans-2a-o-ene**; f) **MECP**. g) **trans-2a-epo-ene**. The hydrogen atoms except the HO type are omitted for clarity. (Purple = Ru; Red = O; Blue = N; Grey = C; White = H).

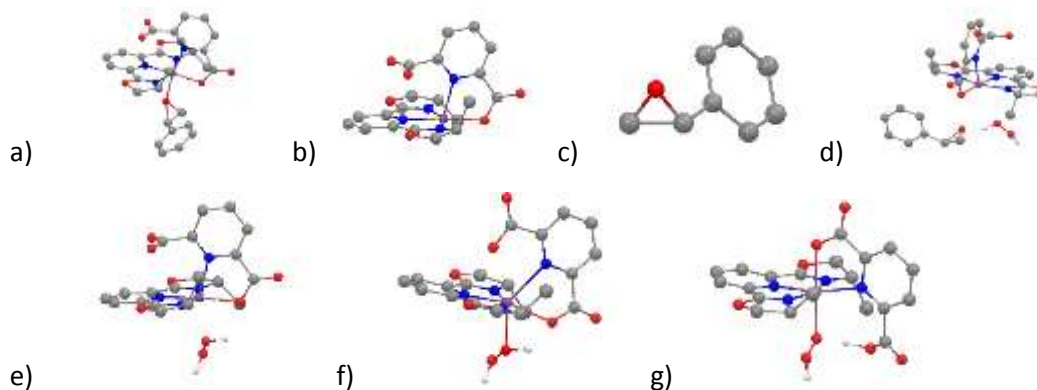


Figure S18. Optimized geometries of **Figure 10**. a) **trans-2a-epo-ene**; b) **D**; c) **styrene epoxide**; d) **Ia**; e) **trans-2a-HOOH-COO**; f) **ts-trans-2a-HOOH-COO**. g) **2a-OOH-COOH**. The hydrogen atoms except the HO type are omitted for clarity. (Purple = Ru; Red = O; Blue = N; Grey = C; White = H).

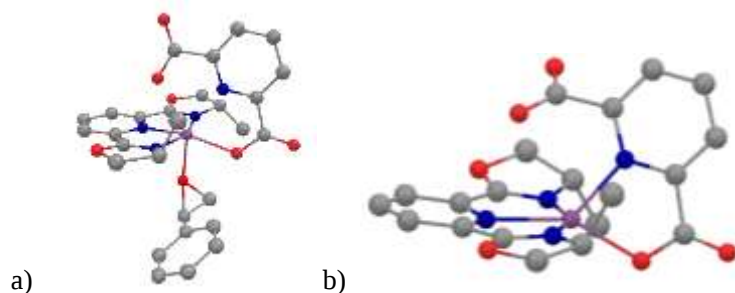


Figure S19. Optimized geometries of **Figure 11**. a) **ts-2'-epo**; b) **ts-D-2'**. The hydrogen atoms except the HO type are omitted for clarity. (Purple = Ru; Red = O; Blue = N; Grey = C; White = H).

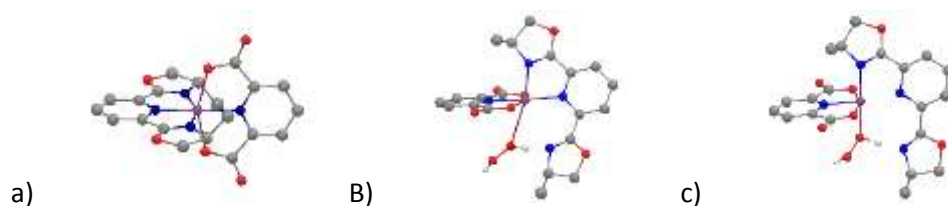


Figure S20. Optimized geometries of **Figure 12**. a) **2'**; b) **ts-2b-HOOH-N**; c) **2b-HOOH-N**. The hydrogen atoms except the HO type are omitted for clarity. (Purple = Ru; Red = O; Blue = N; Grey = C; White = H).

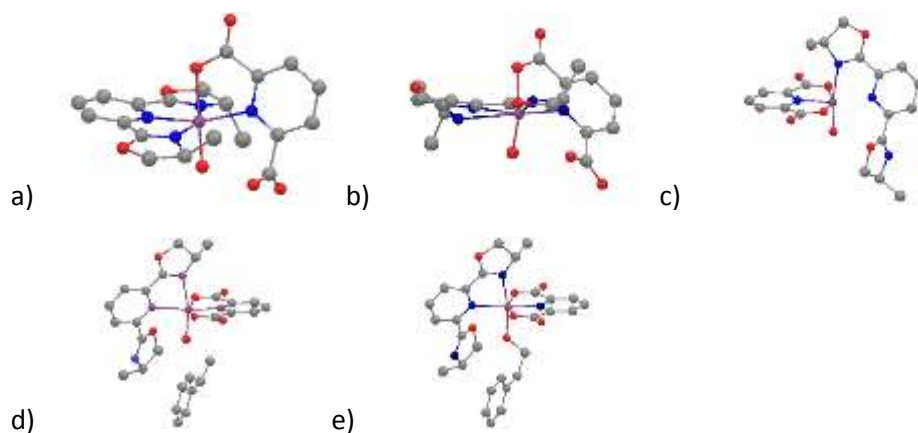
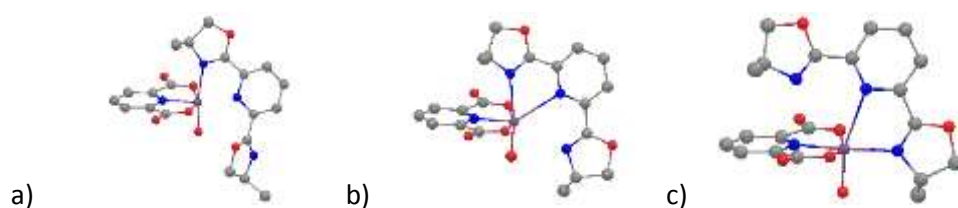


Figure S21. Optimized geometries of **Figure 13**. a) **2a-oxo**; b) **ts-2ab-oxo**; c) **2b-oxo**. d) **ts-2b-o-ene**; e) **2b-o-ene**. The hydrogen atoms except the HO type are omitted for clarity. (Purple = Ru; Red = O; Blue = N; Grey = C; White = H).



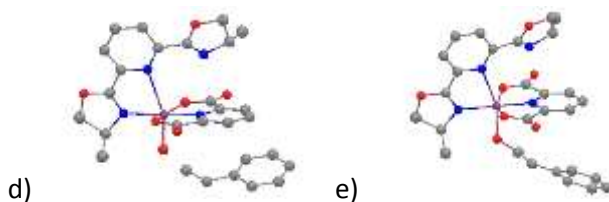


Figure S22. Optimized geometries of **Figure 14**. a) **2b-oxo**; b) **ts-trans-2b-oxo**; c) **trans-2b-oxo**. d) **ts-trans-2b-o-ene**; e) **trans-2b-o-ene**. The hydrogen atoms except the HO type are omitted for clarity. (Purple = Ru; Red = O; Blue = N; Grey = C; White = H).

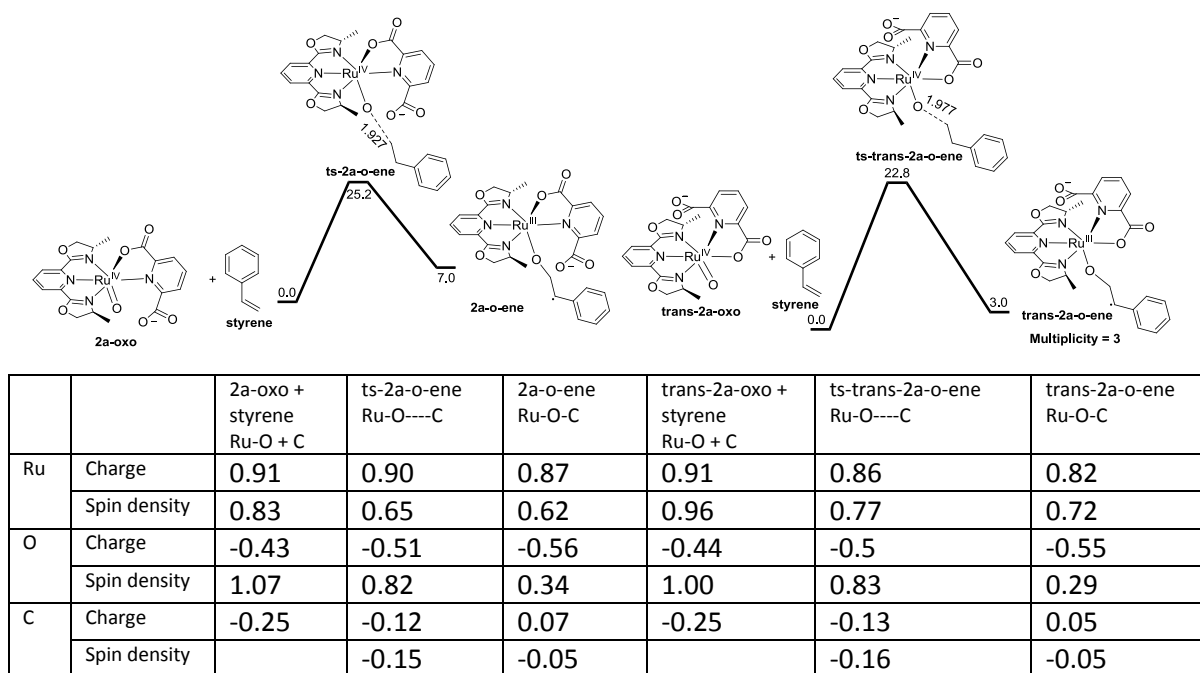


Figure S23. Spin density analysis on reactions between styrene and **2a-oxo** and **trans-2a-oxo**, respectively.

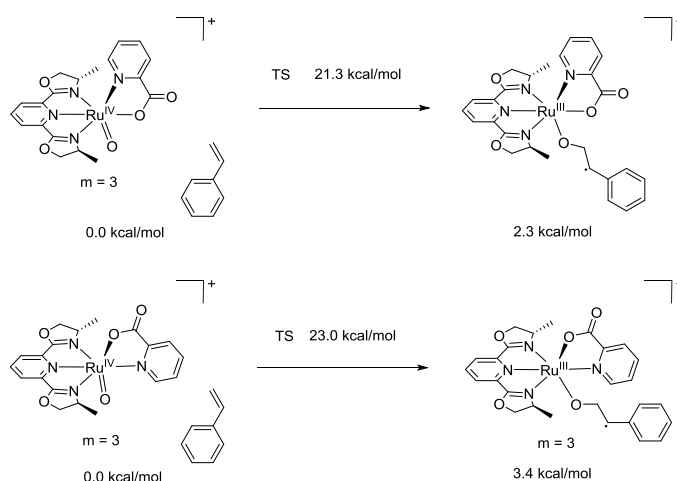


Figure S24. Reaction of two non-carboxylated conformations of **trans-2a-oxo** and **2a-oxo**. The relative Gibbs free energies are given in kcal/mol.

Based on a suggestion from one of the reviewers we calculated the reactivity of the two conformations but with the carboxylate removed. In that way we could distinguish the effect of the carboxylate placement versus the *cis/trans* placement of the picolinate moiety. We found that also here the reactivity is in slight favor of the same conformation that we found more reactive, but the effect is smaller (**Figure S24**). This result indicated that the preference of

reactivity at **trans-2a-oxo** over **2a-oxo** could be due to a combination of the placements of the ligands bound to the metal and the placement of the non-bonded carboxylate group.

	Gsolv(lacvp **) a.u.	E(M06/lacv3p **++(+f)) a.u.	ZPE(lacvp*) kcal/mol	Htot (298) kcal/mol	Stot(298) cal/K/mol
1	-0.0564137	-1460.129885	204.93	15.463	164.116
ts-cis-1-dmso	-0.0620556	-2013.247561	255.812	19.705	197.362
cis-1-dmso	-0.0605185	-2013.275236	256.935	19.705	192.899
ts-1-dmso	-0.0607073	-2013.250457	256.227	19.646	195.984
1-dmso	-0.0618521	-2013.278371	256.479	19.99	196.434
2-oxo-N	-0.053918	-1611.927636	234.299	17.733	182.076
2b-oxo	-0.0517638	-1611.929753	233.018	18.428	191.599
2a-oxo	-0.0671163	-1611.91363	233.13	18.389	189.616
2'	-0.0468176	-1536.780698	231.566	17.284	179.902
ts-2a-HOOH-COO	-0.0463768	-1688.30471	249.86	19.256	194.411
2a-HOOH-COO	-0.0432396	-1688.326029	250.733	19.018	189.358
ts-2a-OOH-COOH	-0.0521517	-1688.309997	247.924	19.027	192.226
2a-OOH-COOH	-0.0460883	-1688.318337	248.464	19.442	196.313
ts-2a-oxo	-0.0476359	-1688.308943	247.223	19.053	191.19
styrene	-0.0051754	-309.4697578	83.865	4.833	82.343
ts-2a-o-ene	-0.054914	-1921.381583	317.21	22.62	219.984
2a-o-ene	-0.0555881	-1921.411151	318.211	22.627	220.791
ts-trans-2a-oxo	-0.0614683	-1611.899333	233.019	17.853	184.439
trans-2a-oxo	-0.0514481	-1611.934264	233.515	18.338	187.648
ts-trans-2a-o-ene	-0.0443622	-1921.398632	317.843	23.083	225.674
trans-2a-o-ene (m = 3)	-0.044192	-1921.432319	318.952	23.034	225.01
MECP	-0.0477979	-1921.423235	319.327	22.964	220.204
trans-2a-o-ene (m = 1)	-0.0463177	-1921.45107	320.102	22.843	219.499
D	-0.0554167	-1536.739797	231.383	17.475	179.095
styrene epoxide	-0.0079818	-384.6660548	87.304	5.101	84.671
I_a	-0.0487468	-2072.96907	337.66	25.381	243.574
trans-2a-HOOH-COO	-0.0510025	-1688.304038	249.848	19.806	195.497
ts-trans-2a-HOOH-COO	-0.050105	-1688.273057	249.079	19.46	196.871
ts-2'-epo	-0.0437094	-1921.413166	319.714	22.482	217.229
ts-D-2'	-0.0486461	-1536.711719	230.582	17.284	178.102
ts-2b-HOOH-N	-0.0524543	-1688.275479	249.474	19.528	197.668
2b-HOOH-N	-0.0544964	-1688.302287	249.541	19.499	196.669
ts-2ab-oxo	-0.0575942	-1611.889495	232.192	17.692	183.829
ts-2b-o-ene	-0.0445714	-1921.385122	316.93	23.271	230.826
2b-o-ene	-0.0440656	-1921.42375	318.112	23.196	229.22
ts-trans-2b-oxo	-0.0448926	-1611.911213	232.826	18.016	187.375
trans-2b-oxo	-0.0457813	-1611.933043	233.278	18.323	189.558
ts-trans-2b-o-ene	-0.0428609	-1921.386466	317.418	23.018	226.407
trans-2b-o-ene	-0.0435269	-1921.425236	318.303	22.411	218.542
Data below are non-carboxylated conformations of trans-2a-oxo and 2a-oxo for Figure S24 .					
non-carboxylated 2a-oxo	-0.082831	-1423.807724	232.692	16.68	176.967
non-carboxylated ts-2a-o-ene	-0.0762259	-1733.272264	316.742	20.937	210.407
non-carboxylated 2a-o-ene	-0.0753087	-1733.307291	317.701	20.868	207.288
non-carboxylated trans-2a-	-0.0875314	-1423.791265	232.351	16.741	176.819

oxo					
non-carboxylated ts-trans-2a-o-ene	-0.0739765	-1733.264436	316.82	21.502	215.506
non-carboxylated trans-2a-o-ene (m = 3)	-0.0752142	-1733.295054	317.847	21.494	215.57

Cartesian coordinates of computed structures

Cartesian coordinates of **1**

atom	x	y	z
Ru1	0.4726405295	8.5347547711	9.1898941345
C2	3.5307606861	8.4184042263	5.5741232815
C3	3.5036902121	7.3655491571	6.4969790180
C4	2.5938762124	7.4266236059	7.5490074922
N5	1.7740554402	8.4841721144	7.6503949364
C6	1.7710373471	9.5113566819	6.7868177100
C7	2.6587514690	9.5051810170	5.7143128702
H8	4.2323983361	8.3918230108	4.7450473866
H9	4.1608977107	6.5057507250	6.4265796022
H10	2.6458737010	10.3411892058	5.0235309322
C11	0.7458135305	10.5954069420	7.1175863821
O12	0.6600585726	11.5778871749	6.3896123591
C13	2.4047729960	6.3895326681	8.6551992840
O14	3.1063469893	5.3844641481	8.6570448418
O15	1.4751553691	6.6918992393	9.5237984437
O16	0.0344427856	10.3554231900	8.1881163662
C17	-2.5835989770	8.6697393382	12.7942714585
C18	-1.3084972475	9.2189147449	12.9396751467
C19	-0.4194865456	9.1700266296	11.8658056234
N20	-0.8039462977	8.5898913609	10.6963808536
C21	-2.0421251235	8.0496383339	10.5319440129
C22	-2.9567513586	8.0811199172	11.5847381127
H23	-3.2846500068	8.7000452456	13.6216561167
H24	-1.0159329045	9.6763575361	13.8780370580
H25	-3.9463369539	7.6535900738	11.4691139285
C26	3.5475697533	10.6056079710	11.5665678848
C27	2.8827469078	9.9644376661	10.5288814206
N28	1.6208068130	9.5138396346	10.6415368704
C29	0.9562775230	9.6913975440	11.8281915219
C30	1.5761180055	10.3298497054	12.9056442439
C31	2.8810026457	10.7918955677	12.7783470982
H32	4.5659543584	10.9496237899	11.4219094885
H33	3.3585726885	9.7968209675	9.5694222266
H34	1.0370458192	10.4631172105	13.8369322636
H35	3.3695758388	11.2891489457	13.6103016575
C36	-2.4544596389	6.4647488838	6.6324203515
C37	-3.5470403899	6.3576401715	7.4939289094
C38	-3.4399082750	6.8690785416	8.7820938942
C39	-2.2506434701	7.4777105502	9.1919945484
N40	-1.1828553850	7.5771724939	8.3369836289
C41	-1.2969081819	7.0792578718	7.0930955195
H42	-2.4928031766	6.0803417391	5.6189491914
H43	-4.4674460153	5.8838931245	7.1675149755
H44	-4.2752409601	6.7987672746	9.4697502438
H45	-0.4224781579	7.1857279569	6.4613637945

Cartesian coordinates of **ts-cis-1-dmso**

atom	x	y	z
Ru1	0.1930159942	8.8630677491	9.2261519267
S2	0.9074262532	6.4124340292	10.2225272490
O3	2.5542813378	7.5808255870	8.3346380133
N4	-0.9340564266	8.8223246228	10.8306933954
N5	1.1327563527	9.6393737359	7.3615778778
N6	-1.5506735822	8.0103189091	8.4335483718
C7	2.2131715283	9.2116488644	6.6780510133
C8	0.9553417082	9.8310868086	11.8569874437
C9	2.6120476041	9.8276866188	5.4871368897
C10	0.4715878800	10.7329236690	6.9154437037
C11	-0.4606561941	9.4278662976	11.9533747028
C12	-2.5776439883	7.9844568738	9.3422098218

C13	1.8932984008	10.9118455427	4.9949621423
C14	-1.7676368817	7.5554756190	7.1864966567
C15	0.8103185561	11.3860878255	5.7352484542
C16	-2.6511875007	9.2390365635	12.9365587612
C17	-0.5921633412	5.3965144950	10.5282564168
C18	-3.1291006711	8.6840934049	11.7500440997
C19	-2.2463599807	8.4947386267	10.6852745216
C20	-4.0472773821	7.0132343907	7.6956146975
C21	1.8522793895	5.1137002330	9.3570504570
C22	-2.9951519690	7.0466693121	6.7783379307
O23	1.5411433321	6.6238181614	11.5789215401
N24	1.5249785885	9.6667574911	10.6269726391
O25	4.0976149564	7.7815725296	6.6779201323
O26	-1.2762285760	12.2565506693	7.4623471020
O27	-0.7430187261	10.6662191526	8.9533797450
C28	2.8265174068	9.9417254949	10.4589156819
C29	-0.6163047894	11.2830324415	7.8063437180
C30	3.0372670592	10.6522025134	12.7403333154
C31	1.6956518445	10.3328571676	12.9273881861
C32	3.6153888052	10.4437800125	11.4898745863
H33	-0.2873808253	4.4899012482	11.0560069864
H34	-1.2654875801	5.9778327224	11.1580312388
H35	-1.0796541202	5.1465386327	9.5822877324
H36	1.9151529974	4.2465084758	10.0191857472
H37	1.3384518733	4.8673161067	8.4245756020
H38	2.8179842132	5.5566576394	9.1246604714
C39	3.0507385742	8.0726459956	7.2751470441
H40	-0.9182275959	7.6155177919	6.5148155980
H41	-5.0196956188	6.6246759151	7.4100729625
H42	-3.1193931957	6.6907588528	5.7614052663
C43	-3.8336963275	7.4855267797	8.9861889374
H44	-4.6353404355	7.4658986301	9.7154973627
H45	-4.1771877895	8.4263900408	11.6515245605
H46	-3.3250005996	9.3949087020	13.7724643101
H47	1.2327778145	10.4600408475	13.8991400967
H48	3.6249069795	11.0436608893	13.5649851807
H49	3.2240128791	9.7233803575	9.4765300495
H50	4.6627517657	10.6578254496	11.3075666982
C51	-1.3146778524	9.6313645039	13.0356860650
H52	-0.9520608663	10.1070157486	13.9392836281
H53	2.1839533519	11.3974613888	4.0671414006
H54	3.4945279105	9.4250499396	5.0033949874
H55	0.2243046284	12.2524127717	5.4501797400

