(ESI)

Electronic supplementary information

Mechanistic Investigation on Radical-Induced Construction of Oxindoles: Radical *versus* Electrophilic Cyclization

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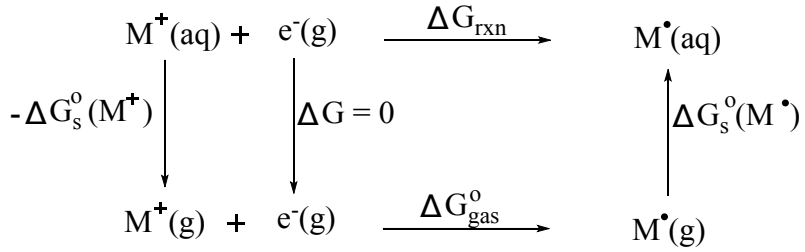
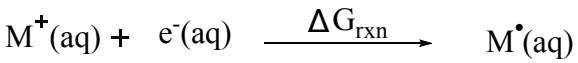
Method A (Born-Haber cycle)



$$E_{cell} = \frac{-\Delta G_{rxn}}{nF} - E_{SHE}$$

Method B



$$\Delta G_{rxn} = G_s(M)^{\bullet} - G_s(M)^{+}$$

$$E_{cell} = \frac{-\Delta G_{rxn}}{nF} - E_{SHE}$$

Note: (1) In method A, gas-phase structures were optimized at the M06-2X/6-31+G(d,p) level of theory. The standard-state free energy of solvation was also obtained at the same level of theory. To refine the energies, single-point energy calculations were performed at the M06-2X/6-311+G(d,p) level of theory.
(2) For some intermediates which could not be optimized in the gas phase, we used the direct method (method B) to calculate their reduction potential.

Fig. S1. Diagrams for calculating reduction potential.

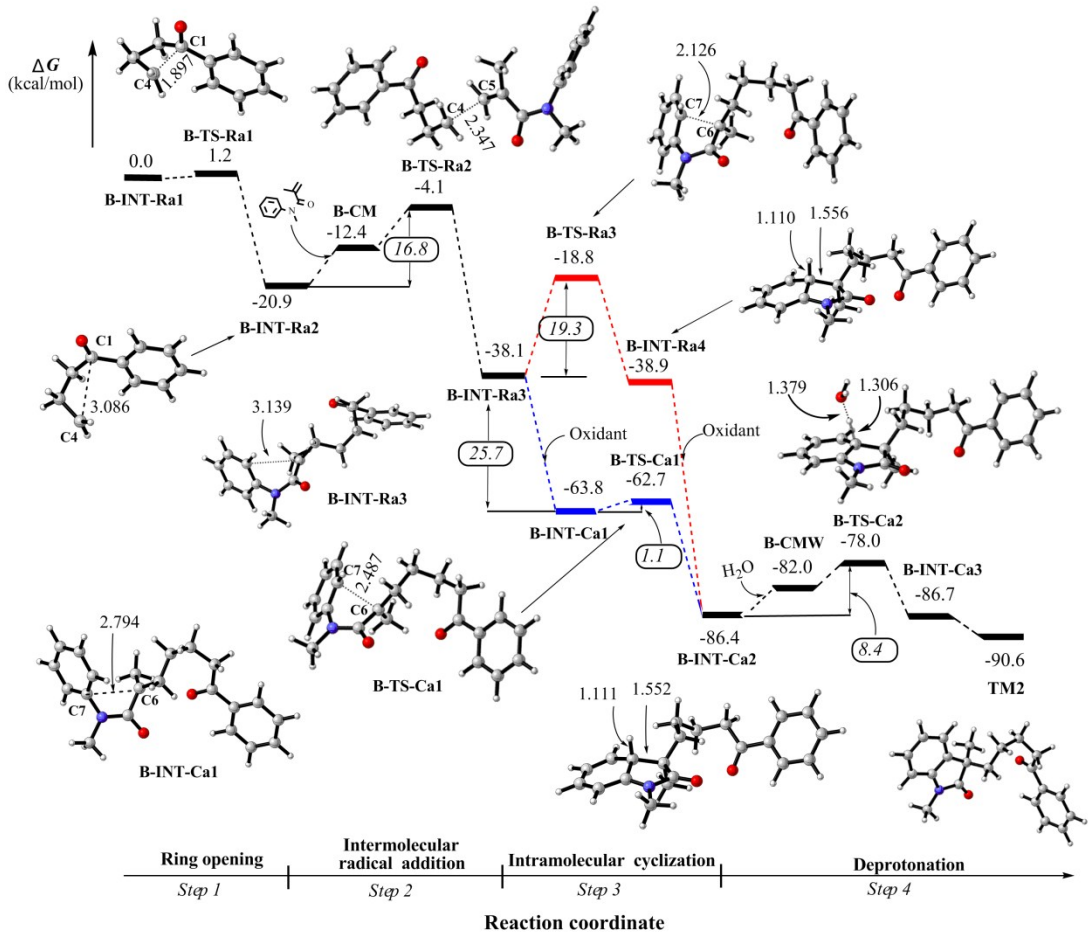


Fig. S2. Relative Gibbs free energy (kcal/mol) profiles for the reaction mechanism of cyclobutanol with acrylamides. Radical (upper) and electrophilic (below) cyclizations in step 3 are labeled as red and blue lines, respectively.

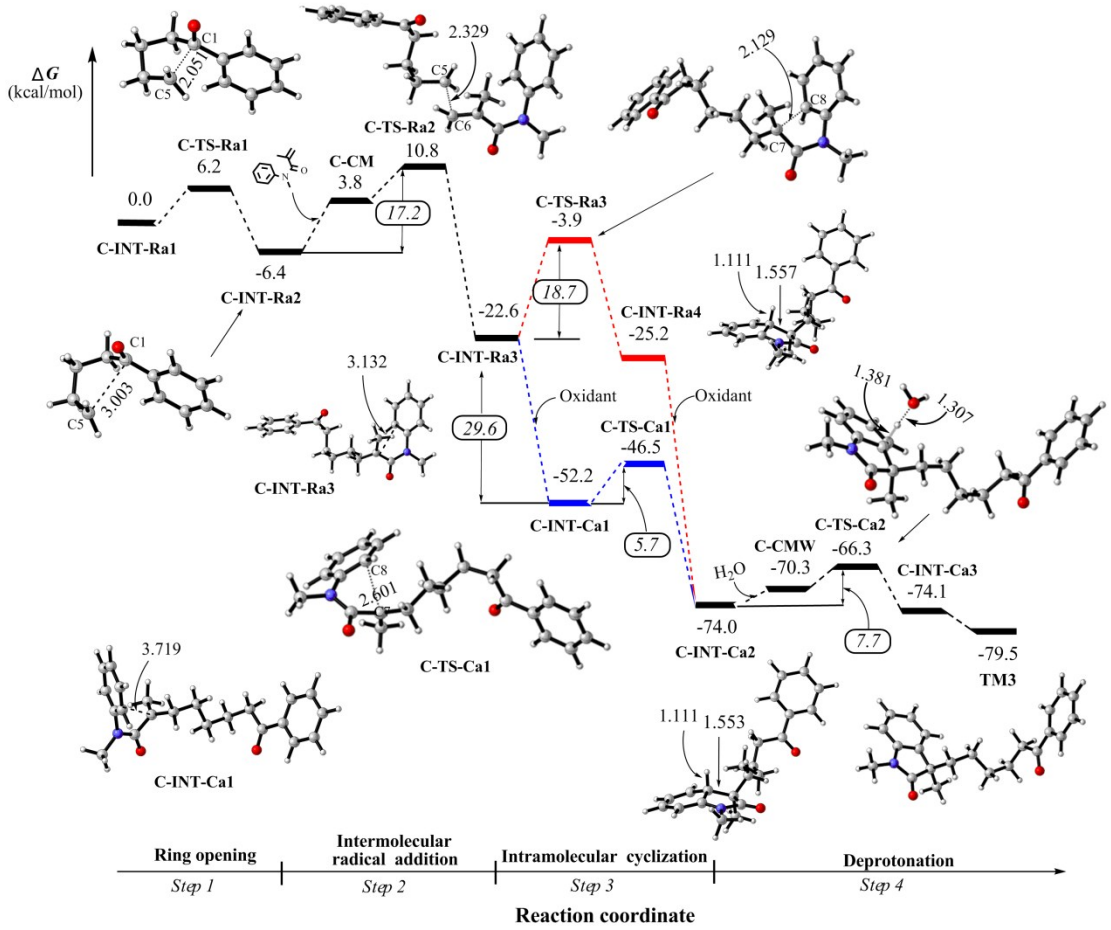


Fig. S3. Relative Gibbs free energy (kcal/mol) profiles for the reaction mechanism of cyclopentanol with acrylamides. Radical (upper) and electrophilic (below) cyclizations in step 3 are labeled as red and blue lines, respectively.

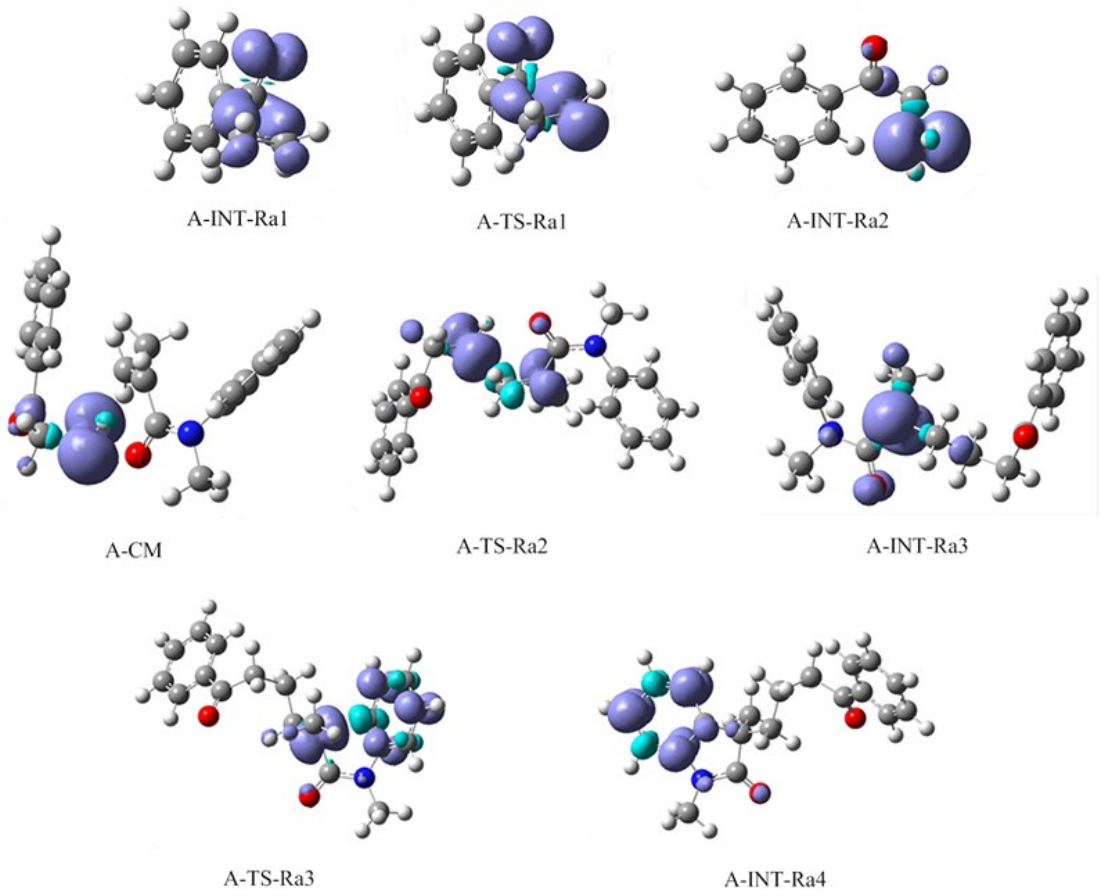


Fig. S4. Spin density distributions (isodensity at 0.004 au) of some intermediates and transition states.

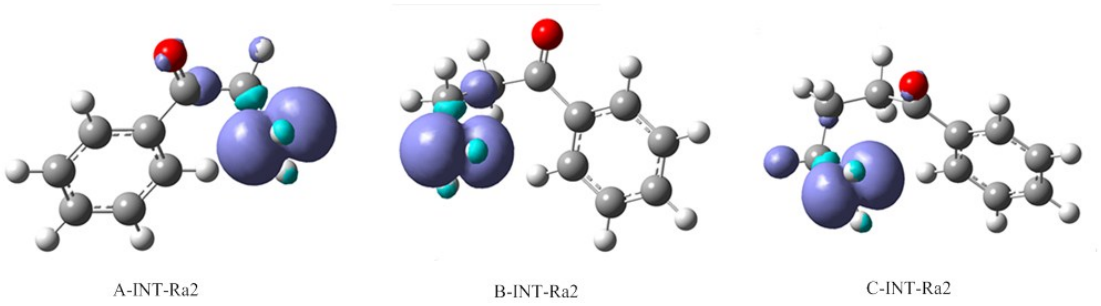


Fig. S5. Spin density distributions (isodensity at 0.004 au) of **A-INT-Ra2**, **B-INT-Ra2** and **C-INT-Ra2**.

Table S1. Gibbs free energy barriers of intermolecular radical addition steps for different radical sources with acrylamide.

Radical source	$\Delta G^{\ddagger}$ (kcal/mol)
β-keto radical	17.6
γ-keto radical	16.8
σ-keto radical	17.2

Table S2. Reduction potential (E_{red}) for some selected intermediates.

Intermediate	E_{red} (eV)
A-INT-Ca1	1.39[a]
B-INT-Ca1	0.89[a]
C-INT-Ca1	1.23[b]

a. using method A

b. using method B

Methods A or B, as shown in Figure S1, were used to calculate the reduction potential.

Table S3. Thermal correction of Gibbs free energies and electronic energies of relevant stationary points in the cyclopropanol-related reaction processes.

	Thermal correction of Gibbs free energies (hartree)	E_{SCF} (hartree)
A-INT-Ra1	0.117332	-423.36355797
A-TS-Ra1	0.116225	-423.36118038
A-INT-Ra2	0.113533	-423.37684415
A-CM	0.308661	-980.14190886
A-TS-Ra2	0.312525	-980.13098465
A-INT-Ra3	0.3166	-980.19099307
A-TS-Ra3	0.317715	-980.16074348
A-INT-Ra4	0.320429	-980.19683511
A-INT-Ca1	0.319003	-979.98958821
A-TS-Ca1	0.320257	-979.98930238
A-INT-Ca2	0.324878	-980.03970759
A-CMW	0.343223	-1056.45284295
A-TS-Ca2	0.342096	-1056.44378817
A-INT-Ca3	0.345246	-1056.46031967
TM1	0.313154	-979.65665749

Table S4. Thermal correction of Gibbs free energies and electronic energies of relevant stationary points in the cyclobutanol-related reaction processes.

