

Supplementary Materials

Role of electronic and steric effects on Ruthenium catalysts with bulky NHC ligands and relationship with the Z-selectivity in olefin metathesis.

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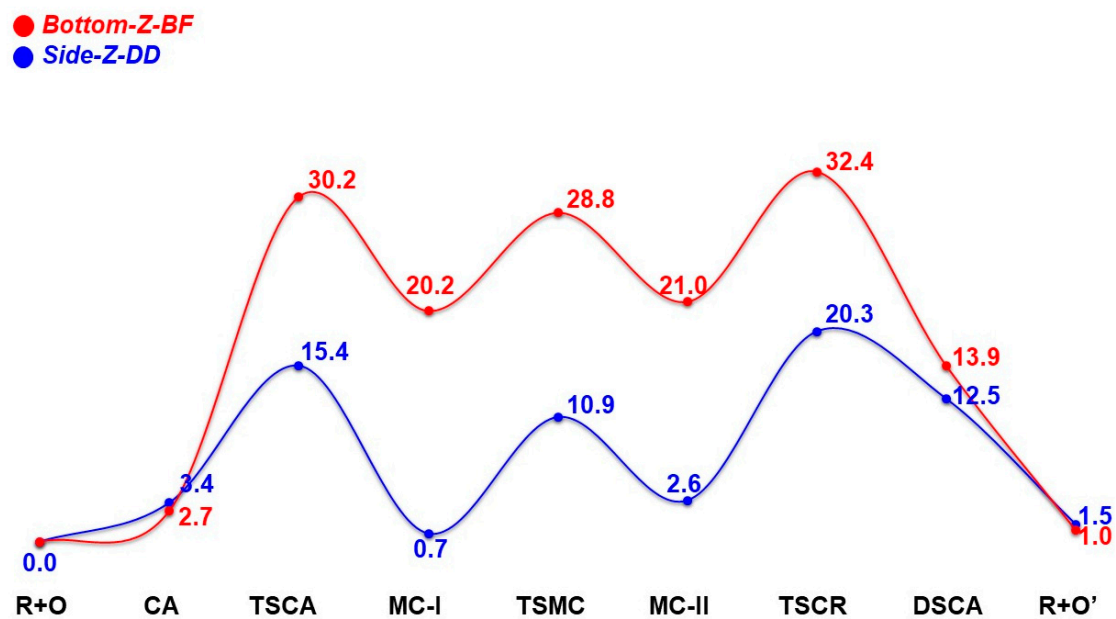


Figure S1. Gibbs energy profile for CM using the **Ru-1** catalyst through the *Bottom-E-BF* and *Side-Z-DD* mechanisms. Values in kcal mol⁻¹.

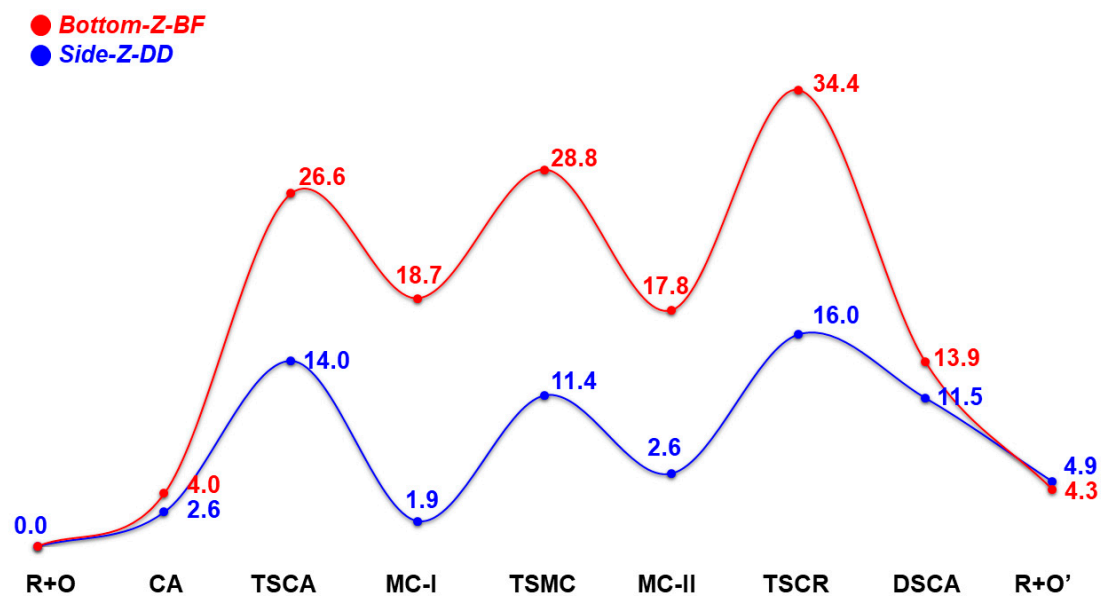


Figure S2. Gibbs energy profile for CM using the **Ru-2** catalyst through the *Bottom-E-BF* and *Side-Z-DD* mechanisms. Values in kcal mol⁻¹.

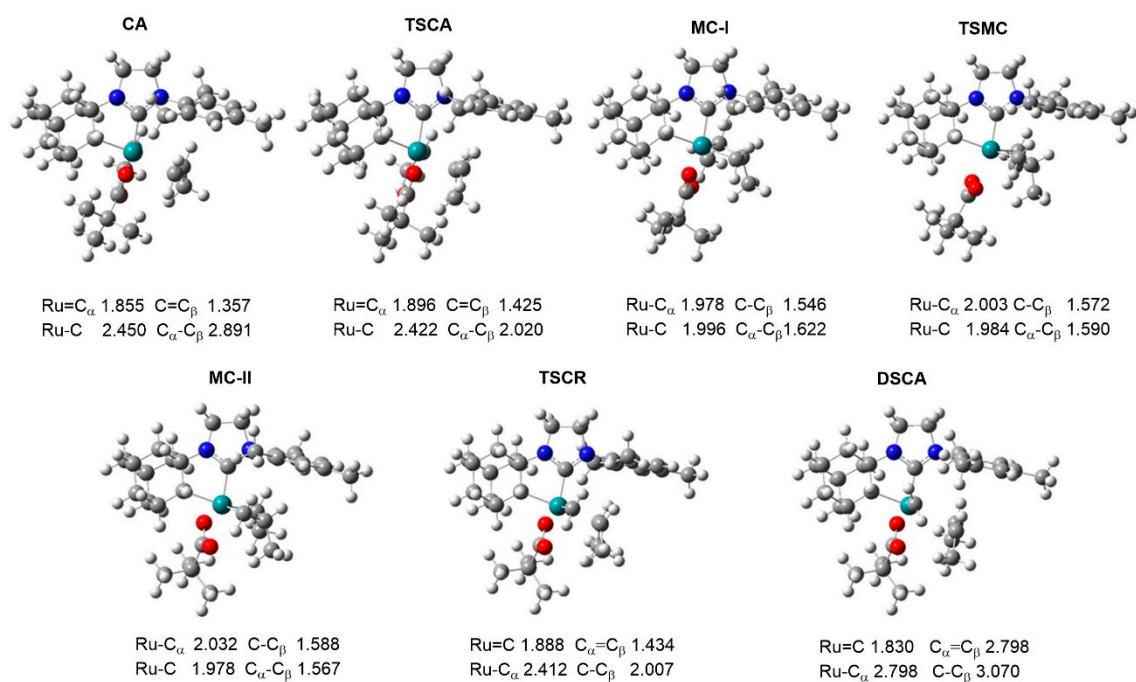


Figure S3. Geometry of the optimized structures associated with the **Side-Z-DD** mechanism for the reaction of CM of propene using the **Ru-1** catalyst. Considering the distances from the Ru=C_α metal center and the C=C_β double bond of the olefin. Values in Å. The colors of the atoms correspond to Ru-Green, N-Blue, O-Red, C-Grey, and H-White.

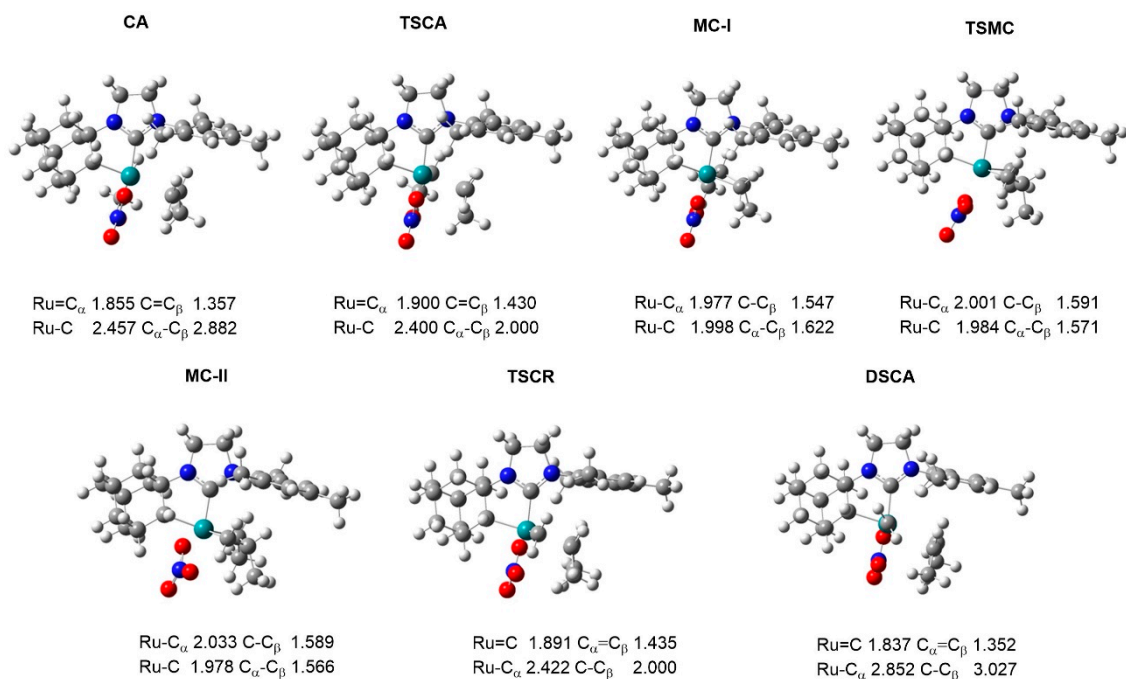


Figure S4. Geometry of the optimized structures associated with the **Side-Z-DD** mechanism for the reaction of CM of propene using the **Ru-2** catalyst. Considering the distances from the Ru=C_α metal center and the C=C_β double bond of the olefin. Values in Å. The colors of the atoms correspond to Ru-Green, N-Blue, O-Red, C-Grey, and H-White.

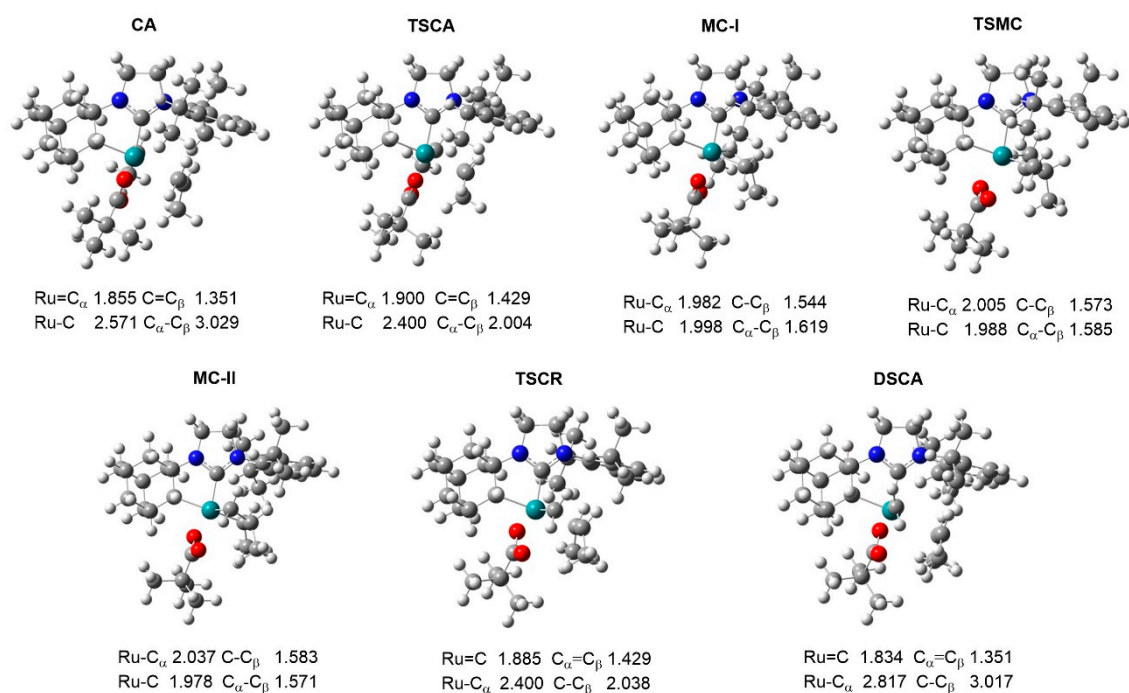


Figure S5. Geometry of the optimized structures associated with the Side-Z-DD mechanism for the reaction of CM of propene using the **Ru-7** catalyst. Considering the distances from the Ru=C_α metal center and the C=C_β double bond of the olefin. Values in Å. The colors of the atoms correspond to Ru-Green, N-Blue, O-Red, C-Grey, and H-White.

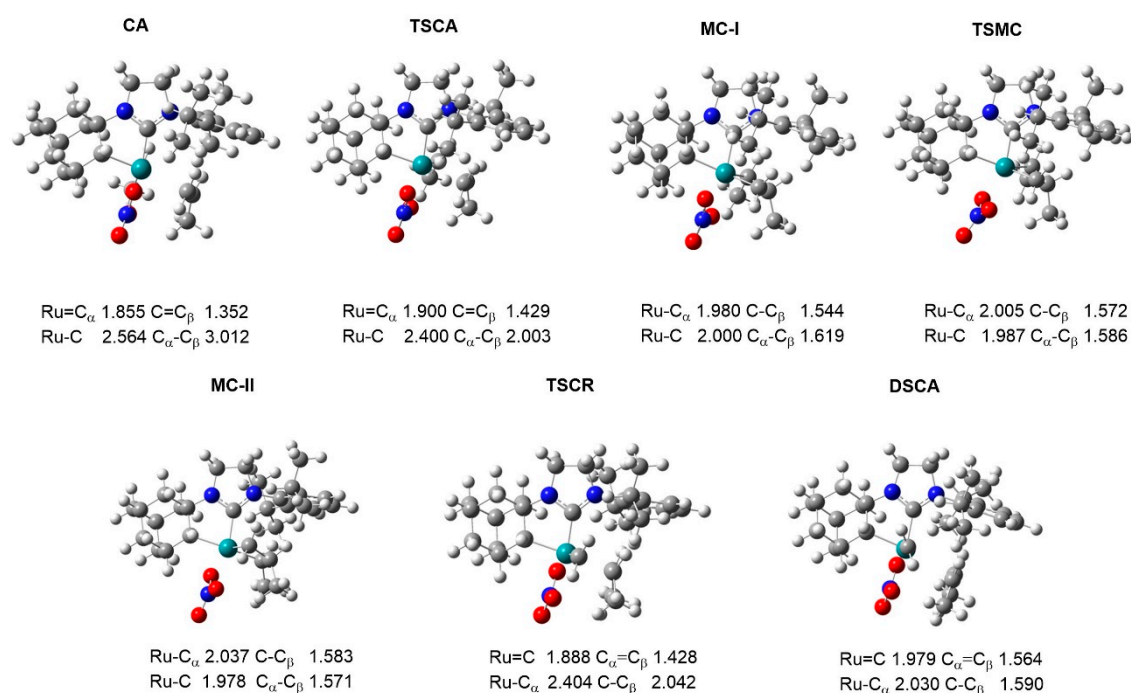


Figure S6. Geometry of the optimized structures associated with the Side-Z-DD mechanism for the reaction of CM of propene using the **Ru-8** catalyst. Considering the distances from the Ru=C_α metal center and the C=C_β double bond of the olefin. Values in Å. The colors of the atoms correspond to Ru-Green, N-Blue, O-Red, C-Grey, and H-White.

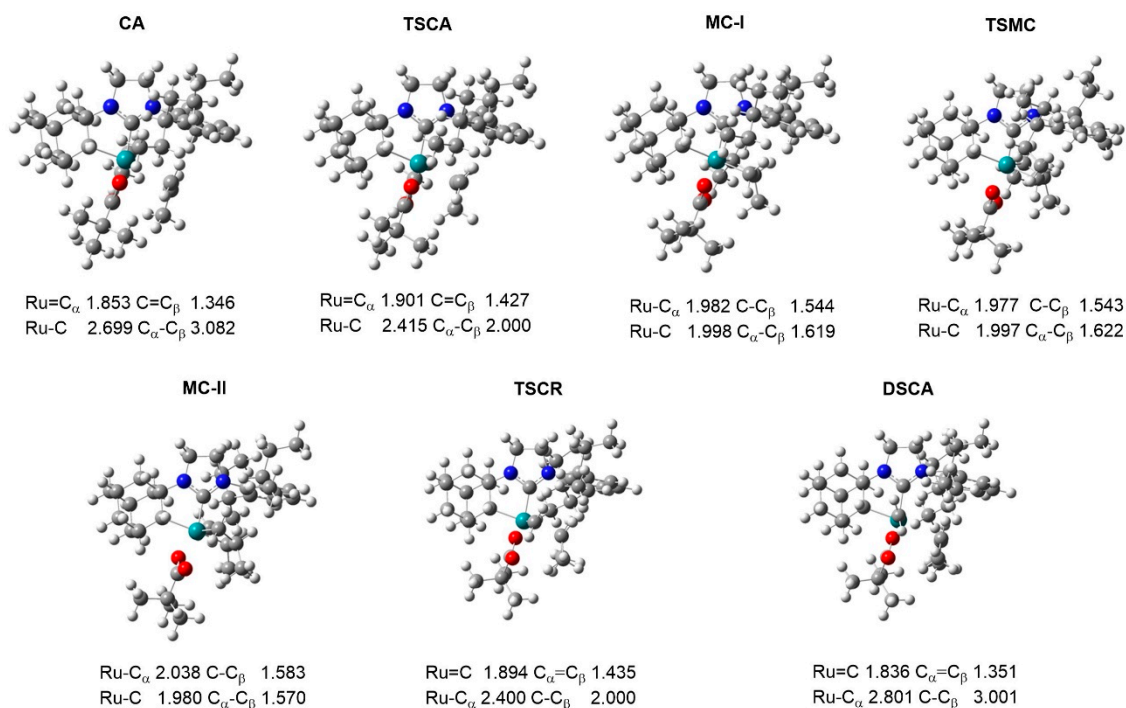


Figure S7. Geometry of the optimized structures associated with the Side-Z-DD mechanism for the reaction of CM of propene using the **Ru-9** catalyst. Considering the distances from the Ru=C_α metal center and the C=C_β double bond of the olefin. Values in Å. The colors of the atoms correspond to Ru-Green, N-Blue, O-Red, C-Grey, and H-White.

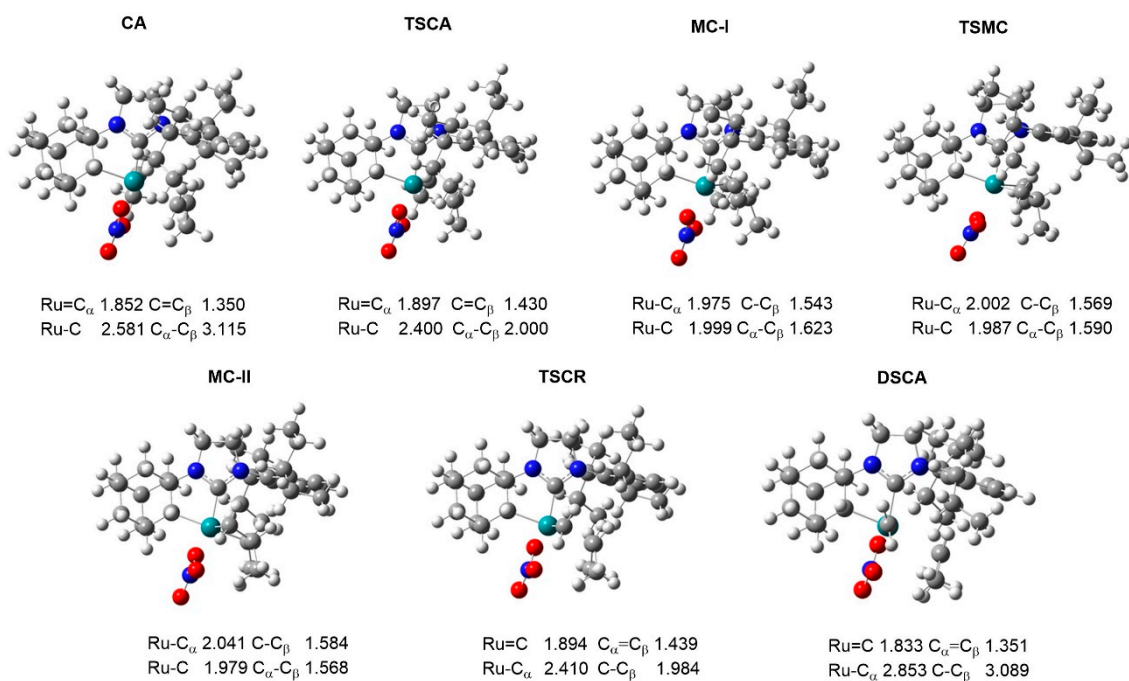


Figure S8. Geometry of the optimized structures associated with the Side-Z-DD mechanism for the reaction of CM of propene using the **Ru-10** catalyst. Considering the distances from the Ru=C_α metal center and the C=C_β double bond of the olefin. Values in Å. The colors of the atoms correspond to Ru-Green, N-Blue, O-Red, C-Grey, and H-White.

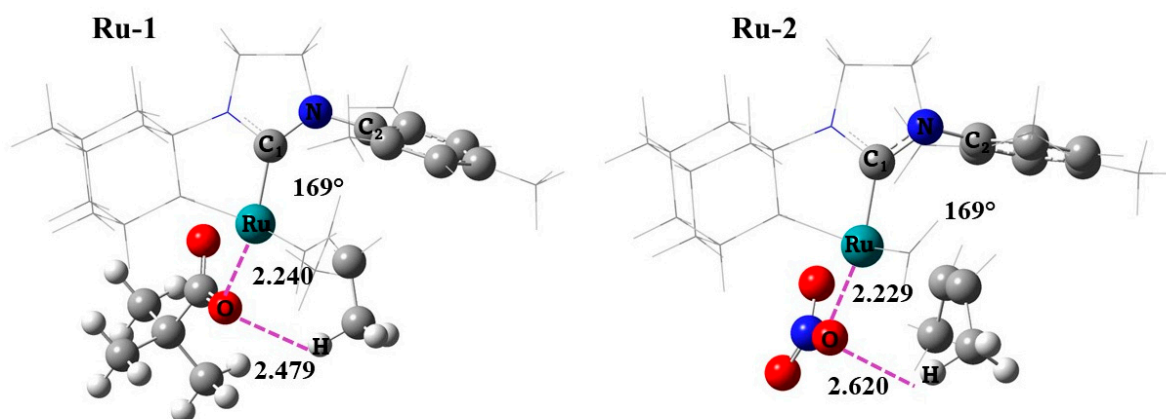


Figure S9. Optimized geometry of the TSCR of the **Ru-1** and **Ru-2** catalysts in the *Side-Z-DD* mechanism. Distances are given in Å.

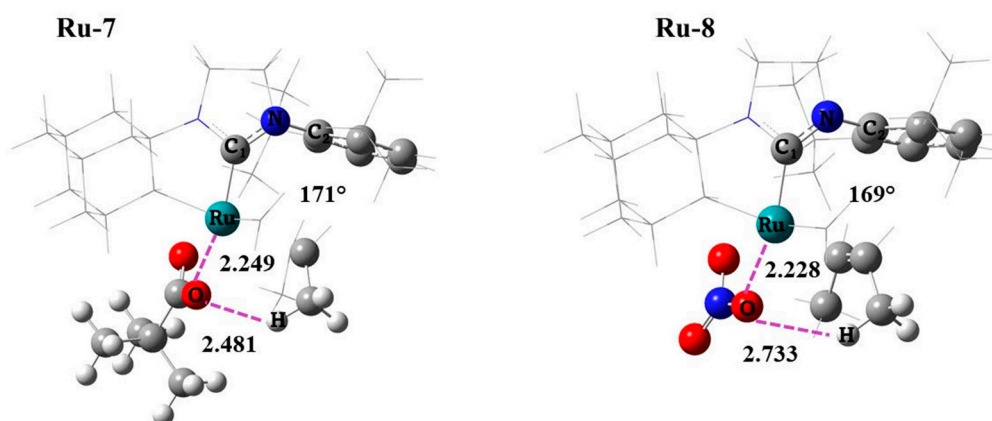


Figure S10. Optimized geometry of the TSCR of the **Ru-7** and **Ru-8** catalysts in the *Side-Z-DD* mechanism. Distances are given in Å.

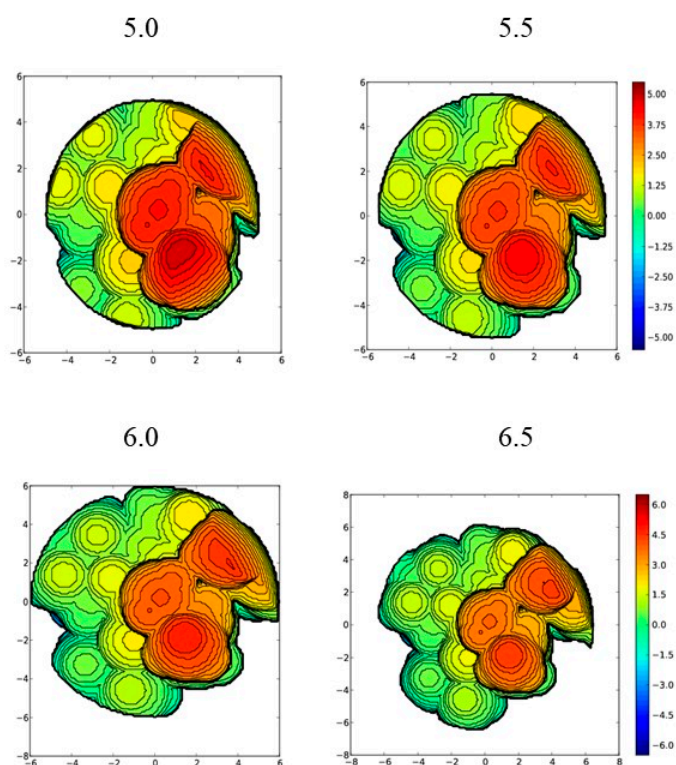


Figure S11. Radius of the sphere built around the metallic atom of the **Ru-1** catalyst.

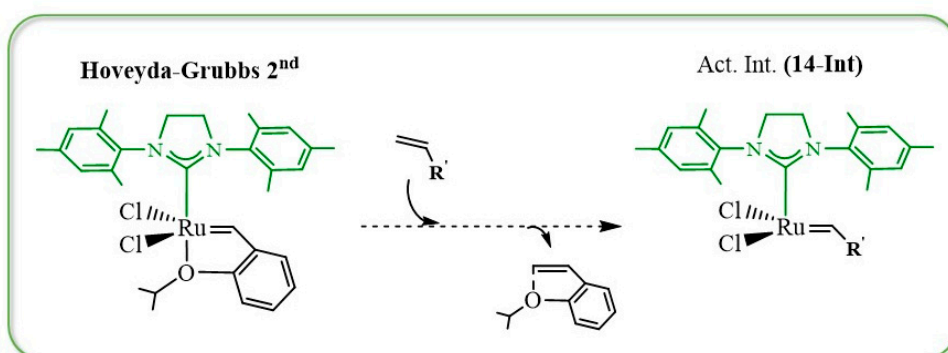


Figure S12. Dissociation mechanism in Hoveyda-Grubbs catalysts.

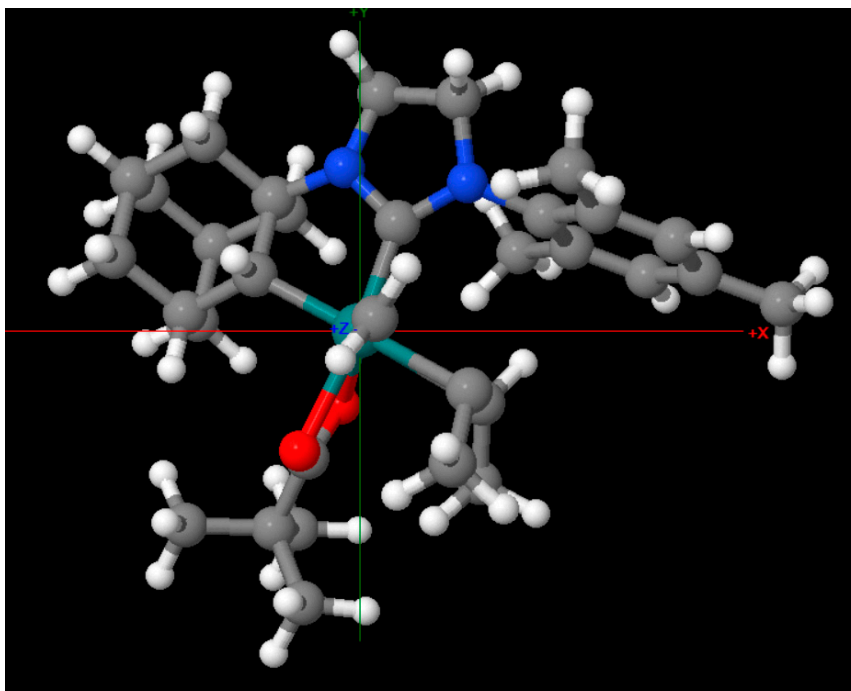


Figure S13. Visualization of the orientation used in steric maps with the **Ru-1** catalyst.

Table S1. Values of %Vfree and %Buried, and of each quadrant that describes the steric map of the **Ru-1** catalyst.

%V Free	%V Buried	% V Tot/V Ex
28.0	72.0	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	46.8	84.0	130.8	35.8	64.2
NW	40.5	90.3	130.8	30.9	69.1
NE	23.0	107.8	130.8	17.6	82.4
SE	36.4	94.4	130.8	27.8	72.2

Table S2. Values of %Vfree and %Buried, and of each quadrant that describes the steric map of the **Ru-2** catalyst.

%V Free	%V Buried	% V Tot/V Ex
31.7	68.3	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	61.2	69.6	130.8	46.8	53.2
NW	41.2	89.7	130.8	31.5	68.5
NE	23.1	107.7	130.8	17.7	82.3
SE	40.2	90.6	130.8	30.7	69.3

Table S3. Values of %Vfree and %Buried, and of each quadrant that describes the steric map of the **Ru-7** catalyst.

%V Free	%V Buried	% V Tot/V Ex
25.2	74.8	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	46.4	84.4	130.8	35.5	64.5
NW	40.7	90.1	130.8	31.1	68.9
NE	15.8	115.0	130.8	12.1	87.9
SE	29.1	101.7	130.8	22.3	77.7

Table S4. Values of %Vfree and %Buried, and of each quadrant that describes the steric map of the **Ru-8** catalyst.

%V Free	%V Buried	% V Tot/V Ex
29.4	70.6	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	62.0	68.8	130.8	47.4	52.6
NW	41.0	89.8	130.8	31.3	68.7
NE	17.1	113.7	130.8	13.1	86.9
SE	33.8	97.0	130.8	25.9	74.1

Table S5. Values of %Vfree and %Buried, and of each quadrant that describes the steric map of the **Ru-9** catalyst.

%V Free	%V Buried	% V Tot/V Ex
24.1	75.9	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	47.5	83.3	130.8	36.3	63.7
NW	41.5	89.3	130.8	31.8	68.2
NE	14.4	116.4	130.8	11.0	89.0
SE	22.5	108.3	130.8	17.2	82.8

Table S6. Values of %Vfree and %Buried, and of each quadrant that describes the steric map of the **Ru-10** catalyst.

