

Supporting Information

Catalytic performance of a series of guanidinium-based ionic liquids on the coupling reaction of carbon dioxide with epoxides

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Table S1 Cartesian coordinates of optimized reactants, intermediates, transition states, and product discussed in the text for Route 1-10.

CO₂			
C	0.000000	0.000000	0.000000
O	0.000000	0.000000	1.169169
O	0.000000	0.000000	-1.169169

EO			
C	-0.152080	-0.037763	0.489352
C	1.044401	0.615467	-0.060917
O	0.827113	-0.789877	-0.242248
H	-0.156286	-0.252558	1.560617
H	1.873002	0.882271	0.595407
C	0.955489	1.222369	-0.962611
H	-1.510618	0.100225	-0.148909
H	-2.079692	-0.830093	-0.050486
H	-1.414316	0.329737	-1.213793

cp1-1			
C	-2.673577	0.939990	0.027833
N	-2.736948	2.234741	-0.415116
N	-3.787281	0.388422	0.578497
C	-3.539805	3.248350	0.258544
H	-2.920463	4.132088	0.451596
H	-4.400184	3.561955	-0.346404
H	-3.900116	2.860854	1.211158
C	-2.022322	2.674524	-1.610327
H	-2.721632	3.193291	-2.276666
H	-1.202733	3.361564	-1.369492
H	-1.619330	1.813506	-2.141490

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C	-5.107698	0.584034	-0.019555
H	-5.475706	-0.372084	-0.408344
H	-5.822694	0.957745	0.721758
H	-5.049484	1.290060	-0.846884
C	-3.683967	-0.750608	1.503450
H	-4.578724	-0.751320	2.132511
H	-3.578111	-1.702296	0.970017
H	-2.803433	-0.623676	2.134683
N	-1.562703	0.228060	-0.042015
H	-1.645137	-0.845028	-0.160503
C	-0.193479	0.739628	-0.092938
H	0.188750	0.729522	-1.118079
H	-0.176126	1.777051	0.252628
C	0.709767	-0.144486	0.771605
H	0.453469	-0.069776	1.833378
H	0.553863	-1.197883	0.494009
Br	-1.580292	-2.822705	-0.500002
C	5.795923	0.198706	-0.536080
C	5.710744	1.471145	0.190317
O	5.522447	0.217166	0.890690
H	4.920773	-0.071367	-1.125890
H	4.808597	2.068700	0.089629
H	6.623435	1.996376	0.466034
C	7.103958	-0.424936	-0.939948
H	7.043058	-1.516619	-0.890423
H	7.352256	-0.147950	-1.970199
H	7.913240	-0.094332	-0.283222
C	2.168608	0.204868	0.588153
N	2.586415	0.933586	-0.302308
N	2.947330	-0.377367	1.497186
H	3.896718	-0.148650	1.299841

cp1-2

Br	-1.370566	-0.031000	1.759821
C	-3.204750	-0.381796	1.039993
C	-3.348345	0.066748	-0.413119
N	-2.418717	-0.599955	-1.247138
H	-3.870404	0.155478	1.715319
H	-3.188053	1.149798	-0.470831
H	-1.734519	0.067908	-1.503533
C	2.579430	0.092635	-0.168289
N	3.330370	0.046116	0.978639
N	2.926033	-0.728000	-1.201883
C	4.778438	-0.120625	0.959514

H	5.250196	0.695397	1.520204
H	5.088498	-1.069375	1.415919
H	5.140085	-0.088541	-0.068018
C	2.708674	0.204610	2.290473
H	3.136700	-0.536229	2.974880
H	2.872705	1.201475	2.717414
H	1.637322	0.017094	2.216878
C	3.349430	-2.109856	-0.968935
H	2.566954	-2.794851	-1.311859
H	4.275951	-2.326293	-1.511652
H	3.510978	-2.282574	0.093726
C	2.399513	-0.470522	-2.544289
H	3.100147	-0.886853	-3.273688
H	1.415792	-0.930187	-2.686260
H	2.306505	0.602690	-2.708451
N	1.563298	0.911841	-0.304088
H	0.720143	0.792800	-1.020255
C	1.338705	2.186642	0.385188
H	0.750689	2.026205	1.295635
H	2.296646	2.636345	0.668499
C	0.542089	3.103408	-0.564215
H	0.231633	4.003060	-0.029807
H	1.184610	3.405924	-1.400801
C	-0.719994	2.409497	-1.140815
N	-0.486389	1.228967	-1.648498
N	-1.805823	2.978261	-1.094092
C	-4.770287	-0.263631	-0.886397
H	-4.936860	-1.346108	-0.872608
H	-5.532569	0.218837	-0.264986
H	-4.890863	0.085533	-1.914979
H	-3.321302	-1.458682	1.151608
C	-0.978439	-2.735123	-0.488752
N	-0.004264	-2.320141	-0.990589
N	-1.888040	-3.256565	0.025704

cp1-3

Br	-5.30766	0.483234	0.13407
C	-3.411216	0.063085	0.557591
C	-2.849153	-0.913638	-0.477392
O	-1.400863	-0.898149	-0.429266
H	-3.407385	-0.345251	1.563139
H	-3.067723	-0.501706	-1.468952
H	-0.63503	0.228802	-1.259783

C	3.595661	-0.101227	0.054666
N	4.788638	0.375994	0.526926
N	3.579235	-1.284269	-0.602107
C	6.045617	0.172335	-0.18491
H	6.562415	1.133473	-0.288082
H	6.71294	-0.517533	0.346515
H	5.847043	-0.223924	-1.18038
C	4.88571	1.069394	1.809161
H	5.639877	0.574131	2.432167
H	5.181356	2.117861	1.6844
H	3.928741	1.026267	2.327927
C	4.387717	-2.420341	-0.158861
H	3.720429	-3.236414	0.138008
H	5.04027	-2.776962	-0.96324
H	4.995552	-2.144922	0.701628
C	2.506652	-1.624105	-1.548943
H	2.943964	-2.233339	-2.345767
H	1.701188	-2.162492	-1.043367
H	2.082221	-0.713721	-1.970586
N	2.463333	0.572585	0.220042
H	1.57964	-0.020179	0.301569
C	2.335685	2.028674	0.301389
H	1.859203	2.293592	1.251196
H	3.327495	2.483194	0.275538
C	1.483626	2.597006	-0.855559
H	1.371103	3.673197	-0.699984
H	1.977583	2.414317	-1.813388
C	0.112708	1.940007	-0.823348
O	0.057737	0.872968	-1.621457
O	-0.769572	2.303313	-0.069353
C	-3.407791	-2.329967	-0.39109
H	-3.166958	-2.771308	0.576474
H	-4.493349	-2.304212	-0.519663
H	-2.976692	-2.948538	-1.183977
H	-2.882292	1.013765	0.512787
C	-0.711147	-1.261673	0.805577
O	0.535356	-1.127802	0.671201
O	-1.389701	-1.642671	1.747583