	Thermal correction of Gibbs free energies (hartree)	E_{SCF} (hartree)
B-INT-Ra1	0.144179	-462.6430325
B-TS-Ra1	0.142465	-462.63937368
B-INT-Ra2	0.139585	-462.67171878
B-CM	0.337675	-1019.43946067
B-TS-Ra2	0.337954	-1019.42648577
B-INT-Ra3	0.344189	-1019.48696989
B-TS-Ra3	0.344317	-1019.4563469
B-INT-Ra4	0.348031	-1019.49207937
B-INT-Ca1	0.344257	-1019.29202021
B-TS-Ca1	0.345454	-1019.29153766
B-INT-Ca2	0.351471	-1019.33535691
B-CMW	0.370254	-1095.74841178
B-TS-Ca2	0.36741	-1095.73931878
B-INT-Ca3	0.370807	-1095.75646527
TM2	0.340005	-1018.9519398

Table S5. Thermal correction of Gibbs free energies and electronic energies of relevant stationary points in the cyclopentanol-related reaction processes.

	Thermal correction of Gibbs free energies (hartree)	E_{SCF} (hartree)
C-INT-Ra1	0.17293	-501.96527847
C-TS-Ra1	0.170329	-501.95280892
C-INT-Ra2	0.166572	-501.96909062
C-CM	0.361033	-1058.73053382
C-TS-Ra2	0.363833	-1058.72216051
C-INT-Ra3	0.370468	-1058.78203911
C-TS-Ra3	0.370483	-1058.75223905
C-INT-Ra4	0.372506	-1058.78825005
C-INT-Ca1	0.37183	-1058.59094025
C-TS-Ca1	0.372663	-1058.58279788
C-INT-Ca2	0.377223	-1058.631073
C-CMW	0.39469	-1135.04409293
C-TS-Ca2	0.392729	-1135.03569162
C-INT-Ca3	0.397469	-1135.05284349
TM3	0.364075	-1058.24813574

Cartesian coordinates for optimized structures

1. Cartesian coordinates of structures in the reaction mechanisim of cycloalkanol with *N*-methyl-*N*-phenylmethacrylamide

A-INT-Ra1

C	-2.276455	1.086069	-0.000107
C	-0.891604	1.238887	-0.000167
C	-0.052503	0.119297	-0.000353
C	-0.627034	-1.158161	-0.000367
C	-2.011923	-1.309849	-0.000285
C	-2.842529	-0.188739	-0.000178
H	-2.913935	1.964819	0.000008
H	-0.445058	2.227728	-0.000100
H	-0.003905	-2.048530	-0.000362
H	-2.441266	-2.306863	-0.000308
H	-3.921163	-0.309322	-0.000115
C	1.430252	0.346216	-0.000361
C	2.349847	-0.753256	0.724256
C	2.350446	-0.753729	-0.722492
H	1.774205	-1.496022	1.266080
H	3.176254	-0.293032	1.251614
H	3.177558	-0.294144	-1.249320
H	1.775784	-1.497288	-1.264268
O	1.906319	1.536530	-0.000363

A-TS-Ra1

C	-2.285606	1.069782	-0.097489
C	-0.904835	1.239079	-0.034862
C	-0.056456	0.131332	0.076826
C	-0.617376	-1.151807	0.122743
C	-1.998581	-1.319932	0.056712
C	-2.837741	-0.210683	-0.052527
H	-2.931491	1.938404	-0.180660
H	-0.466127	2.230758	-0.068655
H	0.012069	-2.033398	0.202722
H	-2.418527	-2.320197	0.091673
H	-3.913729	-0.344556	-0.101957
C	1.417824	0.389544	0.167596
C	2.363457	-0.750139	0.598636
C	2.375393	-0.787175	-0.855624
H	1.881352	-1.570349	1.122817
H	3.248539	-0.354385	1.086662
H	3.125086	-0.232430	-1.404661
H	1.715329	-1.445061	-1.407984
O	1.876378	1.558900	0.095998

A-INT-Ra2

C	-2.392025	0.915924	0.257158
C	-1.042126	1.235083	0.156467
C	-0.097561	0.237234	-0.115538
C	-0.522826	-1.084965	-0.288949
C	-1.875539	-1.404040	-0.188256
C	-2.809935	-0.405517	0.084864
H	-3.119188	1.693615	0.467596
H	-0.699387	2.256545	0.286754
H	0.190897	-1.873975	-0.501974
H	-2.199043	-2.430856	-0.323889
H	-3.863527	-0.655538	0.161989
C	1.343339	0.631823	-0.226213
C	2.597745	-1.232101	0.797364
C	2.395239	-0.451355	-0.460850
H	2.188310	-2.226441	0.918265
H	3.070742	-0.758481	1.648937
H	3.309989	0.075330	-0.749492
H	2.091546	-1.100722	-1.286362
O	1.681473	1.796000	-0.089763

A-TS-Ra2

C	3.642361	-0.748516	1.156845
C	4.240923	-1.986951	1.386317
C	5.070555	-2.554568	0.419976
C	5.300512	-1.878973	-0.780240
C	4.690593	-0.650605	-1.021108
C	3.852885	-0.088434	-0.055326
H	3.002686	-0.295203	1.908823
H	4.064828	-2.501576	2.325608
H	5.539471	-3.516418	0.600901

H	5.946139	-2.315387	-1.535761
H	4.843111	-0.131708	-1.963291
N	3.232659	1.173053	-0.306821
C	4.107411	2.344498	-0.354105
H	4.295021	2.736246	0.652254
H	5.054764	2.054038	-0.808027
H	3.637053	3.124052	-0.952992
C	1.898349	1.391948	-0.062503
O	1.485980	2.535198	0.164944
C	0.955624	0.239225	-0.158412
C	1.202999	-0.907404	-1.107400
H	1.780960	-0.587173	-1.979578
H	1.754658	-1.729020	-0.637390
H	0.244339	-1.302209	-1.455474
C	-5.207273	-2.165965	0.450884
C	-4.418530	-1.168481	1.013609
C	-4.126049	-0.005799	0.289379
C	-4.634729	0.147089	-1.006097
C	-5.433255	-0.848812	-1.565253
C	-5.717790	-2.005020	-0.839470
H	-5.426655	-3.067210	1.014155
H	-4.016409	-1.275768	2.016037
H	-4.421481	1.041939	-1.582389
H	-5.832659	-0.721714	-2.566055
H	-6.336941	-2.781158	-1.278519
C	-3.285220	1.047259	0.941655
C	-1.647937	1.582635	-0.872079
C	-2.666549	2.136626	0.082340
H	-1.930558	0.771617	-1.535689
H	-2.204094	2.858045	0.760677
H	-3.465356	2.666316	-0.460565
O	-3.066907	1.009907	2.141842
H	-0.876464	2.256739	-1.224702
C	-0.218679	0.363827	0.515263
H	-0.925017	-0.462729	0.531106
H	-0.345808	1.144596	1.258676

A-INT-Ra3

C	3.331036	0.586118	1.215340
C	3.745856	1.836721	1.671326
C	4.442937	2.697246	0.824602
C	4.723248	2.301187	-0.484827
C	4.294756	1.061130	-0.950705
C	3.588015	0.202745	-0.103635
H	2.802435	-0.093225	1.878739
H	3.532620	2.130556	2.694325
H	4.771033	3.667784	1.182246
H	5.266662	2.964891	-1.150050
H	4.487088	0.760507	-1.976833
N	3.155676	-1.068066	-0.586960
C	4.197376	-2.039913	-0.918383
H	4.548078	-2.564239	-0.021658
H	5.034525	-1.513854	-1.376570
H	3.798929	-2.772126	-1.620235
C	1.913219	-1.578124	-0.257974
O	1.745372	-2.804275	-0.159435
C	0.786977	-0.657754	-0.104607
C	0.716803	0.696818	-0.731853
H	1.443150	0.823934	-1.537051
H	0.899225	1.487742	0.009550
H	0.289246	0.864097	-1.134587
C	4.473198	2.431899	0.218907
C	4.039947	1.302538	0.905943
C	3.862763	0.088757	0.230361
C	4.129270	0.017838	-1.142347
C	4.576996	1.145927	-1.826916
C	4.744509	2.353138	-1.148862
H	4.599704	3.372546	0.745184
H	3.826756	1.345965	1.969411
H	4.004004	-0.916300	-1.681218
H	4.792724	1.082631	-2.888468
H	5.085341	3.232994	-1.685784
C	3.393225	-1.100385	1.012737
C	1.426414	-1.811363	-0.405858
C	2.731603	-2.248435	0.279957
H	1.645477	-1.100738	-1.210191
H	2.530257	-3.026072	1.021530
H	3.420328	-2.662578	-0.464380
O	3.497556	-1.112449	2.230069
H	0.955805	-2.685978	-0.864038
C	0.433043	-1.175073	0.585743
H	0.920120	-0.334111	1.099129
H	0.161762	-1.920257	1.340896

A-TS-Ra3

C	2.611393	0.862480	-0.894875
C	2.681191	2.241623	-0.572147
C	3.799385	2.758923	0.074417

C	4.899233	1.944212	0.364595
C	4.853073	0.569355	0.078505
C	3.725995	0.046940	-0.527536
H	1.876180	2.902295	-0.878695
H	3.839755	3.818128	0.309891
H	5.781220	2.365289	0.835115
H	5.671184	-0.082549	0.369614
N	3.448126	-1.327832	-0.625705
C	4.484440	-2.337327	-0.760517
H	5.211545	-2.009694	-1.505147
H	4.993423	-2.510569	0.193846
H	4.016686	-3.265238	-1.087627
C	2.159245	-1.656962	-0.279256
O	1.725074	-2.804981	-0.321108
C	1.351228	-0.471752	0.183854
C	1.583763	-0.101915	1.625257
C	-0.050227	-0.427037	-0.369021
H	2.648215	-0.141599	1.877058
H	1.228403	0.914095	1.826986
H	1.050580	-0.789577	2.296789
H	0.004910	-0.535787	-1.459481
H	-0.596846	-1.316405	-0.015704
C	-5.966412	-0.836745	-0.715796
C	-4.828413	-1.058491	0.051929
C	-3.953925	-0.003567	0.344115
C	-4.237263	1.278232	-0.142862
C	-5.380929	1.501224	-0.906955
C	-6.244634	0.445190	-1.195467
H	-6.637002	-1.659700	-0.941369
H	-4.599759	-2.048650	0.433148
H	-3.576127	2.111422	0.072419
H	-5.595761	2.498387	-1.277130
H	-7.133821	0.620465	-1.793179
C	-2.740554	-0.291689	1.176683
C	-0.836745	0.847155	-0.021567
C	-1.649876	0.751338	1.286998
H	-1.519553	1.079730	-0.844901
H	-1.013367	0.456888	2.123677
H	-2.081660	1.729102	1.520365
O	-2.614925	-1.378379	1.722554
H	-0.150520	1.697762	0.057848
H	2.004434	0.560784	-1.747275

A-INT-Ra4

C	-2.404212	-0.748621	-0.423764
C	-2.639055	-2.108163	0.164516
C	-3.882769	-2.672909	0.113528
C	-5.024409	-1.951923	-0.334089
C	-4.927076	-0.562402	-0.597419
C	-3.691210	0.017115	-0.548686
H	-1.793560	-2.685980	0.524101
H	-4.013977	-3.698686	0.446795
H	-5.990894	-2.440555	-0.375221
H	-5.819911	0.031137	-0.768942
N	-3.382483	1.367013	-0.581202
C	-4.352735	2.414023	-0.833986
H	-4.817844	2.261456	-1.810493
H	-5.125599	2.408529	-0.059187
H	-3.827917	3.368399	-0.819797
C	-2.100333	1.608778	-0.145684
O	-1.599216	2.718090	-0.042308
C	-1.447775	0.276481	0.251545
C	-1.526337	0.186356	1.782665
C	-0.009016	0.252755	-0.281155
H	-2.563999	0.272486	2.123066
H	-1.144660	-0.778180	2.129070
H	-0.938251	0.986206	2.242494
H	-0.059826	0.319313	-1.374390
H	0.488132	1.169864	0.057890
C	5.862687	0.854941	-0.910848
C	4.751996	1.076375	-0.104083
C	3.923901	0.010100	0.270596
C	4.225844	-1.282842	-0.174003
C	5.341668	-1.505027	-0.978626
C	6.159589	-0.437847	-1.348408
H	6.497161	1.686737	-1.199455
H	4.508632	2.074800	0.244845
H	3.601979	-2.125599	0.105544
H	5.571371	-2.510581	-1.315612
H	7.027263	-0.613031	-1.976977
C	2.740964	0.299678	1.145433
C	0.825595	-0.978135	0.112432
C	1.699928	-0.775326	1.368881
H	1.474583	-1.250133	-0.725917
H	1.094426	-0.457671	2.219868
H	2.182820	-1.720687	1.633800
O	2.599243	1.409601	1.638057
H	0.179582	-1.845152	0.283191

H	-2.015810	-0.883743	-1.455306

A-INT-Ca1

C	2.459420	0.939227	1.050612
C	2.254640	2.315118	0.907804
C	3.021632	3.035834	0.000619
C	4.004181	2.388267	0.759826
C	4.199561	1.016792	0.644213
C	3.404891	0.296932	0.250253
H	1.515111	2.814839	1.525321
H	2.871766	4.104469	0.110666
H	4.608269	2.956660	1.459027
H	4.935099	0.504313	1.256188
N	3.504731	-1.121467	0.319593
C	4.795179	-1.788236	0.509928
H	5.419153	-1.160723	1.144513
H	5.283692	-1.955693	0.452971
H	4.616637	-2.748390	0.994344
C	2.402774	-1.856365	0.141084
O	2.297825	-3.077591	0.175033
C	1.122217	-1.199310	0.318932
C	1.103872	-0.671078	1.676085
C	-0.124789	-1.478943	0.411743
H	2.042886	-0.216720	1.992441
H	0.217929	-0.067362	1.891362
H	0.975224	-1.599208	2.274097
H	0.048397	-2.275101	1.136866
H	-0.862353	-1.812954	0.331465
C	-5.828631	-0.506801	0.782451
C	-4.518595	-0.238456	1.161947
C	-3.617630	0.321128	0.245577
C	-4.047084	0.610023	1.055963
C	-5.361494	0.343515	1.433505
C	-6.251063	-0.215498	0.516756
H	-6.521202	-0.942747	1.494949
H	-4.173477	-0.459943	2.166646
H	-3.371957	1.050756	1.782306
H	-5.689064	0.573319	2.441933
H	-7.274061	-0.425202	0.813256
C	-2.220963	0.587417	0.704425
C	-0.749389	-0.261637	1.172945
C	-1.151947	0.942859	0.312898
H	-1.628832	-0.681581	1.667979
H	-0.297349	1.357920	0.228549
H	-1.512778	1.728209	0.983471
O	-1.922991	0.475261	1.884976
H	-0.072106	0.061984	1.963274
H	1.956547	0.377328	1.831007