Cartesian coordinates of *cis*-1-dmso

atom	x	y	z
Ru1	0.1679752134	8.9143443580	9.2980897920
S2	0.6054780933	6.5567165710	9.8116153671
O3	3.1868342522	7.7255565535	8.3440840341
N4	-0.9164293783	8.9805184076	10.9555013871
N5	1.1256977495	9.4796585738	7.4012152099
N6	-1.6992829828	8.2630802921	8.5595600084
C7	2.0309754040	8.8413666445	6.6278034180
C8	1.0569273365	9.9193511769	11.8835819229
C9	2.3639241442	9.3192449900	5.3542142246
C10	0.6053481422	10.6543439387	6.9581078956
C11	-0.3698647147	9.5603330577	12.0476445452
C12	-2.6545679567	8.2109070381	9.5369491364
C13	1.8194925933	10.5117137815	4.8960931875
C14	-2.0263179199	7.9159331540	7.3042625835
C15	0.9346826957	11.2011044814	5.7245653186
C16	-2.5040823817	9.4102473193	13.1449125448
C17	0.7396724668	5.3764425632	8.4353784936
C18	-3.0542275077	8.8676876158	11.9837775979
C19	-2.2284994336	8.6696757051	10.8759097448
C20	-4.2810462786	7.4184662854	7.9463040447
C21	2.1702634184	6.1996191413	10.6634232834
C22	-3.3036159728	7.4884386592	6.9550721368
O23	-0.5238793844	6.0477878815	10.6842052473
N24	1.5986816844	9.6329920377	10.6609029196
O25	2.7859667072	6.6208019292	6.3979043533
O26	-0.7878429649	12.4924483348	7.5458591718
O27	-0.4980724496	10.8532641272	9.0553646778
C28	2.8989021350	9.8803056179	10.4311847158
C29	-0.3130058555	11.4168493648	7.8943863960

C30	3.1700091818	10.7921440113	12.6383224674
C31	1.8303668657	10.5023890176	12.8877667203
C32	3.7135636857	10.4680056156	11.3975993432
H33	0.7700818431	4.3827132424	8.8893072111
H34	-0.1782931082	5.4841293877	7.8547956189
H35	1.6152980071	5.5758192707	7.8092230617
H36	2.1567700416	5.1438918643	10.9439287743
H37	2.9774937384	6.4560505181	9.9720299055
H38	2.1936208324	6.8254814678	11.5570758846
C39	2.7388775242	7.6010692684	7.1679509462
H40	-1.2272914665	7.9882309431	6.5743491850
H41	-5.2866545873	7.0850746725	7.7101859758
H42	-3.5181153376	7.2179798204	5.9269484418
C43	-3.9521783419	7.7862465010	9.2478669330
H44	-4.6967226822	7.7406331861	10.0338641704
H45	-4.1089454367	8.6251461206	11.9418704528
H46	-3.1311228867	9.5729239350	14.0155355775
H47	1.3920233320	10.7294351142	13.8528056048
H48	3.7792636798	11.2549139341	13.4087684953
H49	3.2624476264	9.5330513048	9.4668452189
H50	4.7567329017	10.6602069555	11.1710428606
C51	-1.1589344689	9.7766661551	13.1796868563
H52	-0.7394428268	10.2344535940	14.0680165232
H53	2.0849311839	10.9046181722	3.9183025740
H54	3.0555217127	8.7305404205	4.7623783931
H55	0.4846547883	12.1511755082	5.4607435499

Cartesian coordinates of **ts-1-dmso**

atom	x	y	z
Ru1	0.00000000000000	0.00000000000000	0.00000000000000
O27	0.00000000000000	0.00000000000000	2.4892966078000
S2	0.8273619334105	0.00000000000000	-2.1716868631901
O3	-1.8460209069344	0.0178927498466	-1.3536948053749
N4	1.8024751671614	-0.0035235041719	0.7507258307640
N5	-2.2668738855884	-0.0077136889867	1.2018810685121
N6	0.3012015826215	-2.0615615989924	0.2227282051100
C7	-3.3684987004317	-0.0080918479115	0.4499430663160
C8	1.5118624486366	2.3449933255502	0.8031297487336
C9	-4.6460509555170	-0.0142952362521	1.0117847407404
C10	-2.3534411860548	-0.0114057280575	2.5311539096078
C11	2.3774725194584	1.1813862131238	1.0652491324923
C12	1.5138846643516	-2.3523561658527	0.7842974416322
C13	-4.7503774946222	-0.0186736730106	2.4051329909539
C14	-0.5766907899702	-3.0505607326990	-0.0078092349446
C15	-3.5906245124642	-0.0170009127533	3.1814650230079
C16	4.2991243199264	-0.0067526516879	1.8880127030888
C17	0.1195652836493	-1.3721381439219	-3.1330865814194
C18	3.6552767289727	-1.2136180390605	1.6161231657903
C19	2.3790263891757	-1.1902094931745	1.0547722310646
C20	0.9408327906446	-4.6922817942225	0.8538276877462
C21	0.1397872305631	1.3876308512005	-3.1252597671726
C22	-0.2979033467258	-4.3789057322756	0.2939514640958
O23	2.3207782462757	-0.0111513936268	-2.3468551291408
N24	0.3022340340123	2.0579600670639	0.2338869013060
O25	-4.0476644744072	-0.0118890950224	-1.8357244881476
O26	-1.0344748105196	-0.0117321382640	4.5043415374728
C28	-0.5767657876996	3.0467547347135	0.0085468244704
C29	-1.0184762885572	-0.0076425352850	3.2671345985130
C30	0.9337673727835	4.6828439491127	0.8933337079402
C31	1.8464611229319	3.6604276106493	1.1321566594320
C32	-0.3018769250402	4.3725545221832	0.3245091990477
H33	0.4603436432972	-1.2758202291759	-4.1661367674960
H34	0.4984965462626	-2.2965785869262	-2.6963136377527
H35	-0.9647492766680	-1.3010616384915	-3.0387307897088
H36	0.4770958756734	1.2916198017392	-4.1594969742995
H37	-0.9453081828589	1.3319999134847	-3.0294587161466
H38	0.5331353715201	2.3039372437011	-2.6841402674023
C39	-3.1074224016938	-0.0011994367932	-1.0411445982734
H40	-1.5208635239848	-2.7391034845802	-0.4413814277231
H41	1.1912779309978	-5.7181315270056	1.1052357565380
H42	-1.0411287867476	-5.1438822552416	0.0975576540515
C43	1.8522645466234	-3.6703131795433	1.0989652934738
H44	2.8138049138218	-3.8905436872055	1.5482427374952
H45	4.1366331709319	-2.1552843399633	1.8535954958098
H46	5.2922880180035	-0.0079871938328	2.3244138838913
H47	2.8054393722103	3.8781986554645	1.5880839866524

H48	1.1808273552537	5.7066889109756	1.1562231193453
H49	-1.5176003772230	2.7364553036099	-0.4329163790373
H50	-1.0456240745885	5.1381804272604	0.1324541972046
C51	3.6535603688125	1.2015369765571	1.6266955415065
H52	4.1335258817049	2.1417555378953	1.8724770895719
H53	-5.7282467891790	-0.0230312266887	2.8805603623134
H54	-5.5093125178720	-0.0151963504986	0.3556068313180
H55	-3.6044107116659	-0.0194920396826	4.2656763415926

Cartesian coordinates of **1-dmso**

atom	x	y	z
Ru1	0.3904252276	8.4796670266	9.1840662947
S2	0.9540263519	6.3510743702	10.0441555064
O3	1.6418041527	7.9503906001	7.5624081117
N4	-0.7741883069	8.8947833091	10.7504083069
N5	0.2435648999	10.2261657309	7.9708259936
N6	-1.4887515535	7.8231420402	8.4724057644
C7	0.9927440017	10.1235097138	6.8394005947
C8	1.1872927208	9.8846342330	11.6242911677
C9	1.0531198411	11.1462712879	5.9058473117
C10	-0.4665802328	11.3476154345	8.2093593409
C11	-0.2224243327	9.4878005301	11.8280422716
C12	-2.4888038865	8.0016844367	9.3883352313
C13	0.3232168123	12.3152609915	6.1388623994
C14	-1.7938841532	7.3975411854	7.2352555315
C15	-0.4363400465	12.4122296871	7.2942411414
C16	-2.3172655930	9.2635435274	12.9758774990
C17	0.6249820228	5.1380176784	8.7282374494
C18	-2.8773038619	8.7021795027	11.8298036768
C19	-2.0738919776	8.5392010763	10.7016039200
C20	-4.1223983628	7.2629423761	7.7790448515
C21	2.7702931815	6.2337376187	10.0436994934
C22	-3.0970330165	7.1068513038	6.8467846962
O23	0.4290349234	5.8156133416	11.3485697088
N24	1.7572914207	9.4827662735	10.4474817617
O25	2.4608230555	8.7077462590	5.6084544352
O26	-2.4695197900	11.0006810205	9.3749900437
O27	-0.6939355162	11.9238804239	10.4697791981
C28	3.0158654752	9.8555959131	10.1616707666
C29	-1.3030955190	11.4412744061	9.4881778479
C30	3.2179281451	11.0245191440	12.2420714052
C31	1.9126021474	10.6479794190	12.5394371200
C32	3.7809720230	10.6264195191	11.0299439096
H33	1.0591615600	4.1772311938	9.0137360241
H34	-0.4585501659	5.0511477340	8.6386238934
H35	1.0594337740	5.5316739635	7.8065740581
H36	3.0588987104	5.1995599349	10.2442207776
H37	3.1189910799	6.5787518851	9.0676638976
H38	3.1334130761	6.8881262781	10.8370887233
C39	1.7752203821	8.8401087218	6.6168408651
H40	-0.9528320763	7.2952980981	6.5573841373
H41	-5.1525145672	7.0503982895	7.5102380361
H42	-3.2968209485	6.7720186407	5.8347066250
C43	-3.8130376150	7.7121574293	9.0582805559
H44	-4.5974962127	7.8701142446	9.7883870889
H45	-3.9201738223	8.4086348069	11.8166182529
H46	-2.9266792988	9.3986846885	13.8636527350
H47	1.4450813287	10.9722148296	13.4612055515
H48	3.7829352612	11.6318034213	12.9424888935
H49	3.3968081837	9.5148061651	9.2046063963
H50	4.7909130766	10.9094917223	10.7537840526
C51	-0.9844934156	9.6716391416	12.9813691193
H52	-0.5556393558	10.1315973377	13.8635992301
H53	0.3512236803	13.1348781513	5.4255670598
H54	1.6699970462	10.9932400922	5.0281530530
H55	-1.0182109529	13.3003517417	7.5180304586

Cartesian coordinates of **2-oxo-N**

atom	x	y	z
Ru1	0.6380371165	8.6208742025	9.1764310145
C2	3.3031008685	8.1315224624	5.3199189714
C3	3.3722335922	7.1738577365	6.3387729337
C4	2.5918753157	7.3581076277	7.4771750096
N5	1.8163711319	8.4464799394	7.5693294465

C6	1.7003263748	9.3708179222	6.6061117971
C7	2.4548577148	9.2388538201	5.4434291201
H8	3.9022778302	8.0082670242	4.4219060423
H9	4.0004176563	6.2922542939	6.2740918402
H10	2.3572528409	9.9925443222	4.6698587176
C11	0.6940226290	10.4800079664	6.9226517731
O12	0.5397239750	11.3890106015	6.1136431650
C13	2.4830188785	6.4101641816	8.6735926238
O14	3.1831704914	5.4034763759	8.6994192630
O15	1.6141802331	6.7772047045	9.5777552684
O16	0.0740486687	10.3395869676	8.0635294233
C17	-1.9327289205	9.1179703004	13.2386653765
C18	-0.6311914335	9.6089115631	13.1118225397
C19	0.0354366650	9.4329866268	11.9071606991
N20	-0.5254197465	8.7970988986	10.8276610832
C21	-1.7953702537	8.3175006095	10.9591440885
C22	-2.5141259747	8.4673607908	12.1547564468
H23	-2.4815461416	9.2373159048	14.1662236566
H24	-0.1286172450	10.1190488304	13.9261693394
H25	-3.5191710311	8.0685120818	12.2139047104
N26	1.9031464029	9.6633085949	10.4603306081
C27	1.3874625192	9.8751481587	11.6289948205
O28	2.1501063021	10.4874859928	12.5530756979
N29	-1.9402318568	7.3397779864	8.6429716289
C30	-2.4119619239	7.6391904570	9.8396252959
O31	-3.7048335116	7.2360934923	9.9879267683
C32	3.4270186241	10.7561539283	11.9010091901
H33	4.2082864730	10.2686558528	12.4887652584
H34	3.5828241433	11.8389105971	11.9113435274
C35	3.2841187147	10.1847853996	10.4592173726
H36	3.9587727856	9.3341553976	10.3076978524
C37	-2.9975460176	6.7153353055	7.7957118932
H38	-3.3606991025	7.5088707215	7.1303757919
C39	-4.0219289336	6.3619500450	8.8769931996
H40	-3.9091460461	5.3232119090	9.2110135741
H41	-5.0570127452	6.5479361331	8.5889048699
C42	3.5162522348	11.2255276084	9.3642272922
H43	2.8068499996	12.0534061136	9.4570079222
H44	4.5342695887	11.6237821437	9.4386992058
H45	3.3961724055	10.7833585492	8.3736508292
C46	-2.4638801741	5.5465734326	6.9820638030
H47	-2.0749403178	4.7592755206	7.6346254468
H48	-3.2674027894	5.1309567189	6.3659065232
H49	-1.6592483637	5.8835602729	6.3265929177
O50	-0.7827456303	7.5654980606	8.0787519993

Cartesian coordinates of **2b-oxo**

atom	x	y	z
Ru1	0.6060563275	8.4379068931	9.0057184908
C2	3.6323320541	8.2603231853	5.4403302334
C3	3.8573548366	7.4754231342	6.5783779254
C4	2.9580186340	7.5724191073	7.6360040726
N5	1.9204742408	8.4086454522	7.5186227632
C6	1.6716477903	9.1886083517	6.4613717075
C7	2.5384549978	9.1326783580	5.3739014397
H8	4.3186141436	8.1957145107	4.6006694424
H9	4.7001670122	6.7992239012	6.6678781194
H10	2.3418410791	9.7631062369	4.5139636980
C11	0.4475708474	10.0934628716	6.6300089991
O12	0.1646175926	10.8756154891	5.7340176786
C13	3.0345541945	6.8492222072	8.9834779428
O14	3.9780747754	6.1039111281	9.2013138832
O15	2.0665769401	7.1451686765	9.8175476819
O16	-0.1734213580	9.9618274432	7.7760994694
C17	-1.4046498872	8.3091927966	13.5362607423
C18	-0.2879888645	9.0807380353	13.2215090981
C19	0.0991591890	9.1706445302	11.8884064676
N20	-0.5662886715	8.5597554775	10.8744572244
C21	-1.6863868804	7.8754270559	11.1793109266
C22	-2.1127035023	7.7091612493	12.5028160938
H23	-1.7233794518	8.1924562128	14.5669533876
H24	0.2910252526	9.5949477911	13.9793472276
H25	-2.9995924357	7.1133870411	12.6818487059
N26	1.6821365140	9.9808769639	10.2578678447
C27	1.2794361355	9.9379860153	11.4747848838
O28	1.9752789864	10.6196502935	12.3987602374

N29	-3.0211794284	6.1308868079	10.1294739964
C30	-2.5177372576	7.3010828900	10.0924333970
O31	-2.8012499968	8.1297125970	9.0640516102
C32	3.0580629997	11.2820423681	11.6774869505
H33	3.9983204150	10.9806448306	12.1432695216
H34	2.9185770677	12.3609492553	11.7923685960
C35	2.9026950168	10.8068518940	10.2030380271
H36	3.7335501985	10.1491099117	9.9200211727
C37	-3.8033673993	5.9910544123	8.8801991542
H38	-3.4217766369	5.1183777563	8.3393948636
C39	-3.4928543249	7.2988267439	8.0945847277
H40	-4.3814042453	7.8424218692	7.7632418264
H41	-2.8098425590	7.1444233850	7.2562758561
C42	2.7851727522	11.9471997084	9.1925487417
H43	1.9359652743	12.5940214246	9.4324875913
H44	3.6996336646	12.5500469461	9.1985804760
H45	2.6388600299	11.5596473819	8.1819971391
C46	-5.2857794695	5.7777670220	9.1948532960
H47	-5.7007158674	6.6455291477	9.7193376173
H48	-5.8591576398	5.6275297417	8.2735653522
H49	-5.4175648891	4.8980254341	9.8309741467
O50	-0.3456394147	7.1154571484	8.3009151181

Cartesian coordinates of **2a-oxo**

atom	x	y	z
Ru1	0.4033151457	8.7191287543	9.1134960467
C2	4.0286372022	7.8392670852	5.9886961131
C3	3.7816366178	7.0471827092	7.1163302505
C4	2.6896111526	7.3497545602	7.9113342842
N5	1.8569487206	8.3816327644	7.6122646984
C6	2.0450947902	9.1276384976	6.5056906928
C7	3.1626048763	8.8793786037	5.6893005351
H8	4.8866671285	7.6363874350	5.3531199462
H9	4.4015432588	6.2056003965	7.4022980330
H10	3.3161657804	9.5212977462	4.8287023045
C11	1.0156895294	10.2059353046	6.1322688176
O12	-0.0756508832	9.7212464342	5.7438992472
C13	2.3453433757	6.5141944018	9.1330704918
O14	3.0641520228	5.5766649224	9.4560606329
O15	1.2503050450	6.8861235021	9.7430630884
O16	1.4318556611	11.3739625691	6.2424777209
C17	-2.1571816230	8.0588661427	13.0594659275
C18	-0.9306969466	8.7291625435	13.1380945768
C19	-0.2403320308	8.9682942186	11.9512019376
N20	-0.7566634327	8.5705286290	10.7767945272
C21	-1.9174293108	7.9026304939	10.6825395617
C22	-2.6652518759	7.6316198858	11.8272678855
H23	-2.7161324362	7.8575531419	13.9675326798
H24	-0.5171434663	9.0502514157	14.0871727168
H25	-3.6064903862	7.0992899243	11.7526417378
N26	1.6200753485	9.6584194881	10.5907226560
C27	1.0654932514	9.6300929578	11.7563885166
O28	1.6887345586	10.2491764149	12.7601925950
N29	-1.3287938399	7.7514991775	8.3538521069
C30	-2.2094555553	7.5537125599	9.2776813127
O31	-3.4075772777	7.0925015086	8.9167322148
C32	2.9426702154	10.7676294407	12.1880888147
H33	3.7596316252	10.2161743025	12.6595215376
H34	3.0028753272	11.8250507257	12.4517705685
C35	2.8210992327	10.5144645649	10.6558791769
H36	3.6729822402	9.9342071463	10.2878217500
C37	-1.9653949650	7.5079750353	7.0395405342
H38	-2.0893822607	8.4964644005	6.5818355962
C39	-3.3122390691	6.8633821457	7.4629751132
H40	-3.3296991032	5.7798725482	7.3094871479
H41	-4.1915045946	7.3198516983	7.0073732065
C42	2.6389933228	11.7763810403	9.8069703914
H43	1.8159815157	12.3853574525	10.1951783573
H44	3.5583189650	12.3711976885	9.8372452619
H45	2.4109591351	11.5356799877	8.7632573531
C46	-1.1119872561	6.6582875709	6.1066890268
H47	-0.7914860100	5.7290417392	6.5889521156
H48	-1.6894182467	6.4093834257	5.2095483389
H49	-0.2519119876	7.2545443323	5.7971178697
O50	-0.2419969666	10.3229945283	8.6330574819