%V Free	%V Buried	% V Tot/V Ex
28.0	72.0	99.9

Quadrant	V f	V b	V t	%V f	%V b
SW	61.5	69.3	130.8	47.0	53.0
NW	41.6	89.2	130.8	31.8	68.2
NE	14.0	116.8	130.8	10.7	89.3
SE	29.6	101.2	130.8	22.6	77.4

**Cartesian coordinates of the
structures optimized by DFT**

Propene

	x	y	z
C	1.278165	-0.223768	-0.000014
C	0.134566	0.458614	-0.000012
H	1.296153	-1.311893	0.000011
H	2.241059	0.276676	-0.000041
H	0.182483	1.547471	-0.000039
C	-1.232594	-0.156218	0.000023
H	-2.022117	0.598117	0.000038
H	-1.389221	-0.791074	-0.878157
H	-1.389179	-0.791068	0.878214

Cis olefin

	x	y	z
C	0.6686530	0.6644540	0.0000180
C	-0.6686070	0.6644300	0.0000350
C	1.5736410	-0.5197190	0.0000010
H	2.2323220	-0.5167790	-0.8763730
H	2.2331030	-0.5161710	0.8757750
H	1.0317940	-1.4684530	0.0005490
H	1.1688270	1.6329370	-0.0000480
C	-1.5736710	-0.5196930	0.0000240
H	-2.2333220	-0.5160350	0.8756270
H	-2.2320560	-0.5167320	-0.8765780
H	-1.0319390	-1.4685050	0.0006900
H	-1.1688270	1.6329010	-0.0001100

Trans olefin

	x	y	z
C	0.5377480	-0.3950630	-0.0000090
C	-0.5377770	0.3952200	-0.0000440
C	-1.9496570	-0.0785070	0.0000200
H	-2.0058440	-1.1709580	-0.0000340
H	-2.4996640	0.2843640	0.8764840
H	-2.4998210	0.2843980	-0.8763230
H	-0.3856680	1.4770220	-0.0000380
C	1.9497000	0.0784060	0.0000140
H	2.4996640	-0.2844510	0.8765040
H	2.4997240	-0.2847180	-0.8763210
H	2.0061370	1.1708420	-0.0001260
H	0.3853910	-1.4768360	-0.0000350

Ru-1

14-Int

	x	y	z
Ru	-0.3899500	0.5863360	0.6657770
O	0.6702000	2.0812050	-0.7875070
O	1.7476800	1.1678870	0.9067120
N	-1.5624640	-1.4354970	-0.9716670
N	0.4707720	-2.0670850	-0.3846470
C	-0.4393320	-1.0540950	-0.2920730
C	-1.5290140	-2.8508840	-1.3109450
H	-1.9536880	-3.0420810	-2.3018020
H	-2.1015680	-3.4411100	-0.5784780
C	-0.0346820	-3.1573070	-1.2311480
H	0.1857180	-4.1309230	-0.7819690
H	0.4444100	-3.1316950	-2.2201570
C	-2.7669020	-0.6661530	-0.6747540
C	-3.5497650	-1.2972080	0.4877870
H	-2.8753740	-1.4485550	1.3394840
H	-3.9271180	-2.2856060	0.1864980
C	-4.7160370	-0.3898230	0.8811590
H	-5.2674510	-0.8454360	1.7140310
C	-5.6472520	-0.2218510	-0.3225540
H	-6.0628170	-1.1957840	-0.6162200
H	-6.4971800	0.4208740	-0.0571140
C	-4.8689810	0.3971200	-1.4876000
H	-5.5343860	0.5188500	-2.3519010
C	-3.7067600	-0.5304470	-1.8778710
H	-3.1492400	-0.1200210	-2.7298610
H	-4.1007290	-1.5122630	-2.1844270
C	-4.3383040	1.7694310	-1.0517550
H	-3.8062980	2.2532500	-1.8809420
H	-5.1835270	2.4212900	-0.7886550
C	-3.3890210	1.6061740	0.1508410
H	-3.0113410	2.5933420	0.4518790
C	-2.2265340	0.7217760	-0.2970950
H	-1.8117570	1.1607330	-1.2255910
C	-4.1608430	0.9717800	1.3106400
H	-3.5005300	0.8468610	2.1783720
H	-4.9831230	1.6307470	1.6213860
C	1.8806890	-1.8629370	-0.2427040
C	2.5257910	-2.3271460	0.9077440
C	3.9047720	-2.1363510	1.0160670
H	4.4156100	-2.4924890	1.9096220
C	4.6401320	-1.5027620	0.0163440
C	3.9620640	-1.0508840	-1.1190360

H	4.5219750	-0.5546020	-1.9119050
C	2.5852550	-1.2097160	-1.2677440
C	1.7532720	-2.9676840	2.0173340
H	1.1795960	-2.2131630	2.5688890
H	2.4177980	-3.4667850	2.7267850
H	1.0269540	-3.6997360	1.6510840
C	6.1151080	-1.2827490	0.1611090
H	6.6510780	-1.4999670	-0.7678560
H	6.5419390	-1.9057240	0.9512150
H	6.3364780	-0.2392610	0.4153270
C	1.8761140	-0.6542710	-2.4658530
H	1.2354400	-1.3923780	-2.9598160
H	2.5905090	-0.2889320	-3.2079040
H	1.2281000	0.1861560	-2.1856270
C	-0.8407990	-0.2264020	2.2404830
C	1.7206570	1.9706940	-0.0837710
C	2.9398040	2.8285320	-0.4081500
C	3.2843370	2.6518650	-1.8883490
H	2.4193330	2.8691020	-2.5203950
H	3.6093550	1.6262010	-2.0945720
H	4.1023300	3.3241510	-2.1697910
C	2.5522180	4.2896600	-0.1519960
H	1.6944180	4.5782870	-0.7651960
H	3.3908200	4.9512840	-0.3953380
H	2.2925080	4.4538730	0.8993880
C	4.1286040	2.4356830	0.4610340
H	4.9985230	3.0544140	0.2128050
H	4.3934830	1.3851190	0.3074550
H	3.9057770	2.5631980	1.5233230
C	-1.0249590	0.6533020	3.4393130
H	-1.9883020	0.4641510	3.9333560
H	-0.2449150	0.4663070	4.1896350
H	-0.9899240	1.7241870	3.1940750
H	-0.9140960	-1.3033840	2.4685250

CA

Ru	-0.177169	0.336784	0.497038
O	-0.66559	1.942912	-1.146146
O	-1.388874	2.19968	0.930184
N	-0.202124	-2.3042	-0.612063
N	1.908914	-1.82511	-0.259466
C	0.631984	-1.311498	-0.182279
C	0.461526	-3.586495	-0.765457
H	0.093613	-4.13545	-1.638787
H	0.304434	-4.21981	0.12256
C	1.91231	-3.151282	-0.901667
H	2.621633	-3.825597	-0.411647

H	2.214228	-3.054784	-1.956157
C	-1.634785	-2.112911	-0.434481
C	-2.140619	-2.737926	0.875157
H	-1.531375	-2.379684	1.713266
H	-2.023163	-3.83143	0.833718
C	-3.61267	-2.372516	1.081612
H	-3.96634	-2.808824	2.025392
C	-4.433217	-2.932669	-0.08406
H	-4.353653	-4.02852	-0.110307
H	-5.496158	-2.692636	0.052072
C	-3.927369	-2.332698	-1.400132
H	-4.510176	-2.737985	-2.237447
C	-2.449402	-2.705387	-1.593674
H	-2.067927	-2.306206	-2.543094
H	-2.344391	-3.80145	-1.630374
C	-4.090502	-0.808067	-1.347126
H	-3.763498	-0.356524	-2.293474
H	-5.153864	-0.557403	-1.222052
C	-3.261327	-0.236039	-0.183426
H	-3.380364	0.854203	-0.146257
C	-1.799744	-0.590781	-0.441637
H	-1.553287	-0.260867	-1.465754
C	-3.755899	-0.84674	1.128934
H	-3.183487	-0.43259	1.966327
H	-4.80851	-0.579771	1.296262
C	3.076324	-1.023771	-0.433508
C	4.130058	-1.166649	0.482712
C	5.290445	-0.418419	0.287186
H	6.106961	-0.516812	1.001388
C	5.427659	0.454442	-0.793756
C	4.371368	0.554203	-1.700551
H	4.468383	1.216407	-2.560196
C	3.191159	-0.176831	-1.549743
C	3.988812	-2.074363	1.665648
H	4.831772	-1.963469	2.351833
H	3.940424	-3.129961	1.373883
H	3.063352	-1.868141	2.215167
C	6.668096	1.276735	-0.967452
H	6.54939	2.272696	-0.525549
H	6.909678	1.426529	-2.023458
H	7.532558	0.813259	-0.484696
C	2.080697	-0.037324	-2.547692
H	1.620309	-1.000551	-2.792017
H	2.446865	0.409054	-3.47542
H	1.266154	0.595934	-2.170264
C	-0.217876	-0.423135	2.189375
C	-1.358607	2.5717	-0.286332
C	-2.1454	3.801492	-0.736511

C	-1.128707	4.892865	-1.089212
H	-0.440335	4.547189	-1.865704
H	-0.537898	5.18262	-0.212663
H	-1.641044	5.789625	-1.455128
C	-2.950612	3.433803	-1.984904
H	-2.294391	3.056279	-2.772735
H	-3.488668	4.309791	-2.364216
H	-3.692239	2.657057	-1.764808
C	-3.074159	4.286681	0.369992
H	-3.629541	5.171474	0.038929
H	-2.515328	4.546743	1.272446
H	-3.79738	3.513764	0.647485
C	-1.011857	0.141357	3.319696
H	-0.375012	0.358465	4.189114
H	-1.558676	1.047703	3.04468
H	-1.733981	-0.61108	3.671103
H	0.360692	-1.315528	2.505086
C	1.981707	1.387069	1.693961
H	2.649672	0.531366	1.622413
C	1.605312	2.017778	0.552693
H	1.040105	2.945509	0.597696
H	2.013088	1.736255	-0.411355
C	1.701991	1.921111	3.058686
H	1.630417	1.130426	3.810007
H	2.522303	2.579047	3.370764
H	0.778112	2.507212	3.078386

TSCA

	x	y	z
Ru	-0.225404	0.33322	0.330174
O	-0.924881	1.872059	-1.314265
O	-1.479465	2.127011	0.811449
N	-0.105252	-2.368536	-0.637063
N	1.964979	-1.78795	-0.188235
C	0.674031	-1.314769	-0.238528
C	0.604676	-3.636696	-0.593897
H	0.307573	-4.300344	-1.412377
H	0.412505	-4.161644	0.355874
C	2.046982	-3.169121	-0.694402
H	2.746941	-3.765662	-0.101099
H	2.405715	-3.164374	-1.735445
C	-1.540709	-2.220773	-0.420109
C	-1.946232	-2.683521	0.988957
H	-1.301411	-2.188242	1.725337
H	-1.787018	-3.767855	1.087663
C	-3.418282	-2.346502	1.235083
H	-3.700872	-2.666385	2.247191

C	-4.270827	-3.090557	0.201837
H	-4.14253	-4.17577	0.31877
H	-5.335468	-2.875676	0.363918
C	-3.862636	-2.656847	-1.210646
H	-4.471157	-3.193826	-1.949727
C	-2.381193	-2.991149	-1.444453
H	-2.072636	-2.704072	-2.458473
H	-2.223063	-4.07696	-1.346189
C	-4.095087	-1.14673	-1.3496
H	-3.838773	-0.812066	-2.363571
H	-5.161374	-0.925262	-1.198332
C	-3.237928	-0.389495	-0.320355
H	-3.403961	0.689583	-0.426811
C	-1.774541	-0.718365	-0.597037
H	-1.554624	-0.480804	-1.650564
C	-3.627744	-0.83401	1.090986
H	-3.019338	-0.288582	1.824493
H	-4.678328	-0.584218	1.2936
C	3.123364	-0.971888	-0.359063
C	4.102018	-0.965896	0.644302
C	5.252311	-0.197645	0.44918
H	6.009806	-0.177834	1.231568
C	5.457088	0.536884	-0.717711
C	4.470503	0.493982	-1.70697
H	4.611618	1.061797	-2.625951
C	3.300429	-0.248754	-1.55427
C	3.921782	-1.762417	1.899474
H	4.647062	-1.468464	2.662056
H	4.05414	-2.836762	1.723137
H	2.913968	-1.642997	2.311517
C	6.70032	1.349984	-0.913927
H	6.467733	2.407179	-1.078607
H	7.265109	1.014526	-1.790266
H	7.36418	1.287291	-0.048258
C	2.236921	-0.209178	-2.607964
H	1.786774	-1.190716	-2.788638
H	2.63736	0.162734	-3.554038
H	1.41199	0.450767	-2.305266
C	0.189081	-0.110324	2.126863
C	-1.528073	2.512529	-0.40471
C	-2.277688	3.798422	-0.749234
C	-1.244745	4.932441	-0.704016
H	-0.440709	4.760153	-1.427009
H	-0.797805	5.018583	0.293092
H	-1.71777	5.891276	-0.943788
C	-2.865367	3.694511	-2.154447
H	-2.085095	3.491826	-2.891022
H	-3.372694	4.627047	-2.425907

H	-3.59811	2.882452	-2.218486
C	-3.377756	4.064697	0.274009
H	-3.900884	4.997684	0.035949
H	-2.967414	4.143377	1.283308
H	-4.116946	3.256691	0.28252
C	-0.720889	0.22421	3.272
H	-0.194908	0.407648	4.217188
H	-1.378517	1.070261	3.053651
H	-1.35764	-0.654775	3.444106
H	0.93841	-0.869078	2.407552
C	1.458315	1.424184	1.783177
H	2.270651	0.773904	2.11777
C	1.632047	1.883908	0.445351
H	1.177573	2.829995	0.157388
H	2.43125	1.508674	-0.179137
C	1.021997	2.47942	2.777588
H	0.923818	2.100727	3.795499
H	1.769505	3.278526	2.798314
H	0.066812	2.917607	2.474639

MC-I

	x	y	z
Ru	-0.247803	0.323318	0.289674
O	-1.273294	1.795515	-1.430776
O	-1.63547	1.995808	0.746988
N	0.107258	-2.395735	-0.537875
N	2.125026	-1.661072	-0.076
C	0.80853	-1.275762	-0.177338
C	0.886916	-3.613713	-0.383924
H	0.650123	-4.351765	-1.156726
H	0.703057	-4.077591	0.598845
C	2.29981	-3.065574	-0.489558
H	3.022115	-3.578042	0.153306
H	2.67923	-3.10667	-1.522143
C	-1.336526	-2.308194	-0.351749
C	-1.723954	-2.600848	1.109959
H	-1.12154	-1.965056	1.773708
H	-1.485324	-3.646358	1.355681
C	-3.21576	-2.336131	1.313242
H	-3.482463	-2.538059	2.359156
C	-4.009658	-3.263984	0.387765
H	-3.812553	-4.313441	0.647292
H	-5.087063	-3.099641	0.520735
C	-3.620222	-2.994913	-1.07012
H	-4.187462	-3.662212	-1.731547
C	-2.119052	-3.258307	-1.263271
H	-1.824983	-3.089315	-2.307641

H	-1.886801	-4.30723	-1.020062
C	-3.943926	-1.53542	-1.406696
H	-3.701737	-1.321555	-2.45579
H	-5.021979	-1.359231	-1.283838
C	-3.146309	-0.593694	-0.486306
H	-3.383355	0.443722	-0.74423
C	-1.663003	-0.857939	-0.721628
H	-1.411387	-0.70055	-1.779634
C	-3.515249	-0.871668	0.974159
H	-2.943593	-0.199259	1.630464
H	-4.578948	-0.655782	1.144564
C	3.236167	-0.790169	-0.301208
C	4.204224	-0.649433	0.702748
C	5.308781	0.167091	0.451728
H	6.059308	0.288807	1.231511
C	5.477331	0.823935	-0.766951
C	4.507754	0.640465	-1.755822
H	4.626903	1.135824	-2.718649
C	3.38533	-0.161491	-1.551377
C	4.053395	-1.345348	2.020039
H	4.870031	-1.086691	2.698011
H	4.046204	-2.435811	1.911543
H	3.107693	-1.082821	2.507441
C	6.660982	1.709443	-1.011225
H	6.374701	2.767001	-1.012235
H	7.121375	1.508879	-1.983485
H	7.427497	1.58038	-0.243069
C	2.346539	-0.298941	-2.622404
H	2.000149	-1.33107	-2.739931
H	2.731756	0.042235	-3.586002
H	1.452657	0.294044	-2.386198
C	0.425162	0.201209	2.145952
C	-1.837583	2.367828	-0.463471
C	-2.768361	3.560484	-0.690681
C	-1.976147	4.822083	-0.32706
H	-1.090973	4.929123	-0.964042
H	-1.645073	4.79049	0.715823
H	-2.595512	5.715989	-0.461888
C	-3.2043	3.623632	-2.150163
H	-2.342318	3.696131	-2.817114
H	-3.850898	4.492512	-2.317445
H	-3.762084	2.726001	-2.436159
C	-3.985523	3.439117	0.226302
H	-4.650502	4.300394	0.0958
H	-3.68154	3.386387	1.274203
H	-4.563999	2.5351	0.002506
C	-0.549857	0.497595	3.261457
H	-0.044767	0.817709	4.18328

H	-1.273132	1.269789	2.984814
H	-1.109783	-0.411613	3.511181
H	1.104074	-0.61863	2.413212
C	1.306902	1.449294	1.599208
H	2.334814	1.089417	1.725228
C	1.158841	1.725831	0.084355
H	0.71078	2.70029	-0.136156
H	2.061521	1.549618	-0.49775
C	1.054218	2.721815	2.397796
H	1.197684	2.564318	3.470817
H	1.740605	3.51108	2.078258
H	0.032246	3.074476	2.233565

TSMC

	x	y	z
Ru	-0.20129	0.424021	-0.151792
O	-1.671393	1.951838	-1.292007
O	-1.998074	1.614532	0.866435
N	0.241165	-2.416415	-0.219913
N	2.195948	-1.520561	0.242069
C	0.879595	-1.203944	-0.060533
C	1.032098	-3.531978	0.274717
H	0.880534	-4.434948	-0.325105
H	0.772057	-3.769893	1.318811
C	2.43306	-2.968753	0.17002
H	3.102381	-3.291429	0.974565
H	2.908319	-3.228394	-0.788256
C	-1.20924	-2.390783	-0.106401
C	-1.622164	-1.034112	-0.665864
C	0.886172	1.137838	1.371473
C	-2.330672	2.157114	-0.232103
C	-3.528992	3.111174	-0.237692
H	1.687787	0.470023	1.685797
C	1.390211	2.051298	0.171202
H	2.480843	1.973239	0.275684
C	1.130672	1.411906	-1.241396
H	0.603242	2.089007	-1.918214
H	2.027452	0.994928	-1.689451
C	-1.863462	-3.516764	-0.914936
H	-1.562166	-4.500128	-0.521135
H	-1.517728	-3.461257	-1.955695
C	-1.654814	-2.503962	1.365106
H	-1.321159	-3.464694	1.782774
H	-1.167249	-1.703893	1.94313
C	-3.13665	-0.872917	-0.522181
C	-3.176545	-2.390114	1.463856

H	-3.480759	-2.492254	2.513654
C	-3.38594	-3.363836	-0.831909
H	-3.860822	-4.148606	-1.434835
C	-3.599463	-1.021374	0.930738
C	-3.796931	-1.985699	-1.36219
H	-3.508281	-1.884019	-2.416737
C	-3.825299	-3.498314	0.629421
H	-3.543179	-4.486677	1.018892
H	-4.918659	-3.42753	0.700827
H	-3.447135	0.098425	-0.922057
H	-3.173523	-0.219772	1.541285
H	-4.693278	-0.922909	0.980028
H	-4.890296	-1.882089	-1.318256
H	-1.364271	-1.000607	-1.742357
C	3.352013	-0.703914	0.033789
C	4.092306	-0.25687	1.14091
C	3.816704	-0.476704	-1.277786
C	5.237614	0.511498	0.911297
C	4.959204	0.300846	-1.455113
C	5.67754	0.818456	-0.374109
H	5.804581	0.873268	1.768342
H	5.304286	0.499404	-2.469218
C	3.127489	-1.073976	-2.469965
H	3.312111	-0.477495	-3.367233
H	3.504533	-2.082673	-2.678252
H	2.045194	-1.15331	-2.334051
C	3.712288	-0.600329	2.551108
H	4.520632	-1.150814	3.044621
H	3.535577	0.300418	3.149388
H	2.807129	-1.209346	2.594713
C	6.885372	1.676255	-0.59687
H	7.51312	1.288835	-1.404752
H	6.602222	2.696155	-0.880492
H	7.500637	1.750066	0.303363
C	-3.069295	4.409251	0.436656
H	-3.896581	5.12562	0.492952
H	-2.712846	4.216929	1.453752
H	-2.257643	4.882578	-0.127707
C	-3.983016	3.398956	-1.664074
H	-4.307788	2.483602	-2.168921
H	-4.824201	4.101642	-1.661824
H	-3.172722	3.827185	-2.258497
C	-4.670624	2.495554	0.571207
H	-4.347387	2.262635	1.588788
H	-5.51988	3.186431	0.621218
H	-5.025742	1.565196	0.112996
C	0.29311	1.830223	2.567033
H	-0.142316	1.087757	3.243865

H	1.07754	2.357272	3.130558
H	-0.494458	2.539018	2.313223
C	0.928732	3.49717	0.251384
H	1.200484	3.95636	1.206688
H	1.382454	4.08803	-0.549111
H	-0.15681	3.570468	0.139818

MC-II

	x	y	z
Ru	-0.137983	0.412309	-0.406022
O	-1.425687	2.133661	-0.975859
O	-1.874408	1.326622	1.035691
N	0.023744	-2.372804	0.306319
N	2.003469	-1.541638	0.749803
C	0.763574	-1.223904	0.228885
C	0.649053	-3.405514	1.117076
H	0.488581	-4.404612	0.698179
H	0.241824	-3.399504	2.139904
C	2.103057	-2.968958	1.089527
H	2.621116	-3.106544	2.044524
H	2.676837	-3.501926	0.316899
C	-1.412126	-2.286331	0.094203
C	-2.17693	-2.229467	1.428594
H	-1.8103	-1.373938	2.011062
H	-1.975678	-3.14338	2.006247
C	-3.6798	-2.095862	1.16825
H	-4.211627	-2.087747	2.128265
C	-4.169902	-3.269246	0.316949
H	-4.012637	-4.221603	0.8427
H	-5.249623	-3.175707	0.141184
C	-3.41708	-3.278181	-1.016734
H	-3.777679	-4.105939	-1.641005
C	-1.924202	-3.474905	-0.734531
H	-1.348235	-3.533195	-1.667925
H	-1.766459	-4.420466	-0.192591
C	-3.643163	-1.948444	-1.749906
H	-3.125694	-1.960131	-2.71859
H	-4.71379	-1.818738	-1.960867
C	-3.135837	-0.772446	-0.88453
H	-3.298664	0.172735	-1.417899
C	-1.637761	-0.997404	-0.686921
H	-1.17701	-1.112976	-1.696252
C	-3.934029	-0.784971	0.42538
H	-3.654859	0.06185	1.054292
H	-5.004924	-0.692768	0.192435
C	3.222636	-0.884287	0.39599

C	3.929031	-0.161722	1.370593
C	5.109757	0.48347	0.994584
H	5.650625	1.062908	1.741839
C	5.61156	0.40917	-0.303704
C	4.920599	-0.372689	-1.232752
H	5.314434	-0.472622	-2.243643
C	3.743283	-1.04286	-0.90326
C	3.457971	-0.080076	2.791929
H	3.477152	0.951049	3.158994
H	4.111231	-0.661998	3.452571
H	2.441143	-0.461107	2.905456
C	6.853006	1.149775	-0.697295
H	6.61021	2.088359	-1.208298
H	7.470978	0.566873	-1.386347
H	7.464271	1.405607	0.171937
C	3.092465	-1.946465	-1.909948
H	3.420672	-2.984668	-1.775833
H	3.368083	-1.658491	-2.927832
H	2.000986	-1.938776	-1.841436
C	1.030818	1.60816	0.74934
C	-2.097655	2.154875	0.110874
C	-3.195971	3.210506	0.256617
C	-2.660297	4.56195	-0.21929
H	-2.308951	4.500473	-1.252048
H	-1.823116	4.901833	0.401469
H	-3.444759	5.324883	-0.161108
C	-4.365219	2.788315	-0.640745
H	-4.044732	2.697785	-1.683091
H	-5.169301	3.531369	-0.59188
H	-4.782083	1.825264	-0.324844
C	-3.658692	3.303206	1.70616
H	-4.444582	4.060315	1.806704
H	-2.832422	3.578993	2.368914
H	-4.053848	2.347025	2.059377
C	1.682484	1.880279	-0.649643
C	1.189951	0.893029	-1.791874
H	0.690486	1.44679	-2.597077
H	2.004699	0.281256	-2.176458
C	0.532213	2.792956	1.528112
H	-0.03187	2.461489	2.402595
H	1.381269	3.394556	1.885671
H	-0.111574	3.455351	0.944465
H	1.690752	1.005127	1.373512
C	1.554987	3.324168	-1.112698
H	1.955769	4.024609	-0.372605
H	2.105782	3.46836	-2.046795
H	0.507476	3.58059	-1.296361
H	2.734887	1.601879	-0.510359

TSCR

Ru	x	y	z
	-0.190658	0.354239	-0.728602
O	-1.485614	2.164168	-1.074745
O	-1.301921	1.420444	0.997979
N	1.993707	-1.782168	-0.209369
C	0.691879	-1.344147	-0.308096
C	0.636607	-3.655243	0.169103
H	0.320303	-4.536723	-0.397784
H	0.472647	-3.869421	1.238507
C	2.075444	-3.250732	-0.124453
H	2.778859	-3.550214	0.659015
H	2.43228	-3.667089	-1.077049
C	-1.513919	-2.269623	-0.026552
C	-1.822193	-2.17095	1.478434
H	-1.219876	-1.357196	1.905686
H	-1.532794	-3.105398	1.982625
C	-3.312915	-1.895783	1.690114
C	-4.142614	-3.008007	1.044144
H	-3.918146	-3.977188	1.511891
H	-5.212033	-2.816412	1.203731
C	-3.836808	-3.065406	-0.455398
H	-4.442518	-3.85035	-0.926806
C	-2.351268	-3.396187	-0.642999
H	-2.099381	-3.491089	-1.70801
H	-2.122807	-4.362018	-0.164519
C	-4.164603	-1.709285	-1.096604
H	-3.978708	-1.749423	-2.178228
H	-5.233669	-1.48995	-0.963322
C	-3.310588	-0.597347	-0.451298
H	-3.54968	0.364207	-0.923005
C	-1.845119	-0.949432	-0.721544
H	-1.762675	-1.136256	-1.806121
C	-3.65685	-0.553251	1.042682
H	-3.110506	0.250106	1.542684
H	-4.731916	-0.350957	1.160682
C	3.109665	-1.016328	0.228341
C	3.132483	-0.533887	1.552744
C	4.25875	0.163157	1.985018
H	4.277575	0.54609	3.004723
C	5.358114	0.384321	1.149794
C	5.31399	-0.126917	-0.145688
H	6.164112	0.028165	-0.808818
C	4.210275	-0.840321	-0.621673
C	1.954995	-0.718469	2.458998

H	2.208441	-0.46421	3.490742
H	1.580746	-1.7486	2.441974
H	1.111869	-0.084863	2.148536
C	6.55114	1.144442	1.643896
H	6.2831	2.162581	1.944968
H	7.327507	1.219017	0.878606
H	6.9959	0.66625	2.523026
C	4.213697	-1.41187	-2.005391
H	3.218504	-1.371852	-2.458977
H	4.514449	-2.466843	-2.003241
H	4.915371	-0.88107	-2.653771
C	1.523597	1.904297	-0.081567
C	-1.793045	2.237459	0.159248
C	-2.778057	3.3177	0.611806
C	-2.320777	4.673892	0.069187
H	-2.177329	4.631766	-1.01398
H	-1.378307	4.992474	0.527511
H	-3.069768	5.442233	0.290817
C	-4.149128	2.981877	0.013012
H	-4.092354	2.912404	-1.077177
H	-4.874353	3.761279	0.272657
H	-4.531018	2.030339	0.398363
C	-2.872627	3.361269	2.132478
H	-3.576962	4.140178	2.445651
H	-1.901019	3.577532	2.58689
H	-3.216257	2.405364	2.537486
C	1.731832	1.735462	-1.493347
C	0.643079	0.340193	-2.424924
H	0.183762	0.955535	-3.211302
H	1.427925	-0.319607	-2.819376
C	1.0518	3.193887	0.501196
H	0.592037	3.042834	1.48134
H	1.906918	3.871635	0.640468
H	0.333361	3.706927	-0.140814
H	2.167834	1.319058	0.563222
C	1.492234	2.923514	-2.394581
H	2.115899	3.77059	-2.083317
H	1.728529	2.694486	-3.436065
H	0.446945	3.243773	-2.345882
H	2.630234	1.154587	-1.712759

DSCA

Ru	x	y	z
	-0.154694	0.293138	-0.676094
O	-1.299979	2.178088	-1.063265
O	-1.207041	1.441881	1.012592

N	-0.248714	-2.532408	-0.04132	C	1.866441	2.132499	-1.039843
N	1.82005	-1.907538	0.274512	C	0.284801	-0.117087	-2.405129
C	0.58663	-1.453124	-0.09527	H	0.473134	0.699819	-3.128778
C	0.357196	-3.670595	0.639142	H	0.262229	-1.103311	-2.903905
H	0.065257	-4.619411	0.179615	C	1.298487	3.050815	1.265475
H	0.05472	-3.697244	1.698502	H	0.691795	2.594708	2.051957
C	1.836495	-3.359361	0.487214	H	2.141827	3.558472	1.750253
H	2.437546	-3.623457	1.363399	H	0.690802	3.818364	0.779947
H	2.281027	-3.860269	-0.386784	H	2.310765	1.176759	0.755264
C	-1.674342	-2.228521	0.026634	C	1.378722	3.263036	-1.877646
C	-2.096838	-1.934957	1.475999	H	2.224541	3.792591	-2.333011
H	-1.480451	-1.112343	1.864843	H	0.744595	2.905236	-2.695647
H	-1.916808	-2.819408	2.105279	H	0.787325	3.984842	-1.310749
C	-3.578561	-1.556209	1.519146	H	2.407251	1.345809	-1.565166
H	-3.875987	-1.371415	2.55967	C	3.049389	-1.19266	0.276753
C	-4.424238	-2.689312	0.934109	C	3.547715	-0.761566	1.521822
H	-4.304066	-3.606701	1.527883	C	4.773963	-0.106573	1.557907
H	-5.48804	-2.419656	0.974086	H	5.158492	0.24071	2.516017
C	-3.999133	-2.941675	-0.515125	C	5.512857	0.132049	0.393039
H	-4.613251	-3.742785	-0.946902	C	4.99433	-0.311897	-0.819931
C	-2.527953	-3.375578	-0.524638	H	5.560459	-0.138902	-1.734553
H	-2.192885	-3.616461	-1.542445	C	3.769993	-0.985508	-0.905368
H	-2.407162	-4.284964	0.085878	C	3.26638	-1.452407	-2.236132
C	-4.185033	-1.655028	-1.333552	H	4.070143	-1.905521	-2.824273
H	-3.920124	-1.834454	-2.383818	H	2.871621	-0.615344	-2.825482
H	-5.244831	-1.362659	-1.315319	H	2.452848	-2.175209	-2.142165
C	-3.310385	-0.523967	-0.750974	C	6.827932	0.846864	0.459237
H	-3.449587	0.390639	-1.342472	H	7.541516	0.317396	1.099367
C	-1.851955	-0.997623	-0.86903	H	6.716713	1.851792	0.8797
H	-1.748926	-1.374614	-1.896708	H	7.281503	0.950088	-0.529388
C	-3.775212	-0.286011	0.692096	C	2.726481	-0.942187	2.761824
H	-3.223292	0.532723	1.156922	H	3.237206	-0.534832	3.637223
H	-4.839982	-0.009188	0.687119	H	2.502301	-1.995364	2.966134
C	1.807708	2.028869	0.308041	H	1.755637	-0.438568	2.667507
C	-1.606626	2.302165	0.162982	14-Int'	x	y	z
C	-2.493345	3.475608	0.580622				
C	-1.920959	4.773299	0.004361				
H	-1.788386	4.691242	-1.077645				
H	-0.952307	5.025503	0.449983	Ru	-0.2034130	0.2488620	-0.7561550
H	-2.600146	5.608191	0.209198	O	-1.0447510	2.3214120	-1.3571080
C	-3.881007	3.248738	-0.034748	O	0.0328830	1.9471810	0.5350130
H	-3.81286	3.164873	-1.123025	N	-0.4392730	-2.2572130	0.5378540
H	-4.538622	4.091185	0.206832	N	1.6703140	-1.6734820	0.7040050
H	-4.350524	2.337924	0.349284	C	0.4732120	-1.2957090	0.1809060
C	-2.598611	3.562274	2.098199	C	0.0679060	-3.0868800	1.6202820
H	-3.247234	4.396861	2.386567	H	-0.2952780	-4.1167190	1.5532920
H	-1.617514	3.719412	2.557326	H	-0.2234980	-2.6820700	2.6047600
H	-3.01282	2.642507	2.520349	C	1.5728650	-2.9659870	1.3915490