cp1-4

C	2.720866	-0.558704	-0.106803
N	3.993708	-0.079004	-0.225027
N	2.436041	-1.796783	-0.577136
C	4.839246	-0.389039	-1.373554
H	5.229717	0.543548	-1.796218
H	5.691107	-1.021544	-1.095368
H	4.253289	-0.897251	-2.138767
C	4.573180	0.817130	0.773426
H	5.564905	0.445076	1.054388
H	4.682748	1.838906	0.392739
H	3.945254	0.835365	1.663253
C	3.358907	-2.916772	-0.396855
H	2.871983	-3.690973	0.206089
H	3.643569	-3.354955	-1.359874
H	4.256562	-2.588728	0.126159
C	1.068200	-2.158792	-0.990729
H	1.148125	-2.987930	-1.698600
H	0.442160	-2.442035	-0.137788
H	0.592696	-1.314406	-1.492029
N	1.764332	0.170376	0.453393
H	0.939838	-0.328663	0.878022
C	1.625927	1.633174	0.396519
H	1.830011	2.078944	1.374936
H	2.348780	2.042487	-0.312350
C	0.193836	1.940580	-0.031690
H	0.000845	1.544162	-1.034850
H	-0.492261	1.400675	0.634259
Br	-0.876532	-1.029966	1.814817
C	-3.785365	-1.142241	-0.124432
C	-3.725179	0.347964	0.278991
O	-2.910470	-1.204597	-1.283023
H	-3.302813	-1.748589	0.645854
H	-3.305809	0.469793	1.278830
H	-4.683850	0.864458	0.176354
C	-5.162274	-1.656165	-0.497745
H	-5.106531	-2.690040	-0.848155
H	-5.816919	-1.630009	0.379706
H	-5.612121	-1.043637	-1.285684
C	-2.294590	-0.034588	-1.481413
N	-2.800923	0.932089	-0.666641
N	-1.426242	-0.377367	1.497186
H	3.896718	-0.148650	1.299841

cp2-1

Br	-0.306807	-1.828963	-0.090952
C	-3.717162	-0.566109	-0.753526
C	-3.532722	-0.324499	0.679962
O	-3.487501	0.780989	-0.265118
H	-2.883098	-1.003245	-1.298926
H	-2.551529	-0.601806	1.066193
H	-2.118792	1.58769	-1.076178
C	1.978422	0.486634	-0.014918
N	2.448288	0.711566	1.245794
N	2.673058	-0.291966	-0.876282
C	3.867268	0.839011	1.544721
H	4.02115	1.708547	2.194005
H	4.267073	-0.042862	2.062392
H	4.426766	0.989697	0.620795
C	1.531753	0.537186	2.379579
H	2.035436	-0.071533	3.137968
H	1.243379	1.490828	2.836826
H	0.654215	-0.018922	2.037887
C	3.228405	-1.571559	-0.403342
H	2.429358	-2.323183	-0.437276
H	4.065934	-1.853218	-1.046251
H	3.583274	-1.490232	0.621122
C	2.265701	-0.335849	-2.28607
H	3.108034	-0.70833	-2.874078
H	1.405571	-1.006989	-2.400905
H	2.000111	0.66473	-2.628787
N	0.864119	1.08915	-0.433314
H	0.234417	0.495561	-0.984522
C	0.174246	2.204106	0.199654
H	-0.483421	1.83826	0.998538
H	0.903688	2.889459	0.641742
C	-0.673027	2.906257	-0.874001
H	-1.306903	3.659853	-0.380869
H	-0.012095	3.433485	-1.571614
H	-4.716819	-0.726925	-1.155096
C	-4.680845	-0.292692	1.652109
H	-4.807145	-1.276581	2.11694
H	-4.49832	0.433911	2.451298
H	-5.612955	-0.020988	1.148218
O	-1.412444	1.982803	-1.634194

cp2-2			
C	-2.604519	0.352262	0.239735
N	-2.366339	1.532945	-0.458815
N	-3.777094	-0.314682	-0.129317
C	-3.42906	2.460479	-0.805979
H	-3.210524	3.459181	-0.4029
H	-3.551095	2.562786	-1.894884
H	-4.370943	2.112148	-0.382455
C	-1.02428	1.903796	-0.875913
H	-1.053413	2.249372	-1.917933
H	-0.591905	2.710614	-0.26859
H	-0.357171	1.044164	-0.824934
C	-4.001567	-0.596699	-1.546591
H	-3.506226	-1.530769	-1.852611
H	-5.074922	-0.694848	-1.740267
H	-3.610877	0.211804	-2.162994
C	-4.237242	-1.383639	0.746067
H	-5.288468	-1.593025	0.521217
H	-3.660099	-2.310845	0.615368
H	-4.142687	-1.072569	1.786074
N	-1.874787	-0.139328	1.183044
H	-0.859432	-1.71484	1.927963
C	-0.873387	0.64428	1.892595
H	-0.009804	0.906623	1.270572
H	-1.285892	1.582605	2.294137
C	-0.373352	-0.254978	3.029263
H	0.541887	0.137523	3.481781
H	-1.137543	-0.347947	3.813928
O	-0.075742	-1.551612	2.495817
Br	2.641372	1.855576	-0.198469
C	3.425891	0.052077	-0.449499
C	2.867164	-0.947134	0.55267
O	1.493871	-1.13611	0.262541
H	4.501046	0.18883	-0.341608
H	2.991373	-0.529351	1.562344
H	1.013191	-1.360851	1.090474
C	3.63701	-2.272681	0.460875
H	3.549251	-2.696422	-0.54419
H	4.698423	-2.143785	0.699218

H	3.213131	-2.989175	1.170717
H	3.174736	-0.234831	-1.47006
C	0.4666	-2.203344	-2.030617
O	-0.593323	-2.27921	-1.543699
O	1.498688	-2.154397	-2.580155
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cp2-3			
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C	-2.456451	0.017796	0.023229
N	-2.912129	1.308869	0.073425
N	-3.163478	-0.892738	-0.699415
C	-4.332654	1.632212	0.106519
H	-4.529102	2.321539	0.936342
H	-4.668577	2.114628	-0.820502
H	-4.915491	0.72462	0.263088
C	-1.99536	2.446021	0.022978
H	-2.310494	3.123511	-0.779916
H	-1.992308	3.010059	0.963504
H	-0.981628	2.109086	-0.194968
C	-3.724982	-0.554204	-2.007116
H	-3.194714	-1.114562	-2.78552
H	-4.788879	-0.811398	-2.053812
H	-3.60505	0.50874	-2.210417
C	-3.000468	-2.332303	-0.460298
H	-3.945934	-2.826435	-0.703572
H	-2.188124	-2.742748	-1.067002
H	-2.761009	-2.502914	0.589535
N	-1.372807	-0.37453	0.667223
H	-0.789088	-1.149418	0.184332
C	-0.77114	0.264299	1.834657
H	0.158327	0.754562	1.526847
H	-1.445479	1.025816	2.237156
C	-0.471919	-0.777042	2.925339
H	0.105478	-0.261006	3.713533
H	-1.413135	-1.108484	3.382137
O	0.174232	-1.931062	2.450796
Br	2.030715	2.081063	-0.228053
C	3.237233	0.572156	-0.729416
C	3.081475	-0.60346	0.227773
O	1.749689	-1.13001	0.227312
H	4.238421	0.998939	-0.683567