A-TS-Ca1

C	-2.445320	-0.841907	-1.014707
C	-2.197154	-2.212523	-0.858019
C	-2.983293	-2.956564	0.010461
C	-4.035404	-2.343272	0.707940
C	-4.277299	-0.980659	0.583195
C	-3.455757	-0.231894	-0.261492
H	-1.416060	-2.689627	-1.441793
H	-2.803275	-4.018871	0.133269
H	-4.655808	-2.935213	1.372453
H	-5.060082	-0.496987	1.158166
N	-3.532419	1.180152	-0.301550
C	-4.800682	1.901499	-0.407989
H	-5.479850	1.323107	-1.032800
H	-5.236961	2.057685	0.581458
H	-4.602301	2.868522	-0.870648
C	-2.377966	1.850857	-0.162690
O	-2.200344	3.059745	-0.208805
C	-1.146570	1.060165	0.234843
C	-1.117855	0.562604	1.611054
C	0.097685	1.274239	-0.534575
H	-2.073861	0.172882	1.961369
H	-0.272952	-0.095284	1.822034
H	-0.919822	1.492208	2.183936
H	-0.082655	2.015072	-1.314972
H	0.818065	1.694013	0.185261
C	5.754252	0.733207	0.741331
C	4.464061	0.401439	1.139083
C	3.621414	-0.314898	0.278477
C	4.089143	-0.697775	-0.985012
C	5.385030	-0.371137	-1.378753
C	6.216024	0.345748	-0.518568
H	6.400028	1.294493	1.408740
H	4.089434	0.696322	2.113961
H	3.459584	-1.260479	-1.666923
H	5.743959	-0.677151	-2.355752
H	7.223739	0.603565	-0.828946
C	2.242075	-0.640886	0.752572
C	0.765158	0.028201	-1.190517

C	1.198599	-1.101581	-0.248359
H	1.636914	0.428098	-1.714917
H	0.352839	-1.512087	0.309404
H	1.597134	-1.915269	-0.861555
O	1.937119	-0.490561	1.926685
H	0.101437	-0.373273	-1.957609
H	-1.963630	-0.275447	-1.805984

A-INT-Ca2

C	-2.440948	-1.990847	-0.065396
C	-3.676832	-2.514112	0.072195
C	-4.848147	-1.685945	-0.101547
C	-4.798161	-0.333513	-0.324156
C	-3.515033	0.247255	-0.354868
H	-1.556156	-2.615221	0.018043
H	-3.814638	-3.563174	0.304547
H	-5.821637	-2.158008	-0.008040
H	-5.696371	0.270662	-0.363756
N	-3.216148	1.533837	-0.248661
C	-4.163573	2.644852	-0.240459
H	-4.792504	2.593020	-1.129032
H	-4.773444	2.600887	0.663406
H	-3.580983	3.564287	-0.249910
C	-1.811963	1.716076	-0.044152
O	-1.301926	2.798836	0.041444
C	-1.162648	0.340390	0.091675
C	-0.985315	0.107437	1.604442
C	0.151684	0.337554	-0.709516
H	-1.942595	0.192633	2.129201
H	-0.574439	-0.882959	1.800528
H	-0.291772	0.847157	2.010920
H	-0.041180	0.833536	-1.667626
H	0.867429	0.976691	-0.177148
C	5.299010	1.357228	0.322110
C	4.165403	0.785388	0.890008
C	3.577349	-0.344479	0.307732
C	4.142283	-0.900001	-0.846445
C	5.286771	-0.335228	-1.405759
C	5.862162	0.794906	-0.825590
H	5.744866	2.238731	0.771315
H	3.717999	1.207653	1.784427
H	3.708376	-1.782976	-1.305721
H	5.727202	-0.776757	-2.293638
H	6.749515	1.237742	-1.266967
C	2.362358	-0.928255	0.958855
C	0.786052	-1.022449	-1.032469
C	1.428965	-1.794064	0.136524
H	1.555594	-0.831538	-1.786327
H	0.684842	-2.201767	0.823466
H	1.982800	-2.645441	-0.273727
O	2.107195	-0.673373	2.125594
H	0.057608	-1.678461	-1.522397
H	-2.131254	-0.631665	-1.579782

A-CMW

C	2.159775	-0.636788	0.342043
C	2.206563	-2.114748	0.210528
C	3.397561	-2.749888	0.174510
C	4.630064	-1.997164	0.175096
C	4.684613	-0.628227	0.125603
C	3.447763	0.045809	0.056903
H	1.276309	-2.673934	0.249418
H	3.451457	-3.831701	0.153456
H	5.563333	-2.552529	0.174243
H	5.625366	-0.097447	0.042558
N	3.244173	1.311225	-0.273132
C	4.270375	2.327904	-0.477876
H	4.901222	2.396121	0.409092
H	4.871340	2.071972	-1.352217
H	3.758336	3.274281	-0.643567
C	1.848378	1.571689	-0.454145
O	1.415883	2.664307	-0.697841
C	1.102723	0.242595	-0.369374
C	0.910552	-0.223138	-1.827512
C	-0.211783	0.451393	0.401213
H	1.866809	-0.252775	-2.360254
H	0.474617	-1.221985	-1.859691
H	0.234771	0.459574	-2.347855
H	0.005905	1.114879	1.243395
H	-0.898213	1.003565	-0.252872
C	-5.618345	1.223538	-0.452381
C	-4.472224	0.647235	-0.990019
C	-3.797711	-0.365465	-0.295498
C	-4.289029	-0.796770	0.942828
C	-5.443935	-0.227159	1.474869
C	-6.106549	0.784610	0.780503
H	-6.131892	2.013611	-0.990624
H	-4.082257	0.975662	-1.948331

H	-3.788147	-1.586228	1.494232
H	-5.824697	-0.573300	2.430098
H	-7.003108	1.231111	1.199052
C	-2.571202	-0.961007	-0.915886
C	-0.900267	-0.795956	0.970842
C	-1.599957	-1.725470	-0.039769
H	-1.648319	-0.440920	1.686765
H	-0.892358	-2.223218	-0.705659
H	-2.127123	-2.510685	0.511147
O	-2.333497	-0.787370	-2.101167
H	-0.191444	-1.387905	1.561013
H	2.045066	-0.448446	1.433012
O	2.104732	1.616155	2.412356
H	1.505496	1.658431	3.168057
H	2.917190	2.040594	2.715799

A-TS-Ca2

C	2.175492	-0.474175	-0.077585
C	2.395803	-1.835110	-0.477516
C	3.677560	-2.330343	-0.505580
C	4.773555	-1.469930	-0.251814
C	4.624656	-0.115185	-0.001472
C	3.319911	0.388066	0.008441
H	1.546285	-2.485839	-0.664670
H	3.858376	-3.374402	-0.730452
H	5.776314	-1.885079	-0.278764
H	5.483422	0.533024	0.128206
N	2.928840	1.688530	0.101754
C	3.812442	2.817779	0.350823
H	4.327523	2.683906	1.304034
H	4.539556	2.911661	-0.458208
H	3.192538	3.712264	0.390249
C	1.548504	1.808462	-0.081780
O	0.944722	2.856702	-0.037470
C	0.961158	0.417620	-0.352489
C	0.601144	0.381901	-1.850365
C	-0.250782	0.224412	0.582742
H	1.476153	0.626619	-2.460563
H	0.242365	-0.604475	-2.145099
H	-0.188926	1.109558	-2.054708
H	0.028845	0.591775	1.577276
H	-1.045397	0.894274	0.230093
C	-5.252622	1.418074	-0.152462
C	-4.199944	0.816894	-0.833860
C	-3.624968	-0.363143	-0.346134
C	-4.120674	-0.941054	0.828256
C	-5.188200	-0.347407	1.500122
C	-5.749939	0.833425	1.014184
H	-5.686386	2.339121	-0.528232
H	-3.805395	1.254117	-1.745811
H	-3.695430	-1.863910	1.211636
H	-5.579722	-0.805638	2.402464
H	-6.575134	1.298601	1.544302
C	-2.500803	-0.970216	-1.127006
C	-0.797482	-1.196343	0.776279
C	-1.499595	-1.862874	-0.421718
H	-1.504538	-1.137781	1.609267
H	-0.790933	-2.199112	-1.182075
H	-2.020002	-2.758548	-0.061219
O	-2.381398	-0.722935	-2.316758
H	-0.001939	-1.866086	1.120942
H	2.155759	-0.762383	1.205031
O	2.023612	-1.019621	2.538893
H	2.470465	-1.839155	2.804987
H	2.367552	-0.310511	3.105306

TM1

C	-2.189005	0.118499	-0.501630
C	-2.385530	1.355424	-1.087214
C	-3.635061	1.993751	-0.940759
C	-4.667335	1.368903	-0.230187
C	-4.490256	0.104573	0.344867
C	-3.249157	-0.498615	0.186943
H	-1.595783	1.840585	-1.654039
H	-3.810643	2.952067	-1.419705
H	-5.625346	1.868644	-0.129154
H	-5.296502	-0.382076	0.882533
N	-2.851612	-1.754858	0.638075
C	-3.702398	-2.672471	1.368819
H	-4.041795	-2.211242	2.299882
H	-4.568793	-2.952813	0.763768
H	-3.113823	-3.560588	1.595967
C	-1.561213	-2.029403	0.251692
O	-0.967007	-3.070678	0.477843
C	-0.991717	-0.801406	-0.478844
C	-0.542983	-1.236635	-1.880013

C	0.163463	-0.285389	0.422548
H	-1.377690	-1.693172	-2.420281
H	-0.179245	-0.390416	-2.463554
H	0.266094	-1.967009	-1.796449
H	-0.191440	-0.314269	1.460238
H	0.975326	-1.022407	0.358050
C	5.485111	-1.067224	0.630757
C	4.444433	-0.928488	-0.281924
C	3.701089	0.257463	-0.330645
C	4.018288	1.306817	0.539860
C	5.069970	1.172325	1.444043
C	5.799482	-0.015349	1.493951
H	6.051577	-1.992011	0.670827
H	4.189745	-1.735237	-0.962181
H	3.461784	2.238435	0.508163
H	5.317789	1.993312	2.108802
H	6.612657	-0.121775	2.205082
C	2.595018	0.364836	-1.335939
C	0.703498	1.129888	0.188697
C	1.491595	1.378583	-1.110505
H	1.353729	1.355969	1.039786
H	0.847891	1.354229	-1.991987
H	1.930180	2.382070	-1.063510
O	2.574192	-0.377599	-2.305260
H	-0.113971	1.856276	0.239897
H	-3.100597	2.686170	0.795359
O	-2.677055	3.128299	1.598584
H	-3.083742	3.999428	1.775067
H	-2.730914	2.563164	2.394467

B-INT-Ra1

C	2.663460	0.996345	0.006637
C	1.285356	1.212901	-0.013548
C	0.396085	0.135102	-0.022862
C	0.912562	-1.165894	-0.010666
C	2.288818	-1.384433	0.010662
C	3.170076	-0.302471	0.018851
H	3.340905	1.844865	0.012167
H	0.889935	2.223221	-0.022745
H	0.242162	-2.021766	-0.014959
H	2.672257	-2.400066	0.021154
H	4.242137	-0.472102	0.034548
C	-1.098682	0.382533	-0.045136
C	-3.079168	-0.616583	0.034240
C	-2.001560	-0.324780	1.085424
H	-3.561443	-1.593140	0.086740
H	-3.838478	0.165841	0.001550
H	-2.231773	0.315970	1.936982
H	-1.473732	-1.224224	1.410127
O	-1.460250	1.671054	-0.033702
C	-2.007296	-0.427293	-1.051831
H	-1.516284	-1.367620	-1.310666
H	-2.261596	0.128020	-1.955909

B-INT-TS1

C	-2.667322	0.971926	-0.118355
C	-1.299884	1.215073	-0.007110
C	-0.397326	0.154912	0.129007
C	-0.888805	-1.155798	0.144669
C	-2.256369	-1.400004	0.030789
C	-3.150105	-0.336890	-0.099671
H	-3.357058	1.804526	-0.217788
H	-0.915045	2.229358	-0.019213
H	-0.211123	-1.999907	0.234329
H	-2.622671	-2.421742	0.042775
H	-4.215204	-0.527673	-0.186739
C	1.077587	0.471274	0.250744
C	3.034509	-0.656812	-0.189178
C	2.007890	-0.267736	-1.228081
H	3.454191	-1.657205	-0.313263
H	3.842680	0.073607	-0.135431
H	2.202958	0.517592	-1.952653
H	1.338616	-1.053280	-1.575078
O	1.430056	1.694772	0.207237
C	2.045392	-0.500938	0.979076
H	1.565191	-1.448541	1.225324
H	2.443609	-0.044940	1.888496

B-INT-Ra2

C	2.730230	0.708055	0.472660
C	1.432622	1.183824	0.323510
C	0.428208	0.359834	-0.202885
C	0.745753	-0.951370	-0.577891
C	2.046542	-1.429337	-0.424939
C	3.038904	-0.602202	0.098625
H	3.501040	1.354279	0.880179
H	1.177145	2.198181	0.611799
H	-0.012105	-1.612140	-0.983580

H	2.283061	-2.448039	-0.714602
H	4.050957	-0.977134	0.215424
C	-0.954229	0.926233	-0.327586
C	-2.920099	-0.527131	0.278895
C	-2.171062	-1.532390	1.086058
H	-3.803050	-0.990018	-0.175318
H	-3.269834	0.293258	0.914743
H	-1.643636	-1.247889	1.988664
H	-2.040982	-2.543321	0.717339
O	-1.184572	2.063541	0.059516
C	-2.091205	0.094511	-0.881215
H	-1.745781	-0.690538	-1.555873
H	-2.734225	0.774868	-1.446306