H	2.1585060	-2.9605620	2.3158650
H	1.9509210	-3.7770140	0.7504850
C	-1.8262190	-1.8472740	0.3307510
C	-2.2971700	-0.8795500	1.4347710
H	-1.5847910	-0.0400870	1.5177560
H	-2.2939210	-1.3901780	2.4093160
C	-3.6968180	-0.3560900	1.1066880
H	-4.0272960	0.3241440	1.9029930
C	-4.6626330	-1.5409390	1.0013800
H	-4.7192460	-2.0706810	1.9624070
H	-5.6749390	-1.1808360	0.7756510
C	-4.1898500	-2.4942860	-0.1011680
H	-4.8859980	-3.3390090	-0.1800210
C	-2.7938440	-3.0274970	0.2525130
H	-2.4411880	-3.7363780	-0.5084250
H	-2.8307530	-3.5662400	1.2126190
C	-4.1470710	-1.7375260	-1.4356800
H	-3.8354460	-2.4123650	-2.2437380
H	-5.1557110	-1.3807870	-1.6876460
C	-3.1707850	-0.5500790	-1.3375620
H	-3.1412360	-0.0095030	-2.2917270
C	-1.7848700	-1.1117790	-1.0243610
H	-1.5115490	-1.8513590	-1.7851100
C	-3.6481970	0.3926050	-0.2281490
H	-2.9731130	1.2554300	-0.1589080
H	-4.6428620	0.7894750	-0.4723740
C	2.9171700	-1.0473400	0.4130830
C	3.3247030	0.0397280	1.2029760
C	4.5442210	0.6463150	0.9061210
H	4.8704110	1.4906580	1.5120990
C	5.3554010	0.2012420	-0.1406540
C	4.9247380	-0.8898300	-0.8946030
H	5.5460990	-1.2513060	-1.7130560
C	3.7116560	-1.5306030	-0.6356510
C	2.4659680	0.5344250	2.3246890
H	3.0183700	1.2277540	2.9637940
H	2.1014100	-0.2893130	2.9482910
H	1.5814950	1.0576060	1.9449300
C	6.6465710	0.8943180	-0.4540770
H	6.4728590	1.8366760	-0.9856750
H	7.2926710	0.2802560	-1.0866390
H	7.2025380	1.1442070	0.4545800
C	3.2813800	-2.7066920	-1.4593700
H	3.5899080	-3.6554620	-1.0028040
H	3.7304570	-2.6746330	-2.4553700
H	2.1939180	-2.7462620	-1.5784050
C	-0.6617580	2.7271820	-0.2310710
C	-1.0427860	4.0949920	0.3141850

C	0.2205290	4.8095820	0.7996480
H	0.9163050	4.9934990	-0.0253280
H	0.7408580	4.2152520	1.5549930
H	-0.0406190	5.7784900	1.2385550
C	-1.7504800	4.9149220	-0.7572280
H	-1.1042540	5.0807750	-1.6233790
H	-2.0412540	5.8909140	-0.3541930
H	-2.6492540	4.4055180	-1.1143820
C	-1.9821990	3.8574550	1.5048480
H	-2.2725170	4.8146790	1.9509020
H	-1.4953630	3.2509200	2.2738240
H	-2.8992970	3.3443580	1.1934490
C	0.7546420	0.0072260	-2.2691970
H	0.5373680	0.6999340	-3.0987850
H	1.6254280	-0.6451890	-2.4137240

Ru 2

14-Int

	x	y	z
Ru	0.2069700	-1.0413530	0.258545
O	-0.6305870	-1.7756090	-1.785032
O	-1.8325610	-1.8917150	0.01019
N	1.0782340	1.5679600	-0.493313
N	-1.0491320	1.6724980	0.079632
C	0.0148160	0.8328000	-0.056719
C	0.8077500	2.9966040	-0.41043
H	1.2528740	3.5435090	-1.24709
H	1.2088360	3.4170720	0.525559
C	-0.7174550	3.0119920	-0.426151
H	-1.1561300	3.7874020	0.208496
H	-1.1125050	3.1384860	-1.444841
C	2.3841690	0.9334320	-0.356608
C	2.9992760	1.2416750	1.01736
H	2.2758590	0.9867830	1.801647
H	3.2042450	2.3194680	1.096192
C	4.2908770	0.4437850	1.198117
H	4.7234130	0.6677330	2.181809
C	5.2808700	0.8354370	0.097734
H	5.5318850	1.9020200	0.178657
H	6.2188980	0.2772180	0.216453
C	4.6657470	0.5364750	-1.272883
H	5.3737010	0.8152570	-2.063583
C	3.3764850	1.3560600	-1.444791
H	2.9307040	1.1805710	-2.432553
H	3.6060100	2.4307040	-1.373395
C	4.3649310	-0.9657600	-1.361486
H	3.9576390	-1.2158070	-2.349483

H	5.2992500	-1.5331020	-1.246943
C	3.3570240	-1.3639220	-0.26578
H	3.1459620	-2.4399280	-0.340272
C	2.0780010	-0.5643870	-0.509602
H	1.7862670	-0.7148760	-1.56767
C	3.963222	-1.049564	1.104301
H	3.260043	-1.325097	1.900454
H	4.873794	-1.64453	1.256972
C	-2.407548	1.219356	0.106877
C	-3.069252	1.155644	1.339206
C	-4.385808	0.696292	1.358869
H	-4.908085	0.639086	2.312974
C	-5.042512	0.295786	0.195241
C	-4.355308	0.382268	-1.015518
H	-4.84559	0.058852	-1.932568
C	-3.040797	0.841755	-1.08789
C	-2.371983	1.533774	2.608313
H	-1.64385	0.766107	2.895814
H	-3.082127	1.642469	3.431628
H	-1.811534	2.468969	2.511136
C	-6.438201	-0.245917	0.244022
H	-7.04823	0.12764	-0.583718
H	-6.941139	0.01307	1.179382
H	-6.436058	-1.338735	0.166429
C	-2.345705	0.913189	-2.415569
H	-2.516704	1.878921	-2.907795
H	-2.721161	0.138394	-3.088524
H	-1.264976	0.770367	-2.331847
C	0.501414	-0.882466	2.055909
C	0.771204	-2.147903	2.811238
H	1.688045	-2.071299	3.41154
H	-0.045227	-2.369393	3.51122
H	0.88332	-3.023307	2.155949
H	0.437119	0.011998	2.696713
N	-1.756263	-2.091108	-1.263882
O	-2.690405	-2.528973	-1.905701

CA

	x	y	z
Ru	0.399476	-0.368683	0.388009
O	1.505887	-1.824573	-1.107104
O	1.943416	-1.867127	1.061378
N	-0.102202	2.200576	-0.815145
N	-2.060448	1.294205	-0.433125
C	-0.71118	1.048324	-0.38141
C	-1.031279	3.316203	-0.923335
H	-0.805878	3.955083	-1.78342

H	-0.994914	3.942352	-0.01727
C	-2.363444	2.593052	-1.045005
H	-3.184356	3.09192	-0.518957
H	-2.668258	2.45886	-2.095095
C	1.310154	2.358171	-0.482054
C	1.498809	3.10755	0.847444
H	0.895698	2.628588	1.628442
H	1.137375	4.141867	0.747398
C	2.979473	3.108728	1.232772
H	3.10527	3.635484	2.188185
C	3.776677	3.827432	0.139941
H	3.445831	4.872163	0.056681
H	4.842719	3.850148	0.402693
C	3.584013	3.101931	-1.195876
H	4.151039	3.619041	-1.980738
C	2.093668	3.106074	-1.569474
H	1.932801	2.609963	-2.535542
H	1.736513	4.143434	-1.668309
C	4.094058	1.661671	-1.054229
H	3.996298	1.124886	-2.007422
H	5.164041	1.674604	-0.801184
C	3.29235	0.930156	0.037349
H	3.657219	-0.099923	0.134443
C	1.829895	0.922889	-0.397122
H	1.786061	0.514757	-1.421453
C	3.469762	1.662657	1.367919
H	2.911616	1.139286	2.153325
H	4.52733	1.65587	1.66567
C	0.020648	0.404551	2.03113
C	2.17666	-2.267404	-0.124291
C	3.249219	-3.324412	-0.378443
C	2.522499	-4.621965	-0.751764
H	1.894629	-4.47702	-1.635923
H	1.88332	-4.967744	0.069559
H	3.244302	-5.417439	-0.967607
C	4.120134	-2.871445	-1.551487
H	3.510763	-2.688757	-2.439629
H	4.868774	-3.63542	-1.789167
H	4.654203	-1.943803	-1.315023
C	4.100866	-3.543425	0.866432
H	4.861063	-4.30953	0.676884
H	3.489528	-3.865245	1.713703
H	4.611361	-2.622867	1.165516
C	0.739655	0.064321	3.293877
H	0.035225	-0.234785	4.085011
H	1.486877	-0.723462	3.160907
H	1.244389	0.96173	3.683238
H	-0.766461	1.165893	2.210303

C	-1.280957	-2.282479	1.519258
H	-2.143703	-1.662789	1.761828
C	-1.016703	-2.507759	0.213041
H	-0.233198	-3.196463	-0.090798
H	-1.678329	-2.141194	-0.561001
C	-0.584015	-2.955883	2.649094
H	-0.426012	-2.287761	3.500038
H	-1.200908	-3.785299	3.016635
H	0.386724	-3.351858	2.340301
C	-3.048979	0.268002	-0.471675
C	-3.893993	0.097148	0.639581
C	-4.84345	-0.927227	0.59132
H	-5.502288	-1.081739	1.443864
C	-4.961277	-1.741684	-0.5283
C	-4.14815	-1.52498	-1.634696
H	-4.25772	-2.1538	-2.516128
C	-3.185193	-0.512377	-1.636534
C	-3.838951	1.022589	1.839166
H	-3.003869	1.716729	1.681428
C	-2.343525	-0.281002	-2.879287
H	-1.716307	0.602293	-2.714294
H	-5.700312	-2.538033	-0.545342
C	-3.238261	0.004731	-4.086052
H	-3.844528	-0.86848	-4.350949
H	-3.926545	0.835046	-3.89666
H	-2.63315	0.257561	-4.962167
C	-1.395183	-1.444406	-3.169509
H	-0.620793	-1.544451	-2.402711
H	-1.940031	-2.393977	-3.236463
H	-0.887604	-1.288941	-4.126799
C	-5.128709	1.83946	1.933887
H	-5.331298	2.388546	1.009011
H	-5.992155	1.19134	2.122634
H	-5.074611	2.562983	2.753645
C	-3.580952	0.284049	3.150464
H	-4.346426	-0.476203	3.343696
H	-2.606082	-0.213365	3.1502
H	-3.594081	0.982654	3.993364

TSCA

	x	y	z
Ru	-0.460447	-0.36894	-0.307309
O	-1.737175	-1.720992	1.191407
O	-2.082081	-1.743603	-0.992556
N	0.234528	2.224096	0.737528
N	2.132678	1.193909	0.349871
C	0.769027	1.018343	0.354007

C	1.219424	3.295282	0.730779
H	1.050596	4.011734	1.540854
H	1.191267	3.846789	-0.223196
C	2.511061	2.510544	0.881499
H	3.352472	2.933175	0.322431
H	2.8165	2.416685	1.935983
C	-1.175365	2.420454	0.411783
C	-1.351487	2.957098	-1.019796
H	-0.785765	2.31967	-1.711135
H	-0.936495	3.973438	-1.093813
C	-2.838087	2.974586	-1.382361
H	-2.957249	3.345203	-2.409466
C	-3.566871	3.907568	-0.409458
H	-3.177229	4.930666	-0.505876
H	-4.636599	3.949136	-0.653979
C	-3.381854	3.4016	1.025586
H	-3.900689	4.073279	1.721618
C	-1.886026	3.375032	1.377103
H	-1.735236	3.029832	2.40852
H	-1.465925	4.390801	1.304458
C	-3.973702	1.990732	1.130471
H	-3.880613	1.61184	2.156886
H	-5.047573	2.024965	0.897172
C	-3.245	1.044787	0.160262
H	-3.67239	0.038929	0.246099
C	-1.769995	1.017824	0.545988
H	-1.683693	0.726378	1.605556
C	-3.409151	1.555576	-1.272255
H	-2.890343	0.875722	-1.961976
H	-4.469983	1.558494	-1.558737
C	0.244901	-0.067581	-2.046677
C	-2.380976	-2.13528	0.185964
C	-3.50244	-3.157867	0.361263
C	-2.842841	-4.542806	0.328464
H	-2.11566	-4.65064	1.140008
H	-2.323268	-4.709206	-0.622099
H	-3.59702	-5.329526	0.441714
C	-4.190812	-2.946607	1.707222
H	-3.473901	-3.012481	2.528288
H	-4.971467	-3.700315	1.859431
H	-4.662364	-1.95896	1.76014
C	-4.508582	-3.039676	-0.780403
H	-5.309146	-3.778305	-0.660837
H	-4.027594	-3.200221	-1.748007
H	-4.967578	-2.04518	-0.804185
C	-0.593752	-0.138064	-3.288683
H	-0.031799	-0.451937	-4.178123
H	-1.469728	-0.781604	-3.169306

H	-0.954594	0.878553	-3.498176	N	0.334148	2.28336	0.468804
H	1.195263	0.46314	-2.22034	N	2.200362	1.174801	0.155564
C	0.982237	-1.8839	-1.626663	C	0.834116	1.034693	0.204095
H	1.974512	-1.50704	-1.881953	C	1.331039	3.329052	0.298222
C	0.916485	-2.334345	-0.272079	H	1.199242	4.141788	1.019224
H	0.210797	-3.123107	-0.015911	H	1.279656	3.759956	-0.715111
H	1.747231	-2.179905	0.403444	C	2.614194	2.542072	0.507059
C	0.362468	-2.800471	-2.659018	H	3.444443	2.874503	-0.124651
H	0.467432	-2.428003	-3.67938	H	2.950212	2.574676	1.55565
H	0.861085	-3.773827	-2.614539	C	-1.088443	2.448958	0.196077
H	-0.700008	-2.953033	-2.450895	C	-1.34076	2.721456	-1.299467
C	3.07118	0.126335	0.476764	H	-0.837333	1.945289	-1.893337
C	3.967249	-0.119792	-0.580764	H	-0.896767	3.687463	-1.582645
C	4.862809	-1.18431	-0.450374	C	-2.844141	2.727371	-1.57949
H	5.559181	-1.395802	-1.259139	H	-3.013977	2.915438	-2.647913
C	4.884783	-1.964634	0.69917	C	-3.494023	3.838292	-0.748195
C	4.030617	-1.669333	1.75486	H	-3.090244	4.816497	-1.044309
H	4.067253	-2.268035	2.662846	H	-4.575018	3.868934	-0.937725
C	3.117682	-0.614211	1.674837	C	-3.235674	3.585926	0.741246
C	4.042334	0.787622	-1.793432	H	-3.701296	4.382285	1.335833
H	3.167184	1.449413	-1.765695	C	-1.7244	3.577626	1.012387
C	2.233023	-0.306082	2.869003	H	-1.520615	3.417633	2.079481
H	1.647457	0.593671	2.647653	H	-1.286015	4.549136	0.734403
H	5.582765	-2.793411	0.78033	C	-3.839696	2.231434	1.126955
C	3.084188	-0.010988	4.104846	H	-3.69094	2.03766	2.197148
H	3.648989	-0.894547	4.422233	H	-4.924763	2.247121	0.951819
H	3.807096	0.79107	3.922647	C	-3.189479	1.107536	0.298852
H	2.449766	0.287452	4.945124	H	-3.628697	0.149349	0.593886
C	1.235268	-1.428442	3.153085	C	-1.695656	1.103499	0.603824
H	0.523672	-1.559543	2.33252	H	-1.525704	0.949173	1.679387
H	1.751612	-2.381718	3.319977	C	-3.43215	1.366529	-1.190964
H	0.658327	-1.204562	4.05598	H	-2.97024	0.563453	-1.783083
C	5.299127	1.657815	-1.706638	H	-4.508849	1.345673	-1.409281
H	5.345473	2.214948	-0.765506	C	0.370411	-0.478383	-2.065555
H	6.203496	1.041072	-1.76189	C	-2.500913	-2.048993	0.357582
H	5.337299	2.377822	-2.530438	C	-3.673042	-3.024376	0.480827
C	4.019483	0.037549	-3.122754	C	-3.22222	-4.366128	-0.105639
H	4.860087	-0.659178	-3.210407	H	-2.356136	-4.765617	0.434885
H	3.097271	-0.536718	-3.259551	H	-2.944747	-4.25755	-1.158031
H	4.094678	0.740897	-3.957966	H	-4.028013	-5.105485	-0.035992
MC-I				C	-4.077446	-3.194151	1.939656
				H	-3.246746	-3.573126	2.540256
				H	-4.915469	-3.895385	2.023754
				H	-4.383649	-2.239468	2.377474
				C	-4.848618	-2.483961	-0.337835
				H	-5.686982	-3.189421	-0.315116
				H	-4.556111	-2.321749	-1.378611
				H	-5.209242	-1.529483	0.063221

C	-0.532314	-0.608887	-3.269271
H	-0.012691	-1.056759	-4.128336
H	-1.420659	-1.210447	-3.057455
H	-0.867447	0.38436	-3.590853
H	1.235084	0.162965	-2.280263
C	0.90092	-1.861769	-1.411279
H	1.988877	-1.750155	-1.467689
C	0.609546	-2.00469	0.098745
H	-0.035549	-2.855804	0.340541
H	1.492916	-1.967398	0.732936
C	0.4289	-3.089513	-2.178321
H	0.684694	-3.025479	-3.24067
H	0.899505	-3.989882	-1.773207
H	-0.654694	-3.20321	-2.08941
C	3.108976	0.110761	0.446634
C	4.001564	-0.316058	-0.553985
C	4.856783	-1.381211	-0.260812
H	5.54875	-1.732919	-1.023164
C	4.839003	-1.990198	0.988195
C	3.990261	-1.515236	1.980724
H	3.999002	-1.978088	2.965529
C	3.120821	-0.448136	1.74028
C	4.103391	0.392977	-1.89008
H	3.251548	1.081049	-1.963497
C	2.259299	0.077698	2.875839
H	1.702848	0.952009	2.519115
H	5.50341	-2.824674	1.195135
C	3.143743	0.538262	4.036405
H	3.681172	-0.303043	4.487689
H	3.892971	1.269226	3.714632
H	2.537158	0.996608	4.823613
C	1.225409	-0.940103	3.357817
H	0.472245	-1.155523	2.594438
H	1.702712	-1.884088	3.646414
H	0.700507	-0.555974	4.238306
C	5.389413	1.22195	-1.937921
H	5.457849	1.918418	-1.096002
H	6.272114	0.573732	-1.893872
H	5.449427	1.801641	-2.864671
C	4.044618	-0.553054	-3.086811
H	4.86832	-1.275017	-3.072584
H	3.107554	-1.117694	-3.121442
H	4.125503	0.010445	-4.021599

TSMC

x	y	z
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Ru	-0.447443	-0.497817	0.142779
O	-2.080711	-1.606567	1.446512
O	-2.455995	-1.514938	-0.727888
N	0.391456	2.198373	-0.399298
N	2.205921	0.95773	-0.562176
C	0.849818	0.912397	-0.247904
C	1.316253	3.048931	-1.128174
H	1.317017	4.07354	-0.741124
H	1.051963	3.092781	-2.19629
C	2.631695	2.324905	-0.906115
H	3.281354	2.319014	-1.788244
H	3.204068	2.761442	-0.074021
C	-1.049152	2.38025	-0.439356
C	-1.583771	2.288334	-1.880038
H	-1.274646	1.324016	-2.311055
H	-1.135767	3.083887	-2.492812
C	-3.107969	2.414967	-1.882039
H	-3.474379	2.371159	-2.915811
C	-3.514906	3.747542	-1.247245
H	-3.115333	4.589699	-1.829689
H	-4.608497	3.844551	-1.25498
C	-2.992162	3.80957	0.191152
H	-3.295653	4.756807	0.655361
C	-1.462548	3.727512	0.166629
H	-1.044961	3.807754	1.179402
H	-1.051032	4.560248	-0.42501
C	-3.562454	2.635287	0.996029
H	-3.212223	2.684189	2.035641
H	-4.659049	2.703423	1.024146
C	-3.142054	1.295248	0.355425
H	-3.563443	0.473483	0.945959
C	-1.612225	1.23834	0.403491
H	-1.292058	1.388456	1.453554
C	-3.692073	1.256471	-1.074949
H	-3.450414	0.299709	-1.544423
H	-4.78802	1.338689	-1.045537
C	0.478264	-1.587115	-1.264326
C	-2.813827	-1.848691	0.441573
C	-4.137776	-2.598131	0.616684
C	-5.225198	-1.895949	-0.196707
H	-4.940522	-1.823	-1.249369
H	-5.404279	-0.879527	0.172611
H	-6.170307	-2.446102	-0.126024
C	-3.928059	-4.014531	0.06848
H	-3.613506	-3.98557	-0.979528
H	-4.857495	-4.591322	0.132568
H	-3.163982	-4.552347	0.641461
C	-4.533123	-2.661991	2.087318

H	-5.471304	-3.216114	2.205746
H	-4.675939	-1.659734	2.50319
H	-3.761219	-3.153504	2.684071
C	-0.24679	-2.336443	-2.347707
H	0.432869	-3.049183	-2.838554
H	-1.123392	-2.875693	-1.990482
H	-0.586668	-1.637148	-3.118199
H	1.36762	-1.100832	-1.670923
C	0.858345	-2.389772	0.049042
H	1.94515	-2.505846	-0.061522
C	0.753528	-1.518341	1.354712
H	0.153187	-1.999162	2.132394
H	1.725147	-1.19825	1.718715
C	0.17727	-3.741798	0.178613
H	0.364003	-4.370059	-0.698168
H	0.546841	-4.272569	1.060173
H	-0.90503	-3.632433	0.289927
C	3.203618	0.172488	0.105912
C	3.987906	-0.730601	-0.636042
C	4.942552	-1.493034	0.0447
H	5.546205	-2.205348	-0.513744
C	5.142794	-1.341932	1.409934
C	4.415454	-0.388219	2.111617
H	4.600837	-0.242306	3.174052
C	3.448367	0.395573	1.479298
C	3.893405	-0.841852	-2.144333
H	3.017221	-0.266397	-2.466114
C	2.748075	1.479535	2.283972
H	2.012816	1.979884	1.644888
H	5.884822	-1.947698	1.922709
C	3.769962	2.527753	2.73263
H	4.497582	2.096627	3.429355
H	4.334747	2.938436	1.888829
H	3.274529	3.357865	3.245984
C	1.98619	0.939827	3.493677
H	1.152478	0.299066	3.197015
H	2.639779	0.363379	4.158083
H	1.576061	1.768678	4.079424
C	5.129288	-0.213787	-2.79227
H	5.266376	0.827206	-2.483071
H	6.037747	-0.759064	-2.51197
H	5.052738	-0.23635	-3.884119
C	3.722684	-2.282875	-2.619941
H	4.612265	-2.884058	-2.40195
H	2.868136	-2.773412	-2.143155
H	3.566757	-2.316877	-3.702781

MC-II

	x	y	z
Ru	0.44854	-0.48087	-0.593161
O	2.024464	-1.953843	-1.136435
O	2.201734	-1.192976	0.933167
N	-0.290918	2.281531	-0.37754
N	-2.151146	1.18347	-0.050347
C	-0.799118	1.015688	-0.231334
C	-1.241098	3.329433	-0.043951
H	-1.148761	4.187329	-0.717111
H	-1.0904	3.689782	0.987563
C	-2.556884	2.589799	-0.207061
H	-3.313747	2.859298	0.53654
H	-2.99182	2.751687	-1.20474
C	1.146935	2.43745	-0.25344
C	1.554267	2.656187	1.215735
H	1.172055	1.815804	1.813025
H	1.08846	3.576814	1.597396
C	3.078484	2.745721	1.325741
H	3.355696	2.922874	2.372888
C	3.59181	3.895625	0.454951
H	3.178028	4.85415	0.798491
H	4.683735	3.96987	0.541704
C	3.196743	3.647445	-1.003949
H	3.57555	4.462208	-1.634312
C	1.668803	3.603564	-1.104044
H	1.344748	3.463644	-2.144167
H	1.241268	4.555861	-0.753346
C	3.785259	2.313373	-1.479471
H	3.526171	2.141003	-2.53269
H	4.882061	2.348316	-1.421559
C	3.255911	1.158541	-0.601971
H	3.680849	0.21238	-0.955179
C	1.741268	1.130366	-0.757724
H	1.495327	1.026913	-1.842434
C	3.685124	1.426527	0.845678
H	3.37095	0.600851	1.487766
H	4.782154	1.485181	0.891334
C	-0.587723	-1.928387	0.398703
C	2.605559	-1.941551	0.002286
C	3.819457	-2.849988	0.212991
C	3.628501	-4.153856	-0.560365
H	3.480507	-3.960395	-1.62513
H	2.754139	-4.70762	-0.199065
H	4.504214	-4.801325	-0.43888
C	5.047852	-2.110287	-0.330456
H	4.930016	-1.877567	-1.393942
H	5.944954	-2.729201	-0.215821
H	5.216306	-1.172403	0.210646

C	4.009868	-3.133326	1.699983
H	4.893026	-3.762665	1.857433
H	3.143699	-3.65634	2.118566
H	4.137027	-2.205926	2.263698
C	-1.129408	-2.162704	-1.057583
C	-0.747797	-1.012392	-2.076619
H	-0.194381	-1.41311	-2.934185
H	-1.614552	-0.427918	-2.394813
C	0.063955	-3.09321	1.093694
H	0.536809	-2.761881	2.021478
H	-0.695046	-3.844726	1.356997
H	0.822771	-3.596445	0.489491
H	-1.3809	-1.534385	1.028848
C	-0.768133	-3.521965	-1.637188
H	-1.078126	-4.340559	-0.979877
H	-1.260324	-3.660688	-2.604934
H	0.312414	-3.598323	-1.793637
H	-2.216543	-2.060334	-0.936926
C	-3.117571	0.242885	0.414924
C	-3.068542	-0.174143	1.765301
C	-4.07322	-1.026621	2.224055
H	-4.047693	-1.372988	3.253258
C	-5.106738	-1.439718	1.389256
C	-5.145668	-1.009858	0.071734
H	-5.954904	-1.333513	-0.579386
C	-4.155555	-0.165458	-0.441251
C	-1.954181	0.286035	2.68941
H	-1.036083	0.346097	2.08983
C	-4.247002	0.291154	-1.882907
H	-3.312521	0.810372	-2.129888
H	-5.88192	-2.098503	1.770951
C	-5.40438	1.27418	-2.06622
H	-6.363114	0.789256	-1.849832
H	-5.318909	2.136965	-1.397822
H	-5.44619	1.645056	-3.095392
C	-4.389391	-0.883097	-2.849802
H	-3.575424	-1.606083	-2.73473
H	-5.332913	-1.417584	-2.696032
H	-4.38089	-0.530783	-3.885948
C	-2.239569	1.681197	3.246077
H	-2.388993	2.418114	2.451627
H	-3.142874	1.676949	3.866846
H	-1.407498	2.028297	3.867856
C	-1.673257	-0.688188	3.827243
H	-2.482051	-0.702942	4.566776
H	-1.533531	-1.710601	3.462006
H	-0.761099	-0.39496	4.354635

TSCR

	x	y	z
Ru	-0.361426	0.47945	-0.69775
O	-1.896796	2.077111	-1.086773
O	-1.828778	1.212766	0.944669
N	0.162046	-2.323129	-0.387274
N	2.099959	-1.333089	-0.144643
C	0.752888	-1.092708	-0.312587
C	1.030656	-3.41752	0.008957
H	0.913716	-4.282653	-0.65169
H	0.807385	-3.750662	1.036492
C	2.406653	-2.772221	-0.104922
H	3.06278	-3.000294	0.742721
H	2.929048	-3.073397	-1.024221
C	-1.289343	-2.37217	-0.314768
C	-1.754535	-2.437084	1.150995
H	-1.343692	-1.568228	1.685272
H	-1.358366	-3.345525	1.629848
C	-3.283794	-2.427444	1.214549
H	-3.604534	-2.502967	2.261755
C	-3.845586	-3.606989	0.41683
H	-3.506496	-4.560052	0.847136
H	-4.942334	-3.604339	0.471071
C	-3.390464	-3.4983	-1.041593
H	-3.806054	-4.332506	-1.621769
C	-1.859641	-3.569812	-1.083572
H	-1.490917	-3.542049	-2.118007
H	-1.520542	-4.519514	-0.63961
C	-3.877474	-2.167904	-1.63345
H	-3.58261	-2.095133	-2.688825
H	-4.976061	-2.134894	-1.604904
C	-3.290087	-0.985399	-0.834074
H	-3.642364	-0.042254	-1.270713
C	-1.765912	-1.073868	-0.966235
H	-1.551282	-1.16831	-2.044239
C	-3.785874	-1.114166	0.612632
H	-3.439437	-0.273292	1.217441
H	-4.886083	-1.101348	0.62082
C	3.029169	-0.42382	0.43728
C	2.933414	-0.144944	1.81647
C	3.838693	0.768174	2.363624
H	3.765555	1.018904	3.419856
C	4.826699	1.356673	1.583313
C	4.94807	1.015202	0.241773
H	5.747975	1.448746	-0.354414
C	4.062018	0.113729	-0.353463
C	1.896084	-0.79648	2.712949
H	1.398483	-1.590283	2.141623

C	4.272192	-0.334773	-1.785474
H	3.354062	-0.843181	-2.106141
C	0.976692	2.216504	0.277997
C	-2.351118	2.004415	0.100844
C	-3.546742	2.876656	0.489351
C	-3.276697	4.320655	0.059555
H	-3.023536	4.370023	-1.002898
H	-2.451361	4.76169	0.629032
H	-4.16344	4.939836	0.234745
C	-4.773152	2.355864	-0.269701
H	-4.597536	2.365598	-1.34941
H	-5.643387	2.986445	-0.055614
H	-5.022457	1.331905	0.028624
C	-3.798868	2.808812	1.991041
H	-4.654805	3.437896	2.260093
H	-2.929305	3.155825	2.557605
H	-4.01022	1.785213	2.312468
C	1.337208	2.250403	-1.104648
C	0.622346	0.748388	-2.283762
H	0.149709	1.355814	-3.069047
H	1.559197	0.28334	-2.621855
C	0.231103	3.332634	0.929765
H	-0.287707	2.997772	1.831637
H	0.938414	4.119881	1.229
H	-0.500183	3.79187	0.261496
H	1.649641	1.670274	0.928835
C	0.9591	3.4539	-1.931138
H	1.379694	4.365421	-1.48868
H	1.332334	3.37312	-2.955104
H	-0.127744	3.573942	-1.973249
H	2.33486	1.849827	-1.283003
C	5.41812	-1.348874	-1.841646
H	6.364587	-0.880062	-1.548623
H	5.542617	-1.746516	-2.854086
H	5.25006	-2.191784	-1.163848
C	4.539839	0.810883	-2.757024
H	4.653292	0.426442	-3.775309
H	5.463344	1.345855	-2.510826
H	3.726196	1.543275	-2.770206
C	2.55572	-1.451153	3.92641
H	1.813673	-1.99796	4.516198
H	3.009864	-0.706769	4.589371
H	3.342953	-2.153806	3.634372
C	0.809584	0.187609	3.148442
H	1.247783	1.064806	3.640765
H	0.128945	-0.286945	3.863005
H	0.209462	0.533213	2.300366
H	5.518337	2.067259	2.027603

