

**Radical-induced dissociation leading to the loss of CO₂ from the
oxazolone ring of [b₅ – H]^{•+} ions**

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Supporting information

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Figure S1. Structures of $[b_5 - H]^{\bullet+}$ ion and macrocyclic structures optimized at the B3LYP/6-31++G(d,p) level. Upper numbers (black) are energies calculated at the B3LYP/6-31++G(d,p) level while lower numbers (red) are single-point energies calculated at the M06-2X/6-311++G(d,p) level. All enthalpies (ΔH^0_0) and free energies (ΔG^0_{298} , in parentheses) in kJ mol^{-1} are relative to isomer $AAAG^{\bullet}A_{\text{oxa}}^+$.

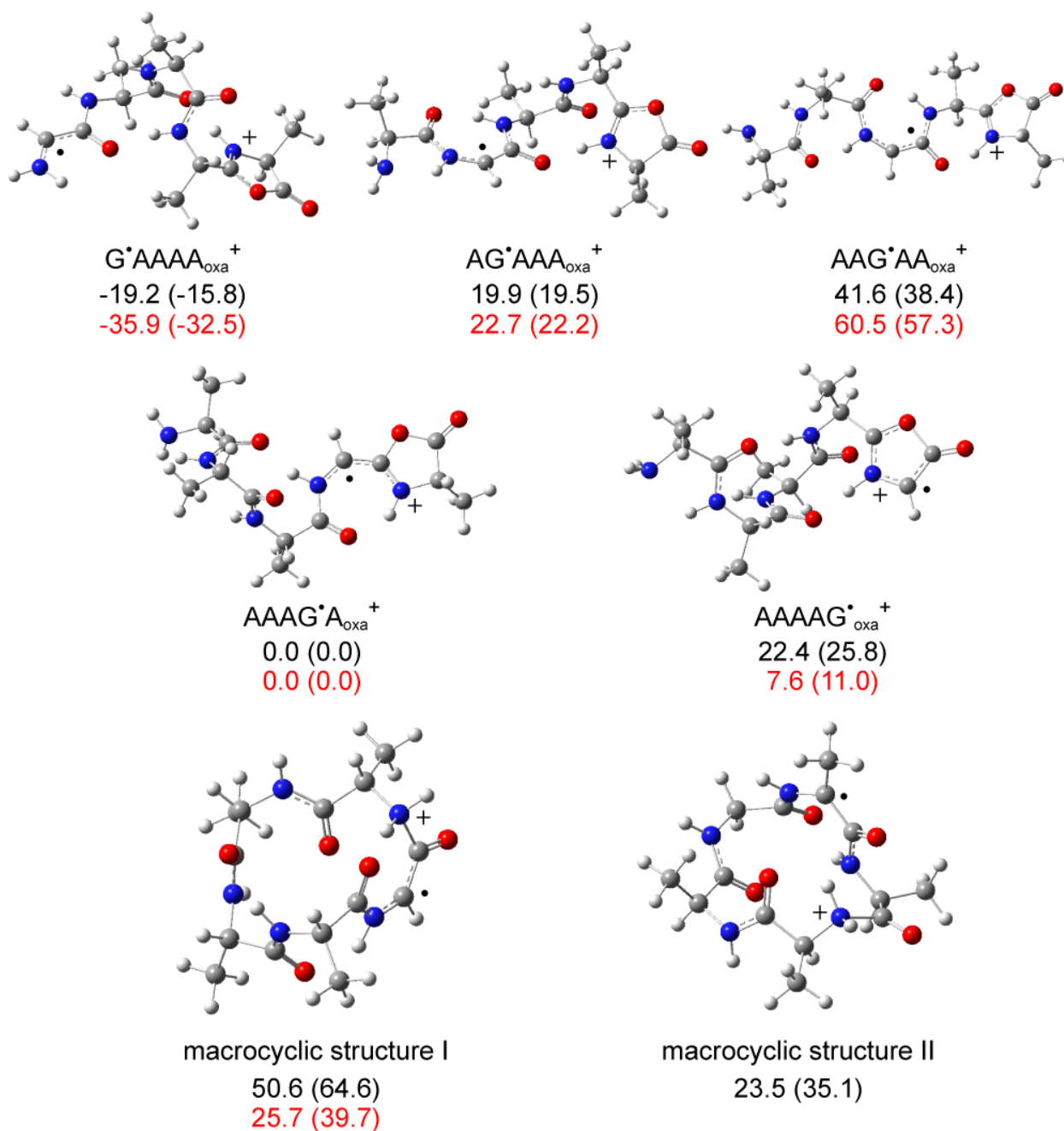
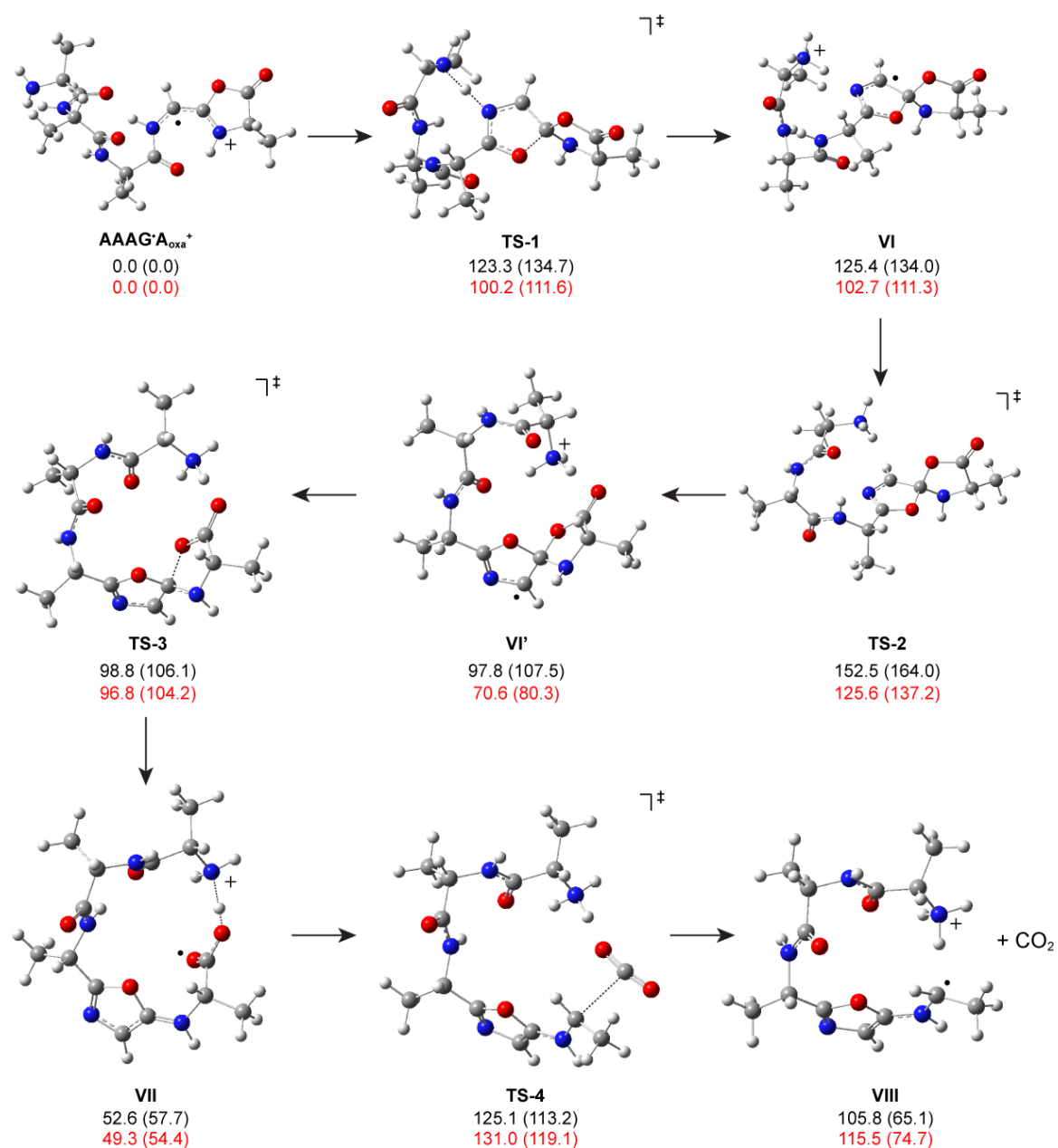