H	3.209448	-0.22817	1.249565
H	0.836307	-1.684981	1.77488
C	4.145357	-1.675913	-0.037593
H	4.059692	-2.058446	-1.054359
H	5.14925	-1.267765	0.122585
H	3.998124	-2.50276	0.663351
H	2.957669	0.302242	-1.743437
C	1.187651	-1.651774	-1.007172
O	-0.016256	-1.977724	-0.8282
O	1.903301	-1.697427	-2.001154

cp2-4

C	2.271314	-0.378224	-0.544891
N	3.545051	-0.040562	-0.196228
N	1.936548	-1.695539	-0.591425
C	4.673531	-0.901623	-0.531406
H	5.470187	-0.287514	-0.966949
H	5.082991	-1.407129	0.352638
H	4.366759	-1.652933	-1.258349
C	3.864328	1.094808	0.673113
H	4.403899	0.722402	1.552826
H	4.513681	1.811711	0.155571
H	2.954576	1.597935	1.006757
C	2.245497	-2.555404	0.561895
H	1.379271	-2.557744	1.234169
H	2.46613	-3.568829	0.2146
H	3.103478	-2.172252	1.110853
C	0.743146	-2.131462	-1.329307
H	0.888377	-3.177053	-1.615411
H	-0.148089	-2.038002	-0.698624
H	0.610386	-1.527201	-2.2266
N	1.361835	0.518513	-0.91143
H	0.397277	0.232507	-0.729454
C	1.506972	1.93794	-1.220889
H	2.563955	2.204406	-1.220669
H	1.109753	2.108052	-2.228208
C	0.699529	2.786716	-0.215896
H	0.905204	3.84364	-0.423843
H	-0.368668	2.613504	-0.395185
Br	-0.55862	-0.359563	1.574231

C	-3.741374	-0.640651	0.157005
C	-3.620406	0.863639	0.494132
O	-2.919647	-0.774359	-1.031207
H	-3.24751	-1.231738	0.931862
H	-3.130515	1.018537	1.456709
H	-4.573988	1.397069	0.439063
C	-5.147723	-1.128609	-0.135793
H	-5.136836	-2.17531	-0.451118
H	-5.762914	-1.051422	0.766927
H	-5.61407	-0.531245	-0.925739
C	-2.28199	0.380602	-1.289567
O	-2.753476	1.387148	-0.528062
O	-1.415989	0.513665	-2.121792
O	1.040133	2.527999	1.129711
H	0.529241	1.734394	1.414098

cp3-1

C	-1.315174	0.637625	0.414432
N	-2.218284	1.130581	-0.48112
N	-1.736776	-0.093848	1.47251
C	-3.561759	1.537367	-0.096903
H	-3.782271	2.512209	-0.547324
H	-4.326846	0.828474	-0.439452
H	-3.626273	1.631302	0.987668
C	-1.946534	1.01866	-1.918808
H	-2.825449	0.578438	-2.401711
H	-1.74781	1.994324	-2.3783
H	-1.116485	0.323398	-2.067507
C	-2.745543	-1.148985	1.288954
H	-2.22968	-2.07447	1.008529
H	-3.310876	-1.263243	2.218222
H	-3.428285	-0.899487	0.481821
C	-0.801871	-0.384871	2.559963
H	-1.380119	-0.641312	3.451165
H	-0.159837	-1.231324	2.290023
H	-0.182395	0.486989	2.770939
N	-0.029491	0.996338	0.325019
H	0.678003	0.299617	0.584741
C	0.48301	2.1491	-0.410411
H	0.920337	1.817911	-1.36127

H	-0.356318	2.807468	-0.646769
C	1.531034	2.907044	0.413428
H	1.059216	3.27392	1.333252
H	2.315084	2.20807	0.72377
Br	-0.33944	-2.080251	-0.970276
C	3.434103	-0.935949	0.285123
C	2.607193	-1.812069	1.125969
O	2.42405	-0.370305	1.159096
H	4.444076	-0.717102	0.638912
H	3.02639	-2.226561	2.042652
H	1.77516	-2.345162	0.66432
C	3.213472	-0.809216	-1.199412
H	3.422571	0.213445	-1.536054
H	3.899334	-1.477445	-1.732582
H	2.185208	-1.083811	-1.45731
C	2.140196	4.073732	-0.369195
H	2.881939	4.605432	0.233845
H	2.640917	3.724656	-1.279026
H	1.375509	4.79934	-0.669352

cp3-2

C	-2.156367	-0.867701	0.347353
N	-3.026297	-1.791001	-0.228844
N	-1.939175	-1.041103	1.706807
C	-4.204177	-2.295063	0.458329
H	-5.098039	-2.136216	-0.159906
H	-4.133031	-3.372044	0.670595
H	-4.333885	-1.762741	1.400367
C	-2.788121	-2.327733	-1.557618
H	-2.811854	-3.425833	-1.524942
H	-3.539135	-1.996814	-2.287795
H	-1.803623	-2.019839	-1.909717
C	-1.60266	-2.356307	2.240852
H	-0.517522	-2.453735	2.39498
H	-2.09613	-2.518827	3.205957
H	-1.919071	-3.138312	1.551435
C	-1.417543	0.075731	2.487876
H	-1.707996	-0.066768	3.534413
H	-0.325594	0.159392	2.428381
H	-1.837907	1.010588	2.11855