DSCA

	x	y	z
Ru	-0.309861	0.336289	-0.720525
O	-1.766285	1.95931	-1.302988
O	-1.673624	1.346769	0.815271
N	0.108786	-2.433101	-0.007843
N	1.980551	-1.390526	0.419119
C	0.702106	-1.199504	-0.02202
C	0.907987	-3.420742	0.706614
H	0.832139	-4.410821	0.247985
H	0.584335	-3.504289	1.757282
C	2.295732	-2.813738	0.593962
H	2.927416	-2.972522	1.473601
H	2.837359	-3.196828	-0.284741
C	-1.349115	-2.415916	0.015958
C	-1.86266	-2.17581	1.446467
H	-1.426937	-1.239796	1.824966
H	-1.531533	-2.992006	2.105955
C	-3.389864	-2.089811	1.443932
H	-3.747969	-1.942731	2.471249
C	-3.983765	-3.377836	0.869663
H	-3.706306	-4.241048	1.491197
H	-5.080259	-3.318248	0.876403
C	-3.475971	-3.575717	-0.561515
H	-3.912295	-4.48936	-0.985926
C	-1.949048	-3.71758	-0.524379
H	-1.544895	-3.911182	-1.527095
H	-1.672171	-4.572816	0.112815
C	-3.880824	-2.367541	-1.419363
H	-3.555289	-2.51558	-2.457387
H	-4.976952	-2.283372	-1.435808
C	-3.258181	-1.075742	-0.846111
H	-3.553942	-0.221064	-1.468812
C	-1.734484	-1.262687	-0.915399
H	-1.530331	-1.62918	-1.930118
C	-3.803368	-0.900372	0.577535
H	-3.434254	0.021726	1.030049
H	-4.901107	-0.835894	0.538899
C	1.077921	2.637987	0.123825
C	-2.203023	2.043168	-0.113214
C	-3.400951	2.952477	0.173708
C	-3.118553	4.363267	-0.350751
H	-2.781591	4.332005	-1.390928
H	-2.355416	4.872768	0.245169
H	-4.030401	4.968521	-0.302048
C	-4.602865	2.387019	-0.595084

H	-4.387931	2.334879	-1.666017
H	-5.476018	3.032189	-0.447422
H	-4.868129	1.383157	-0.249636
C	-3.70724	2.996248	1.666035
H	-4.563937	3.652254	1.856473
H	-2.854743	3.375622	2.238031
H	-3.944219	2.002122	2.055508
C	1.538745	2.381734	-1.120197
C	0.339976	-0.082445	-2.384565
H	0.294547	0.685626	-3.178443
H	0.673745	-1.059616	-2.780368
C	0.213559	3.789442	0.497003
H	-0.529836	3.50894	1.249472
H	0.826833	4.586982	0.936344
H	-0.303765	4.210995	-0.367737
H	1.490003	2.054854	0.941327
C	1.169096	3.157746	-2.343444
H	1.653165	4.141967	-2.34975
H	1.478018	2.641368	-3.255996
H	0.087366	3.320176	-2.400671
H	2.300825	1.612368	-1.219418
C	3.001701	-0.407494	0.545171
C	3.975507	-0.286323	-0.459663
C	5.029666	0.608262	-0.250621
H	5.796645	0.714091	-1.015506
C	5.102403	1.364244	0.910496
C	4.108209	1.256527	1.878681
H	4.161712	1.878107	2.767782
C	3.03898	0.373513	1.720327
H	5.928895	2.0538	1.05914
C	3.901091	-1.074182	-1.751998
H	2.958942	-1.636219	-1.751363
C	1.919497	0.284422	2.746004
H	0.976378	0.221907	2.180463
C	1.824609	1.511823	3.645472
H	2.670914	1.574066	4.339317
H	1.793784	2.446098	3.07553
C	2.019608	-0.974348	3.608455
H	1.978018	-1.889053	3.012899
H	1.193254	-1.012447	4.325554
C	3.86502	-0.155446	-2.97223
H	3.003157	0.519446	-2.938747
H	4.770302	0.45737	-3.044665
C	5.05939	-2.065761	-1.857444
H	4.977584	-2.671556	-2.76541
H	5.095208	-2.744032	-0.998645
H	6.020705	-1.540841	-1.896542
H	3.790281	-0.74304	-3.89287

H	2.956429	-0.984588	4.17713
H	0.914717	1.461463	4.24958

14-Int'

	x	y	z
Ru	-0.2651120	0.8240890	-0.599665
O	-0.7619570	3.0298230	-0.818432
O	0.4381890	2.2719720	0.826667
N	-0.8118070	-1.8691270	0.13276
N	1.3631110	-1.6178230	0.264614
C	0.2113010	-0.9768300	-0.049621
C	-0.3829650	-3.0071830	0.933904
H	-0.8806880	-3.9322420	0.629103
H	-0.5921300	-2.8412910	2.004515
C	1.1182460	-3.0141230	0.648745
H	1.7280220	-3.2901100	1.514213
H	1.3736980	-3.6906920	-0.180245
C	-2.1296520	-1.2373870	0.157404
C	-2.3662630	-0.5116310	1.496599
H	-1.5209000	0.1704080	1.695504
H	-2.3806090	-1.2385210	2.322267
C	-3.6782120	0.2714370	1.442914
H	-3.8427670	0.7758170	2.403291
C	-4.8279100	-0.7026360	1.165739
H	-4.9077550	-1.4349370	1.980886
H	-5.7806220	-0.1584720	1.132124
C	-4.5879940	-1.4175150	-0.167973
H	-5.4154780	-2.1096890	-0.368338
C	-3.2768950	-2.2149110	-0.091713
H	-3.0951750	-2.7597280	-1.027666
H	-3.3381840	-2.9601750	0.716891
C	-4.5112980	-0.3713660	-1.28788
H	-4.3688440	-0.8638140	-2.258659
H	-5.4622780	0.1765120	-1.343537
C	-3.3498010	0.6045030	-1.020563
H	-3.2969560	1.3497590	-1.823996
C	-2.0580400	-0.2109940	-0.989484
H	-1.9626780	-0.7755190	-1.923222
C	-3.5885380	1.3082940	0.319691
H	-2.7732400	2.0171830	0.523444
H	-4.5123390	1.8997380	0.277261
C	2.6643340	-1.0391560	0.222035
C	3.0706070	-0.2274470	1.29445
C	4.3404010	0.3436880	1.240606
H	4.6646590	0.9784890	2.063883
C	5.2050220	0.1204250	0.165808
C	4.7780870	-0.7147700	-0.865954

H	5.4442800	-0.9079420	-1.705723
C	3.5143540	-1.3085560	-0.8582
C	2.166758	0.006325	2.465149
H	2.71226	0.457456	3.297
H	1.712954	-0.926271	2.819572
H	1.343938	0.681103	2.207923
C	6.55235	0.774394	0.122355
H	6.469481	1.835899	-0.136009
H	7.204661	0.309042	-0.620868
H	7.056691	0.726072	1.092138
C	3.094371	-2.223114	-1.9683
H	3.333242	-3.269236	-1.739237
H	3.609738	-1.977667	-2.900276
H	2.016493	-2.175993	-2.15144
C	0.564382	0.69159	-2.198706
H	0.453649	1.540186	-2.892884
H	1.263521	-0.091092	-2.519883
N	-0.119435	3.312673	0.243451
O	-0.020065	4.421646	0.710444

Ru-6

14-Int

	x	y	z
Ru	-0.4942240	-0.7884240	-0.602028
O	0.6381650	-2.1550120	0.930801
O	1.6125820	-1.4358500	-0.910642
N	-1.6209460	1.5368110	0.600027
N	0.4716150	1.9603670	0.040315
C	-0.4909570	0.9897200	0.069546
C	-1.5393400	2.9855640	0.695742
H	-1.9657900	3.3546070	1.634994
H	-2.0878580	3.4619480	-0.131166
C	-0.0306970	3.2279530	0.58903
H	0.2242260	4.0612760	-0.074604
H	0.4232530	3.4330570	1.567739
C	-2.8372690	0.7431120	0.480434
C	-3.6320320	1.1275550	-0.777983
H	-2.971226	1.090651	-1.652355
H	-3.992946	2.162522	-0.682808
C	-4.81225	0.171658	-0.956052
H	-5.372175	0.448204	-1.858975
C	-5.726789	0.271749	0.267831
H	-6.12925	1.290506	0.354783
H	-6.58624	-0.402371	0.15488
C	-4.936675	-0.097379	1.527241
H	-5.589801	-0.025313	2.406311
C	-3.760242	0.87747	1.697004

H	-3.193268	0.649843	2.609437
H	-4.140829	1.90652	1.793861
C	-4.427496	-1.537756	1.383079
H	-3.888625	-1.844506	2.288754
H	-5.284032	-2.218129	1.273752
C	-3.494578	-1.644403	0.161713
H	-3.132906	-2.677964	0.070627
C	-2.315553	-0.7015	0.399121
H	-1.897136	-0.938413	1.398459
C	-4.275441	-1.25655	-1.096815
H	-3.62497	-1.324707	-1.978524
H	-5.108147	-1.955598	-1.254205
C	1.866484	1.638595	0.125303
C	2.645465	1.648316	-1.041664
C	4.002629	1.3379	-0.929827
H	4.620147	1.334157	-1.825816
C	4.567414	1.024592	0.299044
C	3.776821	1.013683	1.442269
H	4.221487	0.764874	2.404378
C	2.414221	1.314502	1.382557
C	2.058783	1.966819	-2.398248
H	0.980441	2.110332	-2.262086
C	1.601868	1.313589	2.665856
H	0.547496	1.479665	2.415303
C	-0.937798	-0.213494	-2.27849
C	1.634914	-2.151087	0.145226
C	2.842906	-3.038211	0.428904
C	3.337638	-2.774321	1.851668
H	2.539886	-2.936505	2.581655
H	3.693735	-1.743696	1.959745
H	4.169545	-3.446041	2.090751
C	2.374807	-4.494386	0.319824
H	1.56858	-4.699457	1.029164
H	3.206254	-5.174783	0.534081
H	2.010503	-4.721144	-0.688115
C	3.957078	-2.765953	-0.576165
H	4.820747	-3.405956	-0.363334
H	4.280389	-1.721521	-0.533011
H	3.626468	-2.961839	-1.599536
C	-1.170986	-1.265212	-3.318856
H	-2.129418	-1.112608	-3.834744
H	-0.38939	-1.235642	-4.090526
H	-1.18332	-2.28291	-2.903791
H	-0.944922	0.814185	-2.680972
H	5.624605	0.781143	0.36718
C	2.059082	2.445708	3.588201
H	3.0955	2.289548	3.9082
H	2.018594	3.424381	3.097579

H	1.439509	2.49089	4.489713
C	1.665925	-0.025812	3.394714
H	1.296208	-0.840321	2.766256
H	2.690559	-0.268309	3.699779
H	1.05798	0.010862	4.304838
C	2.644213	3.261354	-2.960128
H	2.477396	4.108908	-2.287332
H	3.726233	3.171673	-3.111249
H	2.197051	3.505328	-3.929405
C	2.255673	0.805654	-3.371083
H	3.316785	0.660965	-3.605941
H	1.880925	-0.129752	-2.94626
H	1.736047	1.002176	-4.31588

CA

	x	y	z
Ru	-0.685613	-0.001824	0.621779
O	-1.738086	1.961233	0.004579
O	-2.314754	0.950679	1.887319
N	-0.120751	-1.562683	-1.723961
N	1.805181	-0.776784	-1.036569
C	0.456255	-0.749491	-0.779317
C	0.859423	-2.344742	-2.4603
H	0.575389	-2.475122	-3.509376
H	0.98035	-3.345064	-2.012703
C	2.107804	-1.497936	-2.278246
H	3.027268	-2.083523	-2.179893
H	2.243702	-0.786089	-3.108023
C	-1.487751	-1.997429	-1.467517
C	-1.524545	-3.323921	-0.690333
H	-0.895468	-3.242012	0.204272
H	-1.104061	-4.129088	-1.311106
C	-2.967622	-3.65664	-0.306088
H	-2.985508	-4.599375	0.256842
C	-3.801054	-3.803402	-1.58222
H	-3.412669	-4.62977	-2.193812
H	-4.839841	-4.054303	-1.329298
C	-3.759517	-2.492231	-2.374358
H	-4.353933	-2.596805	-3.291205
C	-2.305724	-2.170497	-2.754151
H	-2.251621	-1.245081	-3.343183
H	-1.894144	-2.981259	-3.37579
C	-4.34429	-1.370653	-1.505765
H	-4.355884	-0.424112	-2.0628
H	-5.38784	-1.607737	-1.253589
C	-3.506037	-1.210335	-0.223871
H	-3.922809	-0.405965	0.394824

C	-2.086673	-0.850294	-0.653999
H	-2.150889	0.017195	-1.334223
C	-3.533146	-2.524643	0.558493
H	-2.948353	-2.419831	1.479921
H	-4.563006	-2.764072	0.856929
C	-0.20216	-1.44415	1.680805
C	-2.479222	1.878963	1.035654
C	-3.570574	2.929136	1.22425
C	-2.887013	4.296619	1.326713
H	-2.270367	4.488121	0.443172
H	-2.241064	4.35434	2.210863
H	-3.63334	5.094297	1.410153
C	-4.467167	2.902534	-0.01749
H	-3.879458	3.078176	-0.922888
H	-5.241675	3.674342	0.053112
H	-4.970211	1.934424	-0.123869
C	-4.389203	2.646884	2.477554
H	-5.167628	3.407631	2.603728
H	-3.760874	2.646913	3.372825
H	-4.87242	1.66719	2.421956
C	-0.862195	-1.777857	2.978372
H	-0.144799	-1.705778	3.811522
H	-1.72275	-1.137049	3.195437
H	-1.200407	-2.82501	2.974623
H	0.638683	-2.137702	1.47615
C	0.712985	1.277857	2.800321
H	1.474613	0.505512	2.923034
C	0.747303	2.025644	1.68081
H	0.046282	2.844007	1.532663
H	1.536679	1.913602	0.949667
C	-0.206048	1.497432	3.948784
H	-0.778103	0.598946	4.197734
H	0.372589	1.764292	4.841333
H	-0.922747	2.295052	3.742718
C	2.714079	0.213897	-0.559823
C	2.704052	1.497981	-1.143297
C	3.575603	2.456414	-0.613555
H	3.559162	3.467104	-1.012131
C	4.423458	2.150697	0.444429
C	4.42647	0.873506	0.992984
H	5.088448	0.648617	1.825431
C	3.581977	-0.124972	0.496877
H	5.079757	2.915672	0.850401
C	1.736398	1.864873	-2.249714
H	1.044868	1.023717	-2.380717
C	3.616655	-1.53321	1.050506
H	2.683971	-2.019064	0.736235
C	3.636043	-1.576182	2.581714

H	4.534612	-1.082351	2.974271
H	2.790187	-0.980745	2.949344
C	4.756809	-2.356736	0.414695
H	4.673991	-2.274858	-0.677181
H	4.586088	-3.416445	0.643772
C	0.852949	3.054073	-1.844156
H	0.40543	2.827187	-0.870264
H	1.467285	3.953958	-1.700703
C	2.424474	2.05073	-3.618053
H	1.637158	2.073708	-4.38231
H	3.01841	1.152518	-3.836529
C	3.53999	-2.982979	3.146328
H	4.424562	-3.583203	2.909042
H	3.439857	-2.970564	4.235034
H	2.668656	-3.511454	2.741167
C	6.161804	-1.966822	0.839768
H	6.909471	-2.592857	0.345358
H	6.386996	-0.926351	0.585512
H	6.307442	-2.081749	1.919566
C	-0.267265	3.333315	-2.829476
H	-0.947109	4.097788	-2.443319
H	0.103255	3.677508	-3.80161
H	-0.865232	2.429434	-2.996731
C	3.306026	3.277928	-3.777707
H	4.185483	3.239019	-3.128438
H	3.668489	3.363355	-4.805922
H	2.763675	4.201823	-3.548464

TSCA

	x	y	z
Ru	-0.751725	-0.045635	-0.574848
O	-2.107658	-1.896628	0.021555
O	-2.402344	-0.81225	-1.882975
N	-0.024626	1.569429	1.692226
N	1.856889	0.748582	0.915059
C	0.489638	0.712852	0.751741
C	0.99874	2.390105	2.31897
H	0.782435	2.578605	3.375159
H	1.088074	3.363854	1.809737
C	2.231266	1.531351	2.102486
H	3.143784	2.108266	1.924617
H	2.413877	0.855904	2.953646
C	-1.398653	2.007667	1.473573
C	-1.453603	3.234415	0.547241
H	-0.873677	3.021238	-0.360061
H	-0.986862	4.099389	1.041743
C	-2.91004	3.551473	0.202835

H	-2.945085	4.420738	-0.467643
C	-3.663722	3.868751	1.498743
H	-3.226072	4.753391	1.98213
H	-4.711413	4.111988	1.277311
C	-3.598786	2.661954	2.441674
H	-4.135398	2.892646	3.370966
C	-2.131985	2.347399	2.775569
H	-2.063409	1.494779	3.46459
H	-1.668149	3.213174	3.274375
C	-4.255405	1.460217	1.750259
H	-4.249629	0.58581	2.414649
H	-5.308134	1.692299	1.533992
C	-3.501248	1.129182	0.450979
H	-3.973431	0.267753	-0.035993
C	-2.059623	0.793732	0.820329
H	-2.067025	-0.012	1.571838
C	-3.545494	2.33781	-0.486276
H	-3.010003	2.09763	-1.414692
H	-4.583437	2.568643	-0.762904
C	0.051312	1.068836	-1.890018
C	-2.738783	-1.729993	-1.061595
C	-3.886896	-2.672135	-1.419278
C	-3.251629	-3.922467	-2.041447
H	-2.566201	-4.405187	-1.33718
H	-2.690257	-3.670192	-2.948544
H	-4.024522	-4.648557	-2.317012
C	-4.644316	-3.058839	-0.1505
H	-3.973482	-3.516245	0.580305
H	-5.44669	-3.767316	-0.384788
H	-5.098959	-2.181234	0.322933
C	-4.825803	-2.014476	-2.425701
H	-5.641335	-2.697595	-2.688467
H	-4.294914	-1.738923	-3.339969
H	-5.269179	-1.100268	-2.016992
C	-0.719789	1.710438	-3.005431
H	-0.124002	1.867842	-3.914448
H	-1.629966	1.160248	-3.260553
H	-1.020993	2.709344	-2.660628
H	1.03334	1.548383	-1.745826
C	0.674071	-0.739583	-2.474651
H	1.689191	-0.338582	-2.495217
C	0.551199	-1.826629	-1.557329
H	-0.196438	-2.593784	-1.752305
H	1.363906	-2.088345	-0.893835
C	0.046033	-0.954617	-3.835171
H	0.192302	-0.112719	-4.513453
H	0.50536	-1.831847	-4.301406
H	-1.026487	-1.143517	-3.739661

C	2.717855	-0.317677	0.509004	N	0.046563	-1.667429	-1.587075
C	2.601478	-1.575097	1.139414	N	1.90972	-0.81759	-0.800849
C	3.406857	-2.615593	0.662076	C	0.539896	-0.758321	-0.688268
H	3.30118	-3.607587	1.092472	C	1.072905	-2.563267	-2.094064
C	4.309256	-2.410868	-0.374753	H	0.89785	-2.837607	-3.138899
C	4.444955	-1.150346	-0.944051	H	1.11556	-3.490679	-1.499234
H	5.161494	-0.998788	-1.747202	C	2.315205	-1.712121	-1.896998
C	3.665223	-0.074545	-0.506748	H	3.205571	-2.287801	-1.62637
H	4.913282	-3.237645	-0.738459	H	2.550129	-1.120002	-2.795491
C	1.620432	-1.824327	2.267228	C	-1.352864	-2.029764	-1.4036
H	1.004364	-0.925765	2.386302	C	-1.511436	-3.108853	-0.315633
C	3.867887	1.316894	-1.069422	H	-0.989513	-2.777964	0.593556
H	2.964952	1.893141	-0.825405	H	-1.031873	-4.042768	-0.644811
C	4.016766	1.34452	-2.595071	C	-2.995706	-3.344962	-0.032846
H	4.907551	0.782901	-2.904534	H	-3.100167	-4.109757	0.7481
H	3.167854	0.811471	-3.042837	C	-3.67059	-3.82523	-1.321937
C	5.036565	2.034941	-0.356797	H	-3.230649	-4.778977	-1.645022
H	4.887875	1.946933	0.726951	H	-4.737894	-4.010798	-1.143467
H	4.970302	3.107925	-0.578064	C	-3.50501	-2.765809	-2.417087
C	0.63332	-2.948088	1.921428	H	-3.987844	-3.111922	-3.339879
H	0.147377	-2.689424	0.973173	C	-2.012346	-2.531538	-2.69129
H	1.173693	-3.889313	1.747468	H	-1.873925	-1.786905	-3.486787
C	2.31912	-2.017919	3.630057	H	-1.53996	-3.467512	-3.028945
H	1.547465	-1.935001	4.405941	C	-4.159444	-1.46207	-1.947797
H	2.997166	-1.169939	3.799634	H	-4.079079	-0.69206	-2.726064
C	4.077667	2.750504	-3.166581	H	-5.231459	-1.629399	-1.771536
H	4.972865	3.289201	-2.839021	C	-3.483728	-0.968448	-0.655338
H	4.089786	2.737134	-4.259585	H	-3.959073	-0.034174	-0.340118
H	3.208414	3.341025	-2.853556	C	-2.011214	-0.719619	-0.96274
C	6.425721	1.53057	-0.707525	H	-1.911644	0.015403	-1.773538
H	7.191268	2.071308	-0.144751	C	-3.631272	-2.031586	0.436799
H	6.539954	0.467014	-0.475334	H	-3.148523	-1.677595	1.359234
H	6.65278	1.663407	-1.77084	H	-4.692859	-2.189915	0.671807
C	-0.440711	-3.149771	2.975023	C	0.153505	-0.798944	2.061987
H	-1.197162	-3.860358	2.632263	C	-2.860037	1.73297	0.976648
H	-0.035126	-3.52499	3.921464	C	-4.061431	2.566918	1.426311
H	-0.958784	-2.206253	3.184788	C	-3.589034	3.466116	2.57397
C	3.083918	-3.315185	3.832273	H	-2.786114	4.137129	2.247522
H	3.961654	-3.381909	3.183195	H	-3.213672	2.86741	3.409187
H	3.439354	-3.398307	4.863177	H	-4.414347	4.087354	2.939648
H	2.456657	-4.19163	3.634674	C	-4.584696	3.415486	0.274118
				H	-3.811175	4.086513	-0.107252
				H	-5.438655	4.018989	0.602168
				H	-4.91038	2.788523	-0.561611
				C	-5.156251	1.626734	1.935747
				H	-6.012357	2.201488	2.30694
				H	-4.781548	0.994426	2.744535
				H	-5.5203	0.968879	1.137773

MC-I

	x	y	z
Ru	-0.769848	0.071802	0.539412
O	-2.317005	1.922241	-0.141229
O	-2.425428	0.846098	1.795274

C	-0.6908	-1.408271	3.155761
H	-0.138288	-1.494664	4.102656
H	-1.603131	-0.8352	3.344146
H	-0.985959	-2.425735	2.872891
H	1.043767	-1.408314	1.860235
C	0.614849	0.737446	2.283626
H	1.706451	0.667341	2.239425
C	0.247337	1.689928	1.124754
H	-0.431694	2.495439	1.423209
H	1.1011	2.060815	0.562017
C	0.147681	1.300464	3.619211
H	0.455159	0.665051	4.455749
H	0.575154	2.294653	3.77769
H	-0.941521	1.39284	3.635942
C	2.763112	0.284673	-0.47696
C	2.655783	1.478952	-1.222336
C	3.43766	2.566282	-0.816834
H	3.337	3.514558	-1.337539
C	4.315139	2.462689	0.255699
C	4.450226	1.257444	0.934221
H	5.147449	1.183798	1.764773
C	3.687929	0.140349	0.576907
H	4.902474	3.324656	0.560249
C	1.727045	1.608727	-2.414395
H	1.104225	0.707984	-2.462251
C	3.873861	-1.189181	1.277539
H	2.984673	-1.793241	1.051895
C	3.951194	-1.065463	2.80424
H	4.825988	-0.470699	3.097248
H	3.080438	-0.496978	3.1556
C	5.074154	-1.964016	0.688865
H	4.967422	-1.991223	-0.403369
H	5.005335	-3.008674	1.018357
C	0.741346	2.776238	-2.262765
H	0.185037	2.633756	-1.329673
H	1.285656	3.72447	-2.153824
C	2.500968	1.637205	-3.75093
H	1.772108	1.47293	-4.554739
H	3.174653	0.76977	-3.784122
C	3.988367	-2.408207	3.513334
H	4.899987	-2.970137	3.284575
H	3.946664	-2.287027	4.598958
H	3.136272	-3.032398	3.219033
C	6.445741	-1.413147	1.03863
H	7.236119	-2.008212	0.573382
H	6.56748	-0.381731	0.693206
H	6.626846	-1.423973	2.118873
C	-0.253179	2.876983	-3.40583

H	-1.024339	3.620196	-3.188497
H	0.221192	3.157432	-4.352822
H	-0.764076	1.919469	-3.561942
C	3.296799	2.895455	-4.053909
H	4.131903	3.03086	-3.360721
H	3.718483	2.853081	-5.062031
H	2.672719	3.794531	-4.001888

TSMC

	x	y	z
Ru	0.767416	-0.30162	0.442454
O	2.36385	-1.615811	-0.987525
O	2.392316	-1.58352	1.230327
N	-0.055752	2.243047	-0.589153
N	-1.90876	1.094138	-0.341533
C	-0.540072	1.004342	-0.26298
C	-1.091177	3.264869	-0.590602
H	-0.927025	4.012364	-1.373209
H	-1.126539	3.788922	0.378437
C	-2.33571	2.420734	-0.818262
H	-3.214093	2.770328	-0.263948
H	-2.608957	2.367004	-1.883966
C	1.339121	2.47789	-0.233477
C	2.010483	1.12263	-0.479306
C	-0.197456	-0.259731	2.168354
C	2.861772	-1.985096	0.10589
C	4.053767	-2.942771	0.154574
H	-1.074709	0.393596	2.25783
C	-0.677833	-1.703476	1.603916
H	-1.766397	-1.591865	1.555163
C	-0.255666	-1.99202	0.14777
H	0.416748	-2.850715	0.045058
H	-1.081063	-2.03095	-0.561518
C	2.003328	3.549832	-1.102356
H	1.5222	4.528065	-0.944546
H	1.880208	3.289407	-2.162102
C	1.476935	2.889097	1.245093
H	0.9909	3.862743	1.407426
H	0.950719	2.154888	1.871162
C	3.477312	1.199808	-0.07281
C	2.9562	2.9652	1.62618
H	3.044899	3.250656	2.682755
C	3.490926	3.629689	-0.729473
H	3.976807	4.386073	-1.359009
C	3.604166	1.59442	1.401605
C	4.157095	2.267299	-0.949882
H	4.09186	1.976512	-2.006367

C	3.635453	4.01922	0.745901	H	-5.50757	1.581316	0.410215
H	3.186647	5.006197	0.924926	H	-6.206799	0.309517	1.374439
H	4.699008	4.100791	1.005912	C	-3.848916	-0.252076	2.873345
H	3.959198	0.232727	-0.249316	H	-4.012501	0.499674	3.655702
H	3.119384	0.831992	2.02819	H	-2.796061	-0.535755	2.976742
H	4.662071	1.625227	1.696905	C	-1.601361	0.705905	-5.371069
H	5.225688	2.333971	-0.701008	H	-0.757686	0.094902	-5.705303
H	1.924312	0.87481	-1.547233	H	-2.206977	0.931434	-6.253086
C	3.589254	-4.228193	0.846679	H	-1.19044	1.652944	-5.00142
H	4.410333	-4.951679	0.903499	C	-0.591556	-2.480601	-3.485913
H	3.242732	-4.01965	1.862845	H	0.378046	-2.976101	-3.586805
H	2.766716	-4.700768	0.297133	H	-1.15031	-3.024021	-2.716098
C	4.552055	-3.249941	-1.251893	H	-1.128355	-2.607736	-4.434461
H	4.868782	-2.337856	-1.766173	C	-5.770719	2.107239	2.480174
H	5.405186	-3.936739	-1.21257	H	-6.712381	2.622151	2.271699
H	3.767226	-3.707623	-1.859812	H	-5.870847	1.638207	3.463734
C	5.166436	-2.295148	0.983507	H	-4.988423	2.871267	2.561954
H	4.806342	-2.03498	1.9824	C	-4.716708	-1.46541	3.162801
H	6.016356	-2.979571	1.0846	H	-4.450171	-2.318684	2.531932
H	5.535318	-1.378227	0.50908	H	-4.593855	-1.783932	4.201684
C	0.61681	-0.271538	3.440216	H	-5.78354	-1.261164	3.013199
H	0.919381	0.751173	3.694798				
H	0.041192	-0.649917	4.296975				
H	1.52367	-0.875213	3.345643				
C	-0.279717	-2.847087	2.526931				
H	-0.629709	-2.679023	3.550555				
H	-0.714792	-3.785951	2.172665				
H	0.807432	-2.963037	2.546689				
C	-2.763278	-0.014181	-0.641707				
C	-3.769435	-0.366828	0.28058				
C	-4.60147	-1.44449	-0.044528				
H	-5.404339	-1.721074	0.632476				
C	-4.439015	-2.14419	-1.232713				
C	-3.478494	-1.742403	-2.152256				
H	-3.393983	-2.265687	-3.100753				
C	-2.633804	-0.657862	-1.893192				
H	-5.089346	-2.984328	-1.460488				
C	-4.045391	0.462342	1.521181				
H	-3.317649	1.285522	1.526913				
C	-1.674426	-0.174067	-2.96874				
H	-1.319016	0.824095	-2.680915				
C	-2.422827	0.008334	-4.30094				
H	-2.765065	-0.963149	-4.680409				
H	-3.338791	0.582525	-4.106797				
C	-0.395918	-1.021733	-3.116625				
H	0.180545	-0.962152	-2.188959				
H	0.235843	-0.536252	-3.871194				
C	-5.442231	1.098065	1.394119				

MC-II

	x	y	z
Ru	0.716485	-0.570869	-0.664678
O	2.310253	-2.062022	-1.112314
O	2.574782	-1.026962	0.824388
N	-0.103135	2.177271	-0.740528
N	-1.892295	1.081134	-0.124105
C	-0.5549	0.927323	-0.400275
C	-1.058378	3.236	-0.45881
H	-1.060109	3.99719	-1.245233
H	-0.826568	3.736938	0.495777
C	-2.357021	2.450941	-0.396591
H	-3.042093	2.788775	0.388515
H	-2.896188	2.484844	-1.354663
C	1.334306	2.383832	-0.733369
C	1.825336	2.791596	0.668798
H	1.509916	2.020382	1.387202
H	1.353056	3.739011	0.967901
C	3.34919	2.935009	0.666051
H	3.684855	3.24763	1.663206
C	3.767329	3.981216	-0.370624
H	3.343453	4.96375	-0.119647
H	4.859365	4.094148	-0.365783
C	3.290723	3.544352	-1.759183
H	3.602156	4.284248	-2.507662