Figure S2. Detailed mechanism for the dissociation of CO₂ from AAAG•A_{oxa}⁺ (pathway b in Scheme 1). All enthalpies (ΔH°_0) and free energies (ΔG°_{298} , in parentheses) in kJ mol⁻¹ are relative to isomer AAAG•A_{oxa}⁺. Upper numbers (black) are energies calculated at the B3LYP/6-31++G(d,p) level while lower numbers (red) are single-point energies calculated at the M06-2X/6-311++G(d,p) level.



Cartesian coordinates of the selected structures involved in this work

G*AAA_{oxa}⁺
47

C	-1.294238	1.586252	0.965265
N	-0.185644	0.688022	1.210090
C	-2.308791	0.917348	0.069241
O	-3.525960	1.443080	-0.023234
N	-2.140265	-0.144294	-0.660579
C	-3.380166	-0.519576	-1.349236
C	-4.308472	0.606844	-0.912333
O	-5.436049	0.856626	-1.161440
H	0.685746	0.844684	0.695933
C	-0.427660	-0.473644	1.893944
C	0.703720	-1.511257	1.983523
O	-1.520238	-0.703262	2.404585
N	1.641253	-1.414132	0.864977
H	2.612859	-1.192325	1.049216
H	-1.264585	-0.721038	-0.671072
H	0.189122	-2.475641	1.930895
H	-3.234945	-0.450011	-2.433888
C	1.267495	-1.479436	-0.424310
O	0.090579	-1.686645	-0.777426
C	2.357897	-1.295120	-1.484153
N	3.470625	-0.488543	-0.983707
H	4.391578	-0.771091	-1.296182
C	3.283062	0.870359	-0.736516
O	2.126703	1.326841	-0.536073
C	4.446358	1.699166	-0.682886
H	5.446735	1.324119	-0.860640
N	4.301069	3.008812	-0.376723
H	3.365017	3.377128	-0.269465
H	5.076989	3.650888	-0.408556
H	-1.831017	1.772513	1.903118
H	1.853944	-0.773701	-2.307241
C	2.863652	-2.656902	-1.979929
H	2.023459	-3.261350	-2.328579
H	3.552770	-2.522424	-2.819507
H	3.379173	-3.204870	-1.184683
C	1.452276	-1.405189	3.317086
H	0.741668	-1.485965	4.142170
H	2.178001	-2.218538	3.410871
H	1.977585	-0.448255	3.406392
C	-0.829640	2.923863	0.362437
H	-0.185414	3.424551	1.088726
H	-0.261082	2.766568	-0.557847
H	-1.686110	3.570131	0.158296
C	-3.896954	-1.911982	-0.962952
H	-4.859309	-2.082031	-1.451702
H	-3.189929	-2.673403	-1.300172
H	-4.023042	-1.996454	0.119127

AG*AAA_{oxa}⁺
47

C	3.631840	-1.783099	-0.317162
N	2.593411	-0.829224	0.090016
C	3.101524	0.143463	0.782380
O	4.404095	0.021436	1.016920
C	4.861107	-1.189453	0.359599
C	2.377436	1.350098	1.332133
N	1.102531	1.501076	0.665196
O	5.990987	-1.530206	0.412078
H	3.427471	-2.763496	0.129283
H	0.249670	1.261518	1.153729
C	1.067016	1.704831	-0.692265
O	2.095538	1.902321	-1.328461

C	-0.303400	1.658727	-1.374489
H	-0.088646	1.265403	-2.374984
N	-1.252237	0.772580	-0.696721
H	-2.224457	1.088612	-0.578591
C	-1.040099	-0.565765	-0.595553
O	0.103637	-1.073216	-0.789312
C	-2.107547	-1.485723	-0.246189
H	-1.782553	-2.515385	-0.166693
N	-3.455209	-1.308385	-0.051484
H	-4.016304	-2.153809	0.123146
C	-4.289102	-0.211848	-0.057827
C	-5.764061	-0.555275	0.221145
H	-6.324683	-0.067016	-0.586069
N	-5.968877	-2.012308	0.215956
H	-6.409767	-2.337760	-0.639054
H	1.587788	-0.865126	-0.248351
O	-3.929276	0.951001	-0.249775
H	-6.544636	-2.317136	0.994620
H	3.021172	2.203238	1.086937
C	-6.189278	0.076540	1.555983
H	-5.947685	1.141192	1.568776
H	-7.268729	-0.034994	1.693478
H	-5.678472	-0.407062	2.396454
C	-0.898484	3.068364	-1.499221
H	-1.823801	3.037422	-2.081220
H	-1.119738	3.497341	-0.516868
H	-0.190640	3.720979	-2.014812
C	2.218361	1.251061	2.858552
H	3.192390	1.140110	3.339738
H	1.758040	2.171310	3.226140
H	1.588529	0.401352	3.140950
C	3.781769	-1.906745	-1.839915
H	4.619505	-2.572309	-2.061508
H	2.869435	-2.331311	-2.264878
H	3.966442	-0.931020	-2.295604