B-TS-Ra2

C	4.342704	-0.241319	1.054246
C	5.029892	-1.356009	1.532954
C	5.598701	-2.265262	0.641528
C	5.478089	-2.055974	-0.733843
C	4.777617	-0.953666	-1.216267
C	4.199639	-0.050297	-0.321375
H	3.905689	0.476773	1.742296
H	5.128017	-1.507388	2.603350
H	6.136267	-3.131083	1.014758
H	5.917719	-2.760500	-1.432764
H	4.654779	-0.797939	-2.284494
N	3.482134	1.078718	-0.821654
C	4.268138	2.122890	-1.478532
H	4.685928	2.822042	-0.745027
H	5.082606	1.651740	-2.028496
H	3.631187	2.676571	-2.168020
C	2.248700	1.435832	-0.328187
O	1.869893	2.610901	-0.397559
C	1.359175	0.367570	0.212057
C	1.411453	-1.046590	-0.313201
C	-1.417040	1.429795	-0.289976
H	1.708853	-1.070634	-1.366288
H	2.120508	-1.675069	0.236916
H	0.419955	-1.500411	-0.223442
H	-0.810575	2.101167	-0.887364
H	-1.600698	0.449785	-0.725056
C	-5.428553	-1.924189	-1.367374
C	-4.384963	-1.690320	-0.478633
C	-4.358967	-0.519208	0.289740
C	-5.395189	0.413238	0.160294
C	-6.446110	0.173132	-0.723194
C	-6.461673	-0.991935	-1.489434
H	-5.438761	-2.829129	-1.966190
H	-3.575267	-2.405091	-0.370554
H	-5.399400	1.322059	0.753658
H	-7.250107	0.896128	-0.813803
H	-7.277400	-1.174039	-2.182121
C	-3.210232	-0.309682	1.227289
C	-2.454731	2.022650	0.610982
C	-2.920540	1.081816	1.744390
H	-3.329071	2.316935	0.008870
H	-2.140804	0.983683	2.502795
H	-3.807664	1.502874	2.227915
O	-2.478477	-1.244298	1.520040
H	-2.077686	2.945345	1.064336
C	0.378644	0.763637	1.065735
H	-0.270250	0.022522	1.524891
H	0.391376	1.763161	1.490374

B-INT-Ra3

C	4.085782	-0.252317	1.039136
C	4.721197	-1.361667	1.595990
C	5.325564	-2.311477	0.773723
C	5.290458	-2.147963	-0.612677
C	4.641923	-1.051325	-1.173954
C	4.029639	-0.103386	-0.349155
H	3.629112	0.498023	1.679102
H	4.752385	-1.475009	2.675098
H	5.823255	-3.171828	1.209311
H	5.757342	-2.883486	-1.260218
H	4.588367	-0.933494	-2.252638
N	3.376066	1.021773	-0.934460
C	4.227726	1.994346	-1.618688
H	4.689500	2.686732	-0.904741
H	5.010447	1.458960	-2.155616
H	3.627435	2.567961	-2.324763
C	2.173601	1.493156	-0.436336
O	1.903866	2.703849	-0.496603
C	1.200086	0.537779	0.087885
C	1.160971	-0.910353	-0.279380
C	-1.135653	1.463413	0.038974
H	1.729659	-1.130743	-1.185048
H	1.565562	-1.536586	0.528931

H	0.120282	-1.220911	-0.429827
H	-0.819319	2.230204	-0.675522
H	-1.447495	0.590804	-0.552249
C	-5.122067	-1.891695	-1.513795
C	-4.130674	-1.688923	-0.559413
C	-4.164197	-0.557720	0.266232
C	-5.205768	0.366944	0.125431
C	-6.204475	0.157862	-0.824095
C	-6.161729	-0.968119	-1.645592
H	-5.087505	-2.766865	-2.154542
H	-3.317525	-2.398535	-0.442691
H	-5.253527	1.247233	0.758498
H	-7.012921	0.874775	-0.922923
H	-6.936983	-1.126403	-2.388692
C	-3.075726	-0.382029	1.281118
C	-2.321935	1.987462	0.852316
C	-2.850896	0.982012	1.896125
H	-3.128113	2.262140	0.163877
H	-2.131731	0.851247	2.707862
H	-3.779299	1.361623	2.334367
O	-2.344139	-1.320202	1.562705
H	-2.031875	2.901997	1.381649
C	0.077153	1.079975	0.910525
H	-0.225298	0.309054	1.629906
H	0.402081	1.965676	1.467055

B-TS-Ra3

C	-3.235065	-0.397699	-0.951038
C	-3.959150	-1.584097	-0.671302
C	-5.049205	-1.557018	0.193516
C	-5.487573	-0.352754	0.755158
C	-4.776163	0.835979	0.518349
C	-3.668388	0.801999	-0.307633
H	-3.684570	-2.506625	-1.173560
H	-5.596619	-2.472865	0.395271
H	-6.361244	-0.336518	1.397842
H	-5.062839	1.758711	1.013926
N	-2.725393	1.840604	-0.409526
C	-3.074823	3.243183	-0.265726
H	-3.961290	3.458761	-0.864450
H	-3.273593	3.495947	0.781475
H	-2.236474	3.840643	-0.621918
C	-1.421075	1.409537	-0.347303
O	-0.459378	2.169525	-0.430703
C	-1.297909	-0.078225	-0.135178
C	-1.457052	-0.505158	1.301102
C	-0.265437	-0.740783	-1.010679
H	-2.276296	0.037681	1.783472
H	-1.683216	-1.575510	1.357684
H	-0.532534	-0.321942	1.862275
H	-0.536305	-0.549184	-2.058229
H	0.697175	-0.224562	-0.874751
C	5.175558	1.913211	0.411337
C	4.031517	1.202825	0.758831
C	3.846799	-0.108977	0.304482
C	4.826358	-0.703204	-0.500003
C	5.977279	0.006133	-0.839982
C	6.151368	1.313848	-0.388179
H	5.308950	2.931497	0.762226
H	3.265723	1.652564	1.382662
H	4.707334	-1.720507	-0.858236
H	6.736266	-0.462403	-1.458080
H	7.045875	1.866326	-0.658415
C	2.598340	-0.832853	0.714862
C	-0.097614	-2.252720	-0.805816
C	0.867541	-2.681523	0.309485
H	0.269641	-2.684452	-1.744535
H	0.520027	-2.340340	1.288229
H	0.879782	-3.775522	0.338834
O	1.858079	-0.342806	1.553103
H	-1.081995	-2.704441	-0.627927
H	-2.719313	-0.318210	-1.906718
C	2.298778	-2.183905	0.091281
H	2.538330	-2.150769	-0.978333
H	3.020838	-2.883054	0.535360

B-INT-Ra4

C	-2.857762	-0.418371	-0.608109
C	-3.690433	-1.594314	-0.194605
C	-5.039725	-1.455908	-0.025607
C	-5.681925	-0.187166	-0.068937
C	-4.906959	0.998468	-0.137242
C	-3.556967	0.876341	-0.304033
H	-3.230304	-2.576054	-0.141162
H	-5.643442	-2.337290	0.172758
H	-6.756562	-0.120643	0.054897
H	-5.370548	1.969846	0.005569
N	-2.594730	1.868019	-0.208895

C	-2.896584	3.278270	-0.063323
H	-3.507664	3.615249	-0.903662
H	-3.436058	3.456166	0.872071
H	-1.954079	3.824159	-0.050246
C	-1.331855	1.341131	-0.065095
O	-0.315097	2.004782	0.072549
C	-1.430130	-0.191251	-0.031161
C	-1.359974	-0.601015	1.448307
C	-0.298126	-0.781654	-0.882563
H	-2.144387	-0.097651	2.024614
H	-1.515000	-1.679225	1.548936
H	-0.382346	-0.348358	1.866598
H	-0.495937	-0.504281	-1.925367
H	0.628629	-0.263912	-0.608451
C	4.922472	2.009547	0.327463
C	3.892963	1.181146	0.761775
C	3.760058	-0.113363	0.243693
C	4.676592	-0.571173	-0.710337
C	5.715900	0.254801	-1.134872
C	5.837069	1.545478	-0.620794
H	5.015024	3.014495	0.726613
H	3.176507	1.525049	1.501144
H	4.597672	-1.573977	-1.117348
H	6.428830	-0.109892	-1.867127
H	6.643258	2.189748	-0.957639
C	2.638112	-0.970726	0.748545
C	-0.109165	-2.304780	-0.791562
C	0.898685	-2.793946	0.259996
H	0.235011	-2.666971	-1.767458
H	0.586125	-2.518571	1.270829
H	0.923115	-3.887276	0.219993
O	2.019085	-0.637267	1.746919
H	-1.075459	-2.792897	-0.618326
H	-2.731846	-0.457425	-1.710571
C	2.314860	-2.261039	0.015975
H	2.494895	-2.131332	-1.056679
H	3.063136	-2.988071	0.361455

B-INT-Ca1

C	-3.720937	-0.447041	-0.993949
C	-4.629261	-1.471817	-0.713178
C	-5.561222	-1.312884	0.306162
C	-5.594013	-0.125138	1.046633
C	-4.677737	0.889591	0.795691
C	-3.731167	0.714101	-0.216678
H	-4.616196	-2.376267	-1.311544
H	-6.273695	-2.102539	0.519200
H	-6.328194	0.001605	1.835113
H	-4.675740	1.796667	1.391720
N	-2.723680	1.701613	-0.426845
C	-3.073029	3.111526	-0.613047
H	-4.008011	3.166093	-1.169286
H	-3.180276	3.610976	0.352933
H	-2.274197	3.590958	-1.178629
C	-1.434590	1.337102	-0.389883
O	-0.451436	2.048519	-0.554881
C	-1.123706	-0.101546	-0.022826
C	-1.337234	-0.513021	1.352959
C	-0.335255	-0.867541	-0.987285
H	-2.075801	0.081790	1.887510
H	-1.511439	-1.588716	1.441043
H	-0.331140	-0.332691	1.791802
H	-0.756267	-0.702127	-1.987749
H	0.590124	-0.258862	-1.030289
C	5.388832	1.883364	0.472834
C	4.176232	1.242086	0.700027
C	3.975030	-0.069008	0.250177
C	5.003561	-0.731685	-0.431239
C	6.218633	-0.087978	-0.656910
C	6.411989	1.217383	-0.206119
H	5.538870	2.899491	0.822833
H	3.370822	1.745254	1.224958
H	4.869213	-1.747068	-0.789131
H	7.013045	-0.605744	-1.184172
H	7.359556	1.716249	-0.383940
C	2.651881	-0.713176	0.513961
C	-0.054208	-2.345433	-0.714197
C	1.019285	-2.678971	0.331737
H	0.256805	-2.779199	-1.669577
H	0.723598	-2.355012	1.333191
H	1.088085	-3.769568	0.369438
O	1.783573	-0.105389	1.126337
H	-0.994889	-2.842827	-0.449687
H	-3.056338	-0.526616	-1.848381
C	2.409067	-2.124057	0.015066
H	2.609138	-2.156242	-1.064348
H	3.178679	-2.757087	0.473634

B-TS-Ca1

C	-3.553599	-0.537536	-0.898572
C	-4.212707	-1.712530	-0.502495
C	-5.132847	-1.669200	0.532645
C	-5.425305	-0.448023	1.162964
C	-4.764942	0.719064	0.803154
C	-3.804730	0.659614	-0.209492
H	-4.019924	-2.638606	-1.033468
H	-5.650334	-2.570841	0.841244
H	-6.158679	-0.418049	1.962163
H	-4.951979	1.650582	1.326888
N	-2.950467	1.754131	-0.472599
C	-3.428806	3.131386	-0.573032
H	-4.392247	3.132587	-1.081641
H	-3.525010	3.578796	0.419323
H	-2.701435	3.697981	-1.154324
C	-1.632841	1.475560	-0.507716
O	-0.714060	2.245065	-0.740483
C	-1.261713	0.048729	-0.131711
C	-1.353896	-0.323419	1.283083
C	-0.391024	-0.668553	-1.074458
H	-2.091202	0.252422	1.840474
H	-1.499492	-1.399417	1.410231
H	-0.338914	-0.100709	1.665841
H	-0.707030	-0.458449	-2.100924
H	0.541305	-0.079294	-0.965239
C	5.564446	1.745697	0.667965
C	4.303448	1.178468	0.814154
C	4.021954	-0.073866	0.253322
C	5.018588	-0.751503	-0.459488
C	6.281401	-0.180457	-0.607152
C	6.555149	1.065498	-0.043899
H	5.776502	2.715506	1.106338
H	3.521990	1.694092	1.362516
H	4.822230	-1.721544	-0.904157
H	7.050565	-0.708610	-1.160901
H	7.539838	1.507383	-0.160122
C	2.649631	-0.639121	0.439170
C	-0.134941	-2.160058	-0.834120
C	0.933981	-2.531877	0.203362
H	0.166553	-2.582664	-1.797451
H	0.652127	-2.204635	1.207776
H	0.971450	-3.624332	0.233871
O	1.797232	0.005771	1.035501
H	-1.083184	-2.646694	-0.573653
H	-2.977000	-0.523381	-1.817526
C	2.340371	-2.016666	-0.114199
H	2.520299	-2.004531	-1.198054
H	3.091755	-2.700445	0.297941

B-INT-Ca2

C	-2.946168	-0.463728	-0.484818
C	-3.740010	-1.638719	-0.032635
C	-5.070359	-1.519572	0.162062
C	-5.721347	-0.238849	0.017825
C	-5.050100	0.931155	-0.229720
C	-3.646808	0.839758	-0.320000
H	-3.250965	-2.605594	0.030064
H	-5.673560	-2.381363	0.420737
H	-6.797812	-0.197584	0.155347
H	-5.559860	1.886906	-0.247101
N	-2.776489	1.835977	-0.244619
C	-3.096613	3.260035	-0.209628
H	-3.674689	3.525395	-1.095030
H	-3.659353	3.487240	0.697330
H	-2.152486	3.801816	-0.205537
C	-1.442366	1.340080	-0.107602
O	-0.485373	2.062590	-0.051039
C	-1.496999	-0.182556	-0.005033
C	-1.352039	-0.543544	1.483790
C	-0.389495	-0.768776	-0.897459
H	-2.118943	-0.044799	2.085286
H	-1.471936	-1.622842	1.610696
H	-0.360929	-0.256984	1.841471
H	-0.640308	-0.530856	-1.937401
H	0.528349	-0.214540	-0.675298
C	5.267003	1.888801	0.458088
C	4.137644	1.156350	0.807214
C	3.890015	-0.089182	0.216251
C	4.791234	-0.594646	-0.728608
C	5.926094	0.137723	-1.073783
C	6.163752	1.378694	-0.483611
H	5.449563	2.855207	0.916935
H	3.431718	1.537516	1.537880
H	4.623814	-1.560088	-1.194735
H	6.623587	-0.261130	-1.803019
H	7.046427	1.948517	-0.756610
C	2.659017	-0.837195	0.633290

C	-0.146064	-2.280700	-0.762725
C	0.931289	-2.699785	0.249218
H	0.157105	-2.660408	-1.744721
H	0.658190	-2.404897	1.265995
H	0.986857	-3.792303	0.238571
O	1.964614	-0.408422	1.541679
H	-1.082449	-2.798788	-0.524346
H	-2.914660	-0.589528	-1.588469
C	2.318078	-2.135590	-0.075527
H	2.438722	-1.995661	-1.156900
H	3.100554	-2.848928	0.216524