C	-2.274119	2.528193	0.320241	H	-0.185097	-4.341583	0.751406
H	-2.883836	2.667634	1.220014	H	1.086195	-3.827983	-0.361457
H	-2.8822	2.81742	-0.549174	H	-1.039589	-1.934361	0.843226
C	1.387274	2.465243	-0.29337	C	-0.691621	-3.333555	-2.26942
C	1.968083	2.449064	1.132691	H	-1.010588	-4.306318	-1.875358
H	1.666967	1.511557	1.623749	H	-1.20806	-3.166721	-3.217972
H	1.550156	3.282077	1.717903	H	0.382159	-3.39228	-2.47295
C	3.493825	2.555536	1.076567	H	-2.027197	-1.895729	-1.252205
H	3.894717	2.570699	2.098459	C	-2.69723	0.091431	0.679984
C	3.899768	3.836965	0.344491	C	-3.843202	-0.264627	-0.05945
H	3.52925	4.721901	0.881139	C	-4.691699	-1.242442	0.472832
H	4.994484	3.9171	0.313617	H	-5.563579	-1.557125	-0.094419
C	3.333252	3.811016	-1.078134	C	-4.433532	-1.820192	1.708785
H	3.636754	4.719925	-1.613779	C	-3.303692	-1.448996	2.428124
C	1.803154	3.762498	-0.996227	H	-3.102299	-1.913784	3.389702
H	1.352607	3.789031	-1.997684	C	-2.407934	-0.499243	1.931046
H	1.432521	4.642482	-0.446566	H	-5.111686	-2.568109	2.110559
C	3.864039	2.576316	-1.820676	C	-4.15126	0.382653	-1.392978
H	3.487427	2.566805	-2.852206	H	-3.240713	0.91058	-1.710079
H	4.960604	2.62791	-1.880637	C	-1.140364	-0.155622	2.691883
C	3.434191	1.289375	-1.084752	H	-0.356358	0.021942	1.94225
H	3.816707	0.415608	-1.627514	C	-0.618427	-1.31122	3.558039
C	1.902147	1.265784	-1.088315	H	-1.200137	-1.393421	4.48732
H	1.586045	1.420489	-2.134737	H	-0.78272	-2.258131	3.026186
C	4.039069	1.340747	0.324856	C	-1.289792	1.150689	3.493453
H	3.809066	0.428657	0.879569	H	-1.412588	1.983905	2.790207
H	5.133867	1.41666	0.245752	H	-0.34215	1.347652	4.011053
C	-0.437096	-2.350213	0.046246	C	-4.452599	-0.652198	-2.485776
C	2.79197	-1.830195	-0.343156	H	-3.619022	-1.366623	-2.525625
C	4.070259	-2.633266	-0.093775	H	-5.333605	-1.248246	-2.215271
C	3.896803	-4.051556	-0.641223	C	-5.254707	1.457302	-1.277152
H	3.580339	-4.029024	-1.687492	H	-5.233561	2.066847	-2.189883
H	3.150963	-4.614299	-0.069952	H	-4.992626	2.141208	-0.460126
H	4.842639	-4.600618	-0.575908	C	0.862134	-1.174215	3.875527
C	5.208762	-1.945006	-0.856935	H	1.076956	-0.260347	4.440446
H	4.979153	-1.879711	-1.924609	H	1.219884	-2.014731	4.477663
H	6.138015	-2.513462	-0.738336	H	1.457032	-1.142255	2.95468
H	5.387497	-0.931939	-0.48121	C	-2.4371	1.158542	4.489493
C	4.394284	-2.675013	1.395785	H	-2.471212	2.097088	5.049365
H	5.311141	-3.24967	1.568445	H	-3.403017	1.034294	3.988065
H	3.586583	-3.143962	1.967487	H	-2.347094	0.348947	5.221888
H	4.536966	-1.669054	1.800542	C	-4.654177	-0.036969	-3.8597
C	-0.990985	-2.238368	-1.273851	H	-4.75771	-0.805962	-4.629616
C	-0.496927	-0.627865	-2.351899	H	-5.552587	0.587582	-3.902211
H	-0.068881	-1.117309	-3.238042	H	-3.803407	0.595688	-4.138165
H	-1.489358	-0.20012	-2.553365	C	-6.664925	0.938705	-1.052668
C	0.439122	-3.48774	0.449001	H	-6.751712	0.392254	-0.10883
H	1.065891	-3.225257	1.306527	H	-7.38056	1.764466	-1.01597

H	-6.987971	0.267012	-1.85559	C	-5.047091	1.862331	-1.103663
				H	-4.800343	1.712391	-2.158535
				H	-5.980582	2.432805	-1.044294
DSCA				H	-5.225755	0.882519	-0.650882
	x	y	z	C	-4.270764	2.805635	1.087049
Ru	-0.567451	0.238223	-0.904342	H	-5.193004	3.388157	1.189818
O	-2.140839	1.655965	-1.703733	H	-3.475052	3.333942	1.622991
O	-2.099956	1.242642	0.463444	H	-4.415082	1.843105	1.586323
N	0.071631	-2.406063	0.06456	C	1.102187	2.392074	-1.389683
N	1.797708	-1.140292	0.516788	C	0.235215	-0.267838	-2.476236
C	0.540534	-1.121992	-0.013339	H	0.183117	0.412657	-3.345886
C	0.915499	-3.254435	0.897336	H	0.691464	-1.23927	-2.743399
H	0.990549	-4.268204	0.493124	C	-0.45202	3.831267	-0.027542
H	0.514953	-3.326346	1.921509	H	-1.208542	3.581867	0.723106
C	2.235036	-2.500061	0.856417	H	0.068879	4.728075	0.332447
H	2.784925	-2.509545	1.803902	H	-0.956514	4.095454	-0.959735
H	2.899811	-2.892454	0.073047	H	0.911041	2.259863	0.686428
C	-1.381997	-2.528297	0.025257	C	0.767705	3.014142	-2.707535
C	-1.982586	-2.223011	1.409884	H	1.145938	4.041782	-2.769289
H	-1.657596	-1.21873	1.721642	H	1.206574	2.457293	-3.539214
H	-1.605087	-2.942629	2.151767	H	-0.316046	3.051917	-2.864203
C	-3.509065	-2.288785	1.342621	H	1.926485	1.683821	-1.355341
H	-3.926355	-2.097989	2.33998	C	2.653499	-0.023313	0.735964
C	-3.952461	-3.669403	0.853016	C	3.752935	0.190532	-0.117098
H	-3.624518	-4.450661	1.553383	C	4.61073	1.25606	0.178939
H	-5.048894	-3.715819	0.813029	H	5.449081	1.465465	-0.480144
C	-3.363046	-3.927812	-0.536213	C	4.39813	2.057461	1.293243
H	-3.692952	-4.909198	-0.901249	C	3.297736	1.837268	2.114196
C	-1.833035	-3.920164	-0.427031	H	3.127879	2.486139	2.969313
H	-1.365573	-4.153077	-1.393203	C	2.391751	0.808722	1.845428
H	-1.509029	-4.691749	0.289769	H	5.084628	2.870088	1.514699
C	-3.839234	-2.834338	-1.504469	C	3.980816	-0.683047	-1.332722
H	-3.455186	-3.030558	-2.514032	H	3.064527	-1.272687	-1.479237
H	-4.936627	-2.858184	-1.568544	C	1.136112	0.622128	2.680285
C	-3.365362	-1.448074	-1.015584	H	0.327028	0.365555	1.978052
H	-3.709466	-0.676136	-1.716613	C	0.673348	1.901618	3.392325
C	-1.828995	-1.495937	-1.013728	H	1.279153	2.080788	4.292222
H	-1.549176	-1.921496	-1.986321	H	0.8563	2.767461	2.742518
C	-3.990076	-1.215438	0.366945	C	1.258619	-0.559342	3.66166
H	-3.729362	-0.229558	0.757388	H	1.2806	-1.49617	3.092309
H	-5.086006	-1.25973	0.279688	H	0.338224	-0.607354	4.257327
C	0.52409	2.724628	-0.21454	C	4.156039	0.14871	-2.610975
C	-2.640663	1.805355	-0.546594	H	3.287794	0.813283	-2.708302
C	-3.924184	2.624443	-0.386492	H	5.025051	0.813222	-2.518389
C	-3.763783	3.987196	-1.065761	C	5.125811	-1.697582	-1.122866
H	-3.392261	3.871221	-2.087882	H	5.053902	-2.459154	-1.910168
H	-3.073433	4.635704	-0.5183	H	4.953132	-2.231686	-0.179779
H	-4.731271	4.499459	-1.106606	C	-0.803904	1.860243	3.749835

H	-1.03593	1.046101	4.444938	C	3.168314	1.373365	-1.183415
H	-1.12503	2.790643	4.227265	H	3.325105	0.930341	-2.174485
H	-1.415559	1.711132	2.852016	C	1.672979	1.569814	-0.940009
C	2.467471	-0.491699	4.579804	H	1.281225	2.294858	-1.661353
H	2.47977	-1.327719	5.28438	C	3.787102	0.468771	-0.112579
H	3.404019	-0.51958	4.012292	H	3.327781	-0.527923	-0.157949
H	2.478491	0.43014	5.171624	H	4.858967	0.329621	-0.307877
C	4.287241	-0.69443	-3.867388	C	1.515459	-2.47303	-0.716636
H	4.298249	-0.071148	-4.765394	C	2.228356	-3.761915	-0.335691
H	5.208917	-1.285742	-3.871773	C	1.194867	-4.892031	-0.294812
H	3.449172	-1.394278	-3.962729	H	0.735668	-5.049537	-1.275978
C	6.531466	-1.120955	-1.110221	H	0.399804	-4.669705	0.422228
H	6.676817	-0.421579	-0.281594	H	1.67544	-5.829566	0.004543
H	7.275099	-1.914541	-0.997855	C	3.326238	-4.077323	-1.343922
H	6.765265	-0.588452	-2.038627	H	2.919543	-4.194192	-2.351467

14-Int'

	x	y	z				
Ru	0.4536490	-0.1453070	-0.928956	H	3.338068	-4.484576	1.3826
O	1.8067150	-1.8235260	-1.753104	H	2.043887	-3.337819	1.792341
O	0.6079750	-2.0265170	0.092453	H	3.558218	-2.755825	1.078861
N	0.0019540	2.2084000	0.591569	C	-0.522236	0.105549	-2.42869
N	-1.8898470	1.0918300	0.585895	H	-0.17052	-0.400208	-3.342616
C	-0.6113070	1.0730100	0.12027	H	-1.499118	0.60187	-2.506917
C	-0.7579360	2.7964530	1.68449	C	-2.859599	0.062806	0.385912
H	-0.6581800	3.8851930	1.715607	C	-2.753621	-1.119926	1.148413
H	-0.4397470	2.3890960	2.660635	C	-3.723387	-2.105253	0.955546
C	-2.1644910	2.3372860	1.316754	H	-3.661571	-3.029929	1.521891
H	-2.8158290	2.1557600	2.176509	C	-4.769144	-1.922581	0.057523
H	-2.6599180	3.0679060	0.659097	C	-4.856433	-0.749891	-0.678563
C	1.4569100	2.1643800	0.465312	H	-5.673889	-0.614242	-1.383019
C	2.0804430	1.2375260	1.529437	C	-3.899225	0.258588	-0.539072
H	1.5866290	0.2507000	1.49299	C	-1.657584	-1.297335	2.182024
H	1.8970520	1.6429520	2.535814	H	-0.742745	-0.851772	1.773904
C	3.5809000	1.0850280	1.274285	C	-4.018185	1.530632	-1.352904
H	4.0169780	0.4307670	2.040841	H	-3.054125	2.054024	-1.296239
C	4.2408490	2.4660730	1.333393	H	-5.516769	-2.700953	-0.069298
H	4.1142520	2.9038460	2.333196	C	-5.098727	2.443789	-0.769249
H	5.3210710	2.3740870	1.160093	H	-6.082282	1.965239	-0.839009
C	3.6184440	3.3798140	0.272227	H	-4.923169	2.667866	0.287724
H	4.0962990	4.3669410	0.311861	H	-5.151715	3.392233	-1.313889
C	2.1164710	3.5397870	0.553462	C	-4.303713	1.25808	-2.828037
H	1.6513940	4.2140430	-0.177986	H	-3.574559	0.568389	-3.263051
H	1.9673590	3.9825100	1.550986	H	-5.297928	0.82208	-2.972285
C	3.837914	2.758367	-1.113943	H	-4.274912	2.189379	-3.401949
H	3.424059	3.412549	-1.892459	C	-2.008759	-0.557379	3.474634
H	4.915972	2.670445	-1.309512	H	-2.18323	0.509353	3.30714
				H	-2.916993	-0.972005	3.927179

H	-1.199309	-0.65053	4.20667
C	-1.342195	-2.755645	2.487027
H	-2.153732	-3.24439	3.039118
H	-1.150913	-3.31989	1.57136
H	-0.445129	-2.82004	3.110367

Ru-7

14-Int

	x	y	z
Ru	-0.4658780	0.5753460	-1.034067
O	0.5186320	-1.0558350	-2.350886
O	1.5057630	0.8448830	-2.040823
N	-1.0806740	-0.8657690	1.346873
N	1.0600630	-0.3558820	1.373331
C	-0.0853680	-0.2512360	0.647795
C	-0.6906620	-1.1308630	2.72284
H	-1.0734140	-2.0938370	3.075398
H	-1.0750620	-0.3471560	3.394694
C	0.8342250	-1.0971390	2.621623
H	1.3153620	-0.5881150	3.462918
H	1.2568680	-2.1075000	2.550222
C	-2.4369040	-0.6635900	0.85698
C	-3.0956330	0.5462490	1.537205
H	-2.4384820	1.4187870	1.441551
H	-3.2165010	0.3424960	2.611434
C	-4.4551950	0.8248600	0.895403
H	-4.9180610	1.6923650	1.38334
C	-5.3528630	-0.4034240	1.067011
H	-5.5207130	-0.6016350	2.134553
H	-6.3376860	-0.2183280	0.618198
C	-4.6939860	-1.6139940	0.398735
H	-5.3350140	-2.4963430	0.519884
C	-3.3356320	-1.8881910	1.063806
H	-2.8551940	-2.7708780	0.621831
H	-3.4808540	-2.0947200	2.135697
C	-4.5123150	-1.3147760	-1.095573
H	-4.0766930	-2.1820740	-1.608067
H	-5.4944410	-1.1317760	-1.553695
C	-3.5975370	-0.0877970	-1.276828
H	-3.4724300	0.1168760	-2.349339
C	-2.2458470	-0.4292780	-0.650334
H	-1.9175240	-1.3987240	-1.07538
C	-4.2463420	1.1187660	-0.593449
H	-3.6119010	2.0061850	-0.71108
H	-5.2096690	1.3456670	-1.069874
C	2.3769530	-0.1465320	0.848024
C	2.9368970	1.1398340	0.920371

C	4.2243640	1.3279540	0.414522
H	4.6705650	2.3191610	0.458991
C	4.9327750	0.2774740	-0.150519
C	4.3616620	-0.9863870	-0.215279
H	4.9167740	-1.8046240	-0.667318
C	3.0770250	-1.2286670	0.275649
C	-0.849154	2.230578	-0.361154
C	-1.247364	3.276379	-1.357636
H	-2.186139	3.768587	-1.069321
H	-0.485924	4.065429	-1.423972
H	-1.389221	2.874034	-2.370914
H	-0.73152	2.619559	0.663325
N	1.532813	-0.31453	-2.607187
O	2.454985	-0.671256	-3.313026
H	5.930338	0.443502	-0.547383
C	2.195877	2.3167	1.515553
H	1.170895	1.991707	1.72978
C	2.515937	-2.637854	0.222348
H	1.43699	-2.585131	0.420809
C	3.17623	-3.50415	1.300634
H	2.725561	-4.501474	1.334803
H	4.242581	-3.630897	1.081625
H	3.107166	-3.063475	2.300621

CA

	x	y	z
Ru	0.480232	-0.893166	0.100964
O	1.094963	-2.155455	-1.787209
O	1.514977	-2.865941	0.220164
N	0.707195	1.94802	-0.318437
N	-1.423391	1.530995	-0.035136
C	-0.197796	0.932573	-0.162546
C	0.129498	3.258372	-0.056672
H	0.522124	4.021733	-0.735892
H	0.345045	3.578656	0.975367
C	-1.352415	2.980802	-0.257686
H	-2.000524	3.516776	0.443445
H	-1.684756	3.223955	-1.279329
C	2.113372	1.618223	-0.10978
C	2.549932	1.865471	1.34377
H	1.857306	1.36207	2.028617
H	2.501686	2.941444	1.568461
C	3.977821	1.352407	1.545405
H	4.277134	1.518286	2.588894
C	4.916466	2.122564	0.611724
H	4.898814	3.19339	0.858284
H	5.95071	1.7803	0.74844

C	4.483128	1.904099	-0.841376
H	5.151123	2.458944	-1.51258
C	3.046997	2.415339	-1.031093
H	2.722878	2.287723	-2.072332
H	2.998788	3.491261	-0.800574
C	4.558175	0.406002	-1.160903
H	4.283754	0.224199	-2.207953
H	5.591747	0.054515	-1.03535
C	3.612403	-0.376713	-0.231139
H	3.673849	-1.445467	-0.467458
C	2.197032	0.136453	-0.477386
H	1.999984	0.074817	-1.562495
C	4.032688	-0.145076	1.221024
H	3.371087	-0.707825	1.890552
H	5.050809	-0.522876	1.384703
C	-2.660415	0.856047	-0.251612
C	-3.517463	0.646409	0.843598
C	-4.715055	-0.037466	0.618625
H	-5.38867	-0.218309	1.454197
C	-5.055664	-0.484418	-0.65236
C	-4.216986	-0.223092	-1.729638
H	-4.499937	-0.555021	-2.726664
C	-3.011702	0.462887	-1.557767
C	0.381788	-0.52457	1.916534
C	1.011735	-1.363389	2.977187
H	1.774617	-0.771393	3.505415
H	0.280871	-1.645352	3.749584
H	1.489231	-2.268445	2.590101
H	-0.157535	0.339312	2.356443
N	1.625463	-3.061556	-1.050751
O	2.189502	-4.037906	-1.508088
H	-5.986274	-1.023225	-0.807569
C	-3.19927	1.180912	2.226289
H	-2.208668	1.650682	2.178689
C	-2.153939	0.785688	-2.768909
H	-1.296633	1.383245	-2.438106
C	-2.946805	1.62634	-3.771024
H	-2.309196	1.933562	-4.605627
H	-3.784475	1.059789	-4.192321
H	-3.361882	2.528152	-3.30924
C	-1.587328	-0.46406	-3.441273
H	-0.869834	-0.984754	-2.800399
H	-2.38289	-1.169758	-3.708484
H	-1.063743	-0.195481	-4.363931
C	-4.217278	2.250001	2.626274
H	-3.958875	2.694717	3.592513
H	-4.27426	3.054337	1.886241
H	-5.221947	1.822148	2.71875

C	-3.136149	0.083029	3.28607
H	-2.957644	0.514444	4.27623
H	-4.074228	-0.481295	3.338705
H	-2.328151	-0.627684	3.085756
C	-1.691299	-2.453969	0.888204
H	-2.347742	-1.680503	1.284158
C	-1.468202	-2.468861	-0.445311
H	-1.982266	-1.780292	-1.104276
H	-0.918956	-3.284044	-0.908709
C	-1.241822	-3.519868	1.825288
H	-0.979774	-3.12757	2.811303
H	-2.059218	-4.233862	1.984036
H	-0.382749	-4.066604	1.428219

TSCA

	x	y	z
Ru	0.556612	0.885758	-0.04332
O	1.346346	2.120579	1.829602
O	1.708453	2.777559	-0.205406
N	0.617646	-1.974295	0.294884
N	-1.489014	-1.445075	-0.00654
C	-0.235238	-0.911175	0.156904
C	-0.015164	-3.242974	-0.035807
H	0.336161	-4.05464	0.60862
H	0.195025	-3.522017	-1.08077
C	-1.48215	-2.904883	0.167778
H	-2.150755	-3.388522	-0.551757
H	-1.82942	-3.162549	1.180863
C	2.031321	-1.68926	0.064245
C	2.383366	-1.78895	-1.430055
H	1.673337	-1.179908	-2.004269
H	2.276741	-2.829277	-1.77161
C	3.820095	-1.311853	-1.651416
H	4.062205	-1.373031	-2.720891
C	4.764489	-2.218881	-0.855735
H	4.686352	-3.253798	-1.217033
H	5.805971	-1.906032	-1.006799
C	4.411931	-2.147592	0.634149
H	5.086713	-2.799832	1.203072
C	2.964956	-2.619281	0.846146
H	2.699038	-2.59266	1.911158
H	2.855814	-3.660684	0.504498
C	4.570554	-0.698903	1.111018
H	4.352055	-0.623428	2.183991
H	5.612749	-0.378685	0.973474
C	3.622406	0.221257	0.321245
H	3.74526	1.25232	0.671683

C	2.194651	-0.255602	0.570414
H	2.010018	-0.273545	1.657732
C	3.958133	0.136954	-1.169724
H	3.285067	0.795951	-1.735024
H	4.98113	0.49307	-1.350173
C	-2.699636	-0.743877	0.277897
C	-3.602084	-0.492871	-0.772963
C	-4.76986	0.216452	-0.480571
H	-5.477861	0.428069	-1.279028
C	-5.044478	0.641057	0.813795
C	-4.167971	0.331926	1.847007
H	-4.398923	0.645898	2.862934
C	-2.986811	-0.375543	1.60722
C	0.007938	0.853585	-1.862849
H	-0.73761	0.137592	-2.244381
N	1.877974	2.98924	1.060834
O	2.504703	3.949417	1.469553
H	-5.954086	1.197831	1.021301
C	-3.382091	-1.050288	-2.166104
H	-2.351533	-1.425307	-2.213442
C	-2.077884	-0.71993	2.773098
H	-1.249432	-1.334395	2.401953
C	-2.832805	-1.543538	3.817228
H	-2.158781	-1.855561	4.620791
H	-3.639937	-0.962942	4.277198
H	-3.283116	-2.441988	3.382589
C	-1.459251	0.524756	3.408116
H	-0.810363	1.058282	2.707626
H	-2.234011	1.218932	3.7549
H	-0.851905	0.249226	4.275823
C	-4.328	-2.231455	-2.400323
H	-4.134901	-2.704502	-3.368455
H	-4.22802	-2.995085	-1.622444
H	-5.372489	-1.899575	-2.394668
C	-3.555714	-0.017443	-3.276596
H	-3.403576	-0.482562	-4.255485
H	-4.562647	0.413286	-3.276856
H	-2.842174	0.808843	-3.192067
C	-1.244998	2.216999	-1.098766
H	-2.075049	1.648388	-1.521774
C	-1.337829	2.312681	0.324075
H	-2.096496	1.76421	0.865939
H	-0.910143	3.182916	0.818804
C	-0.911409	3.499874	-1.827919
H	-0.874156	3.379208	-2.911653
H	-1.685554	4.241708	-1.609467
H	0.045442	3.905419	-1.489236
C	0.814193	1.467315	-2.968948

H	1.458744	2.282416	-2.627576
H	0.203014	1.822101	-3.808853
H	1.464939	0.68067	-3.374749

MC-I

	x	y	z
Ru	0.594524	0.864223	0.021714
O	1.604247	1.910709	2.048817
O	1.794989	2.719939	0.039364
N	0.550704	-2.004149	-0.014244
N	-1.543811	-1.392269	-0.229111
C	-0.276543	-0.913711	-0.011862
C	-0.103443	-3.197729	-0.529634
H	0.232031	-4.102352	-0.013497
H	0.100916	-3.322589	-1.605307
C	-1.563157	-2.863311	-0.270932
H	-2.243783	-3.222762	-1.04933
H	-1.911459	-3.260135	0.695497
C	1.968834	-1.707126	-0.179861
C	2.319792	-1.504949	-1.666306
H	1.630798	-0.765067	-2.098874
H	2.171563	-2.44696	-2.214709
C	3.768625	-1.035792	-1.797594
H	4.008505	-0.889013	-2.858871
C	4.689011	-2.105801	-1.201422
H	4.585934	-3.046015	-1.760695
H	5.737736	-1.794468	-1.291733
C	4.337853	-2.323808	0.274361
H	4.996843	-3.090874	0.700328
C	2.880784	-2.79428	0.395786
H	2.615395	-2.976971	1.445486
H	2.743653	-3.741404	-0.14933
C	4.526154	-1.003548	1.029325
H	4.308726	-1.137905	2.096658
H	5.573691	-0.680768	0.954562
C	3.600403	0.078314	0.441414
H	3.74986	1.01152	0.993169
C	2.163118	-0.405924	0.602735
H	1.939885	-0.597326	1.66307
C	3.934762	0.284567	-1.039586
H	3.274961	1.055363	-1.463487
H	4.963038	0.653788	-1.146496
C	-2.729192	-0.726325	0.213399
C	-3.666216	-0.294759	-0.743674
C	-4.802015	0.381688	-0.291399
H	-5.535396	0.732125	-1.014422
C	-5.009311	0.605635	1.064303

C	-4.099631	0.120367	1.995983
H	-4.279885	0.275308	3.057822
C	-2.951168	-0.567459	1.595938
C	-0.188848	1.247853	-1.756743
H	-0.820837	0.483327	-2.226451
N	2.067594	2.828012	1.306996
O	2.737769	3.757592	1.722277
H	-5.893164	1.14271	1.397116
C	-3.507622	-0.610009	-2.218047
H	-2.49024	-0.99429	-2.36527
C	-2.019954	-1.134318	2.654111
H	-1.212048	-1.68206	2.155546
C	-2.774364	-2.129484	3.538248
H	-2.093569	-2.604073	4.251554
H	-3.559518	-1.631901	4.11801
H	-3.254194	-2.917935	2.949013
C	-1.360739	-0.050808	3.507388
H	-0.682881	0.576902	2.922468
H	-2.10972	0.598709	3.975064
H	-0.775278	-0.507199	4.311623
C	-4.493451	-1.710239	-2.619613
H	-4.347349	-2.007236	-3.663053
H	-4.387577	-2.602347	-1.994007
H	-5.527579	-1.362811	-2.514933
C	-3.683763	0.606561	-3.123384
H	-3.55648	0.321356	-4.172265
H	-4.684294	1.041572	-3.026608
H	-2.956131	1.394533	-2.904707
C	-1.117641	2.193119	-0.82624
H	-2.123707	1.809692	-1.025463
C	-0.923503	1.981886	0.69181
H	-1.776458	1.533065	1.196203
H	-0.560818	2.873228	1.213634
C	-1.00229	3.666788	-1.192224
H	-1.191942	3.834172	-2.256935
H	-1.732156	4.251421	-0.625707
H	-0.006661	4.050711	-0.954835
C	0.679112	1.94994	-2.773733
H	1.348344	2.686007	-2.318661
H	0.081978	2.465635	-3.538963
H	1.29917	1.216426	-3.302075

TSMC

	x	y	z
Ru	-0.561892	0.875873	-0.341451
O	-1.80555	2.170852	-1.879328

O	-2.232235	2.54318	0.205623
N	-0.522759	-1.819144	0.639509
N	1.560288	-1.108963	0.740893
C	0.280996	-0.752641	0.331574
C	0.110304	-2.768413	1.538501
H	-0.163745	-3.800847	1.297099
H	-0.184456	-2.57679	2.581992
C	1.581057	-2.469745	1.304732
H	2.184082	-2.501501	2.218565
H	2.031257	-3.167598	0.583182
C	-1.958128	-1.601952	0.585395
C	-2.509686	-1.133433	1.944521
H	-1.96338	-0.230461	2.257504
H	-2.328019	-1.90758	2.704124
C	-4.00808	-0.844155	1.829838
H	-4.392834	-0.533311	2.809466
C	-4.739411	-2.106639	1.365129
H	-4.615717	-2.915805	2.098593
H	-5.81592	-1.905862	1.289876
C	-4.19032	-2.543682	0.00377
H	-4.72363	-3.43894	-0.340712
C	-2.701085	-2.870928	0.150478
H	-2.277944	-3.226688	-0.798736
H	-2.562678	-3.67224	0.892971
C	-4.374934	-1.411616	-1.013543
H	-4.0037	-1.723887	-1.998587
H	-5.443939	-1.188099	-1.131304
C	-3.631651	-0.142226	-0.543333
H	-3.789652	0.647735	-1.284605
C	-2.146312	-0.505802	-0.460225
H	-1.827668	-0.902669	-1.444645
C	-4.214735	0.277064	0.811389
H	-3.748137	1.201827	1.158922
H	-5.287104	0.482773	0.69505
C	2.752059	-0.727822	0.038835
C	3.732774	0.033779	0.701283
C	4.876842	0.40406	-0.012804
H	5.637704	1.004292	0.4815
C	5.063512	0.003372	-1.328704
C	4.121966	-0.815174	-1.94062
H	4.289152	-1.16159	-2.958611
C	2.96118	-1.210055	-1.272418
C	0.57129	1.878366	0.974573
H	1.277397	1.235207	1.504145
N	-2.550226	2.75397	-1.014689
O	-3.494084	3.45822	-1.331605
H	5.955964	0.305835	-1.869418
C	3.632469	0.388703	2.171049

H	2.624344	0.122057	2.510466	C	-2.051414	-1.653797	-0.284274
C	2.012886	-2.176542	-1.964859	C	-2.513477	-1.831339	1.174248
H	1.151458	-2.360093	-1.313659	H	-1.909168	-1.174671	1.816935
C	2.720026	-3.515183	-2.19349	H	-2.334129	-2.86783	1.495851
H	2.030416	-4.250626	-2.619452	C	-4.000248	-1.485404	1.295112
H	3.557061	-3.404781	-2.891852	H	-4.322225	-1.637173	2.33315
H	3.126761	-3.928658	-1.264416	C	-4.81654	-2.386718	0.36467
C	1.461599	-1.643066	-3.286432	H	-4.697828	-3.441994	0.647788
H	0.833846	-0.760769	-3.140428	H	-5.883965	-2.149098	0.459043
H	2.265684	-1.377033	-3.981621	C	-4.357566	-2.177198	-1.08153
H	0.84978	-2.408308	-3.774502	H	-4.950244	-2.810195	-1.754143
C	4.632216	-0.44349	2.977257	C	-2.881348	-2.570076	-1.194731
H	4.536512	-0.240105	4.048605	H	-2.523355	-2.470764	-2.22832
H	4.487474	-1.517162	2.821264	H	-2.748673	-3.623135	-0.901878
H	5.661979	-0.208091	2.685369	C	-4.536186	-0.705111	-1.47245
C	3.84977	1.876908	2.435663	H	-4.232288	-0.551554	-2.516407
H	3.681619	2.110317	3.491635	H	-5.596684	-0.427405	-1.40452
H	4.874828	2.180538	2.19671	C	-3.704298	0.197529	-0.534618
H	3.174693	2.502664	1.843161	H	-3.845756	1.24388	-0.82841
C	1.200183	2.351206	-0.403075	C	-2.245378	-0.206366	-0.711603
H	2.272597	2.185693	-0.231812	H	-1.980471	-0.120028	-1.793445
C	0.901795	1.367201	-1.592568	C	-4.201028	-0.022235	0.899921
H	1.752787	0.741949	-1.84614	H	-3.67422	0.63911	1.590752
H	0.490707	1.88302	-2.465674	H	-5.267462	0.234368	0.953197
C	0.91637	3.802107	-0.75502	C	0.870689	2.009746	0.52074
H	1.236174	4.477796	0.044182	H	1.52941	1.388856	1.122972
H	1.448108	4.083533	-1.667613	N	-2.275427	2.907568	0.27004
H	-0.149565	3.970187	-0.931053	O	-3.064699	3.803965	0.50975
C	0.041424	2.941255	1.897272	C	1.441583	2.140738	-0.938056
H	-0.637457	3.642977	1.414351	H	2.452486	1.721309	-0.847657
H	0.87312	3.508336	2.340766	C	0.729	1.203992	-1.997626
H	-0.501165	2.476525	2.726696	H	1.383269	0.410605	-2.366125