AAG*AA_{oxa}⁺
47

C	-5.236039	0.987973	0.760138
N	-3.916715	0.893625	0.130266
C	-3.759034	-0.247583	-0.464614
O	-4.805688	-1.060045	-0.379803
C	-5.832090	-0.368630	0.392762
C	-2.511264	-0.629106	-1.243173
N	-1.308643	-0.378985	-0.449634
O	-6.877654	-0.872241	0.609303
H	-5.120326	1.029475	1.850387
H	-0.618228	-1.141076	-0.362599
C	-0.854187	0.875217	-0.163118
O	-1.616626	1.885401	-0.256389
C	0.499918	1.120169	0.281841
H	0.690048	2.162414	0.506059
N	1.589978	0.309844	0.468609
H	2.457377	0.811847	0.776205
C	1.787178	-1.042511	0.301861
O	0.912485	-1.834987	-0.062413
C	3.183318	-1.569739	0.679302
H	3.198108	-2.575897	0.256597
N	4.302590	-0.858279	0.047812
H	4.984141	-1.391358	-0.493879
C	4.715632	0.399370	0.304311
C	6.094044	0.775345	-0.269916
H	6.719390	0.930396	0.618728
N	6.654408	-0.335437	-1.056261
H	7.600898	-0.565224	-0.773186
H	-3.069203	1.564410	0.069533
O	4.052380	1.226596	0.958825

H	6.676546	-0.118072	-2.048613
H	-2.514237	0.045371	-2.114699
C	6.009907	2.100718	-1.040041
H	5.541039	2.874079	-0.428407
H	7.012948	2.433208	-1.321456
H	5.416431	1.980017	-1.954289
C	3.329780	-1.677349	2.210905
H	2.502995	-2.261662	2.625234
H	4.265074	-2.191469	2.448477
H	3.343291	-0.693915	2.685872
C	-2.541001	-2.082359	-1.722142
H	-2.537177	-2.780084	-0.880543
H	-3.429787	-2.272864	-2.326671
H	-1.659025	-2.271765	-2.337733
C	-6.079968	2.171257	0.269701
H	-7.067447	2.121959	0.734622
H	-5.602553	3.110500	0.558295
H	-6.197961	2.149898	-0.816551

AAAG*A_{oxa}⁺
47

C	1.477224	0.722069	-0.027040
N	0.559679	-0.239112	-0.305166
C	2.872221	0.632682	0.133454
O	3.517346	1.785411	0.427643
N	3.709886	-0.393959	0.059448
C	5.087809	0.010343	0.328637
C	4.907109	1.508560	0.563600
O	5.694310	2.361083	0.806476
H	-0.410070	0.133931	-0.273463
H	1.056708	1.711325	0.111568
C	0.725139	-1.606769	-0.516198
C	-0.546824	-2.432461	-0.760433
O	1.826864	-2.145121	-0.557719
N	-1.748126	-1.772663	-0.283173
H	-2.456581	-1.482660	-0.943457
H	3.336882	-1.324993	-0.169720
H	-0.380179	-3.347787	-0.182841
H	5.430719	-0.445497	1.267134
C	-1.890713	-1.461777	1.041032
O	-1.042763	-1.781391	1.867268
C	-3.140478	-0.676784	1.457473
H	-2.798041	-0.054132	2.291676
N	-3.663688	0.188624	0.396049
H	-4.671236	0.269416	0.251474
C	-2.961947	1.175046	-0.198522
O	-1.723980	1.289264	-0.114186
C	-3.787250	2.187033	-1.013038
H	-3.285527	2.259996	-1.987281
N	-5.179888	1.739020	-1.146770
H	-5.837162	2.500174	-1.008900
H	-5.371151	1.330044	-2.056003
C	-3.703724	3.559503	-0.325380
H	-4.223441	3.542053	0.639115
H	-2.663457	3.841896	-0.152625
H	-4.169409	4.321250	-0.957637
C	-4.240500	-1.625097	1.952637
H	-3.849151	-2.254253	2.754898
H	-5.084259	-1.052997	2.350166
H	-4.603228	-2.271693	1.147116
C	-0.672689	-2.785158	-2.250277
H	0.234362	-3.286470	-2.593170
H	-1.516020	-3.465696	-2.396027
H	-0.830241	-1.891743	-2.864568
C	6.074605	-0.307706	-0.801595
H	7.054460	0.099563	-0.540681
H	6.168387	-1.389478	-0.924549