Cartesian coordinates of **2'**

atom	x	y	z
Ru1	0.5110330402	8.5341646377	9.1431463920
C2	3.5715159357	8.4120550679	5.5304819197
C3	3.5820462415	7.3902942795	6.4876212256
C4	2.6690147316	7.4518406086	7.5370749135
N5	1.8115542970	8.4810878316	7.6054618946
C6	1.7722669538	9.4781838132	6.7090183122
C7	2.6594957639	9.4691205542	5.6358902551
H8	4.2742089028	8.3845398342	4.7024233940
H9	4.2701472960	6.5531686889	6.4450906833
H10	2.6164211028	10.2811735880	4.9183668041
C11	0.7158361668	10.5399550132	7.0093229878
O12	0.5924779850	11.4940575232	6.2492984443
C13	2.5121571466	6.4386781126	8.6695789811
O14	3.2496540440	5.4598704178	8.7041055232
O15	1.5640729519	6.7275179645	9.5218698317
O16	0.0230352855	10.3171319853	8.0952202480
C17	-2.5655211137	8.6684905060	12.7769667422
C18	-1.2918945304	9.2299455981	12.9178459734
C19	-0.4139536252	9.1765397815	11.8385356445
N20	-0.7742634120	8.5892467002	10.6629880078
C21	-2.0141283571	8.0411401055	10.5256086381
C22	-2.9352316733	8.0671551315	11.5691667592
H23	-3.2663320427	8.6996084749	13.6040755770
H24	-0.9786869273	9.7015605833	13.8426642163
H25	-3.9159260833	7.6253993052	11.4315715192
N26	1.6153601397	9.5570616636	10.6412032239
C27	0.9459491216	9.6844403101	11.7461179617
O28	1.5535952433	10.2815791982	12.7852688585
N29	-1.1852252223	7.5361346969	8.3449001353
C30	-2.1671963442	7.4807466333	9.1920951900
O31	-3.3141283862	6.9078887403	8.7903943279
C32	2.8841985268	10.6510821759	12.3151464139
H33	3.6126771042	10.1778045370	12.9773385348
H34	2.9717304530	11.7388333546	12.3920001877
C35	2.9545743561	10.1431350139	10.8449315951
H36	3.6888038870	9.3348703898	10.7462945145
C37	-1.6314474698	6.9144351214	7.0827965165
H38	-1.6328331847	7.6940928642	6.3118091922
C39	-3.0840281563	6.4655331389	7.4192405733
H40	-3.2064763719	5.3785688878	7.3973269704
H41	-3.8441973937	6.9320276403	6.7887678237
C42	3.2634892089	11.2414792178	9.8282136801
H43	2.5080668659	12.0318700786	9.8679038948
H44	4.2453066787	11.6804515327	10.0364527108
H45	3.2800006873	10.8367292885	8.8143284161
C46	-0.7176917492	5.7688064919	6.6491215244
H47	-0.6534355845	5.0053020492	7.4300833467
H48	-1.1035319058	5.3064318038	5.7340133663
H49	0.2910244012	6.1341645898	6.4462165848

Cartesian coordinates of **ts-2a-HOOH-COO**

atom	x	y	z
Ru1	0.4006739177	8.7429992467	9.1621317627
C2	3.8757566856	7.7743860479	5.7933086461
C3	3.5927434499	6.9683404260	6.8951540769
C4	2.5837559435	7.3572187045	7.7687859869
N5	1.8709190507	8.4947227258	7.5935042350
C6	2.1423635002	9.2813606886	6.5327203071
C7	3.1368664574	8.9391215811	5.6122330742
H8	4.6556468226	7.4967719415	5.0897316128
H9	4.1179704323	6.0444688610	7.1097673349
H10	3.2868793082	9.6136678356	4.7772261434
C11	1.3309137769	10.5603842339	6.3353588639
O12	1.4793255204	11.1716227219	5.2763302124
C13	2.2379692062	6.5124481647	8.9742691865
O14	2.8439927489	5.4714497086	9.1985099097
O15	1.2724054161	6.9886849411	9.7182346324
O16	0.5679279173	10.8509078513	7.3270464149
C17	-2.1972648463	8.0244498909	13.0640918173
C18	-0.9738030568	8.6959603522	13.1544072612
C19	-0.2626226026	8.9421886143	11.9822481818
N20	-0.7388484530	8.5487041523	10.7747631247
C21	-1.9098369444	7.8725276334	10.6865176041
C22	-2.6731795779	7.6006363899	11.8192684516

H23	-2.7717812377	7.8215817186	13.9615400199
H24	-0.5718237460	9.0206730787	14.1076031280
H25	-3.6105789802	7.0649577824	11.7205764040
N26	1.5560060667	9.7285694664	10.6479037634
C33	1.0234999455	9.6142933837	11.8249509777
O30	1.6804071565	10.1479921541	12.8649499617
N29	-1.2966684299	7.7387094205	8.3812711815
C40	-2.1814760781	7.5096105918	9.2995523127
O36	-3.3547338761	6.9779225965	8.9285297703
C37	2.9549832179	10.6226708191	12.3239080220
H38	3.7388742023	9.9678922676	12.7147666424
H39	3.1075058422	11.6407063787	12.6880807395
C39	2.7900283811	10.5307768923	10.7809176251
H40	3.6152311648	9.9691890402	10.3319378447
C38	-1.9054643731	7.4069132410	7.0762020414
H42	-2.1076732816	8.3646813926	6.5823162334
C41	-3.2288695561	6.7130343607	7.4964658877
H41	-3.1925388700	5.6262339699	7.3643479534
H43	-4.1170400221	7.1152785358	7.0072615272
C43	2.6372529791	11.8810181274	10.0770152096
H44	1.8785688214	12.4927861603	10.5788285305
H45	3.5852903910	12.4288409095	10.0923664330
H46	2.3260173739	11.7351623335	9.0390898161
C46	-1.0042447528	6.5440853561	6.1995606090
H47	-0.7485552450	5.6075141314	6.7052649304
H48	-1.5097014446	6.3065074403	5.2575158140
H49	-0.0792396007	7.0744574114	5.9631369378
O50	-1.2338659502	10.7505658928	9.1031905579
H51	-0.5184611592	11.3909321477	8.9273233637
O52	-1.9325730771	10.7863995839	7.8189526199
H53	-1.1199866732	10.8115496192	7.2409519060

Cartesian coordinates of **2a-HOOH-COO**

atom	x	y	z
O16	0.0080505492	-0.1036537047	-0.0765848111
H51	-0.1707279138	0.0846345841	1.4935513142
Ru1	2.2736672051	0.0258916174	2.6077713927
C2	4.1266606147	-1.0490216517	-1.8097545873
C3	4.8877117760	-0.5671615300	-0.7449101060
C4	4.2545457957	-0.2980603893	0.4628065342
N5	2.9228734622	-0.4712756649	0.6229579116
C6	2.1838182808	-0.9562127773	-0.3966295186
C7	2.7602350676	-1.2571722667	-1.6304642628
H8	4.5938904081	-1.2706882670	-2.7651842993
H9	5.9569522725	-0.3996683196	-0.8046387310
H10	2.1374433166	-1.6497246701	-2.4271828137
C11	0.7265411912	-1.1441554653	-0.0201533615
O12	0.4277409734	-2.2625339596	0.4682530579
C13	5.0321606175	0.1628929838	1.6834978717
O14	6.2376295418	0.3711824497	1.5912553134
O15	4.3184043409	0.2791410857	2.7681771931
C17	1.7784191782	1.1492061400	7.1934751502
C18	1.8051291101	2.1614119166	6.2289569998
C19	1.9218982812	1.7961098064	4.8889499987
N20	2.0129670296	0.4964524713	4.5261830731
C21	2.0026986177	-0.4874251993	5.4549242922
C22	1.8775824387	-0.1926939864	6.8108418076
H23	1.6851712070	1.4058012166	8.2434605546
H24	1.7392478791	3.2087718889	6.5006875582
H25	1.8629625681	-0.9953265541	7.5393989927
N26	2.0927290305	2.1459744723	2.5260512056
C33	1.9759522208	2.6605268072	3.7086017096
O30	1.9101252585	3.9956371093	3.8118836709
N29	2.3310382519	-1.8708752765	3.5345248813
C40	2.1386436272	-1.7951370999	4.8113071591
O36	2.0335528856	-2.9368555886	5.5043411198
C37	2.1082071165	4.5069293694	2.4544046459
H38	3.0731494910	5.0208253760	2.4386175051
H39	1.3058708934	5.2197329917	2.2523786501
C39	2.0625155524	3.2482754254	1.5410722974
H40	2.9665746817	3.1781271037	0.9275452930
C38	2.3915429710	-3.2969931259	3.1577516508
H42	1.5933051865	-3.4728236646	2.4298391041
C41	2.1134109599	-4.0116437370	4.5125583829
H41	2.9208979192	-4.6809046135	4.8206987652
H43	1.1613009966	-4.5467858443	4.5368137734

C43	0.8212464022	3.1610059300	0.6511389790
H44	-0.0884479703	3.2913333669	1.2478487243
H45	0.8508096658	3.9492460158	-0.1089090782
H46	0.7617029178	2.1897016722	0.1516256015
C46	3.7396861296	-3.6585970813	2.5349117957
H47	4.5622231195	-3.4394480717	3.2233358801
H48	3.7623659091	-4.7254030674	2.2879598059
H49	3.8992260722	-3.0930619641	1.6146766200
O50	0.0842574605	-0.0550606952	2.4652627790
O52	-0.5690619841	-1.3288392917	2.7732971495
H53	-0.3553885328	-1.8417208955	1.9427070623

Cartesian coordinates of **ts-2a-OOH-COOH**

atom	x	y	z
O16	0.00000000000000	0.00000000000000	0.00000000000000
H51	0.00000000000000	0.00000000000000	1.2122848069000
Ru1	2.1601915579269	0.00000000000000	2.6433110143006
C2	4.3094739817341	-1.1038312583633	-1.6936537335899
C3	4.9661813079123	-0.7019685691340	-0.5343044797642
C4	4.2186824900590	-0.4107184312349	0.5998944451989
N5	2.8568657565607	-0.4628374315712	0.6198090612653
C6	2.2134745793719	-0.8399900423247	-0.5107737132939
C7	2.9249481225814	-1.1884606375381	-1.6676309167036
H8	4.8650589479099	-1.3516704171484	-2.5936712609023
H9	6.0434636850580	-0.6142506420046	-0.4539000439415
H10	2.3440802438019	-1.5205667424702	-2.5189634399652
C11	0.6816359000272	-0.8925873435827	-0.6433386632815
O12	0.2381578960766	-1.7128858422257	-1.4392173326260
C13	4.9580191885136	-0.0451482571482	1.8787834016959
O14	6.1820742348185	0.0453331867350	1.8620526432638
O15	4.2029821021192	0.1287818590236	2.9215310142559
C17	1.9634466763588	1.1796954237078	7.2369062236071
C18	1.9184976787811	2.1706688280392	6.2513241749949
C19	1.9268946297243	1.7835915136289	4.9133605563431
N20	1.9627608528573	0.4739995496931	4.5597874560809
C21	2.0480695645845	-0.4862615582653	5.5135296319042
C22	2.0414365952650	-0.1668563852257	6.8695854164072
H23	1.9566207481160	1.4566909978670	8.2855401212442
H24	1.8895656263054	3.2243640051584	6.5049276820544
H25	2.1065289530019	-0.9565842610196	7.6094250113776
N26	2.0549836438172	2.1067570952427	2.5496842393244
C33	1.9655763514680	2.6360570258474	3.7284082616231
O30	1.9423486294555	3.9727255461926	3.8206055439956
N29	2.2065894732170	-1.9352339991838	3.6108894995031
C40	2.1791839905489	-1.8063651252402	4.9038277824745
O36	2.2818315618543	-2.9115288998435	5.6506774106259
C37	2.1674213581045	4.4617216926339	2.4590449506144
H38	3.1657129421381	4.9079512898593	2.4361150437836
H39	1.4142593379352	5.2256424262759	2.2568770428852
C39	2.0306770510658	3.2037235092537	1.5552098528584
H40	2.9039709077870	3.0921142137822	0.9050012209414
C38	2.4194771818797	-3.3699703186328	3.3021880803805
H42	1.5836592593793	-3.7121492083045	2.6814251900438
C41	2.3755315448623	-4.0295014237732	4.7116393697441
H41	3.2834023876674	-4.5863453555999	4.9553780066784
H43	1.5006431828434	-4.6644296777669	4.8720599028886
C43	0.7484561178842	3.1730685162047	0.7222753130138
H44	-0.1274448254654	3.3336095974680	1.3602318459455
H45	0.7791190284751	3.9673365454857	-0.0316242398823
H46	0.6272381652728	2.2093942103121	0.2208216357703
C46	3.7329091030191	-3.5962765751164	2.5546921261762
H47	4.5803523985124	-3.2106580145297	3.1297440347915
H48	3.8812285257146	-4.6673655483984	2.3802374115810
H49	3.7153684850152	-3.0921577292435	1.5865780576206
O50	0.0593149755842	-0.0060672410192	2.3750472013704
O52	-0.6206733353036	-1.2734436526506	2.6831233745758
H53	0.0783607277793	-1.7195789229217	3.1856581207802

Cartesian coordinates of **2a-OOH-COOH**

atom	x	y	z
O16	-0.0151129451	-0.0941367537	0.0184235566
H51	0.1057078089	-0.1044406904	1.1225321381
Ru1	2.1954074710	0.0207711278	2.6650853933
C2	4.3431096479	-1.2815327266	-1.6279540209

C3	4.9877723197	-0.7950396218	-0.4973128687
C4	4.2311733659	-0.4176296355	0.6071291416
N5	2.8702841933	-0.4742213199	0.6264440807
C6	2.2367579756	-0.9107364031	-0.4923676071
C7	2.9566466728	-1.3416307344	-1.6149070990
H8	4.9047478633	-1.6019003469	-2.5007954173
H9	6.0637819552	-0.6976401658	-0.4126244680
H10	2.3803229953	-1.7078412287	-2.4548134372
C11	0.7117827183	-0.9228176106	-0.6838509726
O12	0.2698687039	-1.6248209498	-1.5814591766
C13	4.9775088613	0.0721802825	1.8450738083
O14	6.1992660287	0.1897767797	1.7904909649
O15	4.2359759012	0.3270734365	2.8755843317
C17	1.9828212200	1.2047062781	7.2504983065
C18	1.9129411950	2.1966141504	6.2675058602
C19	1.9238293862	1.8113679645	4.9287781479
N20	1.9968676012	0.5038754037	4.5723336023
C21	2.0944578542	-0.4588110050	5.5238228362
C22	2.0813480356	-0.1401290682	6.8796159306
H23	1.9760074891	1.4792385945	8.2999325459
H24	1.8607499471	3.2489278055	6.5231947340
H25	2.1572880404	-0.9302249974	7.6181740313
N26	1.9704887745	2.1395535927	2.5620829461
C33	1.9089635775	2.6639494181	3.7448559420
O30	1.8555063165	4.0014990700	3.8412487706
N29	2.3401366003	-1.8736960460	3.6175434181
C40	2.2286200025	-1.7715719215	4.9029205475
O36	2.1953252909	-2.9004195417	5.6286391275
C37	2.0315491027	4.4987208662	2.4774634955
H38	3.0193257234	4.9656195474	2.4254018520
H39	1.2580343520	5.2482439588	2.2978638251
C39	1.8968481928	3.2400209660	1.5750823846
H40	2.7536133853	3.1499038979	0.8999453576
C38	2.3279322746	-3.3109743026	3.2762844250
H42	1.3587233797	-3.5025300942	2.8014137441
C41	2.4135106048	-3.9838372265	4.6731974866
H41	3.4039159317	-4.4062913931	4.8742945532
H43	1.6479690626	-4.7406656333	4.8517203242
C43	0.5938552594	3.1871060578	0.7756212732
H44	-0.2685920948	3.3196939291	1.4381814652
H45	0.5825379660	3.9884758714	0.0287005703
H46	0.4857506191	2.2271095766	0.2651613164
C46	3.4571941728	-3.7117126206	2.3326806842
H47	4.4324705380	-3.4563354302	2.7588430211
H48	3.4268787787	-4.7911479453	2.1491659629
H49	3.3537368744	-3.2032382954	1.3721437068
O50	0.1416447983	-0.1884771041	2.4027222410
O52	-0.2939065460	-1.5883148424	2.5960171627
H53	-1.2508833535	-1.4723881199	2.4860828710

Cartesian coordinates of **ts-2a-oxo**

atom	x	y	z
Ru1	0.3394951433	8.6991381038	9.2362019825
C2	3.8284255431	8.3580975902	5.7643026919
C3	3.6838606063	7.4606711321	6.8212613522
C4	2.6168392202	7.6234008815	7.6977079888
N5	1.7059225463	8.6133024782	7.5451255960
C6	1.8070737365	9.4526571880	6.4939912744
C7	2.8826481310	9.3658752595	5.6050018413
H8	4.6606118718	8.2679669324	5.0715586740
H9	4.3632470385	6.6359342738	7.0024554341
H10	2.9446970278	10.0921943452	4.8022862034
C11	0.7229460905	10.4978750414	6.2792547524
O12	1.0605886939	11.6731577269	6.1730788827
C13	2.4030229024	6.6464090812	8.8475749432
O14	3.1975892968	5.7240533725	8.9999249680
O15	1.3449610273	6.8751730405	9.5680802392
C17	-2.2656353599	8.1247932283	13.1447804749
C18	-1.0039098219	8.7207026201	13.2300191180
C19	-0.2664417289	8.8994443969	12.0620322805
N20	-0.7555240510	8.4971409191	10.8588500020
C21	-1.9781934695	7.9072885494	10.7718673890
C22	-2.7618458535	7.7093643608	11.9018897708
H23	-2.8582885031	7.9782608047	14.0410939727
H24	-0.5917705527	9.0426788803	14.1799616890
H25	-3.7343183383	7.2391130702	11.8069375926

N25	1.6285636142	9.4965573172	10.7397070714
C33	1.0653253674	9.4732070323	11.9053213277
O30	1.7454113173	9.9968644561	12.9351590899
N28	-1.3604625056	7.7210356197	8.4742978967
C40	-2.2569047750	7.5277774380	9.3893187397
O36	-3.4125963099	6.9678434830	9.0212885457
C37	3.0505056113	10.3797755564	12.3917337574
H38	3.7933182786	9.7023935606	12.8216223196
H39	3.2514261838	11.4037541325	12.7133429542
C39	2.9026212149	10.2296486109	10.8504349431
H40	3.7015777824	9.6021708590	10.4421241949
C36	-1.8719829191	7.2006791601	7.1912295205
H42	-1.8451067533	8.0235160264	6.4719167914
C41	-3.3259283972	6.7919846185	7.5662549352
H41	-3.5514448367	5.7443464743	7.3531952067
H43	-4.0884407948	7.4335730881	7.1184483046
C43	2.8403575676	11.5569333292	10.0895449520
H44	2.0778863828	12.2134051102	10.5206357685
H45	3.8103392115	12.0631569214	10.1405386843
H46	2.5830274632	11.3958052811	9.0400510301
C46	-1.0139824306	6.0432184055	6.6787993532
H47	-0.9710358912	5.2284078906	7.4087351524
H48	-1.4304788748	5.6567274884	5.7422403522
H49	0.0043841930	6.3853348160	6.4840676533
O50	-0.1801111671	10.4807805723	8.9726625347
O52	-0.4694368932	9.9943273722	6.2030516849
O51	-1.7159962860	10.8277497875	8.0660964218
H52	-1.5643683222	11.7833122812	8.1273802281
H53	-1.2060498952	10.5093512743	7.0962268625

Cartesian coordinates of **styrene**

atom	x	y	z
C1	-2.9910345113	0.8273536426	-0.2406208245
C2	-3.7133669081	2.0332100104	-0.3001372556
C3	-5.0845773134	2.0559586678	-0.0665781762
C4	-5.7718165957	0.8758708010	0.2323185924
C5	-5.0714767501	-0.3280574053	0.2961379449
C6	-3.6973764937	-0.3491489056	0.0622829999
H7	-3.1981168387	2.9614332772	-0.5283303439
H8	-5.6226755697	2.9985019340	-0.1180742518
H9	-6.8425868435	0.8976286448	0.4138133419
H10	-5.5940431543	-1.2519267697	0.5281728840
H11	-3.1568735831	-1.2913770200	0.1144099361
C12	-1.5404458118	0.7435269148	-0.4804888215
C13	-0.7051950313	1.7374861224	-0.8078618388
H14	-1.0317736800	2.7656483189	-0.9332212623
H15	0.3521836447	1.5479393447	-0.9604070944
H16	-1.1249246157	-0.2588361591	-0.3779379594

Cartesian coordinates of **ts-2a-o-ene**

atom	x	y	z
Ru1	0.5133821074	8.9662062821	9.1979348015
C2	3.6494696161	7.3927890596	5.8339929642
C3	3.3881065021	6.7057807821	7.0243316642
C4	2.4046952279	7.1980958643	7.8673726514
N5	1.6960821535	8.3121455346	7.5592487296
C6	1.8824188649	8.9520514220	6.3868200822
C7	2.8965679124	8.5155694288	5.5190858156
H8	4.4262242168	7.0439986694	5.1584479498
H9	3.9139056521	5.8058498225	7.3213117569
H10	3.0598698297	9.0801673180	4.6077116955
C11	0.9443437331	10.1027337055	5.9764908586
O12	-0.2634803949	9.7534199129	5.9012477089
C13	2.0216977525	6.4807708909	9.1536731222
O14	2.6530611135	5.4948484584	9.5149335659
O15	0.9823363608	6.9927098774	9.7624743054
O16	1.5045275781	11.1882066431	5.7405350500
C17	-1.8705258519	9.2647601629	13.3045850590
C18	-0.4945473117	9.5375785918	13.2808912579
C19	0.1627115199	9.4852723949	12.0576548576
N20	-0.5088617094	9.1913999305	10.9266297748
C21	-1.8209586450	8.8853177695	10.9403581918
C22	-2.5461981075	8.9246728299	12.1324277140
H23	-2.4099855510	9.3045211077	14.2450668509
H24	0.0544390571	9.7779192438	14.1840564797
H25	-3.6048257690	8.6939497716	12.1295835018