N	-1.588143	0.117488	-0.277539
H	0.021915	0.80365	0.140711
C	-2.156926	0.65631	-1.508551
H	-1.57662	0.321614	-2.382691
H	-3.189192	0.310858	-1.667502
C	-2.134861	2.190428	-1.470227
H	-2.742504	2.528716	-0.622049
H	-1.11114	2.519523	-1.259529
Br	3.814588	-1.640934	-0.439477
C	1.975386	0.650753	-0.287821
C	2.165097	-0.772876	0.245812
O	0.884077	1.22297	0.415034
H	2.856442	1.239697	-0.008567
H	2.26987	-0.766491	1.32947
H	1.344514	-1.427922	-0.05071
C	1.794065	0.709308	-1.804016
H	1.654369	1.746538	-2.120309
H	2.665813	0.297445	-2.318895
H	0.91258	0.133989	-2.109284
C	0.893213	3.645669	1.547485
O	2.028154	3.793697	1.307678
O	-0.241649	3.571339	1.822399
C	-2.643122	2.822091	-2.768521
H	-2.61969	3.914781	-2.712726
H	-2.029905	2.521532	-3.626066
H	-3.676476	2.524512	-2.98207

cp3-3

C	-2.497616	-0.876438	-0.022888
N	-3.679847	-1.160654	-0.652295
N	-2.124738	-1.647601	1.024836
C	-4.880443	-1.531617	0.091569
H	-5.695746	-0.847431	-0.170949
H	-5.203452	-2.554177	-0.13827
H	-4.696709	-1.448201	1.162106
C	-3.851228	-0.991685	-2.090163
H	-4.372866	-1.868646	-2.489781
H	-4.443114	-0.101077	-2.335638
H	-2.877127	-0.919546	-2.573347
C	-2.448982	-3.071448	1.087815

H	-1.523287	-3.638384	1.233165
H	-3.119469	-3.292855	1.92603
H	-2.91503	-3.400269	0.159672
C	-1.202794	-1.173296	2.067442
H	-1.615023	-1.459282	3.040952
H	-0.220576	-1.642201	1.947775
H	-1.068837	-0.087809	2.01957
N	-1.718439	0.114737	-0.442415
H	-0.730702	0.137265	-0.113751
C	-2.177651	1.409648	-0.9778
H	-1.260029	1.960008	-1.195882
H	-2.704164	1.273493	-1.927562
C	-3.031897	2.213023	0.010015
H	-3.932451	1.638327	0.267142
H	-2.440314	2.343879	0.920187
Br	4.917506	-0.540517	-0.385541
C	2.118846	0.309609	-0.485903
C	3.143664	-0.293812	0.474364
O	0.912371	0.496712	0.257943
H	2.493102	1.28731	-0.80571
H	3.314589	0.387688	1.303387
H	2.845586	-1.283409	0.823226
C	1.808119	-0.574297	-1.688179
H	1.074046	-0.088299	-2.338174
H	2.714331	-0.767923	-2.266967
H	1.396515	-1.537343	-1.363119
C	0.837769	1.73351	1.14673
O	1.8621	2.399226	1.192119
O	-0.295258	1.79829	1.649239
C	-3.433724	3.571609	-0.570708
H	-4.046551	4.132149	0.141186
H	-2.550651	4.179596	-0.793286
H	-4.011685	3.467178	-1.497072

cp3-4

C	-1.949754	-0.52428	0.521116
N	-2.948833	-0.973129	-0.290317
N	-1.493543	-1.311093	1.527258
C	-3.990729	-1.868632	0.192558
H	-4.963349	-1.504338	-0.157718

H	-3.862637	-2.89429	-0.177296
H	-3.993321	-1.883087	1.282733
C	-2.87281	-0.784428	-1.743431
H	-3.065067	-1.749593	-2.22381
H	-3.614233	-0.061234	-2.102992
H	-1.855781	-0.491959	-2.013651
C	-1.153213	-2.717033	1.25398
H	-0.13729	-2.758916	0.84451
H	-1.241304	-3.287659	2.18252
H	-1.821379	-3.141837	0.509318
C	-0.703056	-0.719722	2.610617
H	-0.775376	-1.378373	3.480109
H	0.34958	-0.608919	2.329194
H	-1.10225	0.260889	2.871023
N	-1.510229	0.731602	0.417183
H	-0.533198	0.901813	0.666992
C	-2.153404	1.817666	-0.319627
H	-1.76874	1.846415	-1.346969
H	-3.226093	1.609608	-0.370551
C	-1.894397	3.163474	0.365117
H	-2.314803	3.136493	1.377885
H	-0.813139	3.297295	0.477252
Br	0.66482	-1.239524	-1.319091
C	3.665052	-0.34837	0.067419
C	3.508845	0.688372	-1.068608
O	2.767427	0.161391	1.091078
H	3.237549	-1.302264	-0.250577
H	3.086335	0.231366	-1.964955
H	4.430376	1.236175	-1.286975
C	5.063591	-0.48693	0.637746
H	5.068129	-1.170239	1.491229
H	5.73495	-0.89412	-0.125698
H	5.456318	0.481575	0.963975
C	2.062574	1.195571	0.609798
O	2.540329	1.628525	-0.562979
O	1.134461	1.711611	1.199598
C	-2.494307	4.328786	-0.426095
H	-2.296492	5.281819	0.07291
H	-2.06647	4.387387	-1.432928
H	-3.58086	4.228627	-0.531331

cp4-1			
C	-1.396284	0.532754	0.344257
N	-2.414888	0.641948	-0.556709
N	-1.577733	-0.160822	1.492472
C	-3.812421	0.694911	-0.15266
H	-4.310241	1.508857	-0.692579
H	-4.34861	-0.235772	-0.379517
H	-3.882686	0.891688	0.917639
C	-2.14507	0.437811	-1.984942
H	-2.883118	-0.270898	-2.375235
H	-2.220558	1.369843	-2.557668
H	-1.162253	-0.028143	-2.094361
C	-2.235643	-1.476497	1.464421
H	-1.473738	-2.239471	1.267859
H	-2.740293	-1.640986	2.420706
H	-2.963056	-1.530617	0.659582
C	-0.593225	-0.039213	2.568046
H	-1.06887	-0.339937	3.504977
H	0.264953	-0.69271	2.373543
H	-0.250672	0.992248	2.652886
N	-0.269592	1.229578	0.160672
H	0.610795	0.800424	0.468484
C	-0.11546	2.372843	-0.736536
H	0.343608	2.044785	-1.67729
H	-1.110434	2.756901	-0.971404
C	0.735776	3.463078	-0.08401
H	0.24292	3.862893	0.807425
H	1.711302	3.07147	0.214759
Br	0.318413	-1.933599	-0.781434
C	3.606233	0.363616	0.205631
C	3.06421	-0.606795	1.166108
O	2.479426	0.719	1.047874
H	4.513496	0.897205	0.497544
H	3.586717	-0.778145	2.107112
H	2.415908	-1.401669	0.795327
C	3.354645	0.251437	-1.275143
H	3.265721	1.245573	-1.729581
H	4.199574	-0.255254	-1.755312
H	2.444995	-0.328019	-1.46462