H 5.748493 0.133497 -1.746906

AAAAG*⁺_{oxa}
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C	-1.885558	-0.960103	-1.390684
N	-0.800043	-0.002300	-1.313998
C	-2.834889	-0.733136	-0.244163
O	-4.049085	-1.210846	-0.257730
N	-2.566738	-0.094823	0.908094
C	-3.665803	-0.116135	1.706630
C	-4.700772	-0.837394	1.022029
O	-5.828877	-1.155364	1.257861
H	0.120123	-0.338888	-1.020865
C	-1.114359	1.328457	-1.344200
C	0.000775	2.350431	-1.072634
O	-2.265290	1.706475	-1.548312
N	1.058490	1.805426	-0.218342
H	2.007560	1.783340	-0.571087
H	-1.661627	0.414529	1.114839
H	-0.502231	3.162035	-0.537841
H	-3.714475	0.350737	2.678659
C	0.832856	1.254457	0.986603
O	-0.303265	1.195369	1.497112
C	2.035956	0.699858	1.756930
H	1.617569	-0.114228	2.359864
N	3.066163	0.166629	0.869771
H	4.055518	0.330138	1.057009
C	2.826858	-0.855542	0.011638
O	1.680215	-1.233795	-0.274902
C	4.070552	-1.528694	-0.593049
H	3.888632	-1.567667	-1.675494
N	5.285508	-0.769569	-0.265748
H	6.056301	-1.381771	-0.017440
H	5.596787	-0.186089	-1.036228
C	4.154932	-2.971293	-0.068340
H	4.367541	-2.981445	1.006557
H	3.215391	-3.499672	-0.241323
H	4.954883	-3.509303	-0.585610
C	2.629542	1.767908	2.686455
H	1.855373	2.156219	3.351998
H	3.419270	1.330036	3.303841
H	3.051260	2.602509	2.117591
C	0.595293	2.890827	-2.378123
H	-0.202417	3.304187	-2.998713
H	1.310318	3.691585	-2.166759
H	1.100015	2.102097	-2.946162
H	-2.480494	-0.783293	-2.294530
C	-1.365923	-2.411372	-1.396965
H	-0.751601	-2.554405	-2.288840
H	-0.751737	-2.619599	-0.517413
H	-2.201978	-3.112915	-1.435483

Structure VI
47

C	-4.577234	0.323844	-0.360025
C	-2.307785	0.408509	-0.044210
C	-4.285659	-0.281342	1.007905
C	-1.151183	1.353913	-0.129462
N	-0.076100	0.776523	-0.720164
H	-1.191639	2.388766	0.179432
H	2.549439	2.186279	-2.062600
C	-0.407745	-0.492107	-0.969270
O	-1.649585	-0.820240	-0.628118
C	0.466263	-1.552812	-1.608007
H	0.630027	-1.239997	-2.647395
N	1.797593	-1.558430	-0.990422

H	2.595047	-1.325241	-1.568778
C	1.977448	-1.606482	0.358274
O	1.054370	-1.749256	1.154793
C	3.423814	-1.299902	0.827118
H	4.148562	-1.584938	0.061102
N	3.463732	0.177721	0.930671
H	3.098930	0.569679	1.789707
C	3.514972	0.951481	-0.168425
C	3.055515	2.423921	-0.067805
H	3.908849	3.051709	-0.342626
N	2.066797	2.512940	-1.216049
H	1.729724	3.466745	-1.363627
O	3.823116	0.544902	-1.294023
H	1.232592	1.839388	-1.053496
N	-2.900849	0.163800	1.216368
O	-3.366365	0.747715	-0.907601
O	-5.613799	0.457858	-0.936280
H	-4.354891	-1.374481	0.890830
H	-2.330213	-0.391089	1.844518
C	2.426339	2.913238	1.230085
H	3.163102	2.872787	2.037688
H	2.121227	3.960791	1.142467
H	1.551102	2.321991	1.516144
C	3.759805	-1.948757	2.161473
H	3.749976	-3.036430	2.055758
H	4.755520	-1.643516	2.493680
H	3.019233	-1.687218	2.922434
C	-0.188398	-2.940689	-1.618593
H	-1.147281	-2.910778	-2.140971
H	0.471414	-3.637437	-2.140785
H	-0.352130	-3.300321	-0.601544
C	-5.255383	0.185332	2.090751
H	-6.275674	-0.095392	1.816962
H	-5.011132	-0.286383	3.046740
H	-5.206501	1.270479	2.212503

Structure VI'
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C	2.227789	-1.568881	0.014834
C	2.439059	0.713816	0.229132
C	3.237397	-1.121155	-1.022740
C	2.641164	1.742644	1.295265
N	1.650274	2.648902	1.270152
H	0.202388	-2.405567	0.953617
C	0.907731	2.360946	0.221845
O	1.352090	1.314807	-0.534631
C	-0.296402	3.122616	-0.252666
H	0.033315	3.764028	-1.082023
N	-1.297605	2.222566	-0.856389
H	-1.642319	2.477280	-1.771672
C	-1.784369	1.100879	-0.287373
O	-1.391538	0.667976	0.804488
C	-2.903331	0.377928	-1.095252
H	-2.568563	0.268555	-2.131027
N	-3.068844	-0.957831	-0.536676
H	-3.677856	-1.015024	0.268715
C	-2.012796	-1.816992	-0.588123
C	-1.863119	-2.823541	0.573803
N	-0.734648	-2.208911	1.394918
H	-0.715996	-2.586001	2.345526
O	-1.122552	-1.747229	-1.424682
H	-0.851864	-1.177628	1.441539
N	3.529004	0.235331	-0.538840
O	1.868822	-0.523045	0.783460
O	1.737074	-2.669648	0.191238
H	2.705238	-1.123977	-1.987941
H	3.886198	0.897174	-1.217884