N26	2.0884289501	9.5241729546	10.6114372034
C33	1.5976304020	9.6899022762	11.7913625404
O30	2.4274661645	10.0545656886	12.7743104466
N29	-1.4274704113	8.4375530178	8.6230648076
C40	-2.2726476146	8.4946312168	9.6052117358
O36	-3.5453423320	8.1698372750	9.3599194873
C37	3.7656907334	10.0845346274	12.1714952280
H38	4.3453741451	9.2820772693	12.6342772727
H39	4.2095466985	11.0524132152	12.4136667162
C39	3.5204930117	9.8764616203	10.6478991700
H40	4.0915325208	9.0203352619	10.2741378724
C38	-2.1534985036	8.0144739464	7.4023925934
H42	-2.1002049231	8.8522403366	6.7018274647
C41	-3.5860069756	7.7595893308	7.9498890134
H41	-3.8694430736	6.7031216403	7.9306521035
H43	-4.3587754170	8.3563903513	7.4614800529
C43	3.8032395782	11.1077833943	9.7846401348
H44	3.2766178800	11.9838772039	10.1759770915
H45	4.8780593466	11.3176810896	9.7749730479
H46	3.4640323889	10.9474128281	8.7586936705
C46	-1.5097641234	6.8018932051	6.7385225216
H47	-1.3782974422	5.9773304630	7.4467085834
H48	-2.1407656792	6.4616860789	5.9099320694
H49	-0.5447667717	7.0997272909	6.3280750760
O50	0.5427788271	10.7409093754	8.6745136037
C60	-2.4438043917	12.4923012251	9.8690864023
C61	-2.6216155918	13.1653593324	11.1009479031
C62	-3.7831711625	13.0134405750	11.8504384047
H66	-1.8274598242	13.8158845906	11.4602867929
H67	-3.8905329007	13.5456967957	12.7922766176
H63	-1.4119746475	11.2363126089	7.5272553397
C64	-0.7850438666	11.9722200066	8.0169302295
H65	-0.0153709300	12.3715008436	7.3657060228
C59	-1.2259957729	12.7022944150	9.1125817242
H60	-0.57113645539	13.4878672686	9.4876315436
C63	-4.8134972077	12.1870557322	11.3926636382
H62	-5.7259742802	12.0746611757	11.9717459122
C65	-4.6648343247	11.5203967311	10.1715343652
H64	-5.4666182989	10.8883924179	7.986833272
C66	-3.5043960723	11.6703698181	9.4200616181
H68	-3.4216025028	11.1735624474	8.4581531542

Cartesian coordinates of 106 **2a-o-ene**

atom	x	y	z
Ru1	0.5254481675	8.8294473027	9.1465281952
C2	3.8765411707	7.5059625584	5.9044746416
C3	3.6012065639	6.7822763489	7.0704957755
C4	2.5555212405	7.2058152047	7.8743067132
N5	1.8010999267	8.2845607016	7.5510969080
C6	2.0025743736	8.9573781849	6.4012042846
C7	3.0787289131	8.5931063591	5.5747533076
H8	4.7002310208	7.2120317058	5.2591307251
H9	4.1624999088	5.9064802812	7.3748277727
H10	3.2520087627	9.1847842560	4.6825984218
C11	1.0189944343	10.0647005815	5.9715181804
O12	-0.1712952689	9.6632862493	5.8852814318
C13	2.1476172181	6.4510513737	9.1278578065
O14	2.7989168832	5.4886017371	9.5097315712
O15	1.0505947375	6.9004243517	9.6941219375
O16	1.5368679523	11.1697324912	5.7352194876
C17	-1.9348244592	8.8775198205	13.2140219709
C18	-0.5842229974	9.2621482034	13.2123747809
C19	0.0883009876	9.2879595045	11.9977327286
N20	-0.5452334977	8.9655233208	10.8511214856
C21	-1.8301583775	8.5597349922	10.8420328963
C22	-2.5691161848	8.5140211730	12.0274953860
H23	-2.4843203465	8.8516777069	14.1491298633
H24	-0.0673798840	9.5279552203	14.1273192134
H25	-3.6047462486	8.1950012535	12.0079313178
N26	2.0232795725	9.5089631073	10.5751195937
C33	1.5043756300	9.6207683635	11.7502533702
O30	2.2831644741	10.0617803070	12.7427888332
N29	-1.3687929965	8.2001060332	8.5253006236
C40	-2.2363513084	8.1828911493	9.4897286353
O36	-3.4946787453	7.8332586691	9.1997874961
C37	3.6200684316	10.2210698000	12.1559037581

H38	4.2644584379	9.4670904775	12.6149571118
H39	3.9719312252	11.2211754068	12.4168406133
C39	3.4094774695	10.0126777185	10.6277035612
H40	4.0722469742	9.2293405765	10.2460770628
C38	-2.0576912055	7.8198007258	7.2692812684
H42	-2.0362788524	8.7049221495	6.6264437572
C41	-3.4814153858	7.4600106490	7.7778391901
H41	-3.6931740456	6.3876612127	7.7249868239
H43	-4.2817834259	8.0184101486	7.2892689090
C43	3.5616738484	11.2802420373	9.7837291031
H44	2.9535279666	12.0923829617	10.1944167995
H45	4.6101230648	11.5963970828	9.7727526080
H46	3.2308746591	11.1063130162	8.7570334840
C46	-1.3454209339	6.6867593004	6.5386764042
H47	-1.1802882984	5.8259764551	7.1949901529
H48	-1.9487618590	6.3683988221	5.6812975205
H49	-0.3940393991	7.0628379542	6.1616978852
O50	0.3913781466	10.6951596818	8.6236663020
C60	-2.1568348416	12.6089708029	10.2382940331
C61	-2.1495618294	13.5660950749	11.2985207652
C62	-3.2527777510	13.7538126516	12.1144418371
H66	-1.2494282221	14.1548853677	11.4585554484
H67	-3.2123134329	14.4901674937	12.9131192562
H63	-1.6488220436	10.8068071389	8.1875226042
C64	-0.7788368402	11.4525646701	8.3435616915
H65	-0.5748909245	11.9557918675	7.3855710850
C59	-0.9989347599	12.4453572240	9.4401551295
H60	-0.1449557395	13.0832204868	9.6615196570
C63	-4.4201902639	13.0034454112	11.9145885528
H62	-5.2864584086	13.1549363386	12.5521522441
C65	-4.4604660718	12.0638124474	10.8765067804
H64	-5.3662816883	11.4869459171	10.7062993307
C66	-3.3611850632	11.8650012151	10.0533480737
H68	-3.4273827678	11.1425639306	9.2461324125

Cartesian coordinates of **ts-trans-2a-oxo**

atom	x	y	z
N5	-0.0804421640	-0.0321508163	0.0826400369
Ru1	-0.0548079391	0.0269130686	2.4322499166
N20	1.1407861794	0.0035055819	4.0451063695
C2	0.0861174611	-0.4916501653	-2.6437170973
C3	1.2350858351	-0.5271306176	-1.8513764798
C4	1.1101992055	-0.2849973684	-0.4861396220
C6	-1.1855579822	0.0403684841	-0.6708541079
C7	-1.1366240469	-0.1930177249	-2.0479262280
H8	0.1489415036	-0.6789995617	-3.7126406235
H9	2.2244941178	-0.7278023836	-2.2465225822
H10	-2.0684658828	-0.1161350520	-2.5967063300
C11	-2.4744801219	0.4735131558	0.0346737857
O12	-3.5000627209	0.5367223151	-0.6567565915
C13	2.3079721936	-0.2553474941	0.4415644667
O14	2.0204486147	0.1345791102	1.6439600314
O15	3.4184261678	-0.5705435554	0.0177097502
O16	-2.2892903022	0.7516884069	1.2603473602
C17	3.0303975774	0.0214072177	6.0262776817
C18	2.5225148233	1.2307844196	5.5406184187
C19	1.5687222515	1.1858386949	4.5269711054
C21	1.6553050723	-1.1650502417	4.4649037895
C22	2.6065267648	-1.1953772641	5.4812937323
H23	3.7754069166	0.0279773947	6.8148630319
H24	2.8618354638	2.1866771910	5.9228542066
H25	3.0120416804	-2.1429210354	5.8166914924
N26	0.1250512350	2.0868106478	2.8400524375
C27	0.9333069641	2.3084255432	3.8230580635
O28	1.1630218785	3.5760854680	4.1698729539
N29	0.3617165587	-2.0906540183	2.6631738137
C30	1.1252803576	-2.2915957456	3.6849996292
O31	1.4086091834	-3.5521513424	4.0250707146
C32	0.4552592585	4.3867448109	3.1642732228
H33	1.2200727857	4.8477596010	2.5334284288
H34	-0.1008974744	5.1550926481	3.7032832107
C35	-0.4536539713	3.3773354157	2.4072547979
H36	-0.3276638511	3.4607085938	1.3245142124
C37	-0.0872729564	-3.4081632179	2.1624795419

H38	-1.1425091069	-3.5079926401	2.4466275554
C39	0.8051766067	-4.3828487232	2.9780547066
H40	1.6237463475	-4.7979387406	2.3816172359
H41	0.2586583293	-5.1868475312	3.4721502313
C42	-1.9370230560	3.4593354126	2.7697387305
H43	-2.0713552231	3.4065148672	3.8559414365
H44	-2.3481981708	4.4098667904	2.4121163708
H45	-2.4704290108	2.6278618279	2.2993174335
C46	0.0492586087	-3.5607644950	0.6516790061
H47	1.0836725528	-3.4004378935	0.3334872009
H48	-0.2589991951	-4.5679966395	0.3521463797
H49	-0.5904114926	-2.8421288085	0.1358343384
O50	-1.4720031881	-0.2078107973	3.4941673739

Cartesian coordinates of **trans-2a-oxo**

atom	x	y	z
Ru1	0.4412030853	8.7098868955	9.0520998804
C2	3.2223540331	4.5849193523	9.6552749562
C3	2.1073503386	4.7009844709	10.4761798903
C4	1.2553779783	5.8049855162	10.3369533925
N5	1.5197437537	6.7626970996	9.4254992788
C6	2.5962562378	6.6467918901	8.6143526579
C7	3.4718691632	5.5733372552	8.7002021858
H8	3.8889058964	3.7316878355	9.7508010210
H9	1.8745407417	3.9519467800	11.2257643446
H10	4.3115733107	5.5442830682	8.0158215757
C11	2.7936115265	7.7295608053	7.5681359152
O12	3.7665726967	7.6793032493	6.8242026536
C13	-0.0035291283	5.9809282638	11.1844088594
O14	0.1750968224	6.5285992927	12.2931017421
O15	-1.0658770074	5.6101890835	10.6179956301
O16	1.8675726676	8.6463466995	7.5403189800
C17	-2.6043894269	8.8247135632	12.7287992977
C18	-1.3220718337	9.3669846359	12.8765926500
C19	-0.4583284418	9.2885268795	11.7919823097
N20	-0.8576901938	8.7341087123	10.6372711182
C21	-2.0636544276	8.1783926962	10.4923589262
C22	-2.9886904904	8.2122689275	11.5358594511
H23	-3.3000464004	8.8612906377	13.5607772075
H24	-0.9946861527	9.8145743206	13.8071955306
H25	-3.9629884283	7.7544120968	11.4139423404
N26	1.6155687555	9.5826806991	10.6067375659
C27	0.9432531910	9.7279945166	11.7024535408
O28	1.5658529496	10.2751927648	12.7444143308
N29	-1.2621241623	7.6534709885	8.2747775315
C30	-2.2084510718	7.5762564995	9.1553941287
O31	-3.3278560520	6.9469126989	8.8181930426
C32	2.9262711064	10.5838311609	12.2901329648
H33	3.6139298174	10.0680702195	12.9616198783
H34	3.0593509757	11.6647215539	12.3802833137
C35	2.9867362438	10.0834341382	10.8165653321
H36	3.6686934981	9.2306432622	10.7229266720
C37	-1.6515167497	6.8229837795	7.1153779211
H38	-1.5614938383	7.4255576457	6.2067690764
C39	-3.1392886395	6.5042752510	7.4360191848
H40	-3.3705007364	5.4381420949	7.4030748566
H41	-3.8495269108	7.0608466127	6.8187683710
C42	3.3578720867	11.1484005472	9.7875203437
H43	2.6901591778	12.0120742683	9.8652448424
H44	4.3883248544	11.4821244777	9.9465464303
H45	3.2730727691	10.7360593363	8.7790483885
C46	-0.7722301261	5.5746212717	7.0241197649
H47	-0.8040970472	5.0318146576	7.9736426924
H48	-1.1283915279	4.9262810742	6.2160205403
H49	0.2621151476	5.8518293578	6.8095730261
O50	-0.1757952037	10.2877903651	8.4941320665

Cartesian coordinates of **ts-trans-2a-o-ene**

atom	x	y	z
Ru1	0.3344456294	8.5844242532	8.7951398901
C2	3.6229250539	5.0002519772	9.8521362376
C3	2.5428217354	5.1310329001	10.7145467246
C4	1.5605847292	6.0990711403	10.4584404590
N5	1.6686604039	6.9140237556	9.3905432984
C6	2.7147597672	6.7835011937	8.5387282469

C7	3.7104663182	5.8378521533	8.7364708132
H8	4.3884398422	4.2515553616	10.0389607381
H9	2.4344088675	4.4962839187	11.5878796863
H10	4.5149338952	5.7845146878	8.0124412799
C11	2.7436419353	7.6977251771	7.3276719857
O12	3.6490860306	7.5948970422	6.5063204279
C13	0.3302087429	6.2669701200	11.3500888971
O14	0.4914303263	7.0263258563	12.3308176489
O15	-0.6899728325	5.6576922656	10.9412438337
O16	1.7524934759	8.5417951220	7.2536603171
C17	-2.8111874570	8.9129935156	12.3587543553
C18	-1.5975816084	9.6001654968	12.4411012580
C19	-0.6912429791	9.4509874263	11.3958753348
N20	-0.9825711124	8.6836253329	10.3331421438
C21	-2.1261369533	7.9903313069	10.2616676574
C22	-3.0858070611	8.0877331933	11.2654023045
H23	-3.5367378004	9.0034577067	13.1604824145
H24	-1.3467891490	10.2176065054	13.2954870099
H25	-4.0047080779	7.5180208210	11.1943949922
N26	1.3624209962	9.7959278570	10.2056043554
C27	0.6527333143	10.0207220131	11.2651367197
O28	1.1939363507	10.7676914603	12.2277807263
N29	-1.1966115924	7.1960483805	8.1805995995
C30	-2.1601156871	7.1657493284	9.0463296764
O31	-3.1861514313	6.3523964112	8.8134962830
C32	2.5310212182	11.1330254289	11.7569635079
H33	3.2449930182	10.7749230334	12.5008220990
H34	2.5696424604	12.2245977308	11.7011729815
C35	2.6746936664	10.4472466030	10.3662322490
H36	3.4359465983	9.6592031504	10.3987763013
C37	-1.4453432828	6.1152282997	7.1978902433
H38	-1.3526965189	6.5227481249	6.1886531550
C39	-2.9138933706	5.7292462839	7.5173495099
H40	-3.0696829191	4.6553122516	7.6339603398
H41	-3.6342621722	6.1378946949	6.8028076719
C42	2.9760519033	11.3994784338	9.2110843788
H43	2.2240301652	12.1934908918	9.1580591124
H44	3.9621599519	11.8567914910	9.3437569600
H45	2.9689782363	10.8502104948	8.2664027860
C46	-0.4607414348	4.9624972619	7.4104548132
H47	-0.4856392125	4.6372712369	8.4554278583
H48	-0.7241465199	4.1240510323	6.7559070131
H49	0.5560791864	5.2776133024	7.1659235045
O50	-0.5588996654	10.0651390245	8.1169246267
C51	-1.1452166188	10.2593165428	5.4594469545
H52	-2.0911634943	10.7992425258	5.4408326758
C53	-1.0955259745	6.7926597248	2.9602692138
C54	-2.2551261923	7.5603244442	3.1005581977
C55	-2.2521925407	8.6823382460	3.9228148103
C56	-1.0927506700	9.0691616229	4.6344363512
C57	0.0720398390	8.2785591396	4.4821731849
C58	0.0627558802	7.1604777575	3.6549876861
H59	-1.0927213338	5.9183890162	2.3150122368
H60	-3.1600677222	7.2851799549	2.5648522271
H61	-3.1549809582	9.2808638203	4.0242048595
H62	0.9729914647	8.5300455086	5.0314839857
H63	0.9688679708	6.5694039242	3.5522294705
C64	-0.1545054951	10.7357866792	6.3011759771
H65	-0.2495247039	11.7457413834	6.6820714777
H66	0.8467933584	10.3236848708	6.2692070577

Cartesian coordinates of **trans-2a-o-ene (m = 3)**

atom	x	y	z
Ru1	0.4227545906	8.5195821734	8.8057112222
C2	3.6342207058	5.0065926905	10.0391698925
C3	2.5404963326	5.1842300237	10.8748486381
C4	1.5742933406	6.1529103180	10.5650091814
N5	1.7126722539	6.9197548452	9.4640387059
C6	2.7735751337	6.7446906901	8.6350172849
C7	3.7531091435	5.7982223528	8.8926908628
H8	4.3872445584	4.2577427717	10.2706049768
H9	2.4084339924	4.5864692934	11.7706463138
H10	4.5715485156	5.7089577956	8.1879782672
C11	2.8351893499	7.6129594328	7.3906959752
O12	3.7655418857	7.4795171137	6.6035456767
C13	0.3372355516	6.3675060797	11.4383865219

O14	0.4965786696	7.1748916651	12.3805785216
O15	-0.6782371993	5.7330456833	11.0608678919
O16	1.8435527906	8.4505161468	7.2647160069
C17	-2.9114982620	9.0642423095	12.1477439025
C18	-1.6912562025	9.7319951874	12.2744794650
C19	-0.7222660243	9.5119931922	11.2992222634
N20	-0.9590434083	8.6927487949	10.2628822286
C21	-2.1136460514	8.0219678339	10.1487523303
C22	-3.1339083651	8.1900475173	11.0800133843
H23	-3.6852037223	9.2101736026	12.8942579244
H24	-1.4834206991	10.3895730873	13.1103850352
H25	-4.0601508650	7.6374021656	10.9766993630
N26	1.3977185193	9.7587365290	10.2106638277
C27	0.6388481226	10.0482162698	11.2206821775
O28	1.1480315651	10.8248356949	12.1748292335
N29	-1.0551174230	7.1113470574	8.1839849394
C30	-2.0813550845	7.1370903380	8.9781751045
O31	-3.0971560354	6.3242304053	8.7077563483
C32	2.5199938025	11.1312743337	11.7637648459
H33	3.1801967204	10.7883977690	12.5623450383
H34	2.5938205918	12.2175196139	11.6612005480
C35	2.7195504347	10.3780686783	10.4155479501
H36	3.4515122447	9.5697419904	10.5279969558
C37	-1.2448011594	5.9789798553	7.2453123777
H38	-1.0533967103	6.3256974684	6.2271466911
C39	-2.7458258919	5.6530333917	7.4532638987
H40	-2.9521790233	4.5898163238	7.5858294554
H41	-3.3884363820	6.0690958326	6.6720876886
C42	3.1158776919	11.2656019047	9.2376421670
H43	2.4012894846	12.0857873087	9.1137127934
H44	4.1128336705	11.6882674301	9.3999273165
H45	3.1303143132	10.6778469687	8.3162338203
C46	-0.3189820821	4.8151763975	7.6107600870
H47	-0.4330094914	4.5614676347	8.6695243673
H48	-0.5607869828	3.9427425361	6.9933801186
H49	0.7242553682	5.0807843691	7.4262809219
O50	-0.5205987168	10.0696367664	8.0557017598
C51	-1.4372207515	10.0019040538	5.8312683042
H52	-2.4114012332	10.4433981492	6.0367454676
C53	-1.3457625502	7.0534498307	2.7643423625
C54	-2.5327815263	7.7311362084	3.0764993304
C55	-2.5498282202	8.6889767521	4.0780511658
C56	-1.3725649446	9.0142564018	4.8181413421
C57	-0.1776297348	8.3051788943	4.4864089037
C58	-0.1769049881	7.3499785576	3.4790636242
H59	-1.3326748661	6.3048671736	1.9772248856
H60	-3.4449985281	7.5080311956	2.5287205842
H61	-3.4727125153	9.2157517553	4.3105053592
H62	0.7329742084	8.4906819116	5.0465476593
H63	0.7461092570	6.8242348029	3.2484629401
C64	-0.3097684995	10.4714296924	6.7003385185
H65	-0.2980711222	11.5739616969	6.7051749144
H66	0.6601563107	10.1241987115	6.3362300882