H	0.893581	4.28511	-0.789164
cp4-2			
C	2.375045	-0.402885	-0.140765
N	3.318824	-1.340606	0.274622
N	2.291755	-0.229801	-1.514399
C	4.6131	-1.489796	-0.37031
H	5.418151	-1.387487	0.370033
H	4.726345	-2.471959	-0.85232
H	4.736191	-0.714881	-1.126624
C	3.054659	-2.239836	1.38462
H	3.241947	-3.277493	1.075286
H	3.686952	-2.030673	2.258361
H	2.010168	-2.159078	1.685848
C	2.204372	-1.382701	-2.404194
H	1.163559	-1.566101	-2.71026
H	2.798054	-1.216163	-3.310334
H	2.574035	-2.277462	-1.904485
C	1.669544	0.981318	-2.039159
H	2.057139	1.162297	-3.047491
H	0.576067	0.907969	-2.084281
H	1.913532	1.828042	-1.39868
N	1.626635	0.306877	0.647101
H	-0.020309	0.912063	0.241589
C	2.016758	0.555883	2.031926
H	1.406644	-0.051868	2.716564
H	3.064266	0.279056	2.21498
C	1.809886	2.034953	2.369887
H	2.465638	2.665726	1.761761
H	0.77826	2.334082	2.16467
Br	-3.49186	-1.990183	-0.116963
C	-1.968641	0.468945	0.420963
C	-1.917054	-0.816395	-0.410826
O	-0.903252	1.298653	-0.013674
H	-2.890122	1.004339	0.165328
H	-1.922025	-0.586456	-1.47506
H	-1.047251	-1.425521	-0.160235
C	-1.939151	0.21747	1.928159
H	-1.960681	1.171643	2.461425
H	-2.796913	-0.382437	2.242909

H	-1.025431	-0.316378	2.213266
C	-1.165771	3.876989	-0.682945
O	-2.322579	3.835757	-0.51699
O	-0.017116	3.996772	-0.870593
H	2.027482	2.226722	3.426113
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cp4-3			
N	-2.385762	-1.152961	1.13964
C	-5.126431	-0.962425	0.180843
H	-5.88825	-0.259284	-0.175355
H	-5.527497	-1.978938	0.088033
H	-4.931365	-0.751176	1.231626
C	-4.070349	-0.796787	-2.048284
H	-4.659649	-1.676214	-2.331332
H	-4.593434	0.096487	-2.411876
H	-3.096111	-0.863854	-2.531982
C	-2.808296	-2.529283	1.392251
H	-1.923428	-3.136285	1.611912
H	-3.484704	-2.589149	2.252477
H	-3.304956	-2.94432	0.516066
C	-1.427165	-0.607597	2.112056
H	-1.84941	-0.73779	3.11402
H	-0.477136	-1.149132	2.055275
H	-1.226305	0.45173	1.922667
N	-1.850798	0.351941	-0.554831
H	-0.864709	0.349726	-0.220454
C	-2.209518	1.591276	-1.271999
H	-1.250697	2.047467	-1.522656
H	-2.71274	1.359229	-2.214863
C	-3.03301	2.562326	-0.426313
H	-3.994538	2.127095	-0.13151
H	-2.460871	2.834507	0.462818
Br	4.712978	-0.771556	-0.244731
C	1.999028	0.281084	-0.552921
C	2.945433	-0.2711	0.51241
O	0.794299	0.658055	0.118007
H	2.461276	1.175738	-0.9823
H	3.152769	0.497436	1.252413
H	2.555892	-1.178903	0.975093
C	1.644901	-0.723665	-1.643129

H	0.963203	-0.270536	-2.36944
H	2.544118	-1.056481	-2.166972
H	1.153698	-1.604631	-1.212711
C	0.798169	2.002033	0.839498
O	1.873061	2.583995	0.839358
O	-0.339132	2.21937	1.286336
H	-3.24153	3.466609	-1.007213

cp4-4

C	-2.105897	0.070102	0.464195
N	-3.141705	-0.362663	-0.308951
N	-1.794116	-0.592508	1.605919
C	-4.313383	-1.009413	0.26556
H	-5.21462	-0.578236	-0.185273
H	-4.32708	-2.090648	0.076464
H	-4.342722	-0.837667	1.341798
C	-3.008067	-0.433239	-1.768505
H	-3.336062	-1.426156	-2.09382
H	-3.622835	0.320412	-2.274506
H	-1.952866	-0.344499	-2.036722
C	-1.65556	-2.057761	1.580505
H	-0.64089	-2.308775	1.250963
H	-1.868269	-2.450471	2.578685
H	-2.34478	-2.500496	0.86628
C	-0.950863	0.056059	2.613872
H	-1.128073	-0.439132	3.572101
H	0.112119	-0.018296	2.360832
H	-1.218138	1.109611	2.70163
N	-1.483901	1.215895	0.17955
H	-0.499319	1.28794	0.447992
C	-1.93975	2.241112	-0.758603
H	-1.537063	2.031006	-1.756571
H	-3.029829	2.185879	-0.818889
C	-1.484753	3.623654	-0.29333
H	-1.937488	3.884888	0.66794
H	-0.397924	3.650058	-0.179292
Br	0.405107	-1.312996	-1.114124
C	3.500241	-0.614424	0.173966
C	3.483819	0.233569	-1.118413
O	2.688418	0.176189	1.084422

H	2.941671	-1.539014	0.008847
H	3.01648	-0.308444	-1.941676
H	4.468223	0.62301	-1.395172
C	4.868023	-0.850893	0.78476
H	4.780099	-1.380259	1.737359
H	5.472956	-1.466143	0.110334
H	5.393466	0.093836	0.958001
C	2.115251	1.19175	0.422835
O	2.634412	1.353349	-0.799966
O	1.263953	1.914242	0.901854
H	-1.776363	4.378042	-1.030139

cp5-1			
C	-1.358915	0.585444	0.399872
N	-2.27608	1.033615	-0.50331
N	-1.753191	-0.160618	1.457967
C	-3.635078	1.396658	-0.130445
H	-3.884553	2.361929	-0.586181
H	-4.373191	0.660955	-0.475752
H	-3.710545	1.492697	0.953257
C	-1.986058	0.930126	-1.93822
H	-2.848178	0.466559	-2.429347
H	-1.808113	1.910116	-2.396347
H	-1.135265	0.258014	-2.07657
C	-2.720178	-1.254664	1.273372
H	-2.170164	-2.15126	0.963939
H	-3.257507	-1.411308	2.212738
H	-3.434744	-1.018168	0.489983
C	-0.804762	-0.420645	2.54205
H	-1.370158	-0.699174	3.434795
H	-0.135393	-1.243586	2.265411
H	-0.215622	0.472049	2.752665
N	-0.08744	0.99563	0.312772
H	0.644743	0.322368	0.564184
C	0.374039	2.168013	-0.421741
H	0.846263	1.857339	-1.363182
H	-0.479744	2.798055	-0.672413
C	1.368543	2.981296	0.415931
H	0.844662	3.373857	1.294918
H	2.160567	2.31342	0.788543