MC-II

	x	y	z				
Ru	-0.541662	0.955497	-0.501485	H	0.307064	1.79079	-2.822245
O	-1.978677	1.999207	1.111362	C	1.484788	3.571318	-1.453108
O	-1.672884	2.82156	-0.873614	H	2.017587	4.236032	-0.766355
N	-0.627929	-1.909172	-0.417232	H	1.993186	3.606248	-2.421568
N	1.475544	-1.407538	-0.109575	H	0.473828	3.966163	-1.590424
C	0.227613	-0.854798	-0.244986	C	0.554009	3.280459	1.261557
C	-0.013643	-3.201222	-0.155746	H	-0.061415	3.982595	0.695072
H	-0.361628	-3.962655	-0.860231	H	1.485017	3.80383	1.523249
H	-0.244665	-3.550608	0.864283	H	0.035727	3.054578	2.196417
C	1.45677	-2.863514	-0.328745	C	2.679573	-0.798213	0.354831
H	2.116212	-3.370238	0.382799	C	2.781505	-0.444966	1.720123
H	1.810576	-3.098678	-1.343558	C	3.996175	0.071104	2.172861
				H	4.094356	0.36507	3.21382
				C	5.083634	0.214705	1.317064
				C	4.968918	-0.150656	-0.015475
				H	5.820753	-0.038397	-0.682684

C	3.769466	-0.660563	-0.522934	H	-5.080927	-2.849386	-1.475468
H	6.021567	0.612766	1.694227	C	-2.993404	-2.623476	-0.976646
C	1.605834	-0.616187	2.667	H	-2.649752	-2.689304	-2.017884
H	0.693101	-0.390274	2.099627	H	-2.904658	-3.629804	-0.537245
C	3.694889	-1.061791	-1.981924	C	-4.584442	-0.741843	-1.491877
H	2.645906	-1.283132	-2.215986	H	-4.299101	-0.746432	-2.552353
C	4.519043	-2.324699	-2.237828	H	-5.634866	-0.422475	-1.444565
H	5.581155	-2.141313	-2.039742	C	-3.696926	0.24693	-0.704967
H	4.207964	-3.15455	-1.595236	H	-3.803778	1.249969	-1.136458
C	4.146183	0.063695	-2.911301	C	-2.251004	-0.240589	-0.867027
H	3.580311	0.985124	-2.740402	H	-2.084027	-0.380485	-1.94829
H	4.009734	-0.224355	-3.958206	C	-4.186604	0.247245	0.749804
C	1.500357	-2.059174	3.161439	H	-3.6414	0.975169	1.352798
H	1.415652	-2.771563	2.335761	H	-5.24579	0.538411	0.769921
H	2.383587	-2.336768	3.74785	C	2.607346	-0.846396	0.447677
C	1.638331	0.344799	3.84958	C	2.674325	-0.332295	1.763108
H	0.694554	0.294213	4.399759	C	3.889003	0.204986	2.192162
H	1.782281	1.381422	3.528761	H	3.963317	0.618173	3.193998
H	2.437121	0.098872	4.558395	C	5.004727	0.22335	1.361194
H	0.620498	-2.186463	3.800833	C	4.919551	-0.286599	0.074094
H	5.207587	0.296015	-2.77417	H	5.792364	-0.265939	-0.57501
H	4.428138	-2.649092	-3.279363	C	3.723386	-0.826994	-0.40772

TSCR

	x	y	z				
Ru	-0.487648	0.889549	-0.6179	O	-2.805068	3.738369	0.654536
O	-1.659592	1.910882	1.057839	H	5.941286	0.640501	1.720822
O	-1.599184	2.796667	-0.922094	C	1.458594	-0.345917	2.674437
N	-0.701248	-1.950873	-0.32056	H	0.581637	-0.134754	2.046679
N	1.408936	-1.485206	0.017325	C	3.666484	-1.381528	-1.816608
C	0.186234	-0.914536	-0.223178	H	2.614929	-1.594809	-2.048472
C	-0.14114	-3.223735	0.106404	C	4.456225	-2.687597	-1.916839
H	-0.487549	-4.047467	-0.524915	H	4.374003	-3.121805	-2.918339
H	-0.424553	-3.45215	1.147234	H	5.519698	-2.513378	-1.717483
C	1.347996	-2.954668	-0.038898	H	4.108637	-3.432764	-1.194329
H	1.959916	-3.398714	0.752884	C	4.169015	-0.377998	-2.852943
H	1.732768	-3.314178	-1.004798	H	3.615534	0.56613	-2.809675
C	-2.116368	-1.619037	-0.220958	H	5.229551	-0.145913	-2.709056
C	-2.556248	-1.564424	1.253066	H	4.05918	-0.782408	-3.863906
H	-1.920514	-0.840367	1.783867	C	1.25515	-1.720199	3.312776
H	-2.406103	-2.547281	1.724842	H	0.345311	-1.732323	3.921819
C	-4.027719	-1.152469	1.345525	H	1.162397	-2.512484	2.564838
H	-4.336301	-1.145146	2.398831	H	2.098481	-1.976558	3.964088
C	-4.89157	-2.144255	0.562111	C	1.493883	0.730866	3.752806
H	-4.803858	-3.153794	0.988223	H	0.526655	0.780875	4.260622
H	-5.9484	-1.856635	0.636939	H	2.250676	0.523539	4.518034
C	-4.451411	-2.154345	-0.904862	H	1.701379	1.722759	3.338276
				C	1.64343	2.130622	-1.024637

H	2.482251	1.44021	-1.125536
C	0.528879	0.895153	-2.208916
H	1.307492	0.196741	-2.545806
H	0.246075	1.608129	-2.996374
C	1.685401	3.345986	-1.918239
H	2.3468	4.108311	-1.488753
H	2.054578	3.102049	-2.917173
H	0.693711	3.79533	-2.025096
C	0.756652	3.602449	0.876834
H	0.185162	4.191591	0.156605
H	1.629725	4.204756	1.166862
H	0.14654	3.469402	1.773195

DSCA

	x	y	z
Ru	-0.419933	0.802101	-0.609479
O	-1.263454	1.826882	1.21878
O	-1.344052	2.835491	-0.696061
N	-0.864465	-2.020771	-0.135806
N	1.259542	-1.655586	0.232121
C	0.095059	-1.051528	-0.135812
C	-0.40035	-3.249441	0.499602
H	-0.804185	-4.137961	0.006515
H	-0.702854	-3.276421	1.559025
C	1.105288	-3.110707	0.348499
H	1.676965	-3.502199	1.195854
H	1.472475	-3.599892	-0.566813
C	-2.243148	-1.54402	-0.054445
C	-2.639462	-1.258335	1.403621
H	-1.922603	-0.547968	1.83761
H	-2.59069	-2.185923	1.993446
C	-4.058611	-0.685255	1.452419
H	-4.339336	-0.50471	2.497846
C	-5.036455	-1.678407	0.81946
H	-5.040435	-2.62505	1.378249
H	-6.057164	-1.276521	0.864382
C	-4.633578	-1.929542	-0.636482
H	-5.341378	-2.627787	-1.101699
C	-3.230209	-2.547999	-0.658631
H	-2.919233	-2.786178	-1.684677
H	-3.230387	-3.48988	-0.087219
C	-4.642545	-0.600783	-1.406049
H	-4.387661	-0.773222	-2.460032
H	-5.655173	-0.174142	-1.386695
C	-3.640572	0.388931	-0.771861
H	-3.656271	1.33215	-1.33192

C	-2.254871	-0.264457	-0.894335
H	-2.175524	-0.602706	-1.936777
C	-4.092306	0.631717	0.673943
H	-3.472659	1.372252	1.180472
H	-5.117205	1.027335	0.666374
C	2.547698	-1.049777	0.304931
C	3.039215	-0.712374	1.582733
C	4.301513	-0.122411	1.66204
H	4.702401	0.157646	2.632205
C	5.051775	0.116024	0.514762
C	4.565289	-0.261269	-0.729484
H	5.173232	-0.100726	-1.617055
C	3.310609	-0.865133	-0.860854
C	1.713114	2.441445	0.391061
H	2.158017	1.575579	0.876811
N	-1.617428	2.877608	0.557286
O	-2.171429	3.822166	1.082629
H	6.029198	0.583668	0.595341
C	2.194998	-0.941746	2.822509
H	1.589214	-1.841229	2.646844
C	2.857217	-1.395079	-2.205816
H	1.784331	-1.613946	-2.13784
C	3.594174	-2.701123	-2.516735
H	3.232311	-3.143069	-3.450587
H	4.669611	-2.521012	-2.627856
H	3.471235	-3.441737	-1.719993
C	3.053195	-0.403293	-3.348315
H	2.537204	0.543496	-3.161609
H	4.112718	-0.18134	-3.516616
H	2.657936	-0.816176	-4.281643
C	3.024148	-1.185084	4.078054
H	2.375805	-1.480197	4.907906
H	3.769938	-1.97265	3.933317
H	3.552289	-0.280078	4.396788
C	1.217907	0.214616	3.0425
H	0.564224	0.017039	3.898238
H	1.761762	1.144947	3.246664
H	0.580903	0.390614	2.168819
C	1.798394	2.491282	-0.956985
H	2.301596	1.655406	-1.440916
C	-0.031689	0.469634	-2.371875
H	-0.153836	-0.475808	-2.931722
H	0.242426	1.29865	-3.051117
C	1.394232	3.622969	-1.836748
H	2.280198	4.107527	-2.264571
H	0.787536	3.280145	-2.68237
H	0.811523	4.380183	-1.30971
C	1.235189	3.527491	1.293335

H	0.64316	4.285399	0.774102
H	2.093082	4.037949	1.748176
H	0.628976	3.132937	2.113314

14-Int'

	x	y	z
Ru	0.5354370	-0.6534860	-0.945284
O	0.0557160	-2.5501290	-0.060502
O	1.3237850	-2.5949080	-1.82573
N	0.6944660	1.7586610	0.560382
N	-1.4082870	1.1225420	0.596312
C	-0.1802220	0.8008560	0.117342
C	0.1099620	2.5335040	1.646907
H	0.4625820	3.5685480	1.647901
H	0.3435690	2.0843860	2.627995
C	-1.3715630	2.4088800	1.309134
H	-2.0312160	2.3956940	2.181238
H	-1.6973410	3.2228460	0.644188
C	2.0927630	1.3452140	0.444042
C	2.4472350	0.3093120	1.529775
H	1.7114920	-0.5134660	1.501343
H	2.3665440	0.7656290	2.527702
C	3.8563330	-0.2341020	1.294362
H	4.1027650	-0.9633910	2.076197
C	4.8517910	0.9293790	1.338759
H	4.8364950	1.4016230	2.330594
H	5.8719690	0.5570880	1.178957
C	4.4956370	1.9544720	0.257034
H	5.2127930	2.7843590	0.286491
C	3.0841610	2.5047600	0.517317
H	2.8160270	3.2626710	-0.230657
H	3.0477870	2.9897030	1.505451
C	4.5579270	1.2705580	-1.115254
H	4.3365040	1.9937960	-1.910873
H	5.5769780	0.9001920	-1.294174
C	3.5507080	0.1071090	-1.171458
H	3.5956610	-0.3774960	-2.154719
C	2.1569250	0.6919010	-0.949361
H	1.9754950	1.4825460	-1.685079
C	3.8994820	-0.9100040	-0.079402
H	3.1916310	-1.7515870	-0.108417
H	4.8952100	-1.3347630	-0.261074
C	-2.5961320	0.3449440	0.428036
C	-2.7530290	-0.8231090	1.205256
C	-3.9309600	-1.5540880	1.043622
H	-4.0746890	-2.4637770	1.618626
C	-4.9240920	-1.1382250	0.163628

C	-4.7494930	0.0147270	-0.587397
H	-5.5264170	0.3321290	-1.279056
C	-3.5793830	0.7710590	-0.480304
N	0.737964	-3.275027	-0.922945
O	0.791464	-4.477384	-0.826483
H	-5.835623	-1.720753	0.061813
C	-1.703195	-1.250482	2.214372
H	-0.720044	-1.063839	1.763901
C	-3.414618	2.025184	-1.313801
H	-2.355683	2.315236	-1.27637
C	-4.248326	3.170621	-0.735493
H	-4.093114	4.096518	-1.298908
H	-5.316039	2.928188	-0.782404
H	-4.007974	3.366855	0.314281
C	-3.774926	1.801497	-2.780904
H	-3.230693	0.954661	-3.209021
H	-4.844496	1.603449	-2.907097
H	-3.540714	2.691324	-3.373224
C	-1.797194	-0.410403	3.490019
H	-1.007948	-0.690773	4.195803

Ru-8

14-Int

	x	y	z
Ru	-0.8181800	-0.2015650	-0.9758660
O	-0.0446390	-2.3941640	-1.0879260
O	1.1421030	-0.7241140	-1.9083820
N	-1.5557310	0.4289020	1.7096890
N	0.5369960	1.0446800	1.3816350
C	-0.5396810	0.4458640	0.7901100
C	-1.2721860	1.3157310	2.8275810
H	-1.6540570	0.9176390	3.7729000
H	-1.7264810	2.3068480	2.6662570
C	0.2507140	1.3824490	2.7807460
H	0.6532000	2.3681160	3.0345710
H	0.7041320	0.6446690	3.4567750
C	-2.8817130	0.1330870	1.1796150
C	-3.6214530	1.4190090	0.7774400
H	-2.9817180	2.0147870	0.1153370
H	-3.8218220	2.0249830	1.6734600
C	-4.9350580	1.0640640	0.0792160
H	-5.4546860	1.9868220	-0.2102450
C	-5.8116620	0.2599360	1.0431720
H	-6.0526440	0.8655370	1.9278370
H	-6.7652420	0.0024000	0.5632700

C	-5.0749870	-1.0175020	1.4579590	H	2.637812	3.611034	-2.138322
H	-5.7011680	-1.5958580	2.1493650	H	1.288858	2.511965	-2.298183
C	-3.7615160	-0.6453680	2.1645640	C	2.024106	4.359379	0.573745
H	-3.2270080	-1.5458660	2.4945630	H	1.962932	4.072763	1.632347
H	-3.9783930	-0.0441630	3.0615440	H	1.272172	5.148001	0.439783
C	-4.7919650	-1.8527360	0.2021110	C	2.247493	-2.729582	1.527785
H	-4.2964800	-2.7936680	0.4736680	H	1.874104	-2.703025	0.500605
H	-5.7424330	-2.1184670	-0.2821140	H	3.316027	-2.973666	1.458088
C	-3.8981720	-1.0548560	-0.7670600	C	2.599553	-1.237828	3.575499
H	-3.6965690	-1.6633040	-1.6598100	H	1.951446	-1.841316	4.224471
C	-2.5897440	-0.7522370	-0.0399960	H	2.491297	-0.2042	3.928467
H	-2.1968520	-1.7101620	0.3529930	C	0.730618	4.596312	-2.191404
C	-4.6253660	0.2308560	-1.1686500	H	1.105708	5.549339	-1.803334
H	-4.0041400	0.8139560	-1.8602910	H	0.667297	4.692719	-3.279159
H	-5.5572610	-0.0122370	-1.6972000	H	-0.291764	4.472695	-1.812613
C	-1.2381290	1.4598530	-1.6138540	C	3.40374	4.926004	0.286636
C	0.9501160	-1.9779090	-1.7558110	H	3.606525	5.800924	0.910503
C	1.9032790	-2.9537290	-2.4411000	H	4.191898	4.19332	0.484805
C	1.5923340	-4.3872990	-2.0247570	H	3.503788	5.243037	-0.757573
H	0.5960730	-4.6877300	-2.3603450	C	1.518846	-3.822759	2.287653
H	1.6062940	-4.5064300	-0.9371500	H	1.639716	-4.790752	1.793433
H	2.3244730	-5.0761510	-2.4602100	H	1.886045	-3.933437	3.314016
C	1.6990160	-2.7935080	-3.9536110	H	0.444289	-3.611132	2.338398
H	0.6676840	-3.0236040	-4.2432050	C	4.04344	-1.66778	3.77113
H	2.3582860	-3.4788770	-4.4976360	H	4.732779	-1.052988	3.184427
H	1.9248070	-1.7718060	-4.2707670	H	4.337273	-1.573486	4.820156
C	3.3487430	-2.5874880	-2.0964960	H	4.203007	-2.712465	3.483573
H	4.0404280	-3.2193060	-2.6650960	C	1.877798	0.903729	0.896062
H	3.5584870	-2.7354840	-1.0321090				
H	3.5524260	-1.5402690	-2.3344100				
C	-1.6214180	1.5391360	-3.0605840				
H	-2.5757720	2.0664840	-3.1981950				
H	-0.8686940	2.0964510	-3.6358970				
H	-1.7229940	0.5508850	-3.5319270				
H	-1.1800040	2.4454150	-1.1231810				
C	2.6192800	-0.2474410	1.2349330				
C	3.9075460	-0.3694030	0.7064370				
H	4.491685	-1.258659	0.928536				
C	4.439945	0.60638	-0.125907				
C	3.692727	1.731413	-0.443713				
H	4.111255	2.481922	-1.108864				
C	2.401484	1.908632	0.063236				
H	5.437856	0.481785	-0.538125				
C	2.057074	-1.332931	2.130698	CA			
H	0.970402	-1.183178	2.19457				
C	1.603944	3.146099	-0.280278		x	y	z
H	0.561472	2.940985	-0.00867	Ru	-0.6856130	-0.0018240	0.6217790
C	1.613858	3.428458	-1.787229	O	-1.7380860	1.9612330	0.0045790
				O	-2.3147540	0.9506790	1.8873190

	x	y	z
Ru	-0.6856130	-0.0018240	0.6217790
O	-1.7380860	1.9612330	0.0045790
O	-2.3147540	0.9506790	1.8873190

N	-0.1207510	-1.5626830	-1.7239610	C	-0.8621950	-1.7778570	2.9783720
N	1.8051810	-0.7767840	-1.0365690	H	-0.1447990	-1.7057780	3.8115220
C	0.4562550	-0.7494910	-0.7793170	H	-1.7227500	-1.1370490	3.1954370
C	0.8594230	-2.3447420	-2.4603000	H	-1.2004070	-2.8250100	2.9746230
H	0.5753890	-2.4751220	-3.5093760	H	0.6386830	-2.1377020	1.4761500
H	0.9803500	-3.3450640	-2.0127030	C	0.7129850	1.2778570	2.8003210
C	2.1078040	-1.4979360	-2.2782460	H	1.4746130	0.5055120	2.9230340
H	3.0272680	-2.0835230	-2.1798930	C	0.7473030	2.0256440	1.6808100
H	2.2437020	-0.7860890	-3.1080230	H	0.0462820	2.8440070	1.5326630
C	-1.4877510	-1.9974290	-1.4675170	H	1.5366790	1.9136020	0.9496670
C	-1.5245450	-3.3239210	-0.6903330	C	-0.2060480	1.4974320	3.9487840
H	-0.8954680	-3.2420120	0.2042720	H	-0.7781030	0.5989460	4.1977340
H	-1.1040610	-4.1290880	-1.3111060	H	0.3725890	1.7642920	4.8413330
C	-2.9676220	-3.6566400	-0.3060880	H	-0.9227470	2.2950520	3.7427180
H	-2.9855080	-4.5993750	0.2568420	C	2.7140790	0.2138970	-0.5598230
C	-3.8010540	-3.8034020	-1.5822200	C	2.7040520	1.4979810	-1.1432970
H	-3.4126690	-4.6297700	-2.1938120	C	3.5756030	2.4564140	-0.6135550
H	-4.8398410	-4.0543030	-1.3292980	H	3.5591620	3.4671040	-1.0121310
C	-3.7595170	-2.4922310	-2.3743580	C	4.4234580	2.1506970	0.4444290
H	-4.3539330	-2.5968050	-3.2912050	C	4.4264700	0.8735060	0.9929840
C	-2.3057240	-2.1704970	-2.7541510	H	5.0884480	0.6486170	1.8254310
H	-2.2516210	-1.2450810	-3.3431830	C	3.5819770	-0.1249720	0.4968770
H	-1.8941440	-2.9812590	-3.3757900	H	5.0797570	2.9156720	0.8504010
C	-4.3442900	-1.3706530	-1.5057650	C	1.7363980	1.8648730	-2.2497140
H	-4.3558840	-0.4241120	-2.0628000	H	1.0448680	1.0237170	-2.3807170
H	-5.3878400	-1.6077370	-1.2535890	C	3.6166550	-1.5332100	1.0505060
C	-3.5060370	-1.2103350	-0.2238710	H	2.6839710	-2.0190640	0.7362350
H	-3.9228090	-0.4059650	0.3948240	C	3.6360430	-1.5761820	2.5817140
C	-2.0866730	-0.8502940	-0.6539990	H	4.5346120	-1.0823510	2.9742710
H	-2.1508890	0.0171950	-1.3342230	H	2.7901870	-0.9807450	2.9493440
C	-3.5331460	-2.5246430	0.5584930	C	4.7568090	-2.3567360	0.4146950
H	-2.9483530	-2.4198310	1.4799210	H	4.6739910	-2.2748580	-0.6771810
H	-4.5630060	-2.7640720	0.8569290	H	4.5860880	-3.4164450	0.6437720
C	-0.2021600	-1.4441500	1.6808050	C	0.8529490	3.0540730	-1.8441560
C	-2.4792220	1.8789630	1.0356540	H	0.4054300	2.8271870	-0.8702640
C	-3.5705740	2.9291360	1.2242500	H	1.4672850	3.9539580	-1.7007030
C	-2.8870130	4.2966190	1.3267130	C	2.4244740	2.0507300	-3.6180530
H	-2.2703670	4.4881210	0.4431720	H	1.6371580	2.0737080	-4.3823100
H	-2.2410640	4.3543400	2.2108630	H	3.0184100	1.1525180	-3.8365290
H	-3.6333400	5.0942970	1.4101530	C	3.5399900	-2.9829790	3.1463280
C	-4.4671670	2.9025340	-0.0174900	H	4.4245620	-3.5832030	2.9090420
H	-3.8794580	3.0781760	-0.9228880	H	3.4398570	-2.9705640	4.2350340
H	-5.2416750	3.6743420	0.0531120	H	2.6686560	-3.5114540	2.7411670
H	-4.9702110	1.9344240	-0.1238690	C	6.1618040	-1.9668220	0.8397680
C	-4.3892030	2.6468840	2.4775540	H	6.9094710	-2.5928570	0.3453580
H	-5.1676280	3.4076310	2.6037280	H	6.3869960	-0.9263510	0.5855120
H	-3.7608740	2.6469130	3.3728250	H	6.3074420	-2.0817490	1.9195660
H	-4.8724200	1.6671900	2.4219560	C	-0.2672650	3.3333150	-2.8294760

H	-0.9471090	4.0977880	-2.4433190
H	0.1032550	3.6775080	-3.8016100
H	-0.8652320	2.4294340	-2.9967310
C	3.3060260	3.2779280	-3.7777070
H	4.1854830	3.2390190	-3.1284380
H	3.6684890	3.3633550	-4.8059220
H	2.7636750	4.2018230	-3.5484640

TSCA

	x	y	z
Ru	-0.751725	-0.045635	-0.574848
O	-2.107658	-1.896628	0.021555
O	-2.402344	-0.81225	-1.882975
N	-0.024626	1.569429	1.692226
N	1.856889	0.748582	0.915059
C	0.489638	0.712852	0.751741
C	0.99874	2.390105	2.31897
H	0.782435	2.578605	3.375159
H	1.088074	3.363854	1.809737
C	2.231266	1.531351	2.102486
H	3.143784	2.108266	1.924617
H	2.413877	0.855904	2.953646
C	-1.398653	2.007667	1.473573
C	-1.453603	3.234415	0.547241
H	-0.873677	3.021238	-0.360061
H	-0.986862	4.099389	1.041743
C	-2.91004	3.551473	0.202835
H	-2.945085	4.420738	-0.467643
C	-3.663722	3.868751	1.498743
H	-3.226072	4.753391	1.98213
H	-4.711413	4.111988	1.277311
C	-3.598786	2.661954	2.441674
H	-4.135398	2.892646	3.370966
C	-2.131985	2.347399	2.775569
H	-2.063409	1.494779	3.46459
H	-1.668149	3.213174	3.274375
C	-4.255405	1.460217	1.750259
H	-4.249629	0.58581	2.414649
H	-5.308134	1.692299	1.533992
C	-3.501248	1.129182	0.450979
H	-3.973431	0.267753	-0.035993
C	-2.059623	0.793732	0.820329
H	-2.067025	-0.012	1.571838
C	-3.545494	2.33781	-0.486276
H	-3.010003	2.09763	-1.414692
H	-4.583437	2.568643	-0.762904
C	0.051312	1.068836	-1.890018

C	-2.738783	-1.729993	-1.061595
C	-3.886896	-2.672135	-1.419278
C	-3.251629	-3.922467	-2.041447
H	-2.566201	-4.405187	-1.33718
H	-2.690257	-3.670192	-2.948544
H	-4.024522	-4.648557	-2.317012
C	-4.644316	-3.058839	-0.1505
H	-3.973482	-3.516245	0.580305
H	-5.44669	-3.767316	-0.384788
H	-5.098959	-2.181234	0.322933
C	-4.825803	-2.014476	-2.425701
H	-5.641335	-2.697595	-2.688467
H	-4.294914	-1.738923	-3.339969
H	-5.269179	-1.100268	-2.016992
C	-0.719789	1.710438	-3.005431
H	-0.124002	1.867842	-3.914448
H	-1.629966	1.160248	-3.260553
H	-1.020993	2.709344	-2.660628
H	1.03334	1.548383	-1.745826
C	0.674071	-0.739583	-2.474651
H	1.689191	-0.338582	-2.495217
C	0.551199	-1.826629	-1.557329
H	-0.196438	-2.593784	-1.752305
H	1.363906	-2.088345	-0.893835
C	0.046033	-0.954617	-3.835171
H	0.192302	-0.112719	-4.513453
H	0.50536	-1.831847	-4.301406
H	-1.026487	-1.143517	-3.739661
C	2.717855	-0.317677	0.509004
C	2.601478	-1.575097	1.139414
C	3.406857	-2.615593	0.662076
H	3.30118	-3.607587	1.092472
C	4.309256	-2.410868	-0.374753
C	4.444955	-1.150346	-0.944051
H	5.161494	-0.998788	-1.747202
C	3.665223	-0.074545	-0.506748
H	4.913282	-3.237645	-0.738459
C	1.620432	-1.824327	2.267228
H	1.004364	-0.925765	2.386302
C	3.867887	1.316894	-1.069422
H	2.964952	1.893141	-0.825405
C	4.016766	1.34452	-2.595071
H	4.907551	0.782901	-2.904534
H	3.167854	0.811471	-3.042837
C	5.036565	2.034941	-0.356797
H	4.887875	1.946933	0.726951
H	4.970302	3.107925	-0.578064
C	0.63332	-2.948088	1.921428

H	0.147377	-2.689424	0.973173
H	1.173693	-3.889313	1.747468
C	2.31912	-2.017919	3.630057
H	1.547465	-1.935001	4.405941
H	2.997166	-1.169939	3.799634
C	4.077667	2.750504	-3.166581
H	4.972865	3.289201	-2.839021
H	4.089786	2.737134	-4.259585
H	3.208414	3.341025	-2.853556
C	6.425721	1.53057	-0.707525
H	7.191268	2.071308	-0.144751
H	6.539954	0.467014	-0.475334
H	6.65278	1.663407	-1.77084
C	-0.440711	-3.149771	2.975023
H	-1.197162	-3.860358	2.632263
H	-0.035126	-3.52499	3.921464
H	-0.958784	-2.206253	3.184788
C	3.083918	-3.315185	3.832273
H	3.961654	-3.381909	3.183195
H	3.439354	-3.398307	4.863177
H	2.456657	-4.19163	3.634674

MC-I

	x	y	z
Ru	-0.769848	0.071802	0.539412
O	-2.317005	1.922241	-0.141229
O	-2.425428	0.846098	1.795274
N	0.046563	-1.667429	-1.587075
N	1.90972	-0.81759	-0.800849
C	0.539896	-0.758321	-0.688268
C	1.072905	-2.563267	-2.094064
H	0.89785	-2.837607	-3.138899
H	1.11556	-3.490679	-1.499234
C	2.315205	-1.712121	-1.896998
H	3.205571	-2.287801	-1.62637
H	2.550129	-1.120002	-2.795491
C	-1.352864	-2.029764	-1.4036
C	-1.511436	-3.108853	-0.315633
H	-0.989513	-2.777964	0.593556
H	-1.031873	-4.042768	-0.644811
C	-2.995706	-3.344962	-0.032846
H	-3.100167	-4.109757	0.7481
C	-3.67059	-3.82523	-1.321937
H	-3.230649	-4.778977	-1.645022
H	-4.737894	-4.010798	-1.143467
C	-3.50501	-2.765809	-2.417087

H	-3.987844	-3.111922	-3.339879
C	-2.012346	-2.531538	-2.69129
H	-1.873925	-1.786905	-3.486787
H	-1.53996	-3.467512	-3.028945
C	-4.159444	-1.46207	-1.947797
H	-4.079079	-0.69206	-2.726064
H	-5.231459	-1.629399	-1.771536
C	-3.483728	-0.968448	-0.655338
H	-3.959073	-0.034174	-0.340118
C	-2.011214	-0.719619	-0.96274
H	-1.911644	0.015403	-1.773538
C	-3.631272	-2.031586	0.436799
H	-3.148523	-1.677595	1.359234
H	-4.692859	-2.189915	0.671807
C	0.153505	-0.798944	2.061987
C	-2.860037	1.73297	0.976648
C	-4.061431	2.566918	1.426311
C	-3.589034	3.466116	2.57397
H	-2.786114	4.137129	2.247522
H	-3.213672	2.86741	3.409187
H	-4.414347	4.087354	2.939648
C	-4.584696	3.415486	0.274118
H	-3.811175	4.086513	-0.107252
H	-5.438655	4.018989	0.602168
H	-4.91038	2.788523	-0.561611
C	-5.156251	1.626734	1.935747
H	-6.012357	2.201488	2.30694
H	-4.781548	0.994426	2.744535
H	-5.5203	0.968879	1.137773
C	-0.6908	-1.408271	3.155761
H	-0.138288	-1.494664	4.102656
H	-1.603131	-0.8352	3.344146
H	-0.985959	-2.425735	2.872891
H	1.043767	-1.408314	1.860235
C	0.614849	0.737446	2.283626
H	1.706451	0.667341	2.239425
C	0.247337	1.689928	1.124754
H	-0.431694	2.495439	1.423209
H	1.1011	2.060815	0.562017
C	0.147681	1.300464	3.619211
H	0.455159	0.665051	4.455749
H	0.575154	2.294653	3.77769
H	-0.941521	1.39284	3.635942
C	2.763112	0.284673	-0.47696
C	2.655783	1.478952	-1.222336
C	3.43766	2.566282	-0.816834
H	3.337	3.514558	-1.337539
C	4.315139	2.462689	0.255699