Cartesian coordinates of **MECP**

atom	x	y	z
O50	0.00000000000000	0.00000000000000	0.00000000000000
C51	0.00000000000000	0.00000000000000	2.20000000000000
Ru1	1.6486614751620	0.00000000000000	-1.2003506796685
C2	5.5650615279099	-1.1599200575122	-3.8927604499331
C3	4.8270436796699	-0.0532069907021	-4.2855968183847
C4	3.7219624898113	0.3611077821271	-3.5258046945852
N5	3.3538948053440	-0.3300586833738	-2.4265401011200
C6	4.0841960255795	-1.4060369854710	-2.0250662645634
C7	5.1926244050330	-1.8448862686073	-2.7320600831325
H8	6.4240349998427	-1.4851982423640	-4.4739494834014
H9	5.0832225400429	0.5135979455088	-5.1747950117915
H10	5.7298371750586	-2.7042905126055	-2.3481150131380
C11	3.6637816205668	-2.0958591714235	-0.7388800331824
O12	4.3177538139844	-3.0446021096580	-0.3127771326780
C13	2.9281252149550	1.6104732071337	-3.9134987675391
O14	2.0524922365726	1.4298160879296	-4.7860202713886
O15	3.2601585348365	2.6453597844970	-3.2820629502413
O16	2.6083999691391	-1.5827713470726	-0.1743060201353
C17	-0.9484199012103	3.3623226134700	-3.3292175107472
C18	-1.1108465929788	2.0231794248089	-3.6958405228472

C19	-0.2971272700334	1.0728936275702	-3.0883825054287
N20	0.6181125384572	1.4246965390170	-2.1636443992584
C21	0.7858503617052	2.7116583943639	-1.8130444057473
C22	0.0097441313683	3.7205292929143	-2.3797575548740
H23	-1.5624828152590	4.1277651049353	-3.7923570921474
H24	-1.8353299342748	1.7195057087806	-4.4424097372822
H25	0.1687163884343	4.7524956652980	-2.0904497847086
N26	0.5046289829199	-1.1343697854387	-2.6125242831629
C27	-0.2671190535299	-0.3719105063500	-3.3179872994233
O28	-1.0163409441071	-0.9466512946394	-4.2670616513523
N29	3.6210290382643	1.7803563377983	-0.3533168725790
C30	1.8587999490642	2.8340631610128	-0.8277199330463
O31	2.2772804958029	4.0316475622471	-0.4110014760215
C32	-0.7244538106619	-2.3763273953321	-4.2011284865640
H33	-0.4029295382119	-2.6909964376589	-5.1958368094447
H34	-1.6536615236721	-2.8904787640118	-3.9347519890511
C35	0.3767418620911	-2.5159652244989	-3.1099905318712
H36	1.3371822987786	-2.7955577518608	-3.5601043293016
C37	3.6210290382686	2.2454055343714	0.4249196564059
H38	3.6074274217683	1.7659473483467	1.4076594378217
C39	3.3506123403206	3.7699117672718	0.5411508572433
H40	4.2043033808254	4.3853466570006	0.2497671634622
H41	2.9943531109620	4.0736257610467	1.5305060744281
C42	0.0423472897397	-3.4977122545906	-1.9888645645205
H43	-0.9185167614136	-3.2453028272809	-1.5274925276040
H44	-0.0165671600538	-4.5188091732312	-2.3805109614796
H45	0.8181972789649	-3.4628664508521	-1.2198549914871
C46	4.9222376421512	1.9218467367684	-0.3139031869940
H47	4.8704450849147	2.3098700964340	-1.3361323904149
H48	5.7719853831307	2.3710672165904	0.2133175235410
H49	5.0797501335329	0.8416477800513	-0.3577726795905
H52	-0.8581134239676	0.6392626736329	2.3971750585654
C53	3.4176292752253	0.7365907281342	4.5740601693569
C54	2.2486699617161	1.4895915967332	4.7560274304577
C55	1.1510764662883	1.2652320636751	3.9427908769959
C56	1.1834694933809	0.2632835440711	2.9312175010115
C57	2.3843830037803	-0.4800221205181	2.7506922840920
C58	3.4795878866367	-0.2358628677264	3.5698309739783
H59	4.2795042893758	0.9142362656614	5.2112205859598
H60	2.2055384690077	2.2484954670102	5.5317991447983
H61	0.2411400663179	1.8442636816536	4.0798946243872
H62	2.4616005528166	-1.2065574971508	1.9463280677867
H63	4.3913901529309	-0.8070020786994	3.4219364811638
C64	-0.1558483637349	-0.9447246802232	1.0492281806888
H65	-1.1583124279748	-1.3937555161788	1.0154087852163
H66	0.5967733315386	-1.7371640602871	1.0220659892570

Cartesian coordinates of **trans-2a-o-ene (m = 1)**

atom	x	y	z
Ru1	0.5228089234	8.4572202038	8.6962338820
C2	3.6562620194	5.0657099915	10.1908474186
C3	2.4752724386	5.2047003143	10.9036951943
C4	1.5174175129	6.1520643676	10.5091955581
N5	1.7456824192	6.9450199826	9.4416187139
C6	2.8977503595	6.8043281740	8.7254179249
C7	3.8684330254	5.8794190245	9.0745869940
H8	4.4009236240	4.3333039191	10.4910143577
H9	2.2616508831	4.5910692200	11.7727052577
H10	4.7561381876	5.8253920767	8.4551623841
C11	3.0769005411	7.6843091946	7.5016960496
O12	4.0994098071	7.5953155191	6.8281742330
C13	0.1987220874	6.2861261450	11.2747558574
O14	0.2366563821	7.0613730002	12.2535185714
O15	-0.7431931402	5.6029316433	10.8004921511
O16	2.0753757359	8.4840161067	7.2692427510
C17	-3.0374880865	9.0286845465	11.8123181416
C18	-1.8375218755	9.7228308820	11.9892304371
C19	-0.8056391563	9.4943931315	11.0849501266
N20	-0.9506589654	8.6342155259	10.0532993556
C21	-2.1025467267	7.9562467150	9.8864246394
C22	-3.1799142458	8.1330489807	10.7511455811
H23	-3.8566235775	9.1781917735	12.5080927008
H24	-1.6916259384	10.4104741243	12.8141677331
H25	-4.0913650853	7.5669829369	10.5984565896
N26	1.3535616177	9.8339598606	10.1050212630

C27	0.5329649337	10.0800738439	11.0778606192
O28	0.9644328951	10.8554236442	12.0818954780
N29	-0.9588081017	7.0652020166	7.9701915172
C30	-2.0100640643	7.0678387671	8.7286883369
O31	-3.0062885019	6.2269064240	8.4340029658
C32	2.3269727121	11.2439376795	11.7327668298
H33	2.9675070560	10.9959069400	12.5808359322
H34	2.3316805588	12.3276142947	11.5734928849
C35	2.6548002459	10.4472800622	10.4389720986
H36	3.3529239322	9.6285302984	10.6537373252
C37	-1.0945854557	5.9129366082	7.0471973395
H38	-0.8908378915	6.2461490133	6.0267055491
C39	-2.5877440870	5.5314533225	7.2217306948
H40	-2.7509867357	4.4639642886	7.3823298791
H41	-3.2211505750	5.8865202968	6.4024681166
C42	3.2120999104	11.2923975574	9.2968252774
H43	2.5405920413	12.1280856731	9.0697492633
H44	4.1916785587	11.7008093381	9.5666334540
H45	3.3267221811	10.6789993100	8.3996806043
C46	-0.1345978752	4.7905689298	7.4519924099
H47	-0.2783826090	4.5433146395	8.5087549524
H48	-0.3162712999	3.9035578437	6.8339632372
H49	0.9025097692	5.1018172237	7.3046597537
O50	-0.4538275807	10.1979985873	7.6701606170
C51	-0.9169149812	10.4974967490	6.2971704403
H52	-1.7982539701	11.1350168912	6.3514384148
C53	-1.3030093734	7.5953452800	3.1577713469
C54	-2.3957245739	8.3596766067	3.5703964046
C55	-2.2459504799	9.2798503729	4.6076555430
C56	-1.0083200389	9.4480477733	5.2460687232
C57	0.0863253397	8.6731659102	4.8314765071
C58	-0.0677584905	7.7547580609	3.7927574521
H59	-1.4118013193	6.8820116247	2.3454656923
H60	-3.3603788920	8.2453925512	3.0837570048
H61	-3.0968293702	9.8805750387	4.9219202478
H62	1.0432500761	8.7542495062	5.3393134184
H63	0.7863675727	7.1612490520	3.4789076855
C64	0.3300022012	11.0719216634	6.8281558031
H65	0.3434403480	12.1091545564	7.1588227813
H66	1.2838236783	10.6463875908	6.5294201467

Cartesian coordinates of **D**

atom	x	y	z
Ru1	0.5622672625	8.4154275439	8.7234128838
C2	3.6240503119	5.0556320407	10.2810696836
C3	2.4184773070	5.1870993251	10.9535515916
C4	1.4659128578	6.1254720766	10.5265572480
N5	1.7341770440	6.9183317285	9.4695861548
C6	2.9067594763	6.7836240105	8.7823787775
C7	3.8676569078	5.8652864910	9.1681026445
H8	4.3631553765	4.3300410795	10.6096947752
H9	2.1801656654	4.5743480323	11.8165688472
H10	4.7738735132	5.8145760897	8.5753455799
C11	3.0965479955	7.6574827480	7.5552159378
O12	4.1441156161	7.5936835643	6.9204939906
C13	0.1136472000	6.2384776654	11.2392129338
O14	0.1077003117	6.9729006959	12.2472391513
O15	-0.8057785317	5.5785267199	10.6922737992
O16	2.0692664660	8.4084420868	7.2880823008
C17	-3.0022395937	9.0334189200	11.8388712054
C18	-1.7981969498	9.7222080784	12.0173449651
C19	-0.7725993694	9.4924092563	11.1073510216
N20	-0.9323619256	8.6392539953	10.0729578745
C21	-2.0891623257	7.9738139772	9.8971220754
C22	-3.1610755113	8.1502049594	10.7687341415
H23	-3.8163799232	9.1815931511	12.5406656823
H24	-1.6481943101	10.4043468188	12.8459095129
H25	-4.0793992993	7.5953141577	10.6168202764
N26	1.3832847189	9.8154533866	10.1046905696
C27	0.5688335424	10.0824167795	11.0782504056
O28	0.9909482370	10.9109272141	12.0385053731
N29	-0.9559022476	7.1098480319	7.9534470413
C30	-2.0060630189	7.1040156642	8.7171885394
O31	-3.0131505134	6.2920787848	8.3984877679
C32	2.3516933449	11.3016698161	11.6687609147
H33	3.0038323209	11.0404265946	12.5041952388

H34	2.3531289411	12.3863194168	11.5257743762
C35	2.6576983619	10.5172402072	10.3600933289
H36	3.4244493862	9.7532906560	10.5348992835
C37	-1.1112325439	5.9978093285	6.9861804218
H38	-0.9297227823	6.3766529295	5.9758279369
C39	-2.6003376797	5.6011615409	7.1797193879
H40	-2.7473118199	4.5321623358	7.3449776945
H41	-3.2532528794	5.9455479878	6.3721463013
C42	3.0718244827	11.3846253030	9.1732382022
H43	2.3290826505	12.1686698920	8.9892255839
H44	4.0383904337	11.8608644046	9.3678118399
H45	3.1595190142	10.7692406656	8.2740926776
C46	-0.1378458924	4.8637984304	7.3168459461
H47	-0.2632846575	4.5655725808	8.3624964088
H48	-0.3262271620	4.0063935544	6.6608616045
H49	0.8937558603	5.1895475193	7.1641512826

Cartesian coordinates of **styrene epoxide**

atom	x	y	z
O50	0.0703583358	10.0977912473	7.4448218280
C51	-0.9756575222	10.3422027698	6.4948015662
H52	-1.9206639366	10.6550343022	6.9433382991
C53	-1.3378970074	7.6685684074	3.1524176377
C54	-2.3744951156	8.5492541390	3.4648149733
C55	-2.2580444968	9.4054309439	4.5596522820
C56	-1.1002648813	9.3971275699	5.3463060392
C57	-0.0673179081	8.5050597650	5.0344664941
C58	-0.1867264863	7.6468532459	3.9425248092
H59	-1.4298974523	6.9973606504	2.3032117080
H60	-3.2767990291	8.5655452381	2.8599086178
H61	-3.0708986596	10.0854738632	4.8043833105
H62	0.8137734612	8.4808596151	5.6682443014
H63	0.6173868334	6.9535867013	3.7115636105
C64	0.1694443105	11.2670375764	6.6283676107
H65	0.0440086249	12.2168671695	7.1490104734
H66	0.9520038713	11.2438441105	5.8700815022

Cartesian coordinates of **I_a**

atom	x	y	z
Ru1	0.4257889828	8.3772362452	8.9355297606
C2	3.7815182375	5.1000015500	10.0487239191
C3	2.6678876064	5.1862752337	10.8687667736
C4	1.6326516360	6.0878679081	10.5727746898
N5	1.7305457394	6.8981037585	9.4982905552
C6	2.8120107989	6.8034394575	8.6684310979
C7	3.8478228962	5.9199927659	8.9189369910
H8	4.5834587192	4.4025812136	10.2754148552
H9	2.5635754290	4.5654259357	11.7524201295
H10	4.6700270966	5.9017284676	8.2128585589
C11	2.8175578901	7.6729254997	7.4277480411
O12	3.7616599145	7.6220228699	6.6442777062
C13	0.3858241062	6.1242826895	11.4634894438
O14	0.4928671433	6.8216790918	12.4915519099
O15	-0.5708906942	5.4367142116	11.0257922144
O16	1.7522753648	8.4090718763	7.2970692412
C17	-2.6676394516	8.8691896492	12.5251854579
C18	-1.4659614882	9.5832576494	12.5384512980
C19	-0.5729086490	9.3816893155	11.4929748350
N20	-0.8516024039	8.5256758632	10.4896550503
C21	-2.0082284785	7.8407663680	10.4680725783
C22	-2.9540205858	7.9897203922	11.4793666600
H23	-3.3799277622	8.9961281671	13.3340084389
H24	-1.2175806899	10.2684703221	13.3404306285
H25	-3.8742131971	7.4181863331	11.4473749874
N26	1.4117559683	9.7722936022	10.2067087993
C27	0.7268733055	10.0188719322	11.2775937469
O28	1.2427346580	10.8724408007	12.1699216302
N29	-1.1467142274	7.0218918338	8.3758687960
C30	-2.0763970720	6.9849059303	9.2792256631
O31	-3.1003491218	6.1488568929	9.0980700926
C32	2.5061741196	11.3343467927	11.6018606356
H33	3.2868904572	11.1451713508	12.3413052840
H34	2.4145722687	12.4110237236	11.4292599423
C35	2.6774310499	10.5281196496	10.2826604917
H36	3.4933550208	9.8006041618	10.3742694671
C37	-1.4100181321	5.9121965649	7.4308172638

H38	-1.3788117248	6.2989786133	6.4085251029
C39	-2.8475170111	5.4789613018	7.8264065327
H40	-2.9474221012	4.4050233787	7.9969475494
H41	-3.6132143027	5.8154242195	7.1205077368
C42	2.9004394185	11.3889561673	9.0413722561
H43	2.0778935647	12.1007661505	8.9217577412
H44	3.8435005237	11.9401878421	9.1255434894
H45	2.9462789455	10.7537213343	8.1532568608
C46	-0.3739395192	4.8001134298	7.6159060354
H47	-0.3436470535	4.4963135990	8.6671213433
H48	-0.6316050004	3.9400035269	6.9870783493
H49	0.6191017656	5.1512625200	7.3239761581
O50	-0.7026229863	10.1683706357	6.5220730249
C51	-0.8125340908	10.2885390093	5.0730806058
H52	-1.5504916632	11.0330812394	4.7725493071
C53	-0.9578887830	6.6988114478	2.7275779238
C54	-1.8470569366	7.7438571022	2.4785293117
C55	-1.7914606876	8.9033211921	3.2530509824
C56	-0.8466704743	9.0298166697	4.2781221540
C57	0.0457782321	7.9758170657	4.5277175850
C58	-0.0146778692	6.8189742959	3.7522390074
H59	-0.9975594072	5.7944783031	2.1262628771
H60	-2.5848654294	7.6575371023	1.6856278881
H61	-2.4881064481	9.7163251407	3.0595149243
H62	0.7734777416	8.0576156891	5.3314131492
H63	0.6836374412	6.0095726687	3.9473267542
C64	0.3786524561	10.7827210872	5.7879961747
H65	0.4866703128	11.8533707537	5.9574565338
H66	1.2911138055	10.1930351737	5.7995446496
O68	-0.6123189203	12.2508227189	9.0686811414
H69	-1.2842347611	12.9202737406	9.2710314237
O69	-1.4617424918	11.0807803742	8.8960476482
H70	-1.3102325354	10.8858584020	7.9406400824

Cartesian coordinates of **trans-2a-HOOH-COO**

atom	x	y	z
Ru1	0.2992160531	8.3208652186	9.0971343979
C2	3.9420844781	5.2349212411	9.9098883998
C3	2.9176044856	5.2599650295	10.8437550504
C4	1.8117237333	6.1042300536	10.6556521864
N5	1.7515010867	6.9088229016	9.5759861629
C6	2.7454423694	6.8795928442	8.6409061742
C7	3.8504055665	6.0562929534	8.7819059689
H8	4.8002567225	4.5827756101	10.0485239709
H9	2.9427018287	4.6346950060	11.7301025986
H10	4.6017527311	6.0834701524	8.0013088517
C11	2.5958704922	7.7638148581	7.4114819869
O12	3.4829632982	7.7944174832	6.5675112727
C13	0.6476296476	6.1193713741	11.6507752957
O14	0.7978217253	6.8832356906	12.6265499602
O15	-0.3090332673	5.3706619720	11.3277047769
O16	1.4728744771	8.4297381182	7.3698300721
C17	-2.5591318203	8.6495316509	12.8943328698
C18	-1.4075473564	9.4390868606	12.8179586289
C19	-0.5820244725	9.2913180679	11.7094463537
N20	-0.8828910199	8.4220555366	10.7195054808
C21	-1.9851428483	7.6502265522	10.7950394894
C22	-2.8577885335	7.7416857647	11.8770816267
H23	-3.2160071041	8.7341690155	13.7537552100
H24	-1.1413180720	10.1380834261	13.6022437365
H25	-3.7314688906	7.1019463361	11.9201713855
N26	1.2928679418	9.7764436740	10.2989766299
C27	0.6694278654	9.9876023679	11.4144598757
O28	1.2057913143	10.8576578485	12.2784180511
N29	-1.2025108868	6.8441439160	8.6720141589
C30	-2.0711877812	6.7671746623	9.6319272029
O31	-3.0431266726	5.8562345169	9.5329796702
C32	2.4237676840	11.3570551936	11.6448069146
H33	3.2508036386	11.1718311465	12.3329073316
H34	2.3008661938	12.4346466295	11.4990487871
C35	2.5342393060	10.5759090919	10.3035254117
H36	3.3774297648	9.8751668142	10.3309287998
C37	-1.4472325082	5.6986996521	7.7657605245
H38	-1.5121018528	6.0648796904	6.7360659199
C39	-2.8236073563	5.1763172179	8.2619334830
H40	-2.8338375914	4.1023189217	8.4579923266

H41	-3.6544220627	5.4398612481	7.5999457291
C42	2.6524785416	11.4593838211	9.0632547643
H43	1.8096292447	12.1550635148	9.0026365771
H44	3.5841801920	12.0342200018	9.0948233431
H45	2.6576370284	10.8411814529	8.1620457523
C46	-0.3286549857	4.6619927293	7.8973263097
H47	-0.2077727857	4.3865878752	8.9498715529
H48	-0.5720622731	3.7727004423	7.3047689803
H49	0.6164909101	5.0686871930	7.5299230427
O68	-0.8184799959	11.1723616485	8.2438698264
H69	-1.7032542612	11.4098793425	7.9197468251
O69	-0.7911830232	9.7559641439	7.8365083543
H70	-0.0651815497	9.7504746563	7.1719831857