N	1.842274	4.116444	-0.38197
H	2.366003	4.75765	0.207703
H	2.496104	3.790248	-1.090798
Br	-0.21966	-2.097185	-0.935206
C	3.491435	-0.757709	0.273785
C	2.714271	-1.664544	1.129468
O	2.453199	-0.234684	1.140313
H	4.488888	-0.479871	0.62207
H	3.15675	-2.041682	2.051308
H	1.911634	-2.248409	0.677415
C	3.263288	-0.666449	-1.212376
H	3.41896	0.360123	-1.566304
H	3.982415	-1.306427	-1.736288
H	2.250246	-0.99718	-1.464426

cp5-2

C	-2.15552	-0.857243	0.339545
N	-3.011437	-1.792652	-0.235756
N	-1.952035	-1.015795	1.70233
C	-4.206067	-2.279768	0.435262
H	-5.089575	-2.107136	-0.194062
H	-4.151978	-3.357665	0.646738
H	-4.340681	-1.74662	1.376129
C	-2.77002	-2.323402	-1.566516
H	-2.811711	-3.42086	-1.539603
H	-3.508063	-1.975642	-2.301801
H	-1.777011	-2.029659	-1.906862
C	-1.635325	-2.325614	2.260555
H	-0.556129	-2.42115	2.452183
H	-2.160953	-2.479371	3.210153
H	-1.928492	-3.11354	1.567724
C	-1.443529	0.10893	2.480055
H	-1.753577	-0.020645	3.522684
H	-0.350442	0.189718	2.439844
H	-1.855246	1.040151	2.09216
N	-1.582878	0.123778	-0.289316
H	0.0217	0.806632	0.144984
C	-2.144997	0.647582	-1.528027
H	-1.552682	0.317067	-2.396636
H	-3.175036	0.312934	-1.703596

C	-2.130689	2.180861	-1.493946
H	-2.793251	2.517877	-0.688823
H	-1.116723	2.518048	-1.225439
N	-2.641388	2.712025	-2.762744
H	-2.76568	3.718448	-2.688344
H	-1.948824	2.5714	-3.495926
Br	3.797093	-1.663662	-0.411798
C	1.977888	0.643679	-0.265194
C	2.14767	-0.785429	0.26022
O	0.88362	1.221737	0.428058
H	2.861174	1.222236	0.028297
H	2.239484	-0.787725	1.345065
H	1.324569	-1.430464	-0.050744
C	1.814945	0.71453	-1.783079
H	1.689354	1.755631	-2.092918
H	2.688538	0.297973	-2.290952
H	0.931475	0.149824	-2.102163
C	0.886581	3.671962	1.493085
O	2.029729	3.801878	1.28383
O	-0.257088	3.61797	1.734547

cp5-3

C	-2.512839	-0.864208	-0.0264
N	-3.700126	-1.137216	-0.648792
N	-2.139749	-1.637116	1.020589
C	-4.897984	-1.505474	0.10127
H	-5.710541	-0.814772	-0.152246
H	-5.228647	-2.524495	-0.132961
H	-4.706732	-1.430187	1.171121
C	-3.88411	-0.948873	-2.083812
H	-4.425568	-1.812644	-2.485264
H	-4.461152	-0.04457	-2.312422
H	-2.914084	-0.889709	-2.576696
C	-2.470387	-3.059385	1.085291
H	-1.546696	-3.630982	1.225241
H	-3.13748	-3.27802	1.926951
H	-2.942967	-3.385542	0.159497
C	-1.208483	-1.166495	2.056567
H	-1.614737	-1.450683	3.033118
H	-0.228523	-1.63835	1.930308

H	-1.071314	-0.081592	2.007456
N	-1.726091	0.119959	-0.449803
H	-0.738097	0.132858	-0.124229
C	-2.175188	1.41476	-0.986811
H	-1.255241	1.964728	-1.196224
H	-2.709877	1.303313	-1.932303
C	-3.029877	2.218642	0.002006
H	-3.963754	1.675439	0.197874
H	-2.468401	2.299299	0.940639
N	-3.376359	3.499152	-0.627743
H	-4.077575	3.973828	-0.064406
H	-2.55814	4.105937	-0.607595
Br	4.922002	-0.549829	-0.368783
C	2.121315	0.288149	-0.491001
C	3.147194	-0.288714	0.484165
O	0.91341	0.490589	0.24763
H	2.493057	1.2585	-0.835064
H	3.315311	0.413019	1.296722
H	2.852068	-1.270636	0.856416
C	1.811875	-0.626168	-1.670521
H	1.077007	-0.157955	-2.332484
H	2.718366	-0.833018	-2.244267
H	1.40186	-1.581303	-1.321069
C	0.836657	1.743429	1.106847
O	1.858468	2.41456	1.138327
O	-0.296999	1.819118	1.608284

cp5-4

C	2.530021	-0.367456	-0.133165
N	3.876723	-0.152402	-0.243655
N	2.066567	-1.636687	-0.209726
C	4.721651	-0.951547	-1.123837
H	5.322508	-0.28429	-1.752374
H	5.406562	-1.59886	-0.561622
H	4.100259	-1.570691	-1.770419
C	4.553931	0.883792	0.531203
H	5.44165	0.451169	1.006707
H	4.873715	1.724729	-0.095267
H	3.891611	1.254061	1.312588
C	2.761541	-2.741644	0.448972

H	2.10193	-3.175495	1.208248
H	3.028471	-3.524931	-0.269348
H	3.664783	-2.384577	0.942453
C	0.693063	-1.934486	-0.647988
H	0.702505	-2.922069	-1.118697
H	-0.002674	-1.916008	0.196297
H	0.362369	-1.195808	-1.378455
N	1.687006	0.646037	0.022751
H	0.798209	0.442884	0.548852
C	1.899885	2.014907	-0.476037
H	2.348713	2.646772	0.299009
H	2.592663	1.951969	-1.320946
C	0.586947	2.670547	-0.91495
H	0.863883	3.536381	-1.530362
H	0.039531	1.971954	-1.565819
N	-0.163889	3.162032	0.243647
H	-1.000073	3.633765	-0.094391
H	-0.508727	2.369662	0.793529
Br	-0.872276	0.046559	1.860126
C	-3.694677	-0.892996	0.015301
C	-3.786315	0.648563	0.067676
O	-2.752357	-1.125335	-1.061739
H	-3.215039	-1.262374	0.924707
H	-3.408919	1.0338	1.016057
H	-4.789227	1.028262	-0.150578
C	-4.999112	-1.608728	-0.283867
H	-4.83551	-2.68444	-0.390968
H	-5.705644	-1.452381	0.538273
H	-5.451449	-1.23159	-1.206773
C	-2.265171	0.042069	-1.525284
O	-2.900595	1.095702	-0.974735
O	-1.393032	0.131828	-2.354073

cp6-1

C	1.533138	-0.969238	0.115188
N	1.423267	-2.290818	-0.22671
N	2.768431	-0.468577	0.381164
C	2.290643	-3.316606	0.339781
H	1.676237	-4.136487	0.730034
H	2.977881	-3.733601	-0.407408