C	4.450226	1.257444	0.934221	N	-1.90876	1.094138	-0.341533
H	5.147449	1.183798	1.764773	C	-0.540072	1.004342	-0.26298
C	3.687929	0.140349	0.576907	C	-1.091177	3.264869	-0.590602
H	4.902474	3.324656	0.560249	H	-0.927025	4.012364	-1.373209
C	1.727045	1.608727	-2.414395	H	-1.126539	3.788922	0.378437
H	1.104225	0.707984	-2.462251	C	-2.33571	2.420734	-0.818262
C	3.873861	-1.189181	1.277539	H	-3.214093	2.770328	-0.263948
H	2.984673	-1.793241	1.051895	H	-2.608957	2.367004	-1.883966
C	3.951194	-1.065463	2.80424	C	1.339121	2.47789	-0.233477
H	4.825988	-0.470699	3.097248	C	2.010483	1.12263	-0.479306
H	3.080438	-0.496978	3.1556	C	-0.197456	-0.259731	2.168354
C	5.074154	-1.964016	0.688865	C	2.861772	-1.985096	0.10589
H	4.967422	-1.991223	-0.403369	C	4.053767	-2.942771	0.154574
H	5.005335	-3.008674	1.018357	H	-1.074709	0.393596	2.25783
C	0.741346	2.776238	-2.262765	C	-0.677833	-1.703476	1.603916
H	0.185037	2.633756	-1.329673	H	-1.766397	-1.591865	1.555163
H	1.285656	3.72447	-2.153824	C	-0.255666	-1.99202	0.14777
C	2.500968	1.637205	-3.75093	H	0.416748	-2.850715	0.045058
H	1.772108	1.47293	-4.554739	H	-1.081063	-2.03095	-0.561518
H	3.174653	0.76977	-3.784122	C	2.003328	3.549832	-1.102356
C	3.988367	-2.408207	3.513334	H	1.5222	4.528065	-0.944546
H	4.899987	-2.970137	3.284575	H	1.880208	3.289407	-2.162102
H	3.946664	-2.287027	4.598958	C	1.476935	2.889097	1.245093
H	3.136272	-3.032398	3.219033	H	0.9909	3.862743	1.407426
C	6.445741	-1.413147	1.03863	H	0.950719	2.154888	1.871162
H	7.236119	-2.008212	0.573382	C	3.477312	1.199808	-0.07281
H	6.56748	-0.381731	0.693206	C	2.9562	2.9652	1.62618
H	6.626846	-1.423973	2.118873	H	3.044899	3.250656	2.682755
C	-0.253179	2.876983	-3.40583	C	3.490926	3.629689	-0.729473
H	-1.024339	3.620196	-3.188497	H	3.976807	4.386073	-1.359009
H	0.221192	3.157432	-4.352822	C	3.604166	1.59442	1.401605
H	-0.764076	1.919469	-3.561942	C	4.157095	2.267299	-0.949882
C	3.296799	2.895455	-4.053909	H	4.09186	1.976512	-2.006367
H	4.131903	3.03086	-3.360721	C	3.635453	4.01922	0.745901
H	3.718483	2.853081	-5.062031	H	3.186647	5.006197	0.924926
H	2.672719	3.794531	-4.001888	H	4.699008	4.100791	1.005912
				H	3.959198	0.232727	-0.249316
				H	3.119384	0.831992	2.02819
				H	4.662071	1.625227	1.696905
				H	5.225688	2.333971	-0.701008
				H	1.924312	0.87481	-1.547233
				C	3.589254	-4.228193	0.846679
				H	4.410333	-4.951679	0.903499
				H	3.242732	-4.01965	1.862845
				H	2.766716	-4.700768	0.297133
				C	4.552055	-3.249941	-1.251893
				H	4.868782	-2.337856	-1.766173
				H	5.405186	-3.936739	-1.21257
TSMC							
	x	y	z				
Ru	0.767416	-0.30162	0.442454				
O	2.36385	-1.615811	-0.987525				
O	2.392316	-1.58352	1.230327				
N	-0.055752	2.243047	-0.589153				

H	3.767226	-3.707623	-1.859812
C	5.166436	-2.295148	0.983507
H	4.806342	-2.03498	1.9824
H	6.016356	-2.979571	1.0846
H	5.535318	-1.378227	0.50908
C	0.61681	-0.271538	3.440216
H	0.919381	0.751173	3.694798
H	0.041192	-0.649917	4.296975
H	1.52367	-0.875213	3.345643
C	-0.279717	-2.847087	2.526931
H	-0.629709	-2.679023	3.550555
H	-0.714792	-3.785951	2.172665
H	0.807432	-2.963037	2.546689
C	-2.763278	-0.014181	-0.641707
C	-3.769435	-0.366828	0.28058
C	-4.60147	-1.44449	-0.044528
H	-5.404339	-1.721074	0.632476
C	-4.439015	-2.14419	-1.232713
C	-3.478494	-1.742403	-2.152256
H	-3.393983	-2.265687	-3.100753
C	-2.633804	-0.657862	-1.893192
H	-5.089346	-2.984328	-1.460488
C	-4.045391	0.462342	1.521181
H	-3.317649	1.285522	1.526913
C	-1.674426	-0.174067	-2.96874
H	-1.319016	0.824095	-2.680915
C	-2.422827	0.008334	-4.30094
H	-2.765065	-0.963149	-4.680409
H	-3.338791	0.582525	-4.106797
C	-0.395918	-1.021733	-3.116625
H	0.180545	-0.962152	-2.188959
H	0.235843	-0.536252	-3.871194
C	-5.442231	1.098065	1.394119
H	-5.50757	1.581316	0.410215
H	-6.206799	0.309517	1.374439
C	-3.848916	-0.252076	2.873345
H	-4.012501	0.499674	3.655702
H	-2.796061	-0.535755	2.976742
C	-1.601361	0.705905	-5.371069
H	-0.757686	0.094902	-5.705303
H	-2.206977	0.931434	-6.253086
H	-1.19044	1.652944	-5.00142
C	-0.591556	-2.480601	-3.485913
H	0.378046	-2.976101	-3.586805
H	-1.15031	-3.024021	-2.716098
H	-1.128355	-2.607736	-4.434461
C	-5.770719	2.107239	2.480174
H	-6.712381	2.622151	2.271699

H	-5.870847	1.638207	3.463734
H	-4.988423	2.871267	2.561954
C	-4.716708	-1.46541	3.162801
H	-4.450171	-2.318684	2.531932
H	-4.593855	-1.783932	4.201684
H	-5.78354	-1.261164	3.013199

MC-II

	x	y	z
Ru	0.7164850	-0.5708690	-0.6646780
O	2.3102530	-2.0620220	-1.1123140
O	2.5747820	-1.0269620	0.8243880
N	-0.1031350	2.1772710	-0.7405280
N	-1.8922950	1.0811340	-0.1241050
C	-0.5549000	0.9273230	-0.4002750
C	-1.0583780	3.2360000	-0.4588100
H	-1.0601090	3.9971900	-1.2452330
H	-0.8265680	3.7369380	0.4957770
C	-2.3570210	2.4509410	-0.3965910
H	-3.0420930	2.7887750	0.3885150
H	-2.8961880	2.4848440	-1.3546630
C	1.3343060	2.3838320	-0.7333690
C	1.8253360	2.7915960	0.6687980
H	1.5099160	2.0203820	1.3872020
H	1.3530560	3.7390110	0.9679010
C	3.3491900	2.9350090	0.6660510
H	3.6848550	3.2476300	1.6632060
C	3.7673290	3.9812160	-0.3706240
H	3.3434530	4.9637500	-0.1196470
H	4.8593650	4.0941480	-0.3657830
C	3.2907230	3.5443520	-1.7591830
H	3.6021560	4.2842480	-2.5076620
C	1.7619380	3.4491790	-1.7518880
H	1.3778810	3.1737860	-2.7433680
H	1.3252120	4.4259670	-1.4914840
C	3.8934230	2.1771440	-2.1062440
H	3.5751200	1.8687180	-3.1110550
H	4.9898540	2.2476920	-2.1257150
C	3.4591050	1.1265140	-1.0612110
H	3.8929750	0.1548680	-1.3231190
C	1.9393350	1.0402680	-1.1133350
H	1.6299480	0.7972940	-2.1587590
C	3.9688780	1.5830220	0.3112860
H	3.7234240	0.8369130	1.0704880
H	5.0639820	1.6753220	0.2761360
C	-0.1939190	-1.9146670	0.5687950

C	2.9498540	-1.8857770	-0.0204900
C	4.1984600	-2.7290340	0.2478730
C	4.0462960	-4.1054650	-0.3963100
H	3.8795020	-4.0201780	-1.4723500
H	3.1961900	-4.6522930	0.0277970
H	4.9462530	-4.7073050	-0.2268660
C	5.3903000	-1.9977570	-0.3816800
H	5.2543950	-1.8767100	-1.4616240
H	6.3133090	-2.5655310	-0.2184910
H	5.5236220	-1.0048030	0.0618820
C	4.4194260	-2.8642270	1.7521420
H	5.3290410	-3.4411870	1.9532760
H	3.5804460	-3.3799430	2.2313890
H	4.5156000	-1.8835900	2.2245570
C	-0.8236720	-2.3445960	-0.8044430
C	-0.5590730	-1.3194510	-1.9819210
H	-0.0508980	-1.8080420	-2.8217960
H	-1.4703890	-0.8093560	-2.3062760
C	0.5357250	-2.9688370	1.3574360
H	1.0498220	-2.5167450	2.2099720
H	-0.1836760	-3.6994800	1.7560060
H	1.2733230	-3.5258670	0.7744460
H	-0.9548150	-1.4636870	1.1995410
C	-0.4512400	-3.7537930	-1.2394970
H	-0.6832800	-4.4938690	-0.4670330
H	-1.0041720	-4.0253040	-2.1442600
H	0.6179570	-3.8169490	-1.4647600
H	-1.9028940	-2.2612600	-0.6177610
C	-2.7595920	0.1889180	0.5755020
C	-3.8554920	-0.3868430	-0.0969530
C	-4.7093800	-1.2216130	0.6341520
H	-5.5412490	-1.7048480	0.1289570
C	-4.5042950	-1.4506800	1.9879520
C	-3.4282580	-0.8580210	2.6384620
H	-3.2684460	-1.0454770	3.6972090
C	-2.5341600	-0.0334210	1.9524740
H	-5.1828690	-2.0967550	2.5381930
C	-4.1097180	-0.1228340	-1.5651020
H	-3.2004040	0.3431860	-1.9689720
C	-1.3370320	0.5689490	2.6618390
H	-0.5251390	0.6324760	1.9257220
C	-0.7905690	-0.3177930	3.7894710
H	-1.4032570	-0.2168680	4.6964170
H	-0.8804280	-1.3701350	3.4889900
C	-1.6169260	2.0093550	3.1297330
H	-1.7752660	2.6406950	2.2456060
H	-0.7076710	2.3999130	3.6055310
C	-4.3185350	-1.4206880	-2.3570020

H	-3.4685770	-2.0865250	-2.1561190
H	-5.2027700	-1.9549020	-1.9862400
C	-5.2468060	0.8990160	-1.7850410
H	-5.1935940	1.2478850	-2.8245790
H	-5.0459490	1.7836140	-1.1671980
C	0.6652590	-0.0145300	4.1039400
H	0.8081940	1.0243260	4.4218760
H	1.0439100	-0.6525210	4.9074360
H	1.2964600	-0.1795400	3.2220190
C	-2.7997370	2.1586400	4.0714840
H	-2.9267660	3.1975210	4.3876990
H	-3.7328720	1.8388560	3.5957440
H	-2.6766950	1.5578960	4.9790680
C	-4.4464350	-1.1989220	-3.8538250
H	-4.4899580	-2.1475680	-4.3950980
H	-5.3507590	-0.6369520	-4.1100990
H	-3.5902470	-0.6365980	-4.2441590
C	-6.6527960	0.4023380	-1.4946870
H	-6.7758020	0.1199590	-0.4448540
H	-7.3912430	1.1793620	-1.7099890
H	-6.9134880	-0.4690810	-2.1053150

TSCR

	x	y	z
Ru	0.6432200	-0.4059480	-0.8557670
O	2.2598680	-1.8467740	-1.4993970
O	2.2789850	-1.1410540	0.5930000
N	-0.0588960	2.3072220	-0.2579590
N	-1.8445530	1.1266730	0.1977690
C	-0.5358790	1.0228480	-0.2060750
C	-0.9523250	3.2787480	0.3510100
H	-0.9825110	4.2114220	-0.2210430
H	-0.6344530	3.5244640	1.3778340
C	-2.2741740	2.5281640	0.3208420
H	-2.8838540	2.6674240	1.2206680
H	-2.8823030	2.8175430	-0.5484900
C	1.3872080	2.4654140	-0.2929770
C	1.9680400	2.4491560	1.1330710
H	1.6668930	1.5116480	1.6241060
H	1.5501490	3.2821620	1.7183170
C	3.4937830	2.5555810	1.0769410
H	3.8946800	2.5706820	2.0988320
C	3.8997490	3.8370450	0.3449320
H	3.5292720	4.7219530	0.8816560
H	4.9944670	3.9171520	0.3140340
C	3.3332000	3.8112130	-1.0776860
H	3.6367090	4.7201580	-1.6132650

C	1.8030920	3.7627150	-0.9957590	H	-3.1021470	-1.9146830	3.3892230
H	1.3525310	3.7893170	-1.9972070	C	-2.4078510	-0.4997390	1.9309230
H	1.4324830	4.6426720	-0.4460390	H	-5.1115720	-2.5686870	2.1099770
C	3.8639850	2.5765590	-1.8202990	C	-4.1512900	0.3830300	-1.3928030
H	3.4873840	2.5671020	-2.8518340	H	-3.2407840	0.9111240	-1.7097400
H	4.9605510	2.6281530	-1.8802470	C	-1.1402430	-0.1563260	2.6917900
C	3.4341150	1.2895840	-1.0844590	H	-0.3562690	0.0213920	1.9421620
H	3.8165970	0.4158550	-1.6273010	C	-0.6182910	-1.3121430	3.5576390
C	1.9020890	1.2660280	-1.0880290	H	-1.2000270	-1.3946360	4.4868790
H	1.5860010	1.4208470	-2.1344350	H	-0.7825360	-2.2589050	3.0255060
C	4.0389600	1.3408020	0.3251630	C	-1.2896020	1.1498080	3.4936570
H	3.8088120	0.4286970	0.8797960	H	-1.4125150	1.9831630	2.7905950
H	5.1337670	1.4166130	0.2460990	H	-0.3419020	1.3466960	4.0111770
C	-0.4369090	-2.3503550	0.0456760	C	-4.4524890	-0.6515590	-2.4858890
C	2.7917790	-1.8300720	-0.3433940	H	-3.6187860	-1.3658260	-2.5259450
C	4.0699510	-2.6332910	-0.0941060	H	-5.3333940	-1.2478250	-2.2155370
C	3.8963000	-4.0514680	-0.6417320	C	-5.2548250	1.4575540	-1.2767230
H	3.5786850	-4.0287050	-1.6876520	H	-5.2337500	2.0672810	-2.1893340
H	3.1512690	-4.6145920	-0.0697740	H	-4.9927720	2.1413160	-0.4595650
H	4.8423540	-4.6003010	-0.5776350	C	0.8622560	-1.1751850	3.8752020
C	5.2085070	-1.9450520	-0.8572170	H	1.0770350	-0.2615070	4.4404440
H	4.9789030	-1.8796690	-1.9248870	H	1.2200270	-2.0158980	4.4770500
H	6.1377220	-2.5135760	-0.7386470	H	1.4571630	-1.1428880	2.9543740
H	5.3873010	-0.9320230	-0.4814110	C	-2.4367860	1.1574190	4.4898410
C	4.3940180	-2.6751760	1.3954310	H	-2.4708900	2.0958690	5.0498740
H	5.3108130	-3.2499490	1.5680400	H	-3.4027570	1.0331930	3.9885110
H	3.5862620	-3.1440780	1.9670970	H	-2.3466310	0.3477070	5.2220880
H	4.5368040	-1.6692570	1.8002580	C	-4.6541820	-0.0359800	-3.8596390
C	-0.9906390	-2.2382560	-1.2744980	H	-4.7575570	-0.8047750	-4.6297730
C	-0.4969390	-0.6273040	-2.3520400	H	-5.5527170	0.5884020	-3.9019820
H	-0.0688010	-1.1164620	-3.2383000	H	-3.8035370	0.5969240	-4.1379230
H	-1.4893780	-0.1995690	-2.5534810	C	-6.6649950	0.9387940	-1.0523160
C	0.4393750	-3.4880040	0.4481920	H	-6.7517330	0.3921850	-0.1085650
H	1.0659670	-3.2259200	1.3059770	H	-7.3807070	1.7644830	-1.0154900
H	-0.1848970	-4.3420240	0.7499870	H	-6.9879740	0.2671970	-1.8553450
H	1.0866350	-3.8277070	-0.3624040				
H	-1.0395560	-1.9347910	0.8426960				
C	-0.6907370	-3.3331490	-2.2702170				
H	-1.0095360	-4.3060870	-1.8764470				
H	-1.2069580	-3.1662480	-3.2188790				
H	0.3831300	-3.3914980	-2.4734360				
H	-2.0269400	-1.8958630	-1.2529810				
C	-2.6972170	0.0912860	0.6800420				
C	-3.8431970	-0.2645970	-0.0594530				
C	-4.6916570	-1.2425780	0.4725890				
H	-5.5635470	-1.5571250	-0.0947220				
C	-4.4334410	-1.8206530	1.7083800				
C	-3.3035780	-1.4496370	2.4277780				

N	0.0716310	-2.4060630	0.0645600	C	1.1021870	2.3920740	-1.3896830
N	1.7977080	-1.1402920	0.5167880	C	0.2352150	-0.2678380	-2.4762360
C	0.5405340	-1.1219920	-0.0133390	H	0.1831170	0.4126570	-3.3458860
C	0.9154990	-3.2544350	0.8973360	H	0.6914640	-1.2392700	-2.7433990
H	0.9905490	-4.2682040	0.4931240	C	-0.4520200	3.8312670	-0.0275420
H	0.5149530	-3.3263460	1.9215090	H	-1.2085420	3.5818670	0.7231060
C	2.2350360	-2.5000610	0.8564170	H	0.0688790	4.7280750	0.3324470
H	2.7849250	-2.5095450	1.8039020	H	-0.9565140	4.0954540	-0.9597350
H	2.8998110	-2.8924540	0.0730470	H	0.9110410	2.2598630	0.6864280
C	-1.3819970	-2.5282970	0.0252570	C	0.7677050	3.0141420	-2.7075350
C	-1.9825860	-2.2230110	1.4098840	H	1.1459380	4.0417820	-2.7692890
H	-1.6575960	-1.2187300	1.7216420	H	1.2065740	2.4572930	-3.5392140
H	-1.6050870	-2.9426290	2.1517670	H	-0.3160460	3.0519170	-2.8642030
C	-3.5090650	-2.2887850	1.3426210	H	1.9264850	1.6838210	-1.3553410
H	-3.9263550	-2.0979890	2.3399800	C	2.6534990	-0.0233130	0.7359640
C	-3.9524610	-3.6694030	0.8530160	C	3.7529350	0.1905320	-0.1170980
H	-3.6245180	-4.4506610	1.5533830	C	4.6107300	1.2560600	0.1789390
H	-5.0488940	-3.7158190	0.8130290	H	5.4490810	1.4654650	-0.4801440
C	-3.3630460	-3.9278120	-0.5362130	C	4.3981300	2.0574610	1.2932430
H	-3.6929520	-4.9091980	-0.9012490	C	3.2977360	1.8372680	2.1141960
C	-1.8330350	-3.9201640	-0.4270310	H	3.1278790	2.4861390	2.9693130
H	-1.3655730	-4.1530770	-1.3932030	C	2.3917510	0.8087220	1.8454280
H	-1.5090290	-4.6917490	0.2897690	H	5.0846280	2.8700880	1.5146990
C	-3.8392340	-2.8343380	-1.5044690	C	3.9808160	-0.6830470	-1.3327220
H	-3.4551860	-3.0305580	-2.5140320	H	3.0645270	-1.2726870	-1.4792370
H	-4.9366270	-2.8581840	-1.5685440	C	1.1361120	0.6221280	2.6802850
C	-3.3653620	-1.4480740	-1.0155840	H	0.3270280	0.3655550	1.9780520
H	-3.7094660	-0.6761360	-1.7166130	C	0.6733480	1.9016180	3.3923250
C	-1.8289950	-1.4959370	-1.0137280	H	1.2791530	2.0807880	4.2922220
H	-1.5491760	-1.9214960	-1.9863210	H	0.8563000	2.7674610	2.7425180
C	-3.9900760	-1.2154380	0.3669450	C	1.2586190	-0.5593420	3.6616600
H	-3.7293620	-0.2295580	0.7573880	H	1.2806000	-1.4961700	3.0923090
H	-5.0860060	-1.2597300	0.2796880	H	0.3382240	-0.6073540	4.2573270
C	0.5240900	2.7246280	-0.2145400	C	4.1560390	0.1487100	-2.6109750
C	-2.6406630	1.8053550	-0.5465940	H	3.2877940	0.8132830	-2.7083020
C	-3.9241840	2.6244430	-0.3864920	H	5.0250510	0.8132220	-2.5183890
C	-3.7637830	3.9871960	-1.0657610	C	5.1258110	-1.6975820	-1.1228660
H	-3.3922610	3.8712210	-2.0878820	H	5.0539020	-2.4591540	-1.9101680
H	-3.0734330	4.6357040	-0.5183000	H	4.9531320	-2.2316860	-0.1797790
H	-4.7312710	4.4994590	-1.1066060	C	-0.8039040	1.8602430	3.7498350
C	-5.0470910	1.8623310	-1.1036630	H	-1.0359300	1.0461010	4.4449380
H	-4.8003430	1.7123910	-2.1585350	H	-1.1250300	2.7906430	4.2272650
H	-5.9805820	2.4328050	-1.0442940	H	-1.4155590	1.7111320	2.8520160
H	-5.2257550	0.8825190	-0.6508820	C	2.4674710	-0.4916990	4.5798040
C	-4.2707640	2.8056350	1.0870490	H	2.4797700	-1.3277190	5.2843800
H	-5.1930040	3.3881570	1.1898180	H	3.4040190	-0.5195800	4.0122920
H	-3.4750520	3.3339420	1.6229910	H	2.4784910	0.4301400	5.1716240
H	-4.4150820	1.8431050	1.5863230	C	4.2872410	-0.6944300	-3.8673880

H	4.2982490	-0.0711480	-4.7653940
H	5.2089170	-1.2857420	-3.8717730
H	3.4491720	-1.3942780	-3.9627290
C	6.5314660	-1.1209550	-1.1102210
H	6.6768170	-0.4215790	-0.2815940
H	7.2750990	-1.9145410	-0.9978550
H	6.7652650	-0.5884520	-2.0386270

14-Int'

	x	y	z
Ru	0.7337700	0.1981910	-1.0279870
O	2.2079960	-1.0566020	-2.2734910
O	1.1609370	-1.8452500	-0.4953410
N	0.0459410	2.1011490	0.9672820
N	-1.6773820	0.7527230	0.7613110
C	-0.4293210	1.0085120	0.2828990
C	-0.7432020	2.3512310	2.1645060
H	-0.7879970	3.4157240	2.4116130
H	-0.3377360	1.8072120	3.0361810
C	-2.0882260	1.7860740	1.7239070
H	-2.6834650	1.3568760	2.5349570
H	-2.6929650	2.5565790	1.2222920
C	1.4913840	2.2635670	0.8307260
C	2.2461120	1.2115590	1.6703720
H	1.8664560	0.2049330	1.4222320
H	2.0432930	1.3671230	2.7408490
C	3.7458740	1.2932620	1.3847680
H	4.2747910	0.5454230	1.9903970
C	4.2449800	2.6975920	1.7388090
H	4.0979790	2.8919670	2.8101780
H	5.3231840	2.7735860	1.5461710
C	3.4919440	3.7378720	0.9024910
H	3.8543590	4.7427550	1.1538170
C	1.9892830	3.6559480	1.2131650
H	1.4309880	4.4120090	0.6451720
H	1.8165460	3.8534460	2.2828970
C	3.7453280	3.4579960	-0.5851330
H	3.2400130	4.2105540	-1.2044960
H	4.8210850	3.5405240	-0.7952730
C	3.2363850	2.0515250	-0.9519930
H	3.4163260	1.8534700	-2.0157230
C	1.7358230	2.0135100	-0.6694370
H	1.2424090	2.8230070	-1.2176440
C	3.9782660	1.0140610	-0.1030460
H	3.6233430	0.0055580	-0.3569440
H	5.0529850	1.0353340	-0.3289340
C	2.0261280	-1.9879120	-1.4469340

C	2.8725670	-3.2523260	-1.4804130
C	3.3344490	-3.5327530	-2.9074310
H	3.8673280	-2.6753560	-3.3235440
H	2.4862260	-3.7468330	-3.5648240
H	4.0007590	-4.4017670	-2.9233910
C	4.0912860	-2.9725890	-0.5870520
H	4.6871750	-2.1427710	-0.9809280
H	4.7331970	-3.8587110	-0.5397610
H	3.7847570	-2.7218480	0.4351360
C	2.0912390	-4.4381800	-0.9209320
H	2.7082230	-5.3426010	-0.9533600
H	1.1828770	-4.6296020	-1.5010990
H	1.7937040	-4.2616020	0.1155530
C	-0.3354580	0.6627300	-2.4091510
H	0.0295400	0.4275860	-3.4221040
H	-1.3643070	1.0448680	-2.3530150
C	-2.4763360	-0.3816580	0.4198350
C	-3.5811670	-0.2200380	-0.4369580
C	-4.3454840	-1.3511300	-0.7420340
H	-5.1936770	-1.2558940	-1.4146190
C	-4.0245810	-2.5942470	-0.2150330
C	-2.9256340	-2.7334450	0.6241960
H	-2.6796010	-3.7131090	1.0232170
C	-2.1264700	-1.6382560	0.9617140
H	-4.6297860	-3.4617950	-0.4639380
C	-3.9349510	1.1321320	-1.0163990
H	-3.0403560	1.7656820	-0.9250420
C	-0.9425210	-1.7940420	1.8964500
H	-0.1482370	-1.1340730	1.5245030
C	-0.3487080	-3.2052330	1.8894260
H	-1.0413550	-3.9200950	2.3540660
H	-0.2303180	-3.5195890	0.8469230
C	-1.2861360	-1.3140250	3.3208060
H	-1.661769	-0.285982	3.263925
H	-0.356913	-1.251433	3.90303
C	-4.258284	1.054659	-2.514041
H	-3.451873	0.502423	-3.012643
H	-5.164239	0.457685	-2.677936
C	-5.048335	1.832177	-0.206237
H	-5.073217	2.891481	-0.493906
H	-4.768652	1.820646	0.854839
C	0.99668	-3.275253	2.590183
H	0.923767	-3.038329	3.657471
H	1.437723	-4.273932	2.513289
H	1.699897	-2.56685	2.136057
C	-2.298468	-2.17773	4.054138
H	-2.57294	-1.739744	5.017732
H	-3.217494	-2.295694	3.469187

H	-1.908782	-3.180831	4.25508
C	-4.425919	2.41783	-3.161781
H	-4.565724	2.332195	-4.242558
H	-5.292264	2.957379	-2.764494
H	-3.54386	3.046473	-2.992763
C	-6.43719	1.235125	-0.355041
H	-6.459801	0.185197	-0.046499
H	-7.161269	1.772501	0.263282
H	-6.79561	1.284273	-1.388778

Ru-9

14-Int

	x	y	z
Ru	-0.6371510	0.6714810	-1.0778660
O	-0.2801660	-0.8535820	-2.8120690
O	1.3185980	0.4241930	-2.1027660
N	-1.3113210	-0.3208330	1.4934990
N	0.8789350	-0.0807630	1.4001470
C	-0.2777810	0.0194970	0.6832300
C	-0.9155140	-0.5464800	2.8746760
H	-1.2630180	-1.5245150	3.2326360
H	-1.3467180	0.2185600	3.5344670
C	0.6160090	-0.4493180	2.8014930
H	1.0281070	0.3140670	3.4729640
H	1.1090430	-1.3984060	3.0457680
C	-2.6603610	-0.0772070	1.0002340
C	-3.2033570	1.2652000	1.5160880
H	-2.4834860	2.0596510	1.2861950
H	-3.3064280	1.2233630	2.6104890
C	-4.5541660	1.5623870	0.8652030
H	-4.9338350	2.5231540	1.2361510
C	-5.5395850	0.4461140	1.2221830
H	-5.6915970	0.4119540	2.3097850
H	-6.5195710	0.6464090	0.7694390
C	-4.9969740	-0.8948920	0.7179040
H	-5.7014660	-1.6968280	0.9722500
C	-3.6458750	-1.1852550	1.3907000
H	-3.2459730	-2.1559740	1.0661660
H	-3.7757310	-1.2316860	2.4832590
C	-4.8374740	-0.8174070	-0.8066570
H	-4.4873950	-1.7787440	-1.2038480
H	-5.8157780	-0.6183160	-1.2661100
C	-3.8349630	0.2939150	-1.1740580
H	-3.7224580	0.3357870	-2.2659990
C	-2.4987810	-0.0691590	-0.5290920
H	-2.2685910	-1.1142030	-0.8218300

C	-4.3631450	1.6330060	-0.6536180
H	-3.6601540	2.4384480	-0.9034640
H	-5.3171180	1.8755460	-1.1408420
C	2.1377460	-0.4253400	0.8025560
C	3.1223780	0.5637940	0.6485040
C	4.3444210	0.1810150	0.0858330
H	5.1311880	0.9209120	-0.0325100
C	4.5680500	-1.1258870	-0.3229290
C	3.5838430	-2.0906720	-0.1478090
H	3.7782040	-3.1152240	-0.4531570
C	2.3519820	-1.7689180	0.4281560
C	-0.7030020	2.3723920	-0.4172360
C	-1.0941260	3.4619660	-1.3658160
H	-1.9238260	4.0603800	-0.9639640
H	-0.2573940	4.1547450	-1.5314190
H	-1.4097590	3.0839340	-2.3482140
H	-0.4064640	2.7399610	0.5807190
N	0.9492960	-0.5034940	-2.9231360
O	1.7164760	-1.0023850	-3.7191450
H	5.5197500	-1.3990550	-0.7701280
C	2.8807800	1.9979170	1.0615000
H	1.9424850	2.0152610	1.6332590
C	1.3078630	-2.8473950	0.6548290
H	0.5691370	-2.4631130	1.3685220
C	1.9178200	-4.0945390	1.3104020
H	2.6383770	-4.5680350	0.6318130
H	2.5053220	-3.7765690	2.1821200
C	0.4887680	-3.1717720	-0.6080860
H	0.0263660	-2.2451000	-0.9647910
H	-0.3487650	-3.8165900	-0.3082090
C	3.9840800	2.5068050	1.9990950
H	4.0579950	1.8155950	2.8491460
H	4.9598970	2.4548700	1.4987170
C	2.6420320	2.9212310	-0.1503750
H	2.2501920	3.8756770	0.2287420
H	1.8383330	2.4837080	-0.7531670
C	0.8784480	-5.1165620	1.7367400
H	0.3661730	-5.5614720	0.8780710
H	1.3292470	-5.9343270	2.3053920
H	0.1092650	-4.6581150	2.3710400
C	1.2521760	-3.8224670	-1.7473550
H	0.5955590	-3.9847170	-2.6058680
H	2.075366	-3.192608	-2.096178
H	1.670119	-4.794948	-1.460811
C	3.750664	3.920213	2.503533
H	4.489603	4.203305	3.258081
H	3.813111	4.656371	1.695692
H	2.758463	4.021984	2.958733

C	3.839893	3.184906	-1.045848
H	4.15924	2.278166	-1.566988
H	3.590985	3.923405	-1.813117
H	4.699906	3.575479	-0.488502

CA

	x	y	z
Ru	0.78051	-0.215312	-0.930624
O	1.64198	1.630777	-2.146805
O	1.87218	-0.404709	-2.864676
N	0.908077	0.123347	1.926378
N	-1.218237	0.057132	1.406574
C	0.042156	0.075568	0.869091
C	0.25296	-0.108433	3.205899
H	0.658856	0.533771	3.994398
H	0.382712	-1.155224	3.523061
C	-1.199589	0.200178	2.869402
H	-1.914996	-0.486834	3.335568
H	-1.48612	1.224099	3.156019
C	2.310524	-0.177149	1.657898
C	2.634538	-1.657593	1.917783
H	1.923577	-2.293524	1.377958
H	2.517741	-1.879917	2.988916
C	4.067382	-1.957403	1.473647
H	4.286027	-3.018982	1.649488
C	5.031099	-1.090792	2.289455
H	4.946696	-1.336136	3.357347
H	6.068351	-1.298196	1.995153
C	4.709495	0.388849	2.056169
H	5.395655	1.01218	2.643722
C	3.267459	0.676098	2.502877
H	3.020858	1.737357	2.366142
H	3.155009	0.446904	3.574284
C	4.878001	0.701266	0.564242
H	4.688368	1.765007	0.371698
H	5.915569	0.501403	0.262368
C	3.905632	-0.158746	-0.264452
H	4.032631	0.072698	-1.328566
C	2.491049	0.195612	0.185512
H	2.388397	1.294099	0.131117
C	4.209775	-1.637623	-0.018422
H	3.526414	-2.258736	-0.610415
H	5.228493	-1.873315	-0.35415
C	-2.398331	0.444677	0.702536
C	-3.383974	-0.529857	0.449895
C	-4.53976	-0.125489	-0.227555
H	-5.321736	-0.852507	-0.430008