Cartesian coordinates of **ts-trans-2a-HOOH-COO**

atom	x	y	z
O15	0.00000000000000	0.00000000000000	0.00000000000000
Ru1	0.00000000000000	0.00000000000000	2.6695408117000
C2	4.7298321001381	0.00000000000000	0.5286309835577
C3	3.6316967147639	-0.0880541842455	-0.3242473379150
C4	2.3441683705923	-0.0180023354706	0.2192617139966
N5	2.1545213738954	0.1390101699034	1.5305485049416
C6	3.2046144324466	0.2330832921773	2.3603368725873
C7	4.5178156632548	0.1611040888057	1.9002498224418
H8	5.7408611658404	-0.0548405754814	0.1330781771728
H9	3.7199353928707	-0.2098149455556	-1.3978737316377
H10	5.3269278505216	0.2339826309647	2.6183227835620
C11	2.8706718189133	0.4131030045551	3.8258561564685
O12	3.7395396032143	0.3393005247540	4.6870208833361
C13	1.0860360362593	-0.1002607078134	-0.6540871928635
O14	1.2600200922583	-0.2438320955511	-1.8727723223523
O16	1.6022181479012	0.6513374532070	4.0304036340943
C17	-3.9641310860372	-1.4422491524586	0.5456428903382
C18	-3.0423234486235	-2.3839119002183	1.0163201903860
C19	-1.8945251959990	-1.9310784228861	1.6580034450662
N20	-1.6699623014053	-0.6050184145259	1.8485954775215
C21	-2.5438214576699	0.3144549315521	1.3589479248067
C22	-3.7106343165576	-0.0778259658816	0.7091033391626
H23	-4.8627112615144	-1.7707155163372	0.0346841971402
H24	-3.1927351334082	-3.4479620976547	0.8719558285433
H25	-4.3879524291722	0.6755817965112	0.3226125456464
N26	0.2501771721035	-2.1221554140237	2.6907254569913
C27	-0.7659579633198	-2.7136610544237	2.1476456986388
O28	-0.7266658088951	-4.0478009255602	2.0235020880594
N29	-0.9206934922392	1.8364906682353	2.2123132485498
C30	-2.0391240147216	1.6610848978145	1.5804424914434
O31	-2.6824742589323	2.7478993736184	1.1299653119889
C32	0.5417055922605	-4.4674189635651	2.6145894464542
H33	1.0767224202369	-5.0526406187279	1.8640792906285
H34	0.3093343769048	-5.1000389281873	3.4767274078525
C35	1.2635434062939	-3.1480470915815	3.0156207384245
H36	2.1296006125626	-2.9672465590509	2.3682776643937
C37	-0.6055667316041	3.2777302526066	2.2113595854921
H38	-0.5621106871779	3.6205786480714	3.2517914166001
C39	-1.8346946749180	3.8869219734695	1.4739712116483
H40	-1.5643658468168	4.3874809982893	0.5402655638459
H41	-2.4279386600662	4.5632791421343	2.0940139988754
C42	1.7055292147908	-3.1063984102953	4.4776649504867
H43	0.8435266140305	-3.2046148111939	5.1440711289026
H44	2.4025378557698	-3.9278416707899	4.6768582414529
H45	2.2154816311915	-2.1683889422821	4.7083215469949
C46	0.7326936787937	3.5511409953122	1.5272866877260
H47	0.7236924581436	3.1643097547983	0.5041842161732
H48	0.9313627380406	4.6280675464131	1.5031276617507
H49	1.5390970514937	3.0584059609991	2.0743227722436
O68	-0.9901407109611	-1.1137278110181	5.3639241053100
H69	-1.6428566643039	-0.7825300042946	6.0030752856331
O69	-0.6574065224312	0.1485926970029	4.6925037447894
H70	0.3104745056566	0.3145620142241	4.9514774891581

Cartesian coordinates of **ts-2'-epo**

atom	x	y	z
O15	0.4349272283	-1.0104645133	0.2481210936

Ru1	-0.1524348990	-0.2651804318	2.5959639741
C2	4.5642111397	1.2568364453	0.8374221994
C3	3.7462267869	0.5070096559	-0.0075890256
C4	2.5107426086	0.0658030933	0.4755126771
N5	2.1139045463	0.3354255500	1.7180146735
C6	2.8937870647	1.0445244928	2.5399287029
C7	4.1342553114	1.5381358902	2.1371895213
H8	5.5276393431	1.6203904913	0.4886603816
H9	4.0200434961	0.2523753762	-1.0253260363
H10	4.7215804311	2.1181146049	2.8405053076
C11	2.3056106251	1.2619211072	3.9155613111
O12	2.8607444686	2.0025337390	4.7322522359
C13	1.5260026653	-0.7431782229	-0.3625454631
O14	1.8624548822	-1.0545040393	-1.5128180238
O16	1.2067731263	0.6044955143	4.1108754516
C17	-3.7593272284	-2.3056604482	0.3258694889
C18	-2.8212668487	-3.0877188465	1.0071702111
C19	-1.7743202385	-2.4558977382	1.6703028182
N20	-1.6588916587	-1.0975085546	1.6732788907
C21	-2.5541149872	-0.3368903830	0.9882196262
C22	-3.6242113328	-0.9133832120	0.3113744140
H23	-4.5804804367	-2.7780843433	-0.2021494754
H24	-2.8838900678	-4.1703874641	1.0147824426
H25	-4.3209988445	-0.2804313953	-0.2270075014
N26	0.2099412002	-2.3013401944	2.9759680989
C27	-0.6624110581	-3.0589828900	2.3863534008
O28	-0.4624760821	-4.3866314734	2.4249287705
N29	-1.1349377478	1.4382393321	1.7244341101
C30	-2.1850580330	1.0682784783	1.0589594060
O31	-2.9046549744	2.0160491885	0.4365828209
C32	0.7270400471	-4.5811678447	3.2509482557
H33	1.3932547760	-5.2592722765	2.7155413014
H34	0.4055843577	-5.0452514645	4.1902292024
C35	1.3072171841	-3.1567463290	3.4630431448
H36	2.1628597515	-2.9814865694	2.7982751780
C37	-0.9586657201	2.8932616656	1.5112489508
H38	-0.8755488487	3.3802003980	2.4861237443
C39	-2.2857023123	3.2860472249	0.8062209702
H40	-2.1394642309	3.8606685015	-0.1111282357
H41	-2.9809462385	3.8122065673	1.4668894583
C42	1.7113319596	-2.8327879128	4.8974314455
H43	0.8846964948	-3.0312984636	5.5888479435
H44	2.5701708454	-3.4400382094	5.2020500612
H45	1.9820249169	-1.7764661123	4.9711123040
C46	0.2858385954	3.1946743897	0.6739064101
H47	0.2362330654	2.6893085546	-0.2959149956
H48	0.3635004183	4.2744430099	0.5040376148
H49	1.1885034941	2.8615011412	1.1878165630
O50	-1.4444789255	-0.2340287900	4.3732069444
C51	-1.9924485459	0.7704095091	5.3257002189
H52	-3.0325928741	0.5146240459	5.5230457905
C53	-1.5511464225	5.0244538470	4.9778068129
C54	-2.7993001557	4.4142375642	4.8373782737
C55	-2.9049497195	3.0274580035	4.9354891343
C56	-1.7710100035	2.2331204387	5.1697194420
C57	-0.5198655421	2.8539361844	5.3130837666
C58	-0.4181979573	4.2415156458	5.2135675207
H59	-1.4630011850	6.1055005047	4.9089772553
H60	-3.6879238832	5.0151897073	4.6637248533
H61	-3.8795834961	2.5533445086	4.8392048408
H62	0.3794602609	2.2686879903	5.4690656870
H63	0.5575400055	4.7056698957	5.3228529701
C64	-0.9911969602	-0.2202555895	5.7496874756
H65	-1.3121938352	-1.0919384259	6.3173168077
H66	0.0457476060	0.0851246441	5.8461994808

Cartesian coordinates of **ts-D-2'**

atom	x	y	z
N5	0.00000000000000	0.00000000000000	0.00000000000000
Ru1	0.00000000000000	0.00000000000000	2.0212968906000
N20	1.5906075171490	0.00000000000000	3.4689844032748
C2	-0.1934696757031	-0.0970280044371	-2.7592423702587
C3	0.9866980317371	0.3045298353552	-2.1404246247353
C4	1.0780388963530	0.3366053496936	-0.7449694804885
C6	-1.1815894081301	-0.3095461419337	-0.5897341648843
C7	-1.3064163870737	-0.3920225849824	-1.9678702595046

H8	-0.2571047076250	-0.1486693039941	-3.8425895053714
H9	1.8567206152814	0.6145214242067	-2.7083919852160
H10	-2.2744088474032	-0.6635609075249	-2.3744959011252
C11	-2.3352225846410	-0.4870940374969	0.3669424271051
O12	-3.4439499212431	-0.8245305222169	-0.0323327651478
C13	2.3354429833144	0.8565793442775	-0.0264146497326
O14	2.7430397186885	1.9533896052540	-0.4685398056954
O15	2.7546090697544	0.1622081312622	0.9354203961586
O16	-2.0098321953525	-0.2220609392587	1.6055228028825
C17	3.8354876367834	-0.0708782664939	4.9938297717146
C18	3.4303721057106	1.1437262542800	4.4229965073496
C19	2.2786807523699	1.1295357306605	3.6372621721591
C21	1.9862398465127	-1.1769030296353	3.9617335299800
C22	3.1288331684507	-1.2552962061652	4.7647486165045
H23	4.7309326688659	-0.0967258481262	5.6072427779139
H24	3.9964511723925	2.0570111710639	4.5612242729949
H25	3.4591018745091	-2.2041836515982	5.1708058872441
N26	0.6218425832827	2.0664924088584	2.1234404811096
C27	1.6942375800655	2.2299577629984	2.8371179673987
O28	2.3247871078992	3.3998930982631	2.7738100818971
N29	0.2091325366088	-2.0360881820878	2.5671102546264
C30	1.1285286310120	-2.2614591130015	3.4595936241683
O31	1.3015953028658	-3.5230816424588	3.8822205073066
C32	1.7011503352014	4.1166582727636	1.6512027501479
H33	2.3998181082656	4.0441577527482	0.8156517903986
H34	1.5466118891026	5.1490085066194	1.9702018366134
C35	0.3952675723604	3.3283695166202	1.3759465753134
H36	0.3397859443070	3.0768908625307	0.3139135571951
C37	-0.3869916798018	-3.3408984235607	2.1967768322997
H38	-1.4687741861327	-3.2680449561449	2.3428416247904
C39	0.2637662012419	-4.3125336988994	3.2206987010077
H40	0.7518195873834	-5.1710917164181	2.7539564335449
H41	-0.4268754664214	-4.6578642008259	3.9948677230404
C42	-0.8922374651450	4.0113280502993	1.8351551183092
H43	-0.8288420731378	4.3011688398589	2.8896713263203
H44	-1.0772751259502	4.9112068098374	1.2390838408419
H45	-1.7430091047793	3.3349433357589	1.7152804998241
C46	-0.0827654729900	-3.6954549598658	0.7403689624754
H47	0.9976915637654	-3.7333931842831	0.5677419880307
H48	-0.5123406453271	-4.6734864770645	0.4988314652137
H49	-0.5142908838496	-2.9572803872549	0.0621275264527

Cartesian coordinates of **ts-2b-HOOH-N**

atom	x	y	z
Ru1	0.0000000000000	0.0000000000000	0.0000000000000
N29	0.0000000000000	0.0000000000000	2.6684918943000
C2	3.9039315796602	0.0000000000000	-2.6351473758468
C3	2.8862331177246	0.9301684626734	-2.8796364710504
C4	1.7489258461874	0.8978668185536	-2.0786311109869
N5	1.6574384228166	-0.0186811784208	-1.1029695404524
C6	2.6095937262046	-0.9221430670852	-0.8368169864983
C7	3.7704180472663	-0.9375433399195	-1.6055302282663
H8	4.8008966275803	0.0064838756842	-3.2482853093693
H9	2.9459008577523	1.6735763905932	-3.6669725789249
H10	4.5333292206403	-1.6739877620855	-1.3784337093433
C11	2.2827939837825	-1.8524391926219	0.3294758078792
O12	3.1028031524711	-2.7054741143625	0.6582136308474
C13	0.5321231303576	1.8158256461186	-2.2051530721823
O14	0.5190714654702	2.6633977055737	-3.0914631220774
O15	-0.4150978470010	1.5885779396164	-1.3344905116373
O16	1.1200361397318	-1.6382266457225	0.8781066397462
C17	-4.6514517317933	0.3209638146885	1.4735865016472
C18	-4.2798086844409	-0.0775508648675	0.1897378247544
C19	-2.9251255483800	-0.2490835361258	-0.0895848868038
N20	-1.9419408507132	0.0161581181090	0.8213880703046
C21	-2.3288399474741	0.2722114267407	2.0941325400671
C22	-3.6653589617198	0.4501384161478	2.4531452636725
H23	-5.6961290779694	0.4786021272928	1.7198441744734
H24	-5.0130200525500	-0.2797923131325	-0.5830338706132
H25	-3.9142180424414	0.6657239063118	3.4858728267873
N26	-1.0960812936511	-1.0908546569478	-1.3244908968456
C33	-2.3705070640003	-0.8572009442214	-1.2813071422551
O30	-3.1182045215093	-1.2889236410495	-2.3101111662246
C40	-1.2250831146692	0.1189802295211	3.0381772694046
O36	-1.5453848894867	-0.1345425230261	4.3257701794368

C37	-2.1645255514777	-1.7806376989447	-3.3025938159823
H38	-2.1541638917664	-1.0658280204907	-4.1302376069845
H39	-2.5239355901339	-2.7502194160133	-3.6533280535944
C39	-0.8056286261685	-1.8584745029619	-2.5519688832303
H40	-0.0237918256892	-1.3387095353887	-3.1138381101040
C38	0.7520332475164	-0.5124580156794	3.8476766389091
H42	0.9951222401725	-1.5530261451874	3.6020817677293
C41	-0.2829733656920	-0.4185190511337	4.9964164257857
H41	-0.0762142876949	0.4065906022518	5.6879085060177
H43	-0.4104891600947	-1.3443799817231	5.5601934842165
C43	-0.3516363433928	-3.2804905287680	-2.2163660891692
H44	-1.1421492636257	-3.8232638703130	-1.6877978895636
H45	-0.1078804179608	-3.8253064873847	-3.1347052687981
H46	0.5314910934521	-3.2632167741023	-1.5743108853874
C46	2.0390661725052	0.2609583225875	4.1234336651963
H47	1.8226601550568	1.3098714850684	4.3589090857635
H48	2.5664271287210	-0.1788949751345	4.9766087039836
H49	2.7014016102965	0.2286419577653	3.2555692249732
O50	1.2326376925872	1.9932571602188	1.1780462117874
H51	0.8921576282193	1.5348448652557	2.0195920039895
O52	2.6837671732098	1.8551615545324	1.2941709639293
H53	2.9345305229295	2.7880169509376	1.2052076851401

Cartesian coordinates of **2b-HOOH-N**

atom	x	y	z
Ru1	0.7597590308	8.4421585943	9.0245134886
C2	3.8032926041	8.7634003203	5.4712453156
C3	4.0764435015	7.9062177948	6.5440874362
C4	3.1659878789	7.8444977553	7.5957886651
N5	2.0659813682	8.6111249587	7.5526375494
C6	1.7565870117	9.4292137128	6.5354486757
C7	2.6327020139	9.5317912008	5.4587503333
H8	4.5006438525	8.8277447883	4.6403764072
H9	4.9639893276	7.2845961145	6.5890158223
H10	2.3761633557	10.1992106593	4.6433198420
C11	0.4219703906	10.1604927411	6.7010817781
O12	0.0758401672	10.9573957677	5.8346866918
C13	3.2665548789	6.9557481886	8.8394879077
O14	4.2618414310	6.2515757155	8.9785183211
O15	2.2491197826	7.0442322178	9.6497256194
O16	-0.2278075245	9.8563399091	7.7892564353
C17	-1.6331151612	8.5066567055	13.4376868677
C18	-0.4192630715	9.1115648159	13.1495116941
C19	0.0703336670	9.0594436032	11.8451264601
N20	-0.5420595798	8.4004881480	10.8021272835
C21	-1.7666352873	7.8713326120	11.1009560826
C22	-2.3212171491	7.9095402597	12.3864568737
H23	-2.0458094813	8.5179968269	14.4405584763
H24	0.1599445062	9.6357573289	13.9012211902
H25	-3.2959282710	7.4650533259	12.5392807518
N26	1.6681907102	9.7892944365	10.2487042184
C33	1.2709984319	9.7754269328	11.4758612996
O30	1.9874675252	10.4830885530	12.3727778718
N29	-2.2645765401	6.7196422629	8.9459071939
C40	-2.6114891975	7.2534107055	10.0552578542
O36	-3.9419387067	7.2531630921	10.3335634375
C37	3.1591439180	10.9589927750	11.6452402633
H38	4.0270898565	10.4078533270	12.0185048671
H39	3.2751955590	12.0230541269	11.8627816119
C39	2.8522763547	10.6665548010	10.1496738035
H40	3.6657450209	10.0962542206	9.6908161454
C38	-3.4820685976	6.3404199192	8.2044332341
H42	-3.6188260426	7.0879376639	7.4118017865
C41	-4.5787846956	6.4761511692	9.2834015722
H41	-4.8720405823	5.5085468991	9.7083559049
H43	-5.4674463819	7.0186920302	8.9580172488
C43	2.5592060063	11.9181980057	9.3200473678
H44	1.7424856986	12.4957654309	9.7640994650
H45	3.4519325495	12.5513966554	9.2749848508
H46	2.2713200316	11.6569257071	8.3004047837
C46	-3.3634846480	4.9589539680	7.5691657103
H47	-3.1808727928	4.1915791605	8.3283246191
H48	-4.2802122139	4.7041968653	7.0274383790
H49	-2.5335797183	4.9501234119	6.8575853228
O50	0.0173676547	6.7736308152	7.8852868582

H51	-0.9153858252	6.6569269936	8.3252457707
O52	-0.4012871797	7.0602061869	6.5042096523
H53	0.1635353668	6.4201522257	6.0426977476

Cartesian coordinates of 87 **ts-2ab-oxo**

atom	x	y	z
Ru1	0.4252527422	8.7673349209	8.8700905125
C2	3.4574518014	7.9367314033	5.1772930714
C3	3.5720261627	7.3141046376	6.4238764159
C4	2.6048131984	7.5744853663	7.3817320654
N5	1.5572057618	8.3970886187	7.1282004891
C6	1.3971555048	8.9700964422	5.9210266892
C7	2.3707383451	8.7659719214	4.9320846183
H8	4.2061692221	7.7664230784	4.4083839787
H9	4.3788274231	6.6374976635	6.6807640889
H10	2.2176191012	9.2853126460	3.9930667764
C11	0.1136001540	9.7736871976	5.5646339803
O12	-0.9101747511	9.4387501809	6.2238941986
C13	2.6377491913	6.9139064627	8.7449255555
O14	3.5347161793	6.1414230415	9.0437239202
O15	1.6264876089	7.2338455549	9.5284265005
O16	0.2560828710	10.5764626076	4.6317646982
C17	-2.3534226321	8.5141681278	12.9810937414
C18	-1.0705126075	9.0337752996	13.1221340933
C19	-0.2417618018	9.1516528221	11.9966332588
N20	-0.6588961125	8.7595668586	10.7804859616
C21	-1.8790029984	8.1801888452	10.6665720648
C22	-2.7677744480	8.0607311950	11.7303692391
H23	-3.0122936417	8.4371049528	13.8399891284
H24	-0.6901349567	9.3519918525	14.0846775173
H25	-3.7373077208	7.6033710003	11.5708691934
N26	1.8366993240	10.2689645933	11.2696976573
C33	1.1439256930	9.6609519222	12.1479430526
O30	1.6824258164	9.4414993994	13.3816468696
N29	-1.1870411651	7.5412494459	8.4590308383
C40	-2.1271606818	7.6030541892	9.3437788906
O36	-3.3108765446	7.0874878060	9.0220396332
C37	3.0742487258	9.8594583720	13.2724958222
H38	3.6982414159	8.9608886233	13.2900322579
H39	3.3106549743	10.4886037747	14.1345352145
C39	3.1248575599	10.6104892280	11.9157369859
H40	3.9386628495	10.2400928176	11.2832162575
C38	-1.6988861033	6.8343392485	7.2600576340
H42	-1.5243413573	7.5182750019	6.4224577134
C41	-3.2082905080	6.7181540659	7.5964672320
H41	-3.6114958469	5.7085144165	7.4976098903
H43	-3.8254473883	7.4296277422	7.0433173701
C43	3.2557322471	12.1300736578	12.0604302581
H44	2.4687276900	12.5269272643	12.7108887427
H45	4.2273733610	12.3928999948	12.4927017083
H46	3.1664281982	12.6117166339	11.0834970022
C46	-0.9884162195	5.4947865752	7.0661830936
H47	-1.1221555523	4.8339940561	7.9297340063
H48	-1.3874091355	4.9926261858	6.1785509424
H49	0.0825333986	5.6472255864	6.9136957788
O50	0.3477040397	10.4841485123	8.6423982010

Cartesian coordinates of **ts-2b-o-ene**

atom	x	y	z
Ru1	0.6526353543	8.4222024565	8.8765403980
C2	3.4986579087	8.9254952496	5.1861959827
C3	3.8892158154	8.1056866710	6.2521203271
C4	3.0315571590	7.9792295141	7.3406360050
N5	1.8652684023	8.6414882982	7.3311327001
C6	1.4694879343	9.4638457738	6.3488556238
C7	2.2844850199	9.6222170701	5.2322412366
H8	4.1476022911	9.0303071436	4.3214293821
H9	4.8290522244	7.5647920951	6.2631194963
H10	1.9564195691	10.2825132068	4.4370204012
C11	0.1514491846	10.1832543422	6.6388972389
O12	-0.2997935464	10.9557649435	5.8048806490
C13	3.2774299942	7.1654890354	8.6110064833
O14	4.3302802413	6.5529606488	8.7323658680
O15	2.3028705153	7.2201412643	9.4857463077
O16	-0.3601871463	9.9196911801	7.8162132983