H	2.872893	-2.896473	1.159507
C	0.44274	-2.750352	-1.207184
H	0.947946	-3.373323	-1.954509
H	-0.354232	-3.344672	-0.745394
H	-0.001781	-1.897269	-1.717281
C	3.919996	-0.799185	-0.457976
H	4.253038	0.100096	-0.988072
H	4.75157	-1.175966	0.147897
H	3.647665	-1.551181	-1.19735
C	2.929624	0.731127	1.216946
H	3.935705	0.705917	1.645444
H	2.768632	1.651888	0.644075
H	2.196705	0.707708	2.024714
N	0.476402	-0.181423	0.215815
H	0.600434	0.868675	-0.021204
C	-0.899585	-0.588962	0.495392
H	-1.48804	-0.662319	-0.424348
H	-0.896587	-1.577432	0.968921
C	-1.565603	0.455105	1.40333
H	-1.000034	0.530028	2.345826
H	-1.480466	1.428658	0.90975
N	-2.981532	0.115309	1.583333
H	-3.09548	-0.559206	2.33617
H	-3.505934	0.94054	1.857924
Br	0.641434	2.802336	-0.561986
C	-4.752337	-0.757612	-0.561272
O	-5.608528	-0.154687	-0.042158
O	-3.948226	-1.389619	-1.131046

cp7-1

C	2.19576	0.330779	-0.81096
H	1.775949	-0.205042	-1.665416
H	2.278484	1.391035	-1.07566
C	1.288524	0.144076	0.409436
H	1.305828	-0.891782	0.751346
H	1.601143	0.798106	1.227929
N	-0.125945	0.43461	0.08646
H	-0.696478	0.402654	0.988907
C	-0.862334	-0.638538	-0.887473
O	-1.825695	-0.116746	-1.456492

O	-0.353578	-1.749548	-0.83689
C	-4.494677	2.195292	0.374851
H	-5.090606	2.462906	1.257144
H	-5.092054	2.428445	-0.50797
C	-3.165642	2.985574	0.418881
H	-2.658601	2.698407	1.34679
H	-3.402073	4.052003	0.496926
N	-2.241506	2.780024	-0.696806
H	-2.498702	3.334804	-1.507502
H	-0.267324	1.37946	-0.289247
H	-2.203044	1.799821	-0.981755
C	4.007239	-1.26535	-0.162864
N	3.401258	-2.420281	-0.56568
N	5.10221	-1.354884	0.636152
C	3.241039	-3.563685	0.328841
H	2.178627	-3.825285	0.387688
H	3.795025	-4.440103	-0.029585
H	3.592156	-3.307153	1.328168
C	2.745785	-2.540768	-1.868781
H	3.006275	-3.516056	-2.295099
H	1.656229	-2.466701	-1.783642
H	3.122292	-1.767959	-2.539671
C	6.107618	-2.398146	0.442457
H	7.070324	-1.932806	0.203565
H	6.230506	-3.003844	1.347482
H	5.823568	-3.046864	-0.385227
C	5.519672	-0.224933	1.479544
H	6.097276	-0.628007	2.315941
H	6.105396	0.513887	0.921654
H	4.63938	0.28923	1.866121
N	3.569485	-0.065392	-0.521543
H	4.245369	0.782642	-0.537614
Br	5.086995	2.573751	-0.696993
C	-4.63176	-0.233196	-0.353345
N	-5.197431	-0.028503	-1.577686
N	-4.545287	-1.511637	0.09759
C	-6.235245	-0.921146	-2.085212
H	-7.039975	-0.315876	-2.517274
H	-5.856174	-1.591464	-2.866652
H	-6.64384	-1.520366	-1.272518

C	-4.714055	0.952168	-2.545599
H	-4.440455	0.434701	-3.472246
H	-5.489902	1.692215	-2.77713
H	-3.827414	1.451422	-2.169506
C	-4.001477	-2.55971	-0.775528
H	-3.038433	-2.894833	-0.376791
H	-4.68803	-3.411123	-0.835431
H	-3.810386	-2.158752	-1.768405
C	-4.510484	-1.81893	1.532383
H	-4.893413	-2.834859	1.665229
H	-3.50097	-1.737839	1.949413
H	-5.157224	-1.12501	2.071765
N	-4.219864	0.755069	0.434613
H	-3.528154	0.503819	1.173198
Br	-1.898612	0.350608	2.71044

cp7-2

C	2.416203	0.391431	-0.913798
H	2.246268	-0.114035	-1.866261
H	2.565823	1.453309	-1.125238
C	1.177273	0.178112	-0.018096
H	1.246105	-0.807034	0.455915
H	1.140477	0.939208	0.765492
N	-0.05844	0.26309	-0.779609
H	-0.721609	0.982419	-0.481019
C	-0.51952	-0.851198	-1.424887
O	-1.698307	-0.710015	-2.071201
O	0.071242	-1.926401	-1.44207
C	-4.712468	0.318154	-1.677543
H	-5.8038	0.212101	-1.709064
H	-4.272942	-0.513713	-2.232662
C	-4.30573	1.622098	-2.372752
H	-4.737053	2.477417	-1.836105
H	-4.757374	1.599188	-3.369336
N	-2.841068	1.743012	-2.501384
H	-2.598635	2.224397	-3.362968
H	-2.488815	2.307897	-1.717196
H	-1.992619	0.243195	-2.221977
C	3.947078	-1.294195	0.082545
N	3.498677	-2.381762	-0.613263

N	4.73194	-1.511496	1.170608
C	2.986958	-3.570883	0.060955
H	1.934253	-3.707412	-0.211988
H	3.549345	-4.467919	-0.227127
H	3.058606	-3.442738	1.141088
C	3.30802	-2.354264	-2.061908
H	3.716614	-3.281555	-2.481127
H	2.246868	-2.282955	-2.321895
H	3.861706	-1.517472	-2.488345
C	5.744686	-2.563546	1.183886
H	6.73769	-2.110559	1.281766
H	5.590679	-3.249561	2.025175
H	5.710902	-3.128419	0.253101
C	4.865585	-0.497743	2.225811
H	5.123731	-1.013175	3.155951
H	5.618274	0.257019	1.968627
H	3.912126	0.016633	2.354046
N	3.645256	-0.048689	-0.259239
H	4.370195	0.72812	-0.056449
Br	5.745139	2.181191	0.088231
C	-4.585914	-0.615038	0.633207
N	-4.876513	-1.89732	0.280636
N	-4.648083	-0.265675	1.941575
C	-5.881427	-2.682483	0.992639
H	-6.546666	-3.153073	0.260577
H	-5.429495	-3.47578	1.600151
H	-6.475576	-2.035156	1.637471
C	-4.16141	-2.601751	-0.787962
H	-3.824663	-3.569442	-0.400282
H	-4.815184	-2.787748	-1.648235
H	-3.285123	-2.03841	-1.109915
C	-4.148075	-1.151357	2.994156
H	-3.348366	-0.638903	3.538857
H	-4.941186	-1.414119	3.702931
H	-3.737079	-2.061725	2.559983
C	-4.904015	1.118714	2.362742
H	-5.442057	1.087286	3.314799
H	-3.973546	1.685612	2.464423
H	-5.525214	1.617132	1.618102
N	-4.27805	0.311774	-0.273529