B-CMW

C	2.861196	-0.527121	0.348579
C	3.598336	-1.789623	0.088299
C	4.922107	-1.755838	-0.176110
C	5.616315	-0.494829	-0.289173
C	4.992326	0.723633	-0.224615
C	3.590962	0.702463	-0.059848
H	3.081446	-2.734745	0.219891
H	5.488868	-2.671506	-0.295577
H	6.686383	-0.519019	-0.473105
H	5.529682	1.649488	-0.390478
N	2.750488	1.705370	-0.249837
C	3.106459	3.101589	-0.471408
H	3.684950	3.469426	0.377502
H	3.681986	3.193806	-1.393899
H	2.176544	3.661193	-0.556756
C	1.394561	1.252560	-0.188037
O	0.457365	2.000139	-0.254232
C	1.406306	-0.272321	-0.126942
C	1.235410	-0.769372	-1.575700
C	0.303340	-0.760682	0.824198
H	1.993665	-0.334108	-2.234735
H	1.348621	-1.856598	-1.605280
H	0.239774	-0.509064	-1.941883
H	0.592927	-0.466770	1.837484
H	-0.601740	-0.191459	0.585793
C	-5.461285	1.825041	-0.608434
C	-4.318556	1.095013	-0.917888
C	-4.052202	-0.114425	-0.263701
C	-4.948158	-0.585587	0.703559
C	-6.095647	0.143928	1.009468
C	-6.352021	1.349056	0.356436
H	-5.659283	2.763479	-1.116282
H	-3.617377	1.450989	-1.665776
H	-4.765838	-1.522548	1.219275
H	-6.788171	-0.229363	1.756754
H	-7.244554	1.917385	0.598755
C	-2.808828	-0.866599	-0.635382
C	0.006457	-2.269607	0.793642
C	-1.093577	-2.727714	-0.175785
H	-0.298285	-2.570420	1.802410
H	-0.832648	-2.497313	-1.212090
H	-1.165889	-3.816950	-0.101108
O	-2.109432	-0.473757	-1.555953
H	0.921847	-2.835136	0.584923
H	2.845403	-0.433071	1.457418
C	-2.467399	-2.127404	0.137043
H	-2.568156	-1.924271	1.210645
H	-3.262546	-2.847046	-0.099509
O	2.000787	1.407436	2.556618
H	1.180658	1.696674	2.975233
H	2.691929	1.955854	2.948585

B-Ts-Ca2

C	2.846577	-0.372303	-0.119313
C	3.571940	-1.536108	-0.550585
C	4.944360	-1.544959	-0.473725
C	5.638913	-0.373779	-0.087713
C	4.996415	0.823033	0.186017
C	3.601538	0.832319	0.086782
H	3.030326	-2.433456	-0.833451
H	5.500625	-2.442293	-0.715892
H	6.722431	-0.406816	-0.028944
H	5.554475	1.723416	0.414135
N	2.773048	1.908406	0.164166
C	3.189560	3.267788	0.473366
H	3.660306	3.298521	1.457808
H	3.886848	3.628535	-0.285738
H	2.295597	3.889491	0.473726
C	1.457841	1.549913	-0.142782
O	0.530498	2.328077	-0.163328
C	1.403848	0.045488	-0.431917
C	1.096655	-0.149052	-1.925483
C	0.319990	-0.562617	0.482044
H	1.825960	0.382782	-2.544136
H	1.146324	-1.211204	-2.180682

H	0.090310	0.217032	-2.144295
H	0.602237	-0.367013	1.522721
H	-0.597372	0.008233	0.306706
C	-5.870738	1.703996	-0.167126
C	-4.681353	1.157463	-0.637756
C	-4.229813	-0.077581	-0.154462
C	-4.988385	-0.758812	0.805090
C	-6.180744	-0.211650	1.274697
C	-6.622171	1.019405	0.790732
H	-6.214587	2.661432	-0.545130
H	-4.088520	1.677164	-1.383641
H	-4.661477	-1.718151	1.191677
H	-6.762798	-0.746351	2.018162
H	-7.550696	1.444823	1.158664
C	-2.942977	-0.631804	-0.691513
C	0.062668	-2.065603	0.284528
C	-1.088742	-2.421426	-0.667089
H	-0.161172	-2.509581	1.261535
H	-0.921601	-1.998046	-1.661373
H	-1.103123	-3.509383	-0.781045
O	-2.324233	-0.023822	-1.550634
H	0.975135	-2.566224	-0.061131
H	2.914520	-0.757906	1.126515
C	-2.460733	-1.968552	-0.157970
H	-2.475414	-1.932562	0.938856
H	-3.232350	-2.698732	-0.435035
O	3.082060	-1.155286	2.436084
H	2.771578	-0.520266	3.099986
H	2.686616	-2.015009	2.648922

TM2

C	2.743214	-0.168470	-0.455318
C	3.533637	-1.293734	-0.608219
C	4.875704	-1.255466	-0.173689
C	5.406461	-0.082077	0.375256
C	4.627905	1.074930	0.502327
C	3.308785	1.006747	0.072650
H	3.140527	-2.203254	-1.051332
H	5.507792	-2.128141	-0.298503
H	6.440620	-0.065898	0.702771
H	5.046052	1.986034	0.915839
N	2.361922	2.028342	0.072892
C	2.619315	3.385833	0.509626
H	2.904883	3.396064	1.564583
H	3.418148	3.832451	-0.088536
H	1.701058	3.956287	0.375176
C	1.172296	1.594775	-0.463157
O	0.183492	2.290779	-0.628502
C	1.287554	0.093088	-0.767116
C	0.922426	-0.187637	-2.226993
C	0.345069	-0.607137	0.249609
H	1.548860	0.405023	-2.899791
H	1.083821	-1.244748	-2.457349
H	-0.129277	0.051091	-2.402168
H	0.735025	-0.395432	1.252609
H	-0.626748	-0.104272	0.185009
C	-5.483627	1.763505	0.187943
C	-4.427153	1.115609	-0.443488
C	-4.049445	-0.173976	-0.047946
C	-4.748092	-0.809589	0.985549
C	-5.813069	-0.163514	1.611039
C	-6.179265	1.122846	1.215909
H	-5.766603	2.765264	-0.118706
H	-3.878671	1.598120	-1.245976
H	-4.477538	-1.811135	1.303049
H	-6.354810	-0.664254	2.406693
H	-7.005408	1.626401	1.708012
C	-2.906038	-0.831815	-0.762362
C	0.176415	-2.124150	0.075138
C	-1.011435	-2.569471	-0.791176
H	0.047226	-2.569155	1.068853
H	-0.921381	-2.188244	-1.811901
H	-0.987084	-3.661430	-0.854916
O	-2.444536	-0.323570	-1.771886
H	1.096996	-2.562656	-0.325574
H	4.136018	-1.461313	1.633961
C	-2.366750	-2.142426	-0.217848
H	-2.324637	-2.088084	0.876288
H	-3.134505	-2.894197	-0.446773
O	3.611845	-1.521727	2.493522
H	3.055865	-2.326255	2.513035
H	4.200459	-1.497736	3.273918

C-INT-Ra1

C	-2.605317	-1.390064	0.002649
C	-1.227823	-1.180560	-0.006408
C	-0.700554	0.116927	-0.010270
C	-1.583550	1.199055	-0.006387

C	-2.964047	0.991647	0.001901
C	-3.480319	-0.302640	0.006681
H	-2.994845	-2.403496	0.007191
H	-0.563554	-2.041162	-0.007991
H	-1.184850	2.207890	-0.009336
H	-3.634815	1.845488	0.004247
H	-4.553567	-0.465168	0.013409
C	0.805193	0.349401	-0.023785
C	3.027845	-0.382654	0.778780
C	1.563661	-0.333846	-1.194217
H	3.453059	-1.321407	1.142854
H	3.621531	0.428196	1.206922
H	1.365607	0.177769	-2.140261
H	1.189803	-1.359206	-1.279777
O	1.143292	1.674908	-0.003692
C	1.555361	-0.266858	1.208581
H	1.103934	-1.248137	1.382250
H	1.395772	0.339687	2.103745
C	3.036172	-0.308722	-0.769319
H	3.592846	-1.132096	-1.223498
H	3.503014	0.622255	-1.099457

C-INT-TS1

C	2.394859	-1.483122	-0.172494
C	1.055614	-1.113294	-0.271231
C	0.677916	0.228624	-0.139307
C	1.664713	1.190979	0.095954
C	3.005902	0.822759	0.188992
C	3.375098	-0.515343	0.054291
H	2.673296	-2.527725	-0.271273
H	0.305151	-1.882700	-0.431689
H	1.366159	2.229227	0.198687
H	3.762973	1.581277	0.362932
H	4.419085	-0.804211	0.125636
C	-0.764971	0.680106	-0.246035
C	-3.031467	-0.280491	-0.559625
C	-1.593448	-0.186896	1.418315
H	-3.707956	-0.876431	-1.177480
H	-3.517891	0.677507	-0.346002
H	-1.902337	0.707011	1.952768
H	-0.743731	-0.699664	1.860402
O	-1.031525	1.888964	0.020521
C	-1.688973	-0.035444	-1.242497
H	-1.257261	-0.985761	-1.567900
H	-1.775178	0.610732	-2.121906
C	-2.677818	-0.987360	0.755351
H	-2.326055	-2.002604	0.543784
H	-3.548608	-1.061479	1.417590

C-INT-Ra2

C	2.296752	-1.491503	-0.454817
C	1.015411	-0.953563	-0.560756
C	0.772426	0.368098	-0.169257
C	1.828530	1.143794	0.325006
C	3.110940	0.611433	0.415721
C	3.345838	-0.708913	0.027115
H	2.475247	-2.521060	-0.747883
H	0.207227	-1.579284	-0.925488
H	1.629041	2.166899	0.627689
H	3.926900	1.222823	0.787752
H	4.344782	-1.127340	0.101501
C	-0.590393	0.989365	-0.239027
C	-2.968463	0.122122	-0.482762
C	-1.924342	-1.076410	1.483952
H	-3.752094	0.015429	-1.238892
H	-3.245574	0.969504	0.154766
H	-1.927095	-0.204061	2.129829
H	-1.379374	-1.950567	1.819821
O	-0.841744	1.982777	0.428314
C	-1.643181	0.442588	-1.186450
H	-1.286160	-0.428183	-1.740208
H	-1.804418	1.241281	-1.920489
C	-2.895256	-1.161512	0.354230
H	-2.639123	-2.007413	-0.295666
H	-3.904987	-1.373234	0.743025

C-TS-Ra2

C	3.070004	0.910300	-0.916498
C	2.718533	2.252133	-1.057627
C	3.444892	3.238207	-0.390975
C	4.525232	2.877762	0.417935
C	4.866124	1.537272	0.577421
C	4.128592	0.551042	-0.080683
H	2.520784	0.134345	-1.441848
H	1.882362	2.524525	-1.694310
H	3.174773	4.283315	-0.502978
H	5.094037	3.642481	0.937292
H	5.686231	1.246107	1.227685

N	4.469744	-0.825561	0.088824
C	5.712031	-1.275052	-0.539375
H	5.564792	-1.470046	-1.608053
H	6.466305	-0.497570	-0.417522
H	6.049466	-2.192082	-0.057167
C	3.505895	-1.776942	0.334006
O	3.679426	-2.944671	-0.031835
C	2.298664	-1.378185	1.117325
C	2.333848	-0.246673	2.113285
C	-1.436545	-1.573432	-0.587128
H	3.327975	-0.126816	2.552700
H	2.061622	0.713711	1.657920
H	1.621599	-0.447775	2.917953
H	-1.335723	-2.665642	-0.616305
H	-1.882317	-1.324919	0.385048
C	-6.160176	0.423355	1.799815
C	-4.888029	0.743547	1.338076
C	-4.543392	0.519235	-0.001089
C	-5.492198	-0.029197	-0.872618
C	-6.769446	-0.341977	-0.411513
C	-7.103728	-0.118604	0.923815
H	-6.418392	0.595363	2.839836
H	-4.144569	1.167328	2.005615
H	-5.248854	-0.206966	-1.915134
H	-7.501525	-0.759677	-1.094842
H	-8.097886	-0.366702	1.282482
C	-3.162736	0.888123	-0.454900
C	-2.401863	-1.160138	-1.715978
C	-2.653141	0.358382	-1.777202
H	-3.349869	-1.693624	-1.585420
H	-1.722152	0.887364	-1.996918
H	-3.365238	0.582945	-2.577418
O	-2.444017	1.569655	0.261618
H	-1.986440	-1.474693	-2.679347
C	-0.087759	-0.936696	-0.707972
H	0.065277	0.061520	-0.308034
H	0.518046	-1.198585	-1.572120
C	1.157706	-2.082624	0.892322
H	0.302046	-1.958140	1.550261
H	1.171115	-2.955727	0.247925

C-INT-Ra3

C	3.024466	1.017394	-0.822852
C	2.946134	2.404009	-0.948446
C	3.951817	3.214349	-0.423845
C	5.038661	2.630898	0.231010
C	5.111225	1.248289	0.376261
C	4.098536	0.436716	-0.142944
H	2.251911	0.382258	-1.248448
H	2.102734	2.848098	-1.468057
H	3.892633	4.293033	-0.526798
H	5.825518	3.255405	0.642201
H	5.939982	0.791160	0.909609
N	4.184194	-0.979720	0.006370
C	5.261711	-1.654197	-0.717579
H	4.987000	-1.824874	-1.765300
H	6.154944	-1.031233	-0.678352
H	5.465944	-2.616222	-0.247982
C	3.066035	-1.740344	0.301784
O	2.973977	-2.901766	-0.127317
C	2.038676	-1.178978	1.181238
C	2.287137	-0.081210	2.162697
C	-1.520492	-1.744155	-0.229511
H	3.349718	0.107488	2.323200
H	1.825574	0.861677	1.832829
H	1.826545	-0.342168	3.122028
H	-1.488355	-2.839785	-0.185275
H	-2.087417	-1.418546	0.654843
C	-6.121296	0.686530	1.591352
C	-4.802027	0.904741	1.208974
C	-4.383775	0.605849	-0.093942
C	-5.305973	0.087974	-1.011380
C	-6.630646	-0.119514	-0.630998
C	-7.038204	0.175883	0.669513
H	-6.436726	0.913323	2.604751
H	-4.077900	1.303571	1.912204
H	-5.003791	-0.145778	-2.027290
H	-7.342450	-0.513198	-1.349145
H	-8.069102	0.007548	0.965356
C	-2.952391	0.861095	-0.459021
C	-2.260352	-1.329950	-1.504446
C	-2.373152	0.196933	-1.688294
H	-3.260821	-1.775750	-1.500354
H	-1.388361	0.639276	-1.856568
H	-2.989951	0.417672	-2.565370