C	-4.709375	1.192751	-0.631342
C	-3.749257	2.148233	-0.32107
H	-3.918416	3.185189	-0.598461
C	-2.581394	1.804605	0.368922
C	0.569228	-2.023439	-0.586185
C	1.092908	-3.108726	-1.465194
H	1.815179	-3.721469	-0.905048
H	0.288468	-3.802893	-1.752552
H	1.583825	-2.738732	-2.369841
H	0.048783	-2.443212	0.297665
N	2.122654	0.849142	-3.041633
O	2.764631	1.250795	-3.994701
H	-5.610179	1.484323	-1.164232
C	-3.233072	-1.959507	0.933631
H	-2.36482	-1.983512	1.60599
C	-1.59441	2.878554	0.795547
H	-0.937667	2.441541	1.558353
C	-2.323773	4.048269	1.474405
H	-2.981276	4.553766	0.755516
H	-2.993067	3.639584	2.243299
C	-0.640317	3.337818	-0.322185
H	-0.090606	2.464809	-0.689401
H	0.127029	3.976793	0.132851
C	-4.454375	-2.380464	1.765778
H	-4.614473	-1.622599	2.543878
H	-5.361242	-2.352678	1.147544
C	-2.899069	-2.965839	-0.185197
H	-2.678819	-3.930382	0.290171
H	-1.956472	-2.658015	-0.653494
C	-1.385052	5.065475	2.099239
H	-0.798546	5.599152	1.345235
H	-1.935677	5.815933	2.672677
H	-0.674907	4.583957	2.781787
C	-1.277369	4.070288	-1.489139
H	-0.522524	4.317543	-2.240549
H	-2.042116	3.465203	-1.98891
H	-1.755315	5.007258	-1.179464
C	-4.318946	-3.751276	2.405477
H	-5.147096	-3.95465	3.089445
H	-4.310946	-4.553469	1.660993
H	-3.389111	-3.832165	2.980497
C	-3.957102	-3.162752	-1.257107
H	-4.12284	-2.25143	-1.841763
H	-3.656664	-3.945849	-1.959266
H	-4.923429	-3.460888	-0.834265
C	-1.446078	-0.687516	-2.550988
H	-2.168564	-0.953379	-1.782117
C	-1.021628	0.593402	-2.592183

H	-1.437231	1.33494	-1.919625
H	-0.388086	0.952754	-3.398588
C	-1.117852	-1.723256	-3.567656
H	-0.202706	-1.47606	-4.112333
H	-1.00307	-2.716434	-3.123868
H	-1.939081	-1.802304	-4.290922

TSCA

	x	y	z
Ru	-0.909316	-0.034256	0.926439
O	-1.944064	1.913335	1.840697
O	-2.151815	-0.037817	2.765879
N	-0.811234	-0.122879	-1.949806
N	1.276435	-0.115722	-1.276827
C	-0.019326	-0.011343	-0.838311
C	-0.071811	-0.571722	-3.121104
H	-0.423048	-0.084957	-4.036303
H	-0.178039	-1.660239	-3.253217
C	1.350366	-0.190234	-2.744683
H	2.102106	-0.922664	-3.060048
H	1.641811	0.789353	-3.155257
C	-2.213335	-0.45173	-1.704536
C	-2.41638	-1.972873	-1.596632
H	-1.698801	-2.376993	-0.871165
H	-2.207936	-2.448476	-2.56647
C	-3.854656	-2.270137	-1.168603
H	-3.990238	-3.356446	-1.080862
C	-4.806584	-1.715277	-2.233301
H	-4.625239	-2.21217	-3.196587
H	-5.847892	-1.926061	-1.956525
C	-4.601282	-0.202411	-2.368062
H	-5.280927	0.19399	-3.133177
C	-3.152061	0.087087	-2.789286
H	-2.989693	1.166399	-2.909502
H	-2.941505	-0.388496	-3.760229
C	-4.90149	0.459504	-1.017993
H	-4.790932	1.548919	-1.093379
H	-5.9452	0.262587	-0.735952
C	-3.946666	-0.086798	0.058734
H	-4.170858	0.393912	1.017749
C	-2.519802	0.237996	-0.373947
H	-2.439256	1.324702	-0.546208
C	-4.133514	-1.601085	0.181977
H	-3.455371	-1.992853	0.952412
H	-5.156259	-1.832698	0.507979
C	2.419702	0.399605	-0.590177
C	3.427786	-0.498884	-0.182854

C	4.553629	0.033419	0.456592
H	5.362193	-0.628748	0.751182
C	4.67404	1.398029	0.681834
C	3.695663	2.26978	0.22035
H	3.824919	3.339668	0.358161
C	2.558097	1.798231	-0.443319
C	-0.195593	-1.77321	1.187969
C	-0.923254	-2.853986	1.931102
H	-1.498014	-3.428769	1.192052
H	-0.25403	-3.571598	2.423164
H	-1.631944	-2.464553	2.66753
H	0.609554	-2.176344	0.554242
N	-2.449192	1.222556	2.786826
O	-3.163275	1.695206	3.65234
H	5.553446	1.788479	1.186487
C	3.384671	-1.969813	-0.554442
H	2.436636	-2.140859	-1.083185
C	1.549012	2.780213	-1.011687
H	0.908866	2.234202	-1.717285
C	2.254905	3.873418	-1.829781
H	2.893945	4.483218	-1.178344
H	2.940674	3.388434	-2.537509
C	0.58088	3.350234	0.042083
H	0.038889	2.516792	0.498401
H	-0.185666	3.931499	-0.485724
C	4.516632	-2.258219	-1.558447
H	4.460896	-1.508117	-2.358489
H	5.488539	-2.085927	-1.076245
C	3.375242	-2.975481	0.614179
H	3.237238	-3.97026	0.172145
H	2.474343	-2.81551	1.218287
C	1.296772	4.77902	-2.583522
H	0.691955	5.389508	-1.906351
H	1.833993	5.463936	-3.245039
H	0.603766	4.197212	-3.202497
C	1.197685	4.201562	1.136568
H	0.421188	4.556147	1.820029
H	1.919763	3.637107	1.736867
H	1.717163	5.083303	0.741954
C	4.477158	-3.651253	-2.161308
H	5.218415	-3.760094	-2.957408
H	4.684363	-4.428786	-1.419718
H	3.493642	-3.86845	-2.594871
C	4.58569	-3.007388	1.53264
H	4.650091	-2.112928	2.15883
H	4.531736	-3.866874	2.206395
H	5.526649	-3.093357	0.976978
C	0.913349	-0.698069	2.458529

H	1.808032	-1.111381	1.988365
C	0.869027	0.726905	2.347048
H	1.595069	1.255839	1.742779
H	0.357622	1.300277	3.118638
C	0.591597	-1.263883	3.82444
H	-0.412263	-0.970981	4.142787
H	0.665773	-2.351704	3.864836
H	1.303988	-0.861624	4.55102

MC-I

	x	y	z
Ru	0.908727	-0.422512	-0.821208
O	2.13232	1.096855	-2.381157
O	2.142516	-1.07333	-2.534365
N	0.765701	0.408875	1.915857
N	-1.321388	0.244248	1.258001
C	-0.020983	0.171644	0.824527
C	0.02258	0.353623	3.165734
H	0.383165	1.092991	3.887669
H	0.10845	-0.643021	3.62751
C	-1.392127	0.629774	2.679045
H	-2.160397	0.049171	3.201596
H	-1.658079	1.694888	2.764533
C	2.172053	0.050939	1.767435
C	2.394064	-1.448382	2.041474
H	1.695463	-2.032032	1.425001
H	2.163832	-1.671295	3.093879
C	3.841072	-1.823843	1.72145
H	3.9898	-2.894333	1.914456
C	4.773563	-1.001432	2.616732
H	4.588113	-1.238773	3.673496
H	5.820052	-1.260896	2.410689
C	4.549479	0.493049	2.360168
H	5.216858	1.08082	3.00299
C	3.093886	0.859775	2.684748
H	2.916114	1.932125	2.528207
H	2.877102	0.639571	3.741878
C	4.852657	0.793924	0.8883
H	4.728466	1.864799	0.682484
H	5.900096	0.545389	0.66864
C	3.915736	-0.023197	-0.021198
H	4.144217	0.205759	-1.066969
C	2.484125	0.387313	0.305445
H	2.358185	1.471039	0.162774
C	4.120935	-1.51783	0.246874
H	3.451966	-2.10426	-0.399317
H	5.147267	-1.810433	-0.01015

C	-2.416549	0.635656	0.421678
C	-3.499086	-0.251904	0.256261
C	-4.557704	0.160404	-0.561782
H	-5.416217	-0.492166	-0.6906
C	-4.543533	1.400957	-1.184954
C	-3.495756	2.283699	-0.956185
H	-3.519829	3.27149	-1.40794
C	-2.418549	1.93461	-0.135013
C	-0.020855	-2.15952	-0.67555
C	0.75654	-3.409008	-1.014589
H	1.325336	-3.738942	-0.137429
H	0.097537	-4.243302	-1.293108
H	1.466504	-3.254512	-1.832243
H	-0.68908	-2.319197	0.179637
N	2.536571	0.071895	-3.009099
O	3.257014	0.123908	-3.991056
H	-5.37174	1.69649	-1.823071
C	-3.598138	-1.552643	1.032466
H	-2.709301	-1.614178	1.675482
C	-1.344324	2.964165	0.176431
H	-0.753448	2.593712	1.024375
C	-1.99147	4.277364	0.650155
H	-2.559218	4.737536	-0.168809
H	-2.736875	4.036844	1.420061
C	-0.319712	3.181566	-0.954092
H	0.229271	2.249302	-1.115703
H	0.431721	3.891343	-0.585652
C	-4.822687	-1.483625	1.964153
H	-4.78056	-0.532877	2.511766
H	-5.740876	-1.425878	1.364066
C	-3.575964	-2.846244	0.193526
H	-3.61651	-3.68478	0.899765
H	-2.598859	-2.940452	-0.292098
C	-0.995819	5.283011	1.201345
H	-0.327111	5.667918	0.425813
H	-1.504437	6.142996	1.645261
H	-0.367035	4.83345	1.979232
C	-0.868637	3.670539	-2.281701
H	-0.053818	3.820848	-2.994871
H	-1.556865	2.94569	-2.729776
H	-1.406255	4.622376	-2.189534
C	-4.924623	-2.63425	2.949926
H	-5.729966	-2.468088	3.670329
H	-5.128671	-3.587927	2.453874
H	-3.99444	-2.754784	3.517876
C	-4.663769	-3.023315	-0.852119
H	-4.553345	-2.316521	-1.680397
H	-4.622839	-4.028813	-1.279969

H	-5.669085	-2.891808	-0.4346
C	-0.869783	-1.478996	-1.880657
H	-1.881856	-1.433229	-1.466361
C	-0.50664	-0.00747	-2.17073
H	-1.298203	0.705467	-1.945875
H	-0.07811	0.154558	-3.16545
C	-0.82912	-2.314087	-3.153379
H	0.179975	-2.335075	-3.574124
H	-1.14838	-3.344628	-2.967538
H	-1.498242	-1.886026	-3.904856

TSMC

	x	y	z
Ru	0.860828	-0.839526	-0.610567
O	2.218438	-1.52263	-2.436257
O	2.420075	-2.675231	-0.61961
N	0.791768	1.265912	1.333123
N	-1.308356	0.700737	0.975445
C	-0.003032	0.458077	0.568942
C	0.10318	1.88327	2.452786
H	0.369697	2.942569	2.553375
H	0.367212	1.38436	3.396648
C	-1.361399	1.670645	2.085522
H	-1.960321	1.27284	2.914039
H	-1.843774	2.599299	1.749192
C	2.221029	1.010818	1.309337
C	2.633432	0.032295	2.424192
H	2.0413	-0.889948	2.321782
H	2.397672	0.468118	3.405922
C	4.129041	-0.274473	2.324225
H	4.414955	-0.952428	3.138461
C	4.927125	1.02775	2.433503
H	4.753503	1.50484	3.408319
H	6.001474	0.811699	2.370931
C	4.516644	1.977305	1.30326
H	5.099551	2.904892	1.368559
C	3.027366	2.307683	1.448393
H	2.698117	3.017704	0.676073
H	2.839378	2.776708	2.426841
C	4.771357	1.303095	-0.050184
H	4.501317	1.983437	-0.868651
H	5.841729	1.081555	-0.159019
C	3.959592	-0.005926	-0.157822
H	4.167093	-0.465039	-1.129812
C	2.482294	0.383213	-0.057927
H	2.270985	1.142952	-0.836148
C	4.403106	-0.938911	0.974803

H	3.88241	-1.897333	0.905741
H	5.476181	-1.148193	0.87217
C	-2.422013	0.757993	0.071342
C	-3.520174	-0.104376	0.26588
C	-4.599857	0.003194	-0.619358
H	-5.470681	-0.628505	-0.473514
C	-4.598004	0.934623	-1.648146
C	-3.539686	1.825922	-1.776025
H	-3.574714	2.592599	-2.545456
C	-2.441705	1.775338	-0.912235
C	-0.424861	-2.189841	0.11953
C	-0.025587	-3.561363	0.589254
H	0.442683	-3.493671	1.576425
H	-0.915423	-4.198053	0.703115
H	0.677721	-4.064536	-0.073215
H	-1.158721	-1.753443	0.801537
N	2.852961	-2.434812	-1.799503
O	3.80144	-3.032371	-2.279692
H	-5.444363	0.996136	-2.326629
C	-3.610325	-1.023752	1.466628
H	-2.653138	-0.942385	1.998459
C	-1.365008	2.845433	-1.000245
H	-0.746459	2.781551	-0.098114
C	-2.005106	4.244414	-0.972755
H	-2.577886	4.421728	-1.892372
H	-2.746169	4.267917	-0.162666
C	-0.368965	2.673587	-2.163383
H	0.189699	1.745157	-2.004454
H	0.375854	3.475266	-2.076372
C	-4.692655	-0.50085	2.425989
H	-4.496468	0.561882	2.620744
H	-5.669988	-0.523786	1.924643
C	-3.781371	-2.525851	1.150726
H	-3.501201	-3.076347	2.058623
H	-3.036705	-2.81888	0.401538
C	-0.998507	5.364269	-0.773324
H	-0.333795	5.480483	-1.634518
H	-1.495859	6.325238	-0.617514
H	-0.365011	5.173688	0.102409
C	-0.960274	2.679545	-3.561613
H	-0.171083	2.616945	-4.315562
H	-1.629484	1.827869	-3.723225
H	-1.532814	3.592115	-3.767266
C	-4.761737	-1.260245	3.73893
H	-5.478912	-0.80541	4.427311
H	-5.065975	-2.301882	3.593693
H	-3.786493	-1.274674	4.239548
C	-5.152187	-3.007033	0.699288

H	-5.406932	-2.66354	-0.306671
H	-5.180378	-4.099873	0.674497
H	-5.950694	-2.680765	1.374566
C	-0.932589	-2.049824	-1.381073
H	-2.010629	-1.892796	-1.239173
C	-0.490755	-0.706212	-2.06132
H	-1.287825	0.032287	-2.107497
H	-0.015197	-0.863447	-3.034604
C	-0.663134	-3.267847	-2.248865
H	0.408931	-3.423369	-2.39712
H	-1.077245	-4.177505	-1.803357
H	-1.115235	-3.139665	-3.235808

MC-II

	x	y	z
Ru	0.750991	-1.246811	-0.15168
O	2.341177	-1.44092	1.637986
O	1.879176	-3.096145	0.312549
N	0.769878	1.289237	-1.488189
N	-1.285216	1.035178	-0.772479
C	-0.030385	0.479283	-0.732821
C	0.149329	2.55042	-1.859236
H	0.347365	2.801075	-2.906289
H	0.533685	3.377072	-1.239527
C	-1.322253	2.262016	-1.589281
H	-1.824834	3.066587	-1.041064
H	-1.889813	2.082269	-2.51382
C	2.206551	1.109595	-1.366189
C	2.763259	1.987355	-0.230189
H	2.218551	1.746798	0.694508
H	2.580736	3.048039	-0.458029
C	4.261459	1.730212	-0.058564
H	4.650027	2.375949	0.73915
C	4.98863	2.035986	-1.370822
H	4.863481	3.093496	-1.642556
H	6.065704	1.863117	-1.24908
C	4.43611	1.139013	-2.482714
H	4.96477	1.344909	-3.422079
C	2.944955	1.438734	-2.670568
H	2.520922	0.83947	-3.487492
H	2.803846	2.498452	-2.93408
C	4.628498	-0.332845	-2.097546
H	4.261306	-0.985839	-2.900314
H	5.698565	-0.548442	-1.975202
C	3.88461	-0.638321	-0.778652
H	4.034908	-1.692795	-0.521152
C	2.407129	-0.361207	-1.029222

H	2.072105	-0.970369	-1.903827
C	4.465366	0.262736	0.318378
H	3.991796	0.044049	1.278267
H	5.537155	0.050354	0.428161
C	-0.557991	-1.655667	1.361047
H	-1.17752	-0.806754	1.648502
N	2.575281	-2.648903	1.308598
O	3.389776	-3.349321	1.88307
C	-1.236793	-2.451878	0.192115
H	-2.247219	-2.024591	0.168917
C	-0.647265	-2.126767	-1.241717
H	-1.347366	-1.567579	-1.869026
H	-0.300525	-3.03951	-1.74054
C	-1.285987	-3.955911	0.411868
H	-1.738472	-4.212283	1.374628
H	-1.877123	-4.430623	-0.377523
H	-0.281381	-4.38797	0.384808
C	-0.15419	-2.431401	2.585356
H	0.42312	-3.332679	2.367715
H	-1.049162	-2.744978	3.141897
H	0.437498	-1.803749	3.256078
C	-2.302579	0.878599	0.218171
C	-2.078382	1.427698	1.501331
C	-3.098111	1.296456	2.448748
H	-2.951681	1.700525	3.446787
C	-4.304744	0.686964	2.127512
C	-4.531542	0.225446	0.837809
H	-5.506407	-0.175801	0.578261
C	-3.538709	0.307847	-0.145641
H	-5.087151	0.606669	2.877096
C	-0.814678	2.195562	1.848595
H	-0.280629	2.405431	0.911283
C	-3.843334	-0.070952	-1.58194
H	-2.918839	0.084481	-2.15468
C	-4.888173	0.911147	-2.142269
H	-5.820073	0.821596	-1.567165
H	-4.533467	1.932856	-1.950991
C	-4.22641	-1.542073	-1.837468
H	-3.412516	-2.188097	-1.490945
H	-4.244175	-1.67525	-2.92662
C	-1.166878	3.568014	2.447059
H	-1.908962	4.047234	1.7947
H	-1.669929	3.445324	3.414962
C	0.189349	1.409581	2.716105
H	1.072414	2.046084	2.856617
H	0.55022	0.545623	2.145088
C	-5.173722	0.737848	-3.623415
H	-5.668442	-0.214294	-3.838682

H	-5.824575	1.532191	-3.998386
H	-4.248776	0.763806	-4.211799
C	-5.540939	-2.044592	-1.26204
H	-5.78458	-3.028897	-1.671183
H	-5.500981	-2.154235	-0.174833
H	-6.380481	-1.381098	-1.500012
C	0.034424	4.483246	2.611674
H	-0.270917	5.495253	2.89051
H	0.720315	4.12783	3.386272
H	0.608362	4.556013	1.67936
C	-0.318921	0.950076	4.071033
H	-1.12956	0.21939	3.975396
H	0.48284	0.4706	4.639237
H	-0.694447	1.782153	4.679219

TSCR

	x	y	z
Ru	-0.727846	1.193848	-0.302944
O	-2.154854	1.430738	1.493112
O	-1.861481	3.068447	0.102814
N	-0.817691	-1.486959	-1.303963
N	1.252532	-1.165038	-0.659165
C	0.003554	-0.590556	-0.686244
C	-0.227214	-2.803071	-1.476824
H	-0.443757	-3.211826	-2.469027
H	-0.619659	-3.514255	-0.730846
C	1.254742	-2.506207	-1.271695
H	1.749992	-3.225001	-0.609191
H	1.811738	-2.487228	-2.21974
C	-2.249779	-1.237814	-1.236307
C	-2.840128	-1.849159	0.047025
H	-2.299774	-1.435867	0.911551
H	-2.68502	-2.939094	0.047073
C	-4.333031	-1.524219	0.142156
H	-4.747959	-1.988794	1.045874
C	-5.058305	-2.062011	-1.094037
H	-4.961543	-3.155382	-1.153888
H	-6.130981	-1.839845	-1.021822
C	-4.470484	-1.414158	-2.35121
H	-5.000313	-1.781971	-3.239396
C	-2.989844	-1.79908	-2.45569
H	-2.539005	-1.391326	-3.370719
H	-2.892645	-2.89542	-2.501918
C	-4.617368	0.111334	-2.261581
H	-4.225072	0.581673	-3.173134
H	-5.682436	0.374434	-2.199
C	-3.869341	0.645419	-1.02085

H	-3.984585	1.735372	-0.971186
C	-2.39151	0.28405	-1.21192
H	-2.100345	0.647685	-2.213255
C	-4.502561	-0.005747	0.216211
H	-4.05681	0.378255	1.135435
H	-5.571853	0.244866	0.24446
C	0.83759	1.983883	1.351362
H	1.310805	1.075359	1.71182
N	-2.477335	2.623328	1.143915
O	-3.29707	3.28569	1.75156
C	1.351662	2.506299	0.112499
H	2.271683	1.997256	-0.178852
C	0.488622	1.903335	-1.569491
H	1.314186	1.391556	-2.080797
H	0.253255	2.8762	-2.022602
C	1.358008	4.00384	-0.083514
H	1.903191	4.493431	0.732268
H	1.837192	4.282155	-1.025451
H	0.341202	4.407142	-0.089343
C	0.250766	2.860122	2.406939
H	-0.300829	3.710452	2.000252
H	1.056876	3.267143	3.034874
H	-0.417186	2.301307	3.066848
C	2.280522	-0.869189	0.286032
C	2.077951	-1.233221	1.637401
C	3.115667	-0.981084	2.540598
H	2.986141	-1.246889	3.586309
C	4.318702	-0.428732	2.118688
C	4.522451	-0.146479	0.774556
H	5.494138	0.209442	0.44607
C	3.512312	-0.357996	-0.171264
H	5.115655	-0.253644	2.836162
C	0.813588	-1.92711	2.110505
H	0.256356	-2.253086	1.2215
C	3.79377	-0.180234	-1.650664
H	2.859106	-0.407487	-2.181285
C	4.826454	-1.234274	-2.089528
H	5.769084	-1.070701	-1.549323
H	4.473052	-2.217952	-1.75278
C	4.177591	1.240464	-2.110699
H	3.367738	1.931986	-1.850923
H	4.184702	1.222534	-3.207884
C	1.151155	-3.208368	2.889642
H	1.857895	-3.799511	2.29204
H	1.688942	-2.963663	3.814831
C	-0.15626	-1.002692	2.872228
H	-1.070822	-1.574356	3.074886
H	-0.469921	-0.196273	2.199661

C	5.084641	-1.268609	-3.585373
H	5.577243	-0.357859	-3.9398
H	5.726964	-2.110048	-3.858407
H	4.148926	-1.372073	-4.147485
C	5.496919	1.816607	-1.621901
H	5.73796	2.733553	-2.16666
H	5.466336	2.076328	-0.560127
H	6.333501	1.124466	-1.771982
C	-0.069709	-4.050093	3.219599
H	0.214625	-5.020183	3.635777
H	-0.719867	-3.561378	3.951354
H	-0.675125	-4.238194	2.324156
C	0.363979	-0.41089	4.170244
H	1.208684	0.266779	4.002073
H	-0.41963	0.167228	4.667762
H	0.697242	-1.181069	4.876578

DSCA

	x	y	z
Ru	0.646179	0.960451	-0.643054
O	1.833582	-0.383059	-2.034856
O	1.657692	1.729639	-2.481463
N	0.929	-0.04498	2.049657
N	-1.125181	-0.478197	1.441125
C	0.052256	0.054746	1.009886
C	0.439381	-0.905936	3.119353
H	0.675569	-0.494691	4.105293
H	0.895637	-1.907056	3.054675
C	-1.058033	-0.941396	2.832542
H	-1.498228	-1.940734	2.928599
H	-1.627734	-0.261586	3.484407
C	2.340623	0.084061	1.700651
C	2.892588	-1.247452	1.16267
H	2.281315	-1.560353	0.304296
H	2.811124	-2.028958	1.933581
C	4.353904	-1.072725	0.739407
H	4.745457	-2.034838	0.384997
C	5.184016	-0.584481	1.929036
H	5.163591	-1.32209	2.743891
H	6.233584	-0.469708	1.62811
C	4.627518	0.755124	2.420053
H	5.231373	1.121347	3.260421
C	3.184979	0.540932	2.894022
H	2.76002	1.468253	3.301493
H	3.166078	-0.211354	3.698683
C	4.667175	1.778837	1.275744

H	4.300197	2.751966	1.627672
H	5.707503	1.926017	0.953445
C	3.811936	1.284556	0.088153
H	3.850082	2.026054	-0.719786
C	2.373633	1.166365	0.619319
H	2.175059	2.10942	1.145564
C	4.420327	-0.041035	-0.388285
H	3.912473	-0.428926	-1.271725
H	5.468638	0.128505	-0.670092
C	-2.264304	-0.786346	0.643352
C	-2.287025	-2.035129	-0.015946
C	-3.418401	-2.347032	-0.775175
H	-3.463566	-3.296636	-1.301859
C	-4.495701	-1.470814	-0.846989
C	-4.477296	-0.278018	-0.136205
H	-5.348809	0.370606	-0.156736
C	-3.363986	0.091625	0.628405
C	-1.144884	0.126924	-2.701472
C	-0.476083	-0.119141	-4.009957
H	0.306643	-0.877631	-3.932715
H	-1.209016	-0.496175	-4.734391
H	-0.035777	0.787301	-4.433954
H	-1.410197	-0.750513	-2.113794
N	2.153674	0.594378	-2.816114
O	2.869153	0.443586	-3.786185
H	-5.368265	-1.734422	-1.438333
C	-1.139066	-3.017792	0.119106
H	-0.567698	-2.73328	1.012967
C	-3.388809	1.349326	1.474306
H	-2.482456	1.339845	2.094772
C	-4.589476	1.308526	2.434458
H	-5.526518	1.297417	1.861849
H	-4.566748	0.347929	2.966045
C	-3.309435	2.663955	0.675058
H	-2.356552	2.678042	0.131189
H	-3.231079	3.483887	1.400135
C	-1.634347	-4.448036	0.368085
H	-2.348363	-4.427463	1.20209
H	-2.205174	-4.81341	-0.495156
C	-0.13262	-2.923975	-1.042614
H	0.769251	-3.483101	-0.762294
H	0.198959	-1.881507	-1.132181
C	-4.61744	2.447088	3.438936
H	-4.792635	3.415297	2.959996
H	-5.410254	2.304876	4.178074
H	-3.668571	2.520097	3.983265
C	-4.446083	2.951821	-0.290571
H	-4.341655	3.95135	-0.722061

H	-4.464792	2.241935	-1.124137
H	-5.426333	2.912666	0.199117
C	-0.50883	-5.420459	0.675893
H	-0.894405	-6.397974	0.977022
H	0.141081	-5.579985	-0.190121
H	0.124319	-5.048734	1.490838
C	-0.635291	-3.423116	-2.385242
H	-1.527252	-2.88078	-2.72003
H	0.131184	-3.295799	-3.154411
H	-0.894189	-4.487778	-2.355756
C	-1.607212	1.317921	-2.261917
H	-2.209247	1.303155	-1.357574
C	0.03266	2.541943	0.052458
H	-0.067132	2.840231	1.111892
H	-0.147796	3.394803	-0.627533
C	-1.484942	2.621034	-2.979593
H	-0.525415	2.717505	-3.495868
H	-2.278064	2.728533	-3.730186
H	-1.583369	3.467473	-2.293531

14-Int'

	x	y	z
Ru	-0.5229040	-1.2823720	-0.9978900
O	1.0239620	-0.2771120	-2.2279820
O	-0.9839300	0.5153040	-2.3770360
N	-1.2068730	-0.5532630	1.6649580
N	0.9039550	0.0061410	1.2929910
C	-0.2054920	-0.5343500	0.7277750
C	-0.8510610	0.2481650	2.8313560
H	-1.1769100	-0.2313660	3.7588460
H	-1.3189190	1.2447120	2.7836070
C	0.6698880	0.3265790	2.7086570
H	1.0751320	1.3146120	2.9505850
H	1.1775990	-0.4129440	3.3436320
C	-2.5445480	-0.5511710	1.0549070
C	-2.8656610	0.8496000	0.5005050
H	-2.0528530	1.1647120	-0.1684760
H	-2.9164710	1.5808640	1.3222430
C	-4.1905780	0.8187240	-0.2607430
H	-4.4142000	1.8234420	-0.6412120
C	-5.3032520	0.3626850	0.6871460
H	-5.4113060	1.0757310	1.5162590
H	-6.2649220	0.3409430	0.1578000
C	-4.9750510	-1.0325590	1.2284930
H	-5.7761780	-1.3654970	1.9006230
C	-3.6542400	-0.9782720	2.0142120
H	-3.4121330	-1.9605650	2.4414940

H	-3.7475300	-0.2686280	2.8512790
C	-4.8591990	-2.0068600	0.0476870
H	-4.6604390	-3.0235240	0.4116920
H	-5.8160200	-2.0404780	-0.4921530
C	-3.7286830	-1.5567090	-0.8987250
H	-3.6543550	-2.2656610	-1.7347450
C	-2.4322530	-1.5746650	-0.0823820
H	-2.3778730	-2.5550740	0.4036680
C	-4.0610470	-0.1603440	-1.4320640
H	-3.2858560	0.1862710	-2.1237890
H	-5.0034600	-0.1934680	-1.9955140
C	2.0133540	0.5853970	0.5941910
C	1.9326000	1.9545380	0.2563670
C	3.0509490	2.5394630	-0.3441130
H	3.0284150	3.5970080	-0.5902680
C	4.1989620	1.8016390	-0.6005650
C	4.2561900	0.4605480	-0.2505840
H	5.1725710	-0.0974390	-0.4186910
C	3.1658650	-0.1801410	0.3465840
N	0.2437830	0.6067270	-2.7500990
O	0.6449300	1.4642510	-3.5068760
H	5.0595830	2.2806200	-1.0590490
C	0.7260600	2.8100990	0.5929840
H	0.0108310	2.1855480	1.1439230
C	3.2592510	-1.6363540	0.7379320
H	2.3175130	-1.8937430	1.2411660
C	4.3817150	-1.8581920	1.7616640
H	5.3450350	-1.5495650	1.3334550
H	4.2121590	-1.1801340	2.6087610
C	3.3514580	-2.5865270	-0.4743760
H	2.5445190	-2.3281680	-1.1701330
H	3.1196710	-3.5983620	-0.1143040
C	1.1294960	3.9489670	1.5443790
H	1.6898510	3.5169130	2.3851350
H	1.8407580	4.6189500	1.0433080
C	-0.0724620	3.3108020	-0.6262830
H	-0.9889580	3.7743740	-0.2366530
H	-0.4205810	2.4460230	-1.1985820
C	4.4758770	-3.2900310	2.2590750
H	4.7787800	-3.9787360	1.4637770
H	5.2050790	-3.3868450	3.0679790
H	3.5101310	-3.6416170	2.6410190
C	4.6690190	-2.6236420	-1.2319800
H	4.6647230	-3.4364870	-1.9634820
H	4.8498990	-1.6994820	-1.7867970
H	5.5265880	-2.7911380	-0.5696380
C	-0.0489140	4.7488520	2.0716470
H	0.2600100	5.4535110	2.8483700

H	-0.5366910	5.3283700	1.2820830
H	-0.8114640	4.0904060	2.5072600
C	0.620426	4.285276	-1.562712
H	1.446619	3.815164	-2.101334
H	-0.082012	4.646024	-2.318647
H	1.011507	5.163766	-1.034853
C	0.141981	-2.888656	-0.466074
H	0.595362	-3.227319	0.477648
H	0.124924	-3.691297	-1.229662