C	-0.888802	4.009327	0.850454
H	-0.124936	4.685546	1.238989
H	-1.711430	4.601129	0.441042
H	-1.258701	3.399163	1.677052
C	4.469249	-2.022492	-1.110224
H	4.171092	-3.036709	-1.388567
H	5.154272	-1.643772	-1.873539
H	4.996541	-2.050835	-0.153382
H	3.429208	1.724830	2.034690
C	-4.233556	1.140562	-1.045948
H	-4.133480	2.135549	-1.486048
H	-4.995998	0.596344	-1.609257
H	-4.580263	1.267548	-0.014448
C	-3.073205	-3.108920	1.455804
H	-3.898254	-3.488100	0.846476
H	-2.836696	-3.882822	2.193112
H	-3.417043	-2.222780	2.000753
H	-1.464124	-3.747646	0.150287

Structure VII
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C	-2.651639	-1.755320	0.979735
N	-3.536185	-0.744746	0.379161
C	-3.097333	0.411894	-0.083282
O	-1.589160	-1.738048	-1.209798
C	-1.543557	-2.118330	-0.052034
C	-3.661285	1.396718	-0.942816
N	-2.751964	2.374058	-1.120699
O	-0.599013	-2.835393	0.503288
H	-4.634132	1.392217	-1.415533
H	1.310871	-2.418420	-1.841305
C	-1.697571	2.036487	-0.403482
O	-1.867287	0.840100	0.265351
C	-0.425644	2.790140	-0.200608
N	0.697841	1.888936	-0.002198
H	1.036337	1.289097	-0.757567
C	1.440196	1.975456	1.141542
O	1.119181	2.689770	2.086772
C	2.777362	1.199860	1.187735
N	2.665768	-0.253909	0.951515
H	2.904124	-0.845656	1.735682
C	2.405248	-0.865956	-0.227088
C	2.634904	-2.384333	-0.271952
N	1.491238	-2.976920	-1.003346
H	1.717531	-3.922655	-1.308363
H	-4.444525	-1.049973	0.043091
O	2.029148	-0.270511	-1.243908
H	0.230543	-2.954046	-0.170174
C	3.993546	-2.683614	-0.927911
H	4.814892	-2.247765	-0.350738
H	4.157888	-3.764814	-0.975757
H	4.028168	-2.276105	-1.942449
C	3.841543	1.865942	0.298937
H	3.923919	2.924715	0.560380
H	4.813804	1.396412	0.473370
H	3.597548	1.782093	-0.761737
C	-0.191218	3.817463	-1.320750
H	-1.053446	4.478981	-1.426770
H	0.684892	4.416880	-1.065916
H	-0.015018	3.321429	-2.279408
C	-3.464471	-2.971477	1.427596
H	-2.791574	-3.703506	1.876742
H	-4.211163	-2.687030	2.174253
H	-3.965381	-3.448412	0.578293
H	2.622963	-2.794642	0.744684
H	3.084250	1.294437	2.230448
H	-0.528945	3.324249	0.760496

H -2.153863 -1.296350 1.839842

Structure VIII
44

C	-1.488688	2.650069	0.762423
N	-0.534733	3.083199	-0.155010
C	0.674378	2.487732	-0.418664
C	1.679568	2.720830	-1.322123
N	2.677627	1.783122	-1.106383
H	1.756144	3.482923	-2.083129
H	-2.308406	0.351622	-1.532690
C	2.265774	1.044773	-0.125418
O	1.025515	1.425960	0.354553
C	2.901445	-0.163222	0.507793
N	2.119738	-1.367337	0.174731
H	2.231683	-1.747621	-0.755742
C	1.075346	-1.777434	0.934814
O	0.769238	-1.264562	2.009364
C	0.209400	-2.955165	0.410681
N	-1.191159	-2.467070	0.433090
H	-1.666013	-2.583109	1.319461
C	-1.607103	-1.455880	-0.349596
C	-2.960021	-0.795606	0.019485
N	-2.921097	0.520521	-0.709669
H	-3.847665	0.835716	-1.001460
H	-0.743287	3.902298	-0.713590
O	-1.004362	-1.028324	-1.339092
H	-2.439124	1.307156	-0.131904
C	-4.168696	-1.629901	-0.414482
H	-4.169276	-2.587814	0.111421
H	-5.105636	-1.119054	-0.170566
H	-4.140608	-1.837271	-1.488826
C	0.593642	-3.620180	-0.911598
H	1.596817	-4.049759	-0.830986
H	-0.096431	-4.441223	-1.124343
H	0.559351	-2.925331	-1.752803
C	4.360193	-0.327860	0.082130
H	4.937860	0.556229	0.360375
H	4.789521	-1.200829	0.579516
H	4.448450	-0.450458	-1.001342
C	-2.509239	3.671440	1.192296
H	-3.302528	3.201423	1.780571
H	-2.062646	4.454190	1.823810
H	-2.980639	4.172498	0.337246
H	-2.998638	-0.577344	1.090856
H	0.255397	-3.707048	1.203680
H	2.827540	-0.057678	1.594039
H	-1.073616	1.991273	1.524053