C-Ts-Ra3

C	3.106785	0.938393	-0.868068

C	2.697825	2.208116	-0.386718
C	3.583751	3.010833	0.325585
C	4.908597	2.609939	0.528280
C	5.339487	1.348701	0.082261
C	4.448591	0.533895	-0.590604
H	1.701451	2.571074	-0.618994
H	3.256338	3.981899	0.684476
H	5.600944	3.258440	1.054477
H	6.343390	0.998239	0.302788
N	4.666916	-0.831020	-0.850202
C	5.985649	-1.389557	-1.094494
H	6.528027	-0.743290	-1.786376
H	6.554302	-1.483188	-0.162756
H	5.861858	-2.377685	-1.536024
C	3.588434	-1.629052	-0.548980
O	3.584700	-2.844896	-0.723051
C	2.433755	-0.863300	0.043990
C	2.581376	-0.595245	1.519194
C	1.081779	-1.241563	-0.504944
H	3.590490	-0.243912	1.757865
H	1.869167	0.169405	1.847427
H	2.393926	-1.506638	2.104038
H	1.132208	-1.201783	-1.600716
H	0.879672	-2.297270	-0.259147
C	-7.095833	-0.623048	-1.022204
C	-6.014342	-0.934747	-0.205202
C	-5.017879	0.016726	0.045456
C	-5.119778	1.288015	-0.531838
C	-6.205764	1.601188	-1.348102
C	-7.192763	0.647524	-1.594392
H	-7.863546	-1.366223	-1.212406
H	-5.924736	-1.916100	0.249303
H	-4.362040	2.042631	-0.348343
H	-6.281318	2.589500	-1.789874
H	-8.037578	0.893951	-2.230015
C	-3.877213	-0.366028	0.943381
C	-0.075975	-0.369752	0.007831
C	-1.609996	0.091856	2.011286
H	-0.825069	-0.277604	-0.785942
H	-2.005543	-0.359229	2.927020
H	-0.978995	0.935753	2.316560
O	-3.862988	-1.462831	1.479282
H	0.291148	0.648623	0.199483
H	2.614949	0.535014	-1.751856
C	-2.773345	0.643509	1.190268
H	-2.428398	1.036242	0.226422
H	-3.234015	1.496891	1.705806
C	-0.740987	-0.928642	1.271786
H	-1.341225	-1.805546	1.002150
H	0.029564	-1.286799	1.963555

C-INT-Ra4

C	2.923719	0.756390	-0.309498
C	2.727573	1.933112	0.599911
C	3.684028	2.906343	0.678745
C	4.955408	2.771406	0.054563
C	5.324575	1.538962	-0.540843
C	4.379614	0.556294	-0.624946
H	1.774736	2.063932	1.102748
H	3.480983	3.803912	1.256400
H	5.682201	3.571822	0.129500
H	6.348072	1.361825	-0.856906
N	4.562238	-0.769554	-0.980581
C	5.811886	-1.308158	-1.480524
H	6.105599	-0.780445	-2.390745
H	6.598965	-1.198263	-0.728289
H	5.659340	-2.364395	-1.698437
C	3.491818	-1.550470	-0.610156
O	3.427274	-2.759774	-0.772388
C	2.446769	-0.670380	0.089956
C	2.605172	-0.906847	1.599144
C	1.052541	-1.040722	-0.434370
H	3.622353	-0.663390	1.925423
H	1.914256	-0.269331	2.158925
H	2.398084	-1.952192	1.845859
H	1.047046	-0.853938	-1.515154
H	0.919656	-2.122689	-0.308637
C	-6.819818	-0.406330	-1.501881
C	-5.826310	-0.870557	-0.646443
C	-4.935007	0.025828	-0.043653
C	-5.054028	1.395606	-0.306518
C	-6.053310	1.860979	-1.159582
C	-6.934667	0.961808	-1.758877
H	-7.505374	-1.107130	-1.967549
H	-5.725407	-1.930178	-0.434644
H	-4.376774	2.108044	0.153013
H	-6.142624	2.924491	-1.355892
H	-7.710034	1.325841	-2.425800

C	-3.885410	-0.520573	0.880019
C	-0.118422	-0.297554	0.231582
C	-1.733802	-0.259427	2.225181
H	-0.866217	-0.067439	-0.535103
H	-2.170651	-0.895070	3.002345
H	-1.150379	0.515773	2.737237
O	-3.883927	-1.706237	1.171281
H	0.217926	0.673065	0.619589
H	2.419139	0.980896	-1.272984
C	-2.857593	0.432444	1.456573
H	-2.458522	1.057359	0.649601
H	-3.401265	1.120655	2.118106
C	-0.787150	-1.094953	1.357654
H	-1.329736	-1.940476	0.918856
H	-0.019325	-1.526927	2.009239

C-INT-Ca1

C	4.005017	1.881934	-1.042213
C	4.216448	3.063324	-0.337509
C	4.767061	3.027398	0.946075
C	5.120156	1.810620	1.525041
C	4.926412	0.621192	0.821677
C	4.358172	0.669362	-0.450069
H	3.939883	4.011872	-0.785412
H	4.921922	3.951880	1.492430
H	5.553866	1.780946	2.518807
H	5.225266	-0.332683	1.246811
N	4.100424	-0.558380	-1.155043
C	4.876430	-0.906623	-2.348206
H	4.727344	-0.145460	-3.115727
H	5.932497	-0.963371	-2.080402
H	4.528830	-1.871692	-2.715163
C	3.141060	-1.350296	-0.712451
O	2.713559	-2.425248	-1.139260
C	2.270364	-1.048595	0.451577
C	2.515385	-1.753431	1.713444
C	1.113489	-0.178549	0.235709
H	3.428873	-2.343863	1.705789
H	2.559812	-0.987199	2.502098
H	1.650118	-2.378249	1.966854
H	1.542255	0.787633	0.586818
H	0.936285	-0.032169	-0.835073
C	-6.466896	1.337386	-1.597720
C	-5.527861	0.327962	-1.414700
C	-4.925675	0.139025	-0.164264
C	-5.280348	0.972385	0.903154
C	-6.224808	1.981258	0.720182
C	-6.816884	2.165753	-0.528835
H	-6.926832	1.480113	-2.570335
H	-5.246224	-0.324775	-2.234621
H	-4.831949	0.840684	1.882393
H	-6.497348	2.621221	1.552993
H	-7.551138	2.952686	-0.669943
C	-3.920683	-0.964821	-0.016408
C	-0.165328	-0.496586	1.013110
C	-2.085061	-2.163267	1.281850
H	-0.812464	0.380599	0.930748
H	-2.473279	-3.105218	0.883185
H	-1.765961	-2.359000	2.312129
O	-3.698122	-1.720556	-0.948825
H	0.057640	-0.620098	2.079091
H	3.554813	1.892864	-2.030336
C	-3.214586	-1.136254	1.315345
H	-2.858770	-0.159979	1.662201
H	-3.978799	-1.442274	2.042411
C	-0.867697	-1.737994	0.455365
H	-1.166465	-1.548064	-0.581722
H	-0.161617	-2.578396	0.423028

C-Ts-Ca1

C	-3.255574	-0.712211	-0.949774
C	-2.837747	-2.048338	-0.873637
C	-3.501925	-2.928203	-0.031762
C	-4.599258	-2.486136	0.723731
C	-5.010900	-1.159901	0.678068
C	-4.313984	-0.272686	-0.144300
H	-2.021257	-2.393577	-1.500310
H	-3.190337	-3.965237	0.026895
H	-5.122068	-3.183070	1.370332
H	-5.830054	-0.807042	1.296093
N	-4.570414	1.118213	-0.113893
C	-5.920312	1.678765	-0.166789
H	-6.539499	1.042426	-0.797543
H	-6.346724	1.746348	0.836867
H	-5.853748	2.677652	-0.598541
C	-3.502394	1.919780	0.025782
O	-3.471751	3.141813	0.018777
C	-2.178868	1.259417	0.362045

C	-2.054045	0.741398	1.728579
C	-0.992835	1.615021	-0.436175
H	-2.949162	0.235086	2.091310
H	-1.146037	0.162337	1.889417
H	-1.944013	1.668947	2.324099
H	-1.277559	2.304926	-1.231861
H	-0.329021	2.141105	0.268609
C	6.877491	0.581826	1.267214
C	5.626284	-0.023357	1.311946
C	4.878678	-0.191563	0.139843
C	5.402092	0.252333	-1.080325
C	6.657331	0.856396	-1.124899
C	7.394595	1.022750	0.046838
H	7.450463	0.710363	2.179966
H	5.211566	-0.373376	2.251710
H	4.842440	0.128890	-2.001705
H	7.057949	1.197679	-2.073869
H	8.371413	1.495070	0.009528
C	3.535971	-0.852108	0.238866
C	-0.153242	0.450365	-1.042664
C	1.320749	-1.591468	-0.762226
H	0.687548	0.955256	-1.526756
H	1.426693	-2.483239	-0.138333
H	0.888133	-1.917039	-1.715471
O	3.132627	-1.267086	1.313612
H	-0.733924	-0.016751	-1.844326
H	-2.864622	-0.052109	-1.718783
C	2.707579	-1.009661	-1.022982
H	2.651084	-0.038511	-1.529024
H	3.274609	-1.660003	-1.701622
C	0.356437	-0.613767	-0.075575
H	0.861547	-0.143638	0.777267
H	-0.486267	-1.189711	0.323356

C-INT-Ca2

C	3.199637	0.627298	-0.416983
C	3.204977	2.021620	0.107378
C	4.304490	2.791254	-0.033953
C	5.511859	2.249246	-0.611653
C	5.660000	0.932098	-0.962156
C	4.557980	0.090816	-0.709495
H	2.282709	2.435601	0.501419
H	4.299246	3.829429	0.275612
H	6.361186	2.915404	-0.730690
H	6.607728	0.537115	-1.307288
N	4.564189	-1.232764	-0.657304
C	5.685558	-2.104024	-0.997026
H	6.048840	-1.855661	-1.994092
H	6.480176	-1.982608	-0.258827
H	5.315741	-3.127617	-0.979048
C	3.343034	-1.729919	-0.104846
O	3.122214	-2.902076	0.028635
C	2.466703	-0.544070	0.291187
C	2.560968	-0.394318	1.818668
C	1.037972	-0.809886	-0.212769
H	3.599509	-0.270767	2.141518
H	1.998459	0.485623	2.141298
H	2.144368	-1.278714	2.307240
H	1.086584	-0.931594	-1.300729
H	0.723466	-1.779390	0.191686
C	-7.099293	-1.113525	-0.815074
C	-6.026335	-1.034696	0.066165
C	-5.118723	0.028660	-0.015780
C	-5.302065	1.015565	-0.991809
C	-6.379249	0.937680	-1.873081
C	-7.276854	-0.125835	-1.786877
H	-7.797560	-1.941540	-0.747044
H	-5.875651	-1.793446	0.827196
H	-4.614484	1.851204	-1.070971
H	-6.516593	1.706967	-2.625882
H	-8.114255	-0.185603	-2.475073
C	-3.979479	0.070636	0.959850
C	-0.004685	0.261565	0.149872
C	-1.789141	1.045933	1.809963
H	-0.691339	0.364423	-0.696339
H	-2.174770	0.848786	2.814845
H	-1.251185	2.000298	1.856437
O	-3.887172	-0.780637	1.829883
H	0.470813	1.244519	0.262692
H	2.750223	0.737013	-1.427395
C	-2.970919	1.199037	0.855056
H	-2.637735	1.279138	-0.186134
H	-3.513638	2.131410	1.060327
C	-0.808327	-0.062769	1.413967
H	-1.354729	-1.001039	1.257498
H	-0.125419	-0.242092	2.251105

C-CMW

C	-2.965736	0.660205	0.421837
C	-2.841895	2.138677	0.337491
C	-3.896699	2.923315	0.645127
C	-5.174655	2.339735	0.979378
C	-5.430873	0.994914	0.922601
C	-4.369718	0.172090	0.487870
H	-1.868874	2.572815	0.132609
H	-3.800425	4.002319	0.659766
H	-5.984184	3.009995	1.252820
H	-6.421227	0.594210	1.102445
N	-4.452945	-1.081393	0.076789
C	-5.619820	-1.949873	0.175184
H	-5.878375	-2.096534	1.225208
H	-6.456592	-1.505324	-0.365426
H	-5.351411	-2.903200	-0.276742
C	-3.207929	-1.522005	-0.470395
O	-3.022144	-2.650158	-0.836453
C	-2.273459	-0.318723	-0.563525
C	-2.379555	0.219950	-2.002277
C	-0.851020	-0.752437	-0.178721
H	-3.413229	0.475296	-2.255883
H	-1.772698	1.124149	-2.102612
H	-2.018819	-0.528384	-2.712422
H	-0.879647	-1.071245	0.867209
H	-0.612941	-1.644083	-0.771716
C	7.001893	-1.283514	0.928074
C	6.008979	-1.108636	-0.030374
C	5.173033	0.014325	0.012557
C	5.347491	0.962699	1.027499
C	6.345551	0.789405	1.985007
C	7.171385	-0.333083	1.937701
H	7.643019	-2.158386	0.891542
H	5.865745	-1.838034	-0.821090
H	4.716681	1.844091	1.076822
H	6.477408	1.530882	2.766132
H	7.945863	-0.468407	2.686137
C	4.119816	0.165385	-1.045743
C	0.251512	0.301701	-0.381553
C	2.017914	1.275272	-1.967026
H	0.964097	0.205133	0.443766
H	2.441175	1.153914	-2.969001
H	1.498083	2.240869	-1.955243
O	4.061057	-0.630400	-1.969579
H	-0.157295	1.317273	-0.300548
H	-2.581498	0.404338	1.434096
C	3.159769	1.335684	-0.954747
H	2.781412	1.409645	0.070643
H	3.755807	2.245097	-1.111535
C	1.000800	0.158685	-1.710555
H	1.506023	-0.814555	-1.728914
H	0.284985	0.148886	-2.539721
O	-2.719859	-1.769701	2.307567
H	-3.365899	-1.791085	3.024592
H	-2.219706	-2.590487	2.394807

C-Ts-Ca2

C	3.003291	0.445621	0.365937
C	2.934436	1.319942	1.506046
C	3.852453	2.335159	1.636554
C	4.927809	2.438767	0.722002
C	5.135230	1.523000	-0.297150
C	4.211218	0.479716	-0.411361
H	2.099367	1.240485	2.195690
H	3.763052	3.053368	2.442406
H	5.638381	3.250487	0.842651
H	6.007900	1.579018	-0.937209
N	4.296787	-0.614022	-1.214561
C	5.339536	-0.850691	-2.201449
H	5.368121	-0.024470	-2.913889
H	6.308849	-0.952921	-1.708731
H	5.093244	-1.776008	-2.720111
C	3.287555	-1.532859	-0.915051
O	3.168267	-2.608975	-1.456588
C	2.375575	-0.940692	0.165497
C	2.494027	-1.785383	1.441465
C	0.945677	-0.937696	-0.417609
H	3.528024	-1.811037	1.797853
H	1.870200	-1.360471	2.232934
H	2.160366	-2.807492	1.242216
H	0.965057	-0.378000	-1.358748
H	0.705760	-1.975085	-0.679426
C	-6.670724	0.018138	-1.767829
C	-5.750785	-0.670551	-0.984470
C	-4.970588	0.012461	-0.043389
C	-5.127027	1.395298	0.107072
C	-6.055482	2.083635	-0.672002
C	-6.825099	1.397394	-1.610682