C17	-1.1204360611	7.6896213178	13.4437401555
C18	-0.0535692623	8.5400487837	13.1607854171
C19	0.2441918055	8.8027577916	11.8274496583
N20	-0.4555844616	8.2815439772	10.7866139202
C21	-1.5396772890	7.5342435138	11.0719561906
C22	-1.8775090008	7.1957619398	12.3886217542
H23	-1.3687728572	7.4364096715	14.4693850999
H24	0.5521668502	8.9864777854	13.9405701820
H25	-2.7379709655	6.5559441400	12.5441483043
N26	1.6480786152	9.8966089168	10.2026720932
C27	1.3537917518	9.6758225820	11.4331457776
O28	2.1030911015	10.2655815061	12.3786866167
N29	-3.0323080452	5.9648482963	9.9538492091
C30	-2.4445024727	7.0966737420	9.9809121645
O31	-2.7269386533	8.0257437868	9.0418935149
C32	3.0821466729	11.0794040082	11.6639543172
H33	4.0730529153	10.7969550992	12.0243089038
H34	2.8839658371	12.1268980956	11.9111904174
C35	2.8417399647	10.7609566189	10.1601500371
H36	3.6670026480	10.1605552244	9.7573090268
C37	-3.8973482158	5.9913868083	8.7544654268
H38	-3.6351467568	5.1328695303	8.1262049475
C39	-3.5141692601	7.3247461070	8.0488015557
H40	-4.3676250923	7.9565331475	7.7894911010
H41	-2.8766872335	7.1787366529	7.1729459581
C42	2.6339929357	11.9957429107	9.2852154514
H43	1.7934645117	12.5943271537	9.6494308517
H44	3.5360758521	12.6169773227	9.2880276153
H45	2.4213987632	11.7072592923	8.2532964548
C46	-5.3715229494	5.8902312321	9.1546645785
H47	-5.6678847533	6.7515964737	9.7634814648
H48	-6.0138393631	5.8605200899	8.2675677288
H49	-5.5465228731	4.9825474557	9.7391226718
O50	-0.2848669572	6.9804969319	8.2174665744
C51	0.3264101125	5.8363103573	6.7327080543
C52	-0.2702137639	4.6007312923	6.9041046338
H53	-0.0444047033	6.4980044391	5.9579435661
H54	1.3707345379	5.9517281817	6.9899244025
H55	-1.2113458021	4.4052330352	6.3920088313
C56	1.1556013266	1.4137810516	9.3575262890
C57	0.1032204149	1.2078613978	8.4618815710
C58	-0.3594971776	2.2593146186	7.6796195379
C59	0.2223466180	3.5440184321	7.7626475700
C60	1.2725534613	3.7407164749	8.6902900559
C61	1.7302701087	2.6841327889	9.4690149286
H62	1.5187343451	0.5935765748	9.9707721469
H63	-0.3558904992	0.2265220436	8.3754383526
H64	-1.1766940257	2.0956766339	6.9804428893
H65	1.7021066218	4.7273727795	8.8279924184
H66	2.5370273368	2.8554547120	10.1763025922

Cartesian coordinates of **2b-o-ene**

atom	x	y	z
Ru1	0.7031532358	8.4755035046	8.9347147740
C2	3.5704415246	8.9750584495	5.2570992715
C3	3.9632864555	8.1757632772	6.3376851455
C4	3.0920538757	8.0412887167	7.4147762451
N5	1.9115560381	8.6753101912	7.3825008372
C6	1.5136884364	9.4782738344	6.3860808177
C7	2.3398794104	9.6437572700	5.2784273448
H8	4.2306859389	9.0876446464	4.4019148673
H9	4.9166007905	7.6597262400	6.3693188496
H10	2.0100200969	10.2899165796	4.4723019690
C11	0.1818058325	10.1743930498	6.6579929292
O12	-0.2885864265	10.9242552531	5.8154115651
C13	3.3405800925	7.2625233944	8.7044842425
O14	4.4001324413	6.6721298427	8.8566032420
O15	2.35744449235	7.3315049567	9.5752316336
O16	-0.3263574644	9.9200964045	7.8430259267
C17	-1.0406559670	7.8389521081	13.5198093033
C18	-0.0090089458	8.7172552536	13.1951619689
C19	0.2764200063	8.9289360611	11.8500419869
N20	-0.4026954353	8.3341040148	10.8327731589
C21	-1.4551079925	7.5580342503	11.1573906719
C22	-1.7768040196	7.2668542732	12.4895253382
H23	-1.2787331981	7.6242277538	14.5566386877

H24	0.5786392437	9.2242989067	13.9516233626
H25	-2.6106539279	6.6006379558	12.6759086862
N26	1.6324008099	9.9898755571	10.1684820182
C27	1.3463284429	9.8261350359	11.4119033552
O28	2.0663694215	10.5038981865	12.3177118148
N29	-2.8907244094	5.8838829924	10.1277860352
C30	-2.3432375821	7.0346739638	10.0927303675
O31	-2.6529559996	7.9012506919	9.1046218726
C32	3.0111449030	11.3158095294	11.5560428912
H33	4.0132034366	11.0907149522	11.9259640287
H34	2.7734229744	12.3661831442	11.7497874907
C35	2.7797032015	10.9122466053	10.0712136133
H36	3.6329759910	10.3379828588	9.6901417720
C37	-3.7452704148	5.8080948371	8.9240702514
H38	-3.4234903254	4.9400655839	8.3382712896
C39	-3.4341778637	7.1291817048	8.1603471770
H40	-4.3202212113	7.7146350077	7.9003937793
H41	-2.8146382646	6.9753197133	7.2736461184
C42	2.5042013860	12.0961868958	9.1460230562
H43	1.6264015579	12.6562981096	9.4819280042
H44	3.3675375997	12.7703853941	9.1326479190
H45	2.3203637231	11.7588166037	8.1239985703
C46	-5.2143438745	5.6371996127	9.3173668493
H47	-5.5662114792	6.5033054011	9.8888667183
H48	-5.8453702001	5.5344278135	8.4276214198
H49	-5.3412411711	4.7446740027	9.9365371084
O50	-0.1904561417	6.8954788700	8.2283615319
C51	0.2725718414	6.1429584950	7.1137138125
C52	-0.4228176429	4.8166577863	7.0486965452
H53	0.0997696888	6.7009883119	6.1803106405
H54	1.3589034468	5.9773938205	7.1924617537
H55	-1.1719886029	4.6650551115	6.2743061372
C56	0.3818715850	1.5455093516	9.6371701623
C57	-0.5473592744	1.4170076176	8.5962849440
C58	-0.8145867841	2.4907314929	7.7618709684
C59	-0.1570635664	3.7423931420	7.9347233460
C60	0.7750161257	3.8533158208	9.0080787451
C61	1.0348395487	2.7693664555	9.8331959523
H62	0.5924168743	0.7020963264	10.2889938989
H63	-1.0595698577	0.4710087786	8.4399020332
H64	-1.5313390451	2.3837181299	6.9504791248
H65	1.2746472998	4.7990466535	9.1914984940
H66	1.7526562848	2.8764192121	10.6422861203

Cartesian coordinates of **ts-trans-2b-oxo**

atom	x	y	z
N5	-0.0804421640	-0.0321508163	0.0826400369
Ru1	-0.0548079391	0.0269130686	2.4322499166
N20	1.1407861794	0.0035055819	4.0451063695
C2	0.0861174611	-0.4916501653	-2.6437170973
C3	1.2350858351	-0.5271306176	-1.8513764798
C4	1.1101992055	-0.2849973684	-0.4861396220
C6	-1.1855579822	0.0403684841	-0.6708541079
C7	-1.1366240469	-0.1930177249	-2.0479262280
H8	0.1489415036	-0.6789995617	-3.7126406235
H9	2.2244941178	-0.7278023836	-2.2465225822
H10	-2.0684658828	-0.1161350520	-2.5967063300
C11	-2.4744801219	0.4735131558	0.0346737857
O12	-3.5000627209	0.5367223151	-0.6567565915
C13	2.3079721936	-0.2553474941	0.4415644667
O14	2.0204486147	0.1345791102	1.6439600314
O15	3.4184261678	-0.5705435554	0.0177097502
O16	-2.2892903022	0.7516884069	1.2603473602
C17	3.0303975774	0.0214072177	6.0262776817
C18	2.5225148233	1.2307844196	5.5406184187
C19	1.5687222515	1.1858386949	4.5269711054
C21	1.6553050723	-1.1650502417	4.4649037895
C22	2.6065267648	-1.1953772641	5.4812937323
H23	3.7754069166	0.0279773947	6.8148630319
H24	2.8618354638	2.1866771910	5.9228542066
H25	3.0120416804	-2.1429210354	5.8166914924
N26	0.1250512350	2.0868106478	2.8400524375
C27	0.9333069641	2.3084255432	3.8230580635
O28	1.1630218785	3.5760854680	4.1698729539
N29	0.3617165587	-2.0906540183	2.6631738137
C30	1.1252803576	-2.2915957456	3.6849996292

O31	1.4086091834	-3.5521513424	4.0250707146
C32	0.4552592585	4.3867448109	3.1642732228
H33	1.2200727857	4.8477596010	2.5334284288
H34	-0.1008974744	5.1550926481	3.7032832107
C35	-0.4536539713	3.3773354157	2.4072547979
H36	-0.3276638511	3.4607085938	1.3245142124
C37	-0.0872729564	-3.4081632179	2.1624795419
H38	-1.1425091069	-3.5079926401	2.4466275554
C39	0.8051766067	-4.3828487232	2.9780547066
H40	1.6237463475	-4.7979387406	2.3816172359
H41	0.2586583293	-5.1868475312	3.4721502313
C42	-1.9370230560	3.4593354126	2.7697387305
H43	-2.0713552231	3.4065148672	3.8559414365
H44	-2.3481981708	4.4098667904	2.4121163708
H45	-2.4704290108	2.6278618279	2.2993174335
C46	0.0492586087	-3.5607644950	0.6516790061
H47	1.0836725528	-3.4004378935	0.3334872009
H48	-0.2589991951	-4.5679966395	0.3521463797
H49	-0.5904114926	-2.8421288085	0.1358343384
O50	-1.4720031881	-0.2078107973	3.4941673739

Cartesian coordinates of **trans-2b-oxo**

atom	x	y	z
Ru1	0.1494334511	8.2280660581	8.7701515205
C2	3.6505126831	8.3113877604	5.6699054709
C3	3.6634794767	7.3566519065	6.6953226758
C4	2.6320706628	7.3845204798	7.6300818711
N5	1.6863751714	8.3181304309	7.5100871309
C6	1.6491326286	9.2695611776	6.5769687130
C7	2.6457136653	9.2863465491	5.6054510260
H8	4.4364964827	8.3016525753	4.9195493598
H9	4.4372845451	6.6024144054	6.7846236663
H10	2.6213181041	10.0509434058	4.8369852325
C11	0.5101773942	10.2735000698	6.7640333691
O12	0.4689619750	11.2598267781	6.0402405605
C13	2.4548976851	6.4745628986	8.8473431861
O14	3.2932867545	5.6175059677	9.0790514402
O15	1.3932323646	6.7386098786	9.5781594498
O16	-0.3209517772	9.9934010016	7.7389635977
C17	1.3174661016	10.2253986724	13.5688808350
C18	2.2653192441	10.5132572510	12.5945385191
C19	2.0036916093	10.1820262813	11.2560595452
N20	0.8821323908	9.5405571278	10.8742108615
C21	-0.0339611055	9.2885380310	11.8334871936
C22	0.1290215338	9.6202807073	13.1808899295
H23	1.4979654677	10.4805749648	14.6082786357
H24	3.1972130259	11.0063452411	12.8384893378
H25	-0.6598924300	9.3895940755	13.8865229096
N26	2.7710350178	10.7170901491	8.9772828411
C27	2.9718940781	10.6395539542	10.2298836737
O28	4.1530535715	11.1072903077	10.7359230473
N29	-1.4125880966	8.1367477749	10.2081247190
C30	-1.2588476739	8.6155965412	11.3871252693
O31	-2.2809739500	8.4817019377	12.2519312890
C32	4.9084735818	11.5906407382	9.5950959175
H33	5.8325156168	11.0089970074	9.5321123342
H34	5.1548212964	12.6421827578	9.7728716145
C35	3.9503369687	11.3793286855	8.3870787162
H36	4.3933880448	10.6957114256	7.6535997424
C37	-2.7266307569	7.4587111225	10.1409129520
H38	-3.2744791984	7.8679836073	9.2874081654
C39	-3.3721676236	7.8804443508	11.4891421319
H40	-3.7552436823	7.0379429921	12.0686372117
H41	-4.1516898484	8.6396279951	11.3798907407
C42	3.5332576160	12.6698129794	7.6771123063
H43	3.1238563044	13.3879699863	8.3959591364
H44	4.3947418358	13.1309336861	7.1812052999
H45	2.7607986601	12.4611038928	6.9321269307
C46	-2.5655978519	5.9465343946	9.9754714389
H47	-2.0078745957	5.5210002816	10.8163061116
H48	-3.5529277747	5.4738963647	9.9331997319
H49	-2.0268410640	5.7285219370	9.0519552666
O50	-0.7493780666	7.1621110533	7.6917777097

Cartesian coordinates of **ts-trans-2b-o-ene**

atom	x	y	z
Ru1	-0.4437484804	7.9547470471	8.5919708841
C2	2.8116601652	7.1619891629	5.3218304591
C3	2.8089190942	6.4010415914	6.4988559130
C4	1.8392167722	6.6751965078	7.4563339742
N5	0.9482678766	7.6459760307	7.2178762272
C6	0.9345561842	8.4169565767	6.1295597985
C7	1.8789231522	8.1875866641	5.1322489854
H8	3.5493586003	6.9574985348	4.5510262298
H9	3.5284205472	5.6125881744	6.6900088239
H10	1.8573106816	8.7965915049	4.2366785005
C11	-0.1416537467	9.4973350345	6.1594224751
O12	-0.2246176393	10.2878118204	5.2244873807
C13	1.6873946227	6.0154241327	8.8251110076
O14	2.4450706562	5.1131185210	9.1481664708
O15	0.7371734501	6.5333083149	9.5744834097
O16	-0.9089722363	9.4784990216	7.2215432217
C17	1.6341821597	10.5731273592	12.6279408696
C18	2.3869272408	10.6380612866	11.4625766123
C19	1.8619303049	10.1299418783	10.2638222106
N20	0.6638946271	9.5107509060	10.2000616174
C21	-0.0635595811	9.4858954171	11.3416778377
C22	0.3679346160	10.0097221062	12.5628450610
H23	2.0222654476	10.9685667002	13.5613286647
H24	3.3681318534	11.0938180835	11.4475894989
H25	-0.2845085890	9.9501071669	13.4255772884
N26	2.2073474086	10.4156986538	7.8368880361
C33	2.6440490633	10.3926649558	9.0298386963
O30	3.9445218330	10.7593471883	9.2583089236
N29	-1.7867307257	8.2209169507	10.2154298835
C40	-1.3804048817	8.8528524488	11.2542858443
O36	-2.2145680968	8.9185573085	12.3116301165
C37	4.4659902676	11.1828280744	7.9731140834
H38	5.3867194599	10.6260271891	7.7819767903
H39	4.6975241484	12.2524034179	8.0351963129
C39	3.3155417656	10.8717039367	6.9752054295
H40	3.5894772762	10.0372604992	6.3183925511
C38	-3.0952785795	7.6064328376	10.5312448914
H42	-3.7936328338	7.8482404831	9.7258319066
C41	-3.4686876941	8.3276517052	11.8521581775
H41	-3.8237437679	7.6537602312	12.6341270045
H43	-4.1839983390	9.1443116387	11.7126626333
C43	2.8799726678	12.0551498693	6.1110607324
H44	2.6167617520	12.9141400822	6.7380051936
H45	3.6880886035	12.3561927769	5.4346840949
H46	2.0021880805	11.7806653107	5.5200003317
C46	-2.9647586376	6.0877844973	10.6717704411
H47	-2.2688128569	5.8313306975	11.4773504025
H48	-3.9436109805	5.6518995781	10.9008682016
H49	-2.5895377674	5.6653784555	9.7386128733
O50	-1.6845106549	6.7948079059	7.8853978266
C57	0.5340656330	6.7603108362	1.8135569308
C58	-0.3180943085	7.7095930996	2.3874116269
C59	-1.0305707646	7.4149619579	3.5440035255
C60	-0.9103059136	6.1513491354	4.1696566648
C61	-0.0474850822	5.2041980034	3.5688711636
C62	0.6651653036	5.5044701668	2.4134854360
H64	-0.4277630291	8.6900538959	1.9322037690
H65	-1.6821900280	8.1729884325	3.9651189594
H66	0.0569168133	4.2246067304	4.0295133128
H67	1.3223320751	4.7572014838	1.9759277021
H63	-2.5624360314	7.6384642529	5.9273401967
C64	-2.4349320282	6.5875324662	6.1682862275
H68	-3.2772000904	6.1339461447	6.6783513805
C65	-1.6712779846	5.7657436105	5.3402269579
H69	-1.6415799709	4.7064008365	5.5901575730
H70	1.0846102433	6.9950476827	0.9065350229

Cartesian coordinates of **trans-2b-o-ene**

atom	x	y	z
Ru1	-0.6320713648	8.2832520101	8.0916340429
C2	2.1575876732	8.2404699343	4.3220380803
C3	2.2569206823	7.2116238750	5.2661442635
C4	1.4343935522	7.2666819562	6.3880487155
N5	0.5946594038	8.2969959595	6.5318784400

C6	0.5001677316	9.3207643092	5.6793092422
C7	1.2797791939	9.3135841643	4.5260825679
H8	2.7707622609	8.2082293101	3.4258659627
H9	2.9296919509	6.3701306538	5.1463356064
H10	1.1913510075	10.1374211041	3.8263292463
C11	-0.4563064701	10.4113398119	6.1486437492
O12	-0.5738016017	11.4366163156	5.4916951224
C13	1.3683366687	6.2660573078	7.5350025884
O14	2.0605062223	5.2594202321	7.5116716444
O15	0.5410412373	6.6092506712	8.5036333079
O16	-1.0754592688	10.1421691951	7.2781918014
C17	1.8280935927	9.6816979281	12.3990632709
C18	2.5290773301	9.9240414803	11.2243353167
C19	1.8988593016	9.7456493299	9.9835030799
N20	0.6380107751	9.2705846226	9.8724376409
C21	-0.0350699106	9.0630397202	11.0331152795
C22	0.5067567508	9.2700641887	12.3034826638
H23	2.2996210452	9.8268823084	13.3657749754
H24	3.5525923392	10.2749878562	11.2383170764
H25	-0.1079656556	9.0859033881	13.1763903205
N26	2.1499952160	10.6281661225	7.6953637345
C33	2.6456583269	10.2125180729	8.7888963164
O30	3.9987432417	10.3155218298	8.9764253386
N29	-1.8933681099	8.1935092112	9.7748742650
C40	-1.4038723446	8.5663480839	10.9001956701
O36	-2.1930082771	8.4722686701	11.9882895329
C37	4.5043722732	11.0121658502	7.8081386025
H38	5.3193191892	10.4183153496	7.3874744427
H39	4.8954371312	11.9831985654	8.1335349135
C39	3.2659269786	11.1421140246	6.8779798093
H40	3.3679766793	10.4849069706	6.0058395502
C38	-3.2438248389	7.6409121877	10.0138019341
H42	-3.9385540748	8.1200184700	9.3190511354
C41	-3.5054025478	8.0753696691	11.4807448984
H41	-3.8751639129	7.2682255313	12.1160861986
H43	-4.1643524057	8.9450012193	11.5639061270
C43	2.9707232656	12.5610943575	6.3923717642
H44	2.8824380038	13.2492593677	7.2400645479
H45	3.7716797740	12.9205410064	5.7365498044
H46	2.0256311372	12.5755404218	5.8427132544
C46	-3.2615592404	6.1252526661	9.8014468176
H47	-2.5656087052	5.6282889801	10.4856864480
H48	-4.2697685411	5.7371271756	9.9839157704
H49	-2.9683292333	5.9016265353	8.7752398252
O50	-2.0487602107	7.3447061252	7.1391128754
C57	0.3913397918	4.5273778098	1.7696471040
C58	-0.4220019233	5.6659435565	1.8293942858
C59	-0.9717878621	6.0823758122	3.0339513685
C60	-0.7250088979	5.3637148819	4.2399391880
C61	0.1038913635	4.2071057473	4.1507146878
C62	0.6487939020	3.8036303639	2.9423721638
H64	-0.6275312122	6.2305668535	0.9233360992
H65	-1.6024138321	6.9662349626	3.0546597142
H66	0.3244047788	3.6547517827	5.0601780133
H67	1.2840904254	2.9222333588	2.9070396978
H63	-1.7249077899	7.8265525880	5.1358577272
C64	-2.0524397703	6.9903381450	5.7732610117
H68	-3.1124491160	6.8150478377	5.5088063260
C65	-1.2420018231	5.7585659739	5.4979571074
H69	-1.0580149197	5.1175973189	6.3566335537
H70	0.8193802870	4.2085319104	0.8233499645

Geometries below are non-carboxylated conformations of **trans-2a-oxo** and **2a-oxo** for **Figure S24**.
Cartesian coordinates of non-carboxylated **2a-oxo**

atom	x	y	z
Ru1	0.4084711150	8.7855753428	9.1436555441
C2	3.7990982612	8.0492765936	5.7217269350
C3	3.5752577447	7.1639795687	6.7742834528
C4	2.5780935431	7.4552746000	7.6998636352
N5	1.8308023096	8.5757697231	7.5946585429
C6	2.0358719334	9.4383385180	6.5819463912
C7	3.0165705455	9.2027395152	5.6241172353