TS-1
47

C	-4.553935	0.325616	-0.345578
C	-2.288828	0.441531	-0.042950
C	-4.244843	-0.291368	1.013042
C	-1.130270	1.380696	-0.118505
N	-0.061875	0.793696	-0.724170
H	-1.149664	2.413639	0.195098
H	2.401015	2.066228	-2.093161
C	-0.381222	-0.478609	-0.999357
O	-1.612505	-0.798914	-0.678433
C	0.514922	-1.517862	-1.644774
H	0.714523	-1.167146	-2.665711
N	1.816343	-1.545833	-0.973346
H	2.643396	-1.311781	-1.511286

C	1.925600	-1.584148	0.385302
O	0.949984	-1.696848	1.124058
C	3.347844	-1.293277	0.924427
H	4.104138	-1.630312	0.211744
N	3.416289	0.183775	0.965577
H	3.032456	0.622626	1.792631
C	3.526755	0.911123	-0.168539
C	3.048939	2.375641	-0.161462
H	3.884077	2.981298	-0.529613
N	1.969662	2.366359	-1.214408
H	1.609253	3.310918	-1.361607
O	3.883129	0.436290	-1.251405
H	0.983870	1.521497	-0.970982
N	-2.858797	0.155410	1.206756
O	-3.344609	0.777453	-0.894056
O	-5.590417	0.453290	-0.918878
H	-4.309970	-1.383507	0.888611
H	-2.272798	-0.373107	1.842917
C	2.524184	2.958545	1.146507
H	3.312384	2.962618	1.905151
H	2.220333	4.000701	1.005908
H	1.661760	2.405753	1.533625
C	3.593266	-1.893639	2.300607
H	3.558527	-2.984351	2.241729
H	4.578779	-1.599296	2.670571
H	2.824167	-1.578487	3.011353
C	-0.149066	-2.898824	-1.723892
H	-1.088702	-2.847086	-2.278849
H	0.526154	-3.581370	-2.244666
H	-0.348911	-3.289866	-0.724972
C	-5.202448	0.164662	2.111677
H	-6.224514	-0.119157	1.848184
H	-4.944433	-0.313438	3.060694
H	-5.157235	1.249076	2.240433

TS-2
47

C	-4.079980	0.561780	-0.777567
C	-2.298160	-0.255558	0.440083
C	-4.606768	-0.538123	0.135734
C	-1.143500	0.267547	1.239700
N	0.025163	-0.283984	0.841123
H	-1.239814	0.935127	2.086573
H	0.503659	2.472456	-1.417243
C	-0.286198	-1.210539	-0.053125
O	-1.602792	-1.338656	-0.317329
C	0.648741	-2.152569	-0.776485
H	0.227672	-2.279252	-1.780255
N	1.960566	-1.534704	-0.969812
H	2.008123	-0.880408	-1.741910
C	2.926162	-1.381275	-0.011624
O	2.961303	-1.961463	1.062171
C	3.981681	-0.297986	-0.376082
H	4.080022	-0.201229	-1.460193
N	3.418320	0.982768	0.114892
H	3.566082	1.181822	1.096424
C	2.455360	1.637866	-0.541745
C	1.767700	2.838517	0.157231
H	2.237262	3.749241	-0.230087
N	0.373706	2.814250	-0.443578
H	-0.087273	3.726665	-0.435693
O	2.070597	1.367299	-1.689552
H	-0.230170	2.128808	0.040147
N	-3.486920	-0.670794	1.079156
O	-2.717548	0.706805	-0.528466
O	-4.648242	1.238479	-1.582163
H	-4.729994	-1.435695	-0.491550

H	-3.412910	-1.547140	1.583034
C	1.723215	2.857647	1.680177
H	2.729190	3.017792	2.078481
H	1.114639	3.691486	2.043683
H	1.329212	1.920045	2.082035
C	5.334249	-0.566099	0.267692
H	5.754599	-1.491375	-0.133887
H	6.029904	0.250120	0.054769
H	5.233023	-0.697544	1.348626
C	0.688158	-3.545706	-0.117012
H	-0.316435	-3.977329	-0.125331
H	1.348198	-4.195658	-0.697323
H	1.060959	-3.491008	0.904977
C	-5.935302	-0.185838	0.799793
H	-6.692807	-0.000831	0.033826
H	-6.275007	-1.013467	1.428626
H	-5.832652	0.706949	1.421921