H	-7.267081	-0.516516	-2.500239
H	-5.620784	-1.742601	-1.092884
H	-4.537142	1.942773	0.835014
H	-6.176947	3.154616	-0.545858
H	-7.544496	1.936202	-2.219536
C	-3.995027	-0.774542	0.781526
C	-0.142285	-0.370781	0.510395
C	-1.932012	-0.911283	2.271087
H	-0.828822	0.229874	-0.095396
H	-2.401142	-1.748718	2.797131
H	-1.389894	-0.325701	3.023387
O	-4.003193	-1.994528	0.738802
H	0.290608	0.323309	1.244535
H	2.332994	1.294332	-0.368603
C	-3.025663	-0.026338	1.676319
H	-2.600744	0.816255	1.120091
H	-3.623216	0.426176	2.479571
C	-0.931865	-1.457764	1.247751
H	-1.457147	-2.074759	0.509210
H	-0.236307	-2.126065	1.768267
O	1.566935	2.121327	-1.165737
H	2.078662	2.613135	-1.826810
H	1.058062	2.772083	-0.657349

TM3

C	-3.162282	-0.195355	0.532972
C	-2.985597	-1.143061	1.526402
C	-3.806060	-2.290942	1.535533
C	-4.805853	-2.451985	0.568475
C	-5.018566	-1.484041	-0.420079
C	-4.193626	-0.366302	-0.407910
H	-2.229263	-1.020166	2.295044
H	-3.683761	-3.034410	2.315903
H	-5.430338	-3.338933	0.587838
H	-5.801757	-1.605414	-1.160278
N	-4.244507	0.734215	-1.260615
C	-5.216941	0.906668	-2.321018
H	-5.112256	0.111014	-3.063043
H	-6.230935	0.893213	-1.912081
H	-5.026851	1.870908	-2.791172
C	-3.300495	1.669814	-0.909005
O	-3.153732	2.755364	-1.446610
C	-2.441971	1.098695	0.229860
C	-2.418075	2.065410	1.415573
C	-1.041003	0.856302	-0.393827
H	-3.432122	2.253971	1.779424
H	-1.834587	1.643533	2.239100
H	-1.969165	3.016504	1.115635
H	-1.171116	0.145260	-1.218740
H	-0.720210	1.804474	-0.844009
C	6.756704	-0.029869	-1.751446
C	5.813374	0.670282	-1.007055
C	5.012827	0.003691	-0.071547
C	5.172159	-1.374642	0.113288
C	6.123769	-2.074519	-0.626972
C	6.913840	-1.404508	-1.560280
H	7.369425	0.492158	-2.479440
H	5.680408	1.738936	-1.141688
H	4.565938	-1.909679	0.837071
H	6.247334	-3.141820	-0.474487
H	7.651844	-1.952147	-2.138184
C	4.011853	0.804708	0.708485
C	0.046260	0.350250	0.567189
C	1.941318	0.976967	2.178275
H	0.679877	-0.356773	0.020734
H	2.417490	1.839082	2.655579
H	1.414539	0.426498	2.966981
O	4.008901	2.022738	0.627715
H	-0.401371	-0.225386	1.387430
H	-2.632375	-2.914692	0.094181
C	3.029970	0.073216	1.603903
H	2.602118	-0.769185	1.048755
H	3.616944	-0.379236	2.414709
C	0.921350	1.468007	1.145667
H	1.441982	1.974999	0.324346
H	0.286180	2.224442	1.619214
O	-2.029671	-3.110915	-0.690636
H	-2.221615	-3.988711	-1.075899
H	-1.086517	-3.048147	-0.441277

H_2O

O	0.000000	0.000000	0.117031
H	0.000000	0.765865	-0.468124
H	0.000000	-0.765865	-0.468124

H_3O

H	-0.068637	-0.928478	0.219061
O	0.000027	0.000032	-0.082170

H -0.770499 0.523439 0.219112
H 0.838922 0.404783 0.219185

2. Cartesian coordinates of structures in the intramolecular cyclization mechanisim for β-, γ-, and δ-keto radicals

A-TS'

C	2.136611	-1.088159	0.380714
C	2.595847	0.207729	0.098776
C	1.743159	1.174143	-0.416662
C	0.368913	0.885043	-0.608720
C	-0.082202	-0.438930	-0.313646
C	0.790020	-1.401857	0.179628
H	2.818733	-1.834682	0.772939
H	3.642026	0.449212	0.262350
H	2.128138	2.151858	-0.688166
H	0.397728	-2.377277	0.455070
C	-1.135722	1.695064	0.703365
C	-2.191656	0.760188	0.176112
C	-1.546699	-0.586477	-0.170481
H	-0.718560	1.475238	1.683078
H	-1.193493	2.748353	0.446910
H	-3.006391	0.569487	0.884069
H	-2.646199	1.161639	-0.738785
O	-2.164207	-1.634634	-0.240593
H	-0.177954	1.492784	-1.327233

A-IM'

C	-2.148613	-1.164427	-0.084392
C	-2.554097	0.212336	-0.134284
C	-1.666405	1.225707	0.045949
C	-0.245991	0.938639	0.405617
C	0.134885	-0.493741	0.196931
C	-0.797507	-1.500476	0.031632
H	-2.892150	-1.941165	-0.224379
H	-3.595777	0.436565	-0.343096
H	-1.991306	2.262075	0.002875
H	-0.470594	-2.530732	-0.083776
C	0.891660	1.709294	-0.310207
C	2.127337	0.835898	-0.029116
C	1.582873	-0.587948	0.026338
H	0.685857	1.737939	-1.385464
H	0.995239	2.733947	0.052283
H	2.928347	0.924593	-0.765898
H	2.548802	1.071978	0.957438
O	2.248443	-1.614781	-0.073436
H	-0.140809	1.171358	1.486705

B-TS'

C	-2.777024	-0.394372	0.026246
C	-1.834214	-1.162830	-0.639448
C	-0.161305	0.561096	-0.233219
C	-1.129363	1.333170	0.405457
C	-2.433538	0.858051	0.555191
H	-3.797506	-0.754821	0.116644
H	-2.118152	-2.110964	-1.085263
H	-0.845448	2.303041	0.804428
H	-3.177662	1.459482	1.066383
C	-0.484915	-0.738357	-0.718236
C	2.105714	-1.415780	0.120655
H	2.210503	-1.727302	-0.925663
H	2.921334	-1.919689	0.659157
C	2.339307	0.095057	0.246027
H	2.455223	0.346553	1.310862
H	3.270440	0.392307	-0.243908
C	0.780061	-1.874813	0.653253
H	0.446325	-1.484787	1.612800
H	0.475613	-2.895410	0.436490
C	1.245337	1.045679	-0.219409
O	1.513217	2.219388	-0.433485
H	0.153229	-1.204916	-1.463147

B-IM'

C	-2.772531	-0.423725	0.103763
C	-1.778051	-1.326932	-0.081505
C	-0.116342	0.548008	-0.131784
C	-1.175638	1.431429	0.019852
C	-2.492742	0.981244	0.105204
H	-3.791541	-0.760189	0.269064
H	-1.993431	-2.392877	-0.081270
H	-0.953988	2.488829	0.132096
H	-3.301070	1.691209	0.240118
C	-0.366416	-0.918944	-0.373034

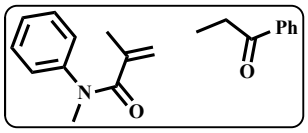
C	2.083834	-1.377279	-0.151395
H	2.146411	-1.484966	-1.241489
H	2.847597	-2.032669	0.277130
C	2.378936	0.071036	0.243941
H	2.543323	0.125305	1.329863
H	3.289271	0.450465	-0.228561
C	0.691824	-1.801758	0.309947
H	0.602490	-1.701022	1.399418
H	0.503660	-2.850581	0.058322
C	1.258978	1.058380	-0.035377
O	1.507896	2.264130	-0.093891
H	-0.227005	-1.095286	-1.461223

C-TS'

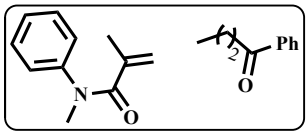
C	-2.897731	-0.131298	0.203231
C	-2.195365	-0.673307	-0.859024
C	-0.278056	0.715896	-0.267676
C	-0.978778	1.215434	0.824549
C	-2.289639	0.795960	1.066372
H	-3.933049	-0.415482	0.367217
H	-2.666630	-1.390475	-1.523890
H	-0.519764	1.958814	1.471840
H	-2.846640	1.211375	1.899583
C	-0.824019	-0.345669	-1.042555
H	-0.333039	-0.604541	-1.977120
C	1.143755	1.062060	-0.546973
C	2.115296	0.856531	0.590985
C	0.194133	-1.972145	-0.047507
C	1.919467	-0.540630	1.220252
C	1.651282	-1.664357	0.196092
H	-0.440709	-1.999842	0.837910
H	1.964205	1.631234	1.352389
H	1.090986	-0.508553	1.936614
H	3.123921	0.970051	0.184464
H	-0.020133	-2.751702	-0.776440
H	2.821356	-0.771359	1.793574
H	2.119889	-2.589904	0.562647
H	2.158432	-1.444844	-0.754306
O	1.514888	1.349297	-1.675120

C-IM'

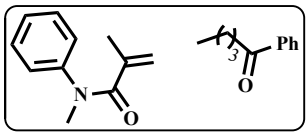
C	2.971981	-0.644269	0.221757
C	1.879936	-1.444695	0.110761
C	0.432474	0.582217	-0.122868
C	1.584560	1.347262	-0.081621
C	2.854353	0.766319	0.042390
H	3.939682	-1.070762	0.468311
H	1.966634	-2.519894	0.247433
H	1.484259	2.428862	-0.056539
H	3.734270	1.396822	0.103341
C	0.544158	-0.912778	-0.324406
H	0.553645	-1.030554	-1.432262
C	0.854192	1.306053	0.006290
C	1.943989	0.693548	0.862889
C	0.631686	-1.802052	0.123296
C	2.783443	-0.379104	0.151273
C	1.947873	-1.439977	-0.577882
H	0.742605	-1.779255	1.214218
H	1.472441	0.256161	1.749654
H	3.408829	-0.858903	0.911478
H	2.588456	1.511659	1.194280
H	0.356030	-2.829338	-0.136654
H	3.462923	0.103309	-0.558719
H	2.559090	-2.338664	-0.704732
H	1.710947	-1.089506	-1.591633
O	1.001855	2.423115	-0.484932



A-CM



B-CM



C-CM

A-CM

C	3.437503	-0.449526	0.989348
C	4.223533	-1.590500	0.830355
C	4.460683	-2.105362	-0.443472
C	3.910304	-1.476346	-1.562541
C	3.111808	-0.346775	-1.407490
C	2.867012	0.158111	-0.129282
H	3.254219	-0.033873	1.976223
H	4.656488	-2.070384	1.702269
H	5.075014	-2.991735	-0.565709
H	4.091636	-1.875053	-2.555585
H	2.654949	0.135308	-2.267529
N	2.044294	1.317362	0.023300
C	2.616403	2.592555	-0.410765
H	3.234852	3.032403	0.379818
H	3.231759	2.414557	-1.292425
H	1.814052	3.288360	-0.655794
C	0.984387	1.360968	0.886543
O	0.557938	2.443124	1.296529
C	0.304546	0.066893	1.265249
C	0.214951	-1.086042	0.293235
H	0.141093	-0.729435	-0.738526
H	1.087765	-1.743396	0.353843
H	-0.677813	-1.676280	0.517322
C	-3.462965	-2.117452	1.091427
C	-3.362982	-0.734428	0.985955
C	-3.062054	-0.138281	-0.244702
C	-2.867541	-0.945447	-1.371140
C	-2.971768	-2.331286	-1.266872
C	-3.267283	-2.918037	-0.036856
H	-3.689004	-2.573766	2.050024
H	-3.504931	-0.098022	1.853812
H	-2.627675	-0.505064	-2.333760
H	-2.817730	-2.951096	-2.144259
H	-3.344160	-3.997936	0.044172
C	-2.959869	1.354880	-0.304571
C	-1.046202	1.838980	-1.791954
C	-2.519288	2.017957	-1.609323
H	-0.643710	1.113386	-2.487275
H	-2.774815	3.076952	-1.510783
H	-3.077848	1.601724	-2.452120
O	-3.187897	2.035350	0.682027
H	-0.362131	2.447769	-1.214365
C	-0.271468	0.027056	2.470815
H	-0.822714	-0.851711	2.794440
H	-0.207947	0.870463	3.150909

B-CM

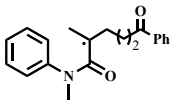
C	2.816736	0.400359	-1.232751
C	2.879549	1.762808	-1.523883
C	3.068255	2.689119	-0.499109
C	3.192456	2.251754	0.820808
C	3.130420	0.891492	1.116690
C	2.938821	-0.032864	0.088110
H	2.682553	-0.331672	-2.024204
H	2.783713	2.098191	-2.552028
H	3.115435	3.749550	-0.726605
H	3.333655	2.970948	1.621309
H	3.220160	0.537484	2.139953
N	2.941205	-1.436073	0.381041
C	4.252145	-2.044725	0.611463
H	4.769603	-2.230136	-0.336876
H	4.849734	-1.365690	1.220141
H	4.120134	-2.990855	1.135090
C	1.915297	-2.257383	0.002866
O	2.087399	-3.466758	-0.154665
C	0.544585	-1.642970	-0.118724
C	0.034074	-0.847824	1.054430
C	-3.296447	-2.540781	0.541512
H	0.275341	-1.350689	1.997057
H	0.476210	0.153460	1.089657
H	-1.049751	-0.735888	0.982954
H	-2.591672	-3.121724	1.124515

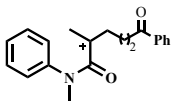
H	-3.623955	-2.945052	-0.410812
C	-0.559551	2.327282	-0.647482
C	-1.524612	1.436497	-1.103792
C	-2.613384	1.093738	-0.291256
C	-2.728096	1.668088	0.980882
C	-1.757516	2.556657	1.440302
C	-0.670017	2.882170	0.629858
H	0.285523	2.582305	-1.277892
H	-1.443744	0.989775	-2.089896
H	-3.570800	1.430098	1.621900
H	-1.852284	2.993817	2.428971
H	0.091372	3.568172	0.989818
C	-3.605174	0.096503	-0.807208
C	-4.044039	-1.413981	1.169715
C	-4.659350	-0.455406	0.129346
H	-3.387293	-0.865860	1.855966
H	-5.379509	-0.998705	-0.488061
H	-5.188584	0.357428	0.635818
O	-3.530171	-0.303654	-1.960082
H	-4.868762	-1.795568	1.792170
C	-0.172309	-1.899796	-1.215543
H	-1.182826	-1.513669	-1.328731
H	0.238435	-2.494351	-2.026921