H8	4.5701212870	7.8452023663	4.9851239186
H9	4.1410148077	6.2490307086	6.9104791060
H10	3.1592043876	9.9143665816	4.8181624441
H11	1.3932952709	10.3127566997	6.5677943367
C13	2.2674253709	6.5266695705	8.8688568513
O14	2.9104222309	5.4996326942	9.0031731731
O15	1.2960082402	6.9468369426	9.6384865711
C17	-2.3310514660	8.2680311803	13.0170944992
C18	-1.0889834168	8.9038441928	13.1256103549
C19	-0.3374431571	9.0708254828	11.9641468216
N20	-0.8027739966	8.6422841057	10.7809805250
C21	-1.9727405488	7.9968581787	10.6662974883
C22	-2.7849141127	7.7950148324	11.7806723345
H23	-2.9399426198	8.1241237203	13.9035137663
H24	-0.7071447231	9.2504221389	14.0791092932
H25	-3.7310772650	7.2754569443	11.6811864709
N26	1.6116058780	9.6725639722	10.6795031588
C27	1.0151223492	9.6414476573	11.8279143558
O28	1.6620550064	10.1046388841	12.8868685241
N29	-1.2921062225	7.7119141730	8.3698131896
C30	-2.1907731697	7.5328293658	9.2839421430
O31	-3.3099008719	6.9035537836	8.9561716393
C32	2.9868880610	10.5273379845	12.4051238816
H33	3.7257318931	9.9216623076	12.9322662611
H34	3.1045953386	11.5790762437	12.6733238940
C35	2.9491980225	10.2819567198	10.8667033503
H36	3.6971176655	9.5373096326	10.5746891105
C37	-1.7968619181	7.1249584312	7.1051984967
H38	-1.9373643074	7.9490622930	6.3966987828
C39	-3.1680229186	6.5281808690	7.5412553240
H40	-3.1936636713	5.4367658486	7.4965765091
H41	-4.0250261532	6.9439185013	7.0102357279
C42	3.1194302142	11.5487017999	10.0294953297
H43	2.3668790050	12.2978973212	10.2937541630
H44	4.1130764617	11.9751840057	10.1993611804
H45	3.0218105884	11.3235518830	8.9650132485
C46	-0.8365757212	6.0931467342	6.5181306523
H47	-0.6337689924	5.2925029560	7.2355928965
H48	-1.2727340076	5.6527117603	5.6160326812
H49	0.1112905063	6.5592018995	6.2403227849
O50	-0.1935042024	10.3604630511	8.5312933862

Cartesian coordinates of non-carboxylated ts-2a-o-ene

atom	x	y	z
Ru1	0.5805674542	9.0502938584	9.2513563324
C2	3.2092984441	7.2131297523	5.5697069713
C3	2.9325892407	6.5092045981	6.7401928066
C4	2.1644388732	7.1190960703	7.7272042838
N5	1.6864584975	8.3724805195	7.5719891678
C6	1.9440109895	9.0588687011	6.4461824088
C7	2.7053719410	8.5073669374	5.4202235921
H8	3.8066276787	6.7617667924	4.7833591745
H9	3.2861230342	5.5006357989	6.9231371128
H10	2.8964312273	9.0865080116	4.5230748141
H11	1.5203393591	10.0573564206	6.4021145898
C13	1.8147869995	6.4062840169	9.0260682723
O14	2.2010289281	5.2628266065	9.2052134940
O15	1.1019322865	7.1210717191	9.8608414173
C17	-1.5121698046	9.2666662889	13.5127973149
C18	-0.1768584019	9.6570671956	13.3719307443
C19	0.3784080529	9.6591699132	12.0938534407
N20	-0.3555298600	9.3103201960	11.0155076115
C21	-1.6257220036	8.8777536915	11.1510830751
C22	-2.2483818610	8.8561621209	12.3949895393
H23	-1.9702635743	9.2533345290	14.4959560330
H24	0.4292601483	9.9334318777	14.2274431646
H25	-3.2721118516	8.5107608089	12.4826319510
N26	2.1596011666	9.7587799271	10.4886275867
C33	1.7714381187	9.9194624566	11.7153013501
O30	2.6779646141	10.2832587747	12.6157185903
N29	-1.3981801981	8.3266777892	8.8217254995
C40	-2.1561661811	8.3929950781	9.8698626601
O36	-3.4139478165	7.9813168515	9.7649612449
C37	3.9623759967	10.3410041429	11.9041310005
H38	4.6099959076	9.5838416890	12.3500438009

H39	4.3805617321	11.3352577042	12.0733474509
C39	3.6058670646	10.0641733297	10.4132538667
H40	4.1191876675	9.1672431816	10.0514202595
C38	-2.2018002130	7.7809211510	7.7041896506
H42	-2.2945521776	8.5714142319	6.9505217233
C41	-3.5734576152	7.5021402600	8.3872068773
H41	-3.8156569682	6.4378538434	8.4424935970
H43	-4.4081288854	8.0513920780	7.9495541678
C43	3.8886750889	11.2367991149	9.4744915654
H44	3.4009290358	12.1496756365	9.8315203471
H45	4.9662479666	11.4201659234	9.4178311223
H46	3.5225212348	11.0208905573	8.4680978453
C46	-1.5640306103	6.5438062344	7.0764748200
H47	-1.4073379151	5.7610153388	7.8246079272
H48	-2.2139502408	6.1498143674	6.2886694267
H49	-0.6006612163	6.7920180644	6.6257970407
O50	0.3053835712	10.6763497473	8.3912962872
C60	-2.5233739150	12.3142615694	10.0969542251
C61	-3.2033054202	12.4369610034	11.3305694524
C62	-4.5885779724	12.3451457940	11.4026416353
H66	-2.6267058658	12.6263980242	12.2330170497
H67	-5.0894061591	12.4569808608	12.3600561855
H63	-0.7005894953	12.6233839115	7.9706556125
C64	-0.2704309386	12.4594193780	8.9515640785
H65	0.7574275626	12.7859262864	9.0583967472
C59	-1.0813775144	12.4463762802	10.0739909409
H60	-0.6019274312	12.5376031332	11.0475713527
C63	-5.3362734195	12.1196447134	10.2439361236
H62	-6.4187323349	12.0521162933	10.2968663970
C65	-4.6825111525	11.9875854225	9.0135201828
H64	-5.2615257141	11.8188827028	8.1098209030
C66	-3.2980746522	12.0810017228	8.9366839810
H68	-2.8079582533	11.9767486448	7.9737848100

Cartesian coordinates of non-carboxylated **2a-o-ene**

atom	x	y	z
Ru1	0.5431487489	8.9201599697	9.1121977244
C2	3.8044230428	7.3673563270	5.8510772582
C3	3.4250355650	6.6307054465	6.9724319484
C4	2.4700362776	7.1622515297	7.8326593302
N5	1.9101279627	8.3701461025	7.6024339766
C6	2.2676342060	9.0888644226	6.5260498443
C7	3.2166387507	8.6139318046	5.6247264661
H8	4.5465160371	6.9767652591	5.1615441504
H9	3.8388284554	5.6565122584	7.2079892904
H10	3.4860334576	9.2151268966	4.7629225501
H11	1.7687907313	10.0471966408	6.4203115035
C13	1.9971494212	6.4153862190	9.0699044538
O14	2.4686935735	5.3236595608	9.3377057758
O15	1.0710429457	7.0399691177	9.7669689455
C17	-2.1170083671	9.0959848265	13.0557804200
C18	-0.7933036601	9.5552444277	13.0811998628
C19	-0.0709897968	9.5497640906	11.8934599252
N20	-0.6310288281	9.1347832056	10.7386186463
C21	-1.8837993335	8.6421848068	10.7151479218
C22	-2.6711888205	8.6183856858	11.8672989215
H23	-2.7041057032	9.0903368748	13.9675910369
H24	-0.3263103307	9.8919076635	13.9997943745
H25	-3.6799052546	8.2232661940	11.8270471437
N26	1.9128645616	9.7342157673	10.5407443133
C33	1.3456567449	9.8886257140	11.6967840588
O30	2.0911992475	10.3228150451	12.7047999112
N29	-1.3079270345	8.0979543889	8.4472693912
C40	-2.2063951331	8.1168850048	9.3855381560
O36	-3.4118752580	7.6331012103	9.1076753289
C37	3.4607617007	10.4388416562	12.1837349313
H38	4.0703676798	9.7119898116	12.7241654019
H39	3.8050669052	11.4510794823	12.4037820976
C39	3.3315001569	10.1427516682	10.6606654528
H40	3.9536915177	9.2871542307	10.3786935389
C38	-1.9164641927	7.4975810740	7.2360462028
H42	-1.9601748316	8.2789365744	6.4682191873
C41	-3.3447666231	7.1260508309	7.7315073503

H41	-3.5134533617	6.0471876892	7.7777873692
H43	-4.1496076477	7.6032511653	7.1706193446
C43	3.6535953799	11.3370741433	9.7629242810
H44	3.0544242454	12.2096377435	10.0417817782
H45	4.7124547255	11.5988262542	9.8551719361
H46	3.4464857758	11.0992981799	8.7171678437
C46	-1.1184531024	6.3067187227	6.7108922033
H47	-1.0102934542	5.5372505028	7.4810004705
H48	-1.6297740678	5.8692931196	5.8474900050
H49	-0.1229000382	6.6205678066	6.3895120576
O50	0.2208701276	10.6120551434	8.1741513217
C60	-2.0288364548	12.4090028323	10.4745303008
C61	-1.8413007669	13.1541551482	11.6781342469
C62	-2.8832196896	13.3699516923	12.5646442432
H66	-0.8564559376	13.5641649142	11.8890872642
H67	-2.7103519511	13.9448063988	13.4702632711
H63	-1.8398932511	10.8553885979	8.2004285158
C64	-0.9201821439	11.4470606469	8.3185019945
H65	-0.8925658272	12.1554038012	7.4731634140
C59	-0.9273142259	12.2023506704	9.6096176288
H60	0.0176719408	12.6740867352	9.8728514802
C63	-4.1605228161	12.8589389016	12.2942527285
H62	-4.9785623277	13.0366764298	12.9858521255
C65	-4.3775502949	12.1335423296	11.1154287724
H64	-5.3708568578	11.7530865657	10.8926733982
C66	-3.3412695865	11.9077651689	10.2206717217
H68	-3.5447138833	11.3651466196	9.3030523890

Cartesian coordinates of non-carboxylated **trans-2a-oxo**

atom	x	y	z
Ru1	0.4020385599	8.4970354572	8.7970745359
C2	3.3993447878	4.8282959607	10.4228566073
C3	2.3285539986	5.1641166771	11.2561507384
C4	1.4610448995	6.1739714164	10.8563706202
N5	1.6182566547	6.8351820191	9.6949751489
C6	2.6498128635	6.5133742453	8.8881789631
C7	3.5614303226	5.5141007028	9.2226543867
H8	4.0933006053	4.0438026973	10.7090001627
H9	2.1662879031	4.6542623742	12.1997937831
H10	4.3666534480	5.3100277183	8.5257911478
C11	2.7826283248	7.2842659951	7.5821758425
O12	3.7132849401	7.0285533876	6.8358490752
H13	0.6175302421	6.4662618088	11.4749065271
O16	1.8519628886	8.1763424225	7.3667053926
C17	-2.6578150349	8.8496812175	12.4504240267
C18	-1.4816299440	9.6101077388	12.4566898208
C19	-0.6139141544	9.4795817054	11.3733759307
N20	-0.9117854693	8.6475889618	10.3609258723
C21	-2.0328009423	7.9077224880	10.3394464042
C22	-2.9479057947	7.9837774953	11.3887101587
H23	-3.3530070723	8.9321661977	13.2795293122
H24	-1.2437820658	10.2837428088	13.2723195206
H25	-3.8542153755	7.3889984503	11.3706215042
N26	1.3925927475	9.8779958264	10.0968910339
C27	0.6824405170	10.1525681844	11.1437915113
O28	1.1494149759	11.0472577417	12.0031092390
N29	-1.1390537209	7.0995115780	8.2476476491
C30	-2.1036894659	7.0875654350	9.1116531892
O31	-3.1688766870	6.3394660146	8.8555293425
C32	2.4065925908	11.5547879286	11.4183162596
H33	3.1845929074	11.4224957657	12.1709147335
H34	2.2556486731	12.6181606622	11.2188079456
C35	2.6165785674	10.7130940375	10.1240280301
H36	3.4724402797	10.0370885891	10.2318863462
C37	-1.5605105679	6.2908529394	7.0775516792
H38	-1.7769570852	7.0031538148	6.2721802685
C39	-2.8650080294	5.6280849271	7.5993271957
H40	-2.7344727383	4.5728331711	7.8555611178
H41	-3.7266618731	5.7501712348	6.9434663236
C42	2.7681200329	11.5304854989	8.8434301840
H43	1.9151007302	12.2014523881	8.7046401795
H44	3.6831317540	12.1288235123	8.8914472681
H45	2.8323767482	10.8659743640	7.9782832303

C46	-0.4868590254	5.3131473801	6.6135748129
H47	-0.2193665608	4.6132070017	7.4116350387
H48	-0.8506617100	4.7384525128	5.7563548630
H49	0.4068256725	5.8579442602	6.3003400764
O50	-0.3946329435	9.8050300337	7.8886034574

Cartesian coordinates of non-carboxylated **ts-trans-2a-o-ene**

atom	x	y	z
Ru1	0.3537875748	8.5543340191	8.8530402291
C2	3.5047565301	4.8905023628	10.0405723399
C3	2.5259435239	5.2030958394	10.9873942686
C4	1.6201733920	6.2191209428	10.7029936934
N5	1.6593826898	6.9098873244	9.5494898759
C6	2.6038688827	6.6123676761	8.6321141517
C7	3.5410178891	5.6040441950	8.8456290577
H8	4.2254104518	4.1018816659	10.2349232320
H9	2.4621985411	4.6708394292	11.9305732463
H10	4.2677884002	5.4141500858	8.0638167650
C11	2.6050309597	7.4188443128	7.3396603513
O12	3.3921890391	7.1201212734	6.4524279674
H13	0.8409981058	6.4943970118	11.4075341313
O16	1.7302865726	8.3841873114	7.2941707406
C17	-2.6614201289	8.7801659435	12.5365063692
C18	-1.4873743321	9.5404159828	12.5509242492
C19	-0.6256746494	9.4446435087	11.4591851039
N20	-0.9145191539	8.6366222574	10.4174128426
C21	-2.0446058556	7.9006180813	10.3930740022
C22	-2.9512968913	7.9464106294	11.4494938897
H23	-3.3510287890	8.8366082686	13.3719704770
H24	-1.2420978524	10.1921927533	13.3820645068
H25	-3.8555107142	7.3489018847	11.4163679994
N26	1.3640350726	9.8778525813	10.1877855774
C27	0.6638940004	10.1150026177	11.2529598053
O28	1.1599342383	10.9560309732	12.1553378782
N29	-1.1656608126	7.1294166801	8.2878462791
C30	-2.1229793601	7.1025151003	9.1608239074
O31	-3.1802390103	6.3358832214	8.9151345142
C32	2.4099677227	11.4762650080	11.5800689727
H33	3.1931471555	11.3338850947	12.3254476613
H34	2.2589882667	12.5437346834	11.3985923829
C35	2.6177133154	10.6625340818	10.2697614909
H36	3.4441915282	9.9500518528	10.3791174547
C37	-1.5587941568	6.2667946848	7.1466684522
H38	-1.7135889588	6.9245994618	6.2847925957
C39	-2.9033290745	5.6581892248	7.6399749611
H40	-2.8366078557	4.5879092261	7.8538612414
H41	-3.7496509514	5.8520611883	6.9799679816
C42	2.8432719703	11.5135168733	9.0233138704
H43	2.0207105451	12.2214579075	8.8820157667
H44	3.7772790930	12.0763678173	9.1171771683
H45	2.9114089443	10.8734541847	8.1403587662
C46	-0.4984101258	5.2249402497	6.8016850878
H47	-0.2825114007	4.5823056093	7.6616124040
H48	-0.8532042065	4.5958060618	5.9793963576
H49	0.4240140215	5.7086593772	6.4745192932
O50	-0.5783688974	9.9623497858	8.0870626746
C51	-1.0313266571	10.2790208969	5.3815065938
H52	-1.9466807428	10.8681555570	5.3544077296
C53	-1.0540871893	6.9447761948	2.7216673967
C54	-2.1797995320	7.7634503089	2.8541055507
C55	-2.1548578417	8.8400967182	3.7331177050
C56	-1.0054409444	9.1257457751	4.5083729721
C57	0.1237357869	8.2816956001	4.3652110225
C58	0.0926119020	7.2104198045	3.4805202033
H59	-1.0665938024	6.1099884613	2.0266949599
H60	-3.0705322686	7.5660372828	2.2645604512
H61	-3.0259425219	9.4844566408	3.8254301194
H62	1.0175396631	8.4611938368	4.9525549841
H63	0.9721167696	6.5816651553	3.3746239812
C64	-0.0407850652	10.6830088814	6.2582689834
H65	-0.1055666568	11.6745022231	6.6896122949
H66	0.9353862229	10.2149048316	6.2523207896

Cartesian coordinates of non-carboxylated **trans-2a-o-ene**

atom	x	y	z
Ru1	0.4030033740	8.4804032728	8.8594775930
C2	3.5090689688	4.9005094774	10.1704342785
C3	2.4920763918	5.2178877289	11.0747193889
C4	1.5908343486	6.2216502566	10.7434801207
N5	1.6719910686	6.8963697438	9.5806251061
C6	2.6520603318	6.5933184449	8.7010446516
C7	3.5866398067	5.5967870281	8.9675981406
H8	4.2273574021	4.1207651360	10.4035947170
H9	2.3962821211	4.6982487057	12.0216903122
H10	4.3446918829	5.4028866371	8.2173272774
C11	2.6922404411	7.3825833872	7.3979930540
O12	3.5294562519	7.0947698585	6.5580027853
H13	0.7832384371	6.5031800405	11.4115697680
O16	1.7899038633	8.3210498533	7.3056983093
C17	-2.7912087751	8.9743374626	12.3507600596
C18	-1.5950382101	9.6971621657	12.3969405385
C19	-0.6699121983	9.5069206767	11.3710927788
N20	-0.9198338415	8.6431021172	10.3665324736
C21	-2.0723450504	7.9484395895	10.3074672561
C22	-3.0425048222	8.0875956202	11.2976197926
H23	-3.5299382049	9.1049047801	13.1339108977
H24	-1.3819746980	10.3926558198	13.2006826462
H25	-3.9653611156	7.5218122001	11.2389842172
N26	1.3911382688	9.8180950674	10.1796099233
C27	0.6497684462	10.1297267781	11.1979171539
O28	1.1292358447	11.0020314878	12.0768783728
N29	-1.1040613314	7.0607538166	8.2871916620
C30	-2.1032973867	7.0893189497	9.1142869416
O31	-3.1550278634	6.3208204682	8.8604198290
C32	2.4286414470	11.4459620736	11.5445579939
H33	3.1671489618	11.2974336863	12.3331309711
H34	2.3343355488	12.5111160917	11.3189709925
C35	2.6627817910	10.5737054564	10.2762697674
H36	3.4656175783	9.8462556413	10.4467424068
C37	-1.4530138753	6.1364207898	7.1771773546
H38	-1.5555421744	6.7464486998	6.2742530569
C39	-2.8265861254	5.5698084375	7.6383064828
H40	-2.7861946994	4.5126708362	7.9146628366
H41	-3.6371771504	5.7373693417	6.9286176452
C42	2.9559237117	11.3637524535	9.0033328751
H43	2.1670694196	12.0973323737	8.8106232436
H44	3.9088800648	11.8925915742	9.1018285202
H45	3.0209394776	10.6866204301	8.1477883117
C46	-0.3929019427	5.0638514244	6.9426890683
H47	-0.2185075523	4.4733738919	7.8484387473
H48	-0.7233795228	4.3880973294	6.1478427821
H49	0.5480351655	5.5164445179	6.6217073076
O50	-0.5769672591	9.9512351080	8.0506039808
C51	-1.3675226194	10.0209709424	5.7628796529
H52	-2.3296915618	10.5093340828	5.9028122855
C53	-1.1731207308	7.1705747681	2.6097447843
C54	-2.3524288543	7.8836237614	2.8665540570
C55	-2.3992646728	8.8094779438	3.8952053126
C56	-1.2600411905	9.0642777374	4.7203681620
C57	-0.0717321769	8.3210178520	4.4406555019
C58	-0.0418992554	7.3986125429	3.4040916278
H59	-1.1359372752	6.4502754595	1.7981462229
H60	-3.2327331872	7.7157798256	2.2522162718
H61	-3.3130720099	9.3681471117	4.0825149888
H62	0.8142851038	8.4610860760	5.0514370779
H63	0.8762735549	6.8512663590	3.2084937797
C64	-0.2870266411	10.4229042220	6.7180743329
H65	-0.2735538219	11.5205082749	6.7974433330
H66	0.6992791760	10.0830079667	6.3976138113