TS-3

47

C	3.125411	-1.562745	-0.831916
N	3.622378	-0.369326	-0.126169
C	2.571458	0.347486	0.412337
O	1.432472	-0.952138	0.700081
C	1.805074	-1.890391	-0.114393
C	2.615440	1.178014	1.618946
N	1.812773	2.244482	1.454367
O	1.154794	-2.929247	-0.317859
H	3.137597	0.956474	2.539444
H	-1.231124	-2.404923	1.652866
C	1.355210	2.173627	0.219966
O	1.832126	1.105977	-0.492056
C	0.358198	3.074607	-0.456428
N	-1.003984	2.580017	-0.201175
H	-1.447767	2.858656	0.663666
C	-1.578962	1.620041	-0.974808
O	-1.022538	1.119208	-1.947321
C	-3.026732	1.177814	-0.630759
N	-3.050901	-0.298787	-0.671418
H	-3.161629	-0.698290	-1.594609
C	-2.434131	-1.062747	0.252792
C	-2.311951	-2.572557	-0.071911
N	-1.232516	-3.063792	0.851151
H	-1.404421	-4.016242	1.175668
H	4.338098	-0.578661	0.563256
O	-2.000596	-0.654830	1.331828
H	-0.254475	-3.016022	0.396664
C	-3.624634	-3.327453	0.161067
H	-4.400525	-2.950267	-0.509407
H	-3.500959	-4.395603	-0.044092
H	-3.975935	-3.197464	1.189664
C	-3.687332	1.760966	0.620640
H	-3.784698	2.846076	0.516811
H	-4.697043	1.354500	0.723937
H	-3.135321	1.524459	1.531872
C	0.497676	4.528115	-0.000581
H	1.498203	4.903174	-0.229721
H	-0.233824	5.147698	-0.525258
H	0.345048	4.623478	1.078367
C	4.129824	-2.709191	-0.853347
H	3.684971	-3.574229	-1.349542
H	5.028112	-2.417194	-1.403227
H	4.415418	-3.009116	0.160855
H	-1.955923	-2.716873	-1.096109
H	-3.613395	1.489755	-1.500928
H	0.517883	2.983251	-1.534039

H 2.860100 -1.286080 -1.860444

TS-4
47

C	3.575642	-0.305922	1.122427
N	3.502821	-1.055984	-0.043029
C	2.370890	-1.605914	-0.591385
O	4.469856	2.461278	0.069422
C	3.322036	2.255904	0.054415
C	2.054366	-2.090848	-1.833212
N	0.767195	-2.607655	-1.784432
O	2.141833	2.258978	-0.068629
H	2.658791	-2.128150	-2.727013
H	-0.742992	2.283485	-1.924232
C	0.352433	-2.413691	-0.573650
O	1.292127	-1.787461	0.226686
C	-0.971030	-2.752268	0.044827
N	-1.838928	-1.561012	0.058696
H	-1.980306	-1.061687	-0.811470
C	-2.521211	-1.172919	1.167396
O	-2.436453	-1.725668	2.258873
C	-3.456102	0.057160	1.011890
N	-2.664711	1.309435	0.870820
H	-2.531838	1.840551	1.722305
C	-2.010928	1.714584	-0.220463
C	-1.249659	3.064558	-0.117365
N	-0.332829	3.038144	-1.319137
H	-0.309020	3.928426	-1.819981
H	4.348267	-1.167159	-0.588807
O	-1.973663	1.119856	-1.308713
H	0.628644	2.771903	-1.054750
C	-2.180255	4.279274	-0.169327
H	-2.847943	4.276236	0.695395
H	-1.607793	5.211585	-0.138186
H	-2.801424	4.264972	-1.070714
C	-4.547979	-0.090596	-0.052273
H	-5.134751	-0.985768	0.171761
H	-5.221663	0.770977	-0.022187
H	-4.147519	-0.183347	-1.062526
C	-1.644394	-3.929940	-0.670220
H	-1.010535	-4.819035	-0.617365
H	-2.598493	-4.150988	-0.185322
H	-1.818387	-3.703263	-1.725414
C	4.909935	-0.187478	1.787762
H	4.878755	0.566148	2.578420
H	5.221838	-1.137610	2.249565
H	5.695049	0.109292	1.081697
H	-0.617961	3.089481	0.774430
H	-3.929103	0.142863	1.991140
H	-0.809214	-3.001670	1.096976
H	2.670694	-0.325034	1.719822