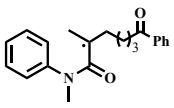
C-CM

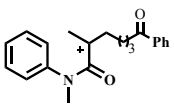
C	3.308693	0.975211	-0.720783
C	3.055871	2.327269	-0.487811
C	3.780786	3.020562	0.480134
C	4.762560	2.357436	1.219866
C	5.005944	1.004067	1.004457
C	4.270182	0.310656	0.040692
H	2.749022	0.429797	-1.475930
H	2.295291	2.839636	-1.068980
H	3.584192	4.072962	0.657441
H	5.328349	2.891656	1.976417
H	5.747524	0.473100	1.594695
N	4.519577	-1.081094	-0.165005
C	5.808034	-1.453393	-0.751013
H	5.759060	-1.432437	-1.845271
H	6.562467	-0.744108	-0.411830
H	6.075664	-2.459226	-0.428546
C	3.523911	-2.017123	-0.183977
O	3.703744	-3.113300	-0.719201
C	2.226671	-1.710608	0.524872
C	2.215807	-0.923757	1.813891
C	-1.351617	-0.094002	-1.198700
H	3.107935	-1.130863	2.412657
H	2.185879	0.155708	1.635385
H	1.333566	-1.195808	2.397842
H	-0.979055	-0.961567	-1.765652
H	-1.743646	-0.497948	-0.256420
C	-5.922196	-1.144060	1.719095
C	-4.895397	-0.228255	1.515376
C	-4.727846	0.380921	0.265122
C	-5.604891	0.062903	-0.778549
C	-6.640481	-0.846438	-0.570698
C	-6.797518	-1.452718	0.675404
H	-6.042286	-1.617524	2.688254
H	-4.208349	0.024289	2.316853
H	-5.495110	0.527381	-1.753297
H	-7.321991	-1.081862	-1.381627
H	-7.600150	-2.166228	0.833625
C	-3.609840	1.365613	0.095509
C	-2.494831	0.536403	-2.011996
C	-3.153175	1.732742	-1.299153
H	-3.244167	-0.231305	-2.231681
H	-2.435202	2.549757	-1.191880
H	-3.999131	2.097219	-1.891089
O	-3.045699	1.824397	1.077922
H	-2.104764	0.887795	-2.973651
C	-0.237124	0.858298	-0.920623
H	0.195015	0.968135	0.066458
H	0.193031	1.433883	-1.734763
C	1.118116	-2.235954	-0.003366
H	0.151797	-2.097745	0.473508
H	1.153690	-2.810438	-0.923746

4. Cartesian coordinates of structures in computations of reduction potential


A-INT-Ra3-Va


A-INT-Ca1-Va


B-INT-Ra3-Va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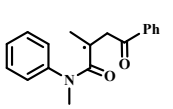
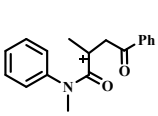

D-INT-Ra2-Va


D-INT-Ca1-Va

A-INT-Ra-Va

C	2.641298	-0.782699	-1.088235
C	2.765993	-2.147920	-1.340447
C	3.709708	-2.903917	-0.648411
C	4.530048	-2.287826	0.297606
C	4.393169	-0.929625	0.566313
C	3.438322	-0.173064	-0.117384
H	1.928093	-0.177715	-1.642779
H	2.131945	-2.616930	-2.086735
H	3.808789	-3.966231	-0.846357
H	5.268020	-2.870969	0.839600
H	5.004079	-0.446511	1.324056
N	3.307391	1.218904	0.162144
C	4.364291	2.077294	-0.371311
H	4.246073	2.230093	-1.451346
H	5.328682	1.605690	-0.176662
H	4.317517	3.048720	0.120305
C	2.044049	1.805808	0.255337
O	1.859749	2.949125	-0.169746
C	0.974614	1.075033	0.941471
C	1.202292	-0.088434	1.849581
C	0.402527	1.641583	0.774121
H	2.231644	-0.133565	2.210926
H	0.974749	-1.042783	1.351949
H	0.523271	-0.024283	2.706058
H	0.356137	2.725843	0.927207
H	1.068611	1.217299	1.533437
C	5.806140	-0.726768	0.912096
C	4.435399	-0.951848	0.958315
C	3.605642	-0.476678	-0.063838
C	4.169054	0.224175	-1.135595
C	5.543398	0.447797	-1.182868
C	6.361786	-0.025759	-0.159453
H	6.444003	-1.095737	1.709008
H	3.979363	-1.496255	1.779083
H	3.543740	0.597978	-1.940370
H	5.974481	0.990607	-2.018044
H	7.432395	0.150826	-0.196421
C	2.132587	-0.752071	0.039987
C	0.984097	1.394839	-0.630156
C	1.181104	-0.100921	-0.943289
H	1.939374	1.924690	-0.715771
H	0.230009	-0.633996	-0.850033
H	1.542143	-0.225634	-1.969699
O	1.703561	-1.454080	0.937934
H	0.306153	1.832168	-1.370959

A-INT-Ca1-Va

C	3.045021	0.827880	-1.065782
C	3.369340	2.170948	-0.843691
C	4.312121	2.503738	0.120338
C	4.949952	1.495178	0.855269
C	4.619850	0.159524	0.660643
C	3.648669	-0.169085	-0.288306
H	2.910177	2.943764	-1.451827
H	4.575820	3.542344	0.288806
H	5.699358	1.758348	1.594718
H	5.089025	-0.620140	1.252919
N	3.184888	-1.507503	-0.422038
C	4.092466	-2.635775	-0.637651
H	4.815106	-2.371383	-1.410433
H	4.612950	-2.894321	0.287946
H	3.494133	-3.488948	-0.958706
C	1.857582	-1.707500	-0.310840
O	1.229216	-2.742329	-0.429632
C	1.029403	-0.507104	0.101064
C	1.128378	-0.044993	1.483427
C	-0.086522	-0.150961	-0.780391
H	1.994699	-0.440722	2.011227
H	1.113277	1.051151	1.518431
H	0.177979	-0.363616	1.961456
H	0.164988	-0.401030	-1.815731

H	-0.811010	-0.942778	-0.483860
C	-5.841758	-1.108216	0.190365
C	-4.570356	-0.923262	0.716810
C	-3.820863	0.208820	0.363831
C	-4.360678	1.148864	-0.524902
C	-5.632268	0.956354	-1.056386
C	-6.372000	-0.169662	-0.697916
H	-6.422201	-1.981195	0.469022
H	-4.139019	-1.641099	1.406855
H	-3.802294	2.035194	-0.809616
H	-6.047137	1.684603	-1.744940
H	-7.365374	-0.315410	-1.110182
C	-2.457851	0.348007	0.932606
C	-0.732397	1.240616	-0.676897
C	-1.581595	1.539905	0.577723
H	-1.369884	1.335270	-1.561105
H	-0.954002	1.734842	1.449190
H	-2.162278	2.445300	0.393253
O	-1.966364	-0.528804	1.632080
H	0.049508	2.003584	-0.774267
H	2.400193	0.548143	-1.894354

B-INT-Ra3-Va

C	4.181074	-0.212041	1.010066
C	4.865946	-1.284158	1.578949
C	5.468585	-2.243347	0.767677
C	5.380204	-2.126434	-0.620067
C	4.681294	-1.067788	-1.191720
C	4.071071	-0.107822	-0.379263
H	3.723729	0.547301	1.638541
H	4.937519	-1.361399	2.659336
H	6.005526	-3.075002	1.211982
H	5.845077	-2.870369	-1.259414
H	4.582718	-0.986049	-2.270558
N	3.368198	0.976480	-0.978126
C	4.179943	1.970024	-1.679218
H	4.664356	2.656062	-0.973784
H	4.943381	1.452664	-2.261450
H	3.538839	2.553015	-2.339762
C	2.180172	1.450292	-0.422842
O	1.904009	2.651752	-0.476597
C	1.237610	0.488500	0.145679
C	1.217044	-0.969738	-0.180965
C	-1.068230	1.458549	0.047300
H	1.742372	-1.195375	-1.111875
H	1.688782	-1.565258	0.613854
H	0.179176	-1.313506	-0.257905
H	-0.711652	2.229623	-0.642489
H	-1.374677	0.596880	-0.561771
C	-5.365787	-1.936652	-1.372148
C	-4.316172	-1.725925	-0.485695
C	-4.240500	-0.538161	0.251419
C	-5.232734	0.434684	0.089670
C	-6.286733	0.221792	-0.796517
C	-6.353146	-0.962039	-1.528389
H	-5.417690	-2.858933	-1.941914
H	-3.539475	-2.470471	-0.343442
H	-5.194033	1.360522	0.654691
H	-7.054671	0.979428	-0.914672
H	-7.173863	-1.126333	-2.219764
C	-3.084789	-0.363721	1.194376
C	-2.272375	1.992755	0.826877
C	-2.851121	0.985446	1.843420
H	-3.051536	2.284886	0.113833
H	-2.148859	0.821538	2.663811
H	-3.777882	1.379201	2.272685
O	-2.308022	-1.282769	1.385696
H	-1.984448	2.899862	1.370781
C	0.110595	1.046547	0.952064
H	-0.222871	0.279700	1.661017
H	0.443199	1.930205	1.508317

B-INT-Ca1-Va

C	-3.705664	-0.575922	-0.874486
C	-4.468413	-1.685091	-0.494470
C	-5.368432	-1.579171	0.559083
C	-5.520205	-0.359962	1.230321
C	-4.748346	0.741776	0.879524
C	-3.826456	0.623325	-0.163132
H	-4.380775	-2.613939	-1.048695
H	-5.971719	-2.433316	0.846861
H	-6.236492	-0.274418	2.040764
H	-4.842028	1.679186	1.419227
N	-2.946377	1.698553	-0.470596
C	-3.434435	3.063248	-0.683020
H	-4.357876	3.022955	-1.260953
H	-3.611610	3.563897	0.272455
H	-2.669654	3.612539	-1.232929

C	-1.623676	1.448651	-0.513125
O	-0.719270	2.218588	-0.781664
C	-1.164059	0.064802	-0.103284
C	-1.230328	-0.293539	1.306366
C	-0.347614	-0.663223	-1.075508
H	-1.968589	0.274282	1.870637
H	-1.341611	-1.372969	1.445006
H	-0.203557	-0.052961	1.658670
H	-0.706045	-0.443349	-2.087543
H	0.588949	-0.070023	-0.996669
C	5.560613	1.774808	0.658642
C	4.302947	1.197803	0.779399
C	4.058931	-0.075382	0.247440
C	5.088623	-0.762655	-0.408926
C	6.346847	-0.180861	-0.530159
C	6.582714	1.085511	0.003456
H	5.746997	2.759777	1.073477
H	3.495162	1.717056	1.284199
H	4.921542	-1.749645	-0.828742
H	7.142762	-0.714132	-1.038869
H	7.565444	1.536311	-0.092001
C	2.697141	-0.649252	0.400272
C	-0.083069	-2.157840	-0.849579
C	0.999845	-2.554433	0.165748
H	0.199651	-2.570004	-1.823970
H	0.730954	-2.247612	1.180357
H	1.027818	-3.648001	0.172097
O	1.807898	-0.016253	0.957341
H	-1.030247	-2.644958	-0.582122
H	-3.087354	-0.615369	-1.767000
C	2.407851	-2.039922	-0.146224
H	2.601583	-2.040577	-1.228149
H	3.153428	-2.719285	0.282593

D-INT-Ra2-Va

C	-3.157010	-0.475779	-0.854062
C	-4.178535	-1.407329	-0.680596
C	-4.972488	-1.372887	0.463651
C	-4.738202	-0.400751	1.436882
C	-3.705771	0.518729	1.277555
C	-2.903933	0.479878	0.133676
H	-2.550766	-0.485322	-1.756069
H	-4.359689	-2.152675	-1.448572
H	-5.770164	-2.096250	0.596425
H	-5.351886	-0.368392	2.331626
H	-3.499198	1.258095	2.046375
N	-1.848289	1.424736	-0.025133
C	-2.234824	2.821595	-0.222736
H	-2.548259	3.001166	-1.257931
H	-3.059189	3.056588	0.451119
H	-1.381021	3.462412	-0.004281
C	-0.644270	1.042707	-0.599690
O	-0.004647	1.832498	-1.298956
C	-0.124014	-0.296626	-0.295065
C	-0.474506	-1.067753	0.935075
C	0.800291	-0.918000	-1.298242
H	-0.973130	-0.444845	1.679141
H	-1.138724	-1.912091	0.699732
H	0.429656	-1.494863	1.384013
H	0.300395	-1.772263	-1.775503
H	1.057831	-0.181627	-2.064719
C	5.215079	-0.286045	1.010315
C	4.214693	-1.112644	0.514511
C	3.099196	-0.560585	-0.127314
C	2.991249	0.827560	-0.269004
C	3.998367	1.652225	0.230863
C	5.107119	1.099256	0.867610
H	6.079722	-0.716944	1.505255
H	4.275609	-2.192276	0.609358
H	2.131221	1.273783	-0.762215
H	3.914269	2.728517	0.118448
H	5.889347	1.746635	1.252601
C	2.055387	-1.497980	-0.649221
O	2.180276	-2.702027	-0.535309

D-INT-Ca1-Va

C	0.472000	1.233480	-1.298236
C	-0.399580	2.225304	-0.856975
C	-0.094458	2.968720	0.284780
C	1.090452	2.736224	0.981144
C	1.974655	1.753964	0.540322
C	1.651849	1.000263	-0.588531
H	-1.321937	2.409754	-1.398321
H	-0.779601	3.737263	0.627625
H	1.330122	3.321672	1.862181
H	2.914758	1.574915	1.055897
N	2.537149	-0.053217	-1.009575
C	3.429086	0.121462	-2.159186

H	2.838196	0.328763	-3.053767
H	4.107968	0.954901	-1.967674
H	3.996163	-0.799955	-2.295557
C	2.532350	-1.180318	-0.306127
O	3.165034	-2.219951	-0.443022
C	1.580629	-1.393983	0.821904
C	2.047080	-1.340291	2.194358
C	0.210934	-1.772616	0.499873
H	3.120971	-1.192480	2.294170
H	1.490983	-0.451462	2.574444
H	1.680839	-2.176079	2.798098
H	0.080509	-1.929511	-0.570349
H	-0.099459	-2.663078	1.063048
C	-4.230239	0.542462	0.084278
C	-2.974054	0.448069	0.666486
C	-2.114395	-0.600669	0.306435
C	-2.526916	-1.557776	-0.627874
C	-3.791429	-1.461476	-1.201705
C	-4.638528	-0.411300	-0.850724
H	-4.895546	1.353001	0.361977
H	-2.637762	1.172743	1.401185
H	-1.892832	-2.393209	-0.906637
H	-4.116074	-2.207681	-1.918739
H	-5.622526	-0.338376	-1.302685
C	-0.802469	-0.636213	0.996841
O	-0.502363	0.092365	1.905445
H	0.242007	0.640192	-2.179620