H	-3.640283	1.084682	0.045535
Br	-2.169007	2.585089	0.608763
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cp7-3			
C	1.573462	1.408786	-1.501859
H	1.296457	0.421354	-1.883595
H	2.392367	1.823325	-2.102827
C	0.364769	2.350846	-1.60431
H	0.633433	3.356343	-1.272566
H	0.082212	2.409514	-2.66079
N	-0.790498	1.926641	-0.829529
H	-1.079688	0.957493	-1.005913
C	-0.85565	2.305348	0.492432
O	-1.891622	1.825727	1.180016
O	-0.018438	3.030837	1.036018
C	2.41035	0.070174	0.404364
N	3.23104	-0.726151	-0.329024
N	2.09714	-0.284386	1.665898
C	3.032627	-2.17981	-0.356752
H	3.085074	-2.510524	-1.397845
H	3.798688	-2.711732	0.21977
H	2.028066	-2.411808	0.00072
C	4.171429	-0.176603	-1.2997
H	5.116462	-0.724733	-1.223417
H	3.803207	-0.266905	-2.328468
H	4.362387	0.873777	-1.078354
C	2.988472	-1.10711	2.478114
H	3.050793	-0.673186	3.480591
H	2.624627	-2.137219	2.566871
H	3.987509	-1.11803	2.042786
C	0.795598	0.077422	2.254976
H	0.015569	-0.155342	1.525248
H	0.645706	-0.548112	3.136205
H	0.746746	1.127971	2.553597
N	1.984636	1.24205	-0.095511
H	1.550752	1.90715	0.550234
Br	-0.47074	-1.399548	-0.818134
C	-3.971947	-0.546729	-1.137175
C	-3.929586	-1.031468	0.247041
O	-3.828797	0.389779	-0.041258

H	-3.082232	-0.683988	-1.748002
H	-4.927081	-0.468618	-1.654617
H	-2.976211	-1.463405	0.551452
C	-5.159698	-1.455464	1.002012
H	-5.295558	-2.53966	0.922677
H	-5.069387	-1.205566	2.064277
H	-6.051871	-0.96097	0.607354
H	-2.526445	1.316886	0.613391

cp7-4

C	2.837722	1.406649	-1.469965
H	2.499246	0.498383	-1.981904
H	3.714468	1.793409	-2.005004
C	1.731409	2.482006	-1.486086
H	2.126836	3.397979	-1.036392
H	1.493537	2.700896	-2.532848
N	0.5253	2.116485	-0.784872
H	-0.162505	1.542366	-1.257624
C	0.477277	2.088941	0.618911
O	-0.539865	1.562295	1.15103
O	1.490234	2.561046	1.234867
C	3.675146	-0.08109	0.329685
N	4.536689	-0.7871	-0.466358
N	3.362228	-0.594048	1.544301
C	4.490539	-2.244425	-0.545241
H	4.442726	-2.545461	-1.597693
H	5.375717	-2.710982	-0.095137
H	3.595309	-2.611345	-0.044486
C	5.496193	-0.123692	-1.341582
H	6.466522	-0.624662	-1.250139
H	5.191422	-0.155794	-2.394689
H	5.616944	0.915788	-1.037175
C	4.360422	-1.282321	2.361323
H	4.449443	-0.771773	3.326442
H	4.075326	-2.323881	2.548445
H	5.333085	-1.261663	1.870957
C	2.101496	-0.261258	2.226952
H	1.280105	-0.218082	1.513804
H	1.899662	-1.058632	2.946251
H	2.145217	0.702726	2.740449

N	3.164631	1.075176	-0.071329
H	2.626314	1.704068	0.620084
Br	-5.666072	-0.149139	0.554201
C	-3.707879	-0.46653	0.433425
C	-3.061085	0.304006	-0.72117
O	-1.660926	0.076056	-0.636107
H	-3.307459	-0.139392	1.392222
H	-3.584697	-1.542988	0.314908
H	-3.281165	1.373175	-0.584232
C	-3.545597	-0.146191	-2.093496
H	-4.626721	-0.019743	-2.187668
H	-3.050708	0.439132	-2.873864
H	-3.300738	-1.20226	-2.248835
H	-1.28983	0.626297	0.131626
C	-0.2944	-2.22289	-0.865221
O	-1.255407	-2.878011	-0.967509
O	0.727845	-1.656453	-0.771276

cp7-5

C	2.834578	1.175477	-1.547456
H	2.242568	0.330572	-1.907132
H	3.685798	1.332698	-2.221484
C	1.976733	2.44904	-1.547954
H	2.55079	3.296064	-1.164685
H	1.711092	2.670605	-2.586662
N	0.763147	2.345709	-0.761408
H	0.080833	1.656586	-1.066974
C	0.85355	2.500063	0.60119
O	-0.206579	2.076433	1.298329
O	1.833276	2.998509	1.156134
C	3.418747	-0.421713	0.2473
N	3.793889	-1.408481	-0.609984
N	3.216463	-0.720925	1.542632
C	3.077662	-2.691164	-0.615906
H	2.91032	-2.979864	-1.65767
H	3.645795	-3.488969	-0.123585
H	2.098117	-2.551013	-0.156562
C	4.756827	-1.181027	-1.682051
H	5.454514	-2.024711	-1.714808
H	4.275382	-1.096939	-2.663721

H	5.327459	-0.272915	-1.484563
C	3.896697	-1.844231	2.183715
H	4.279118	-1.514846	3.154306
H	3.21736	-2.68872	2.344614
H	4.736927	-2.172647	1.572868
C	2.27595	0.044155	2.376913
H	1.351216	0.193307	1.822477
H	2.060667	-0.552402	3.26444
H	2.682594	1.0097	2.691042
N	3.306304	0.84281	-0.190228
H	3.15402	1.575996	0.503993
H	-0.75371	1.456584	0.747179
Br	-5.44082	-0.336675	0.390693
C	-3.483954	-0.678173	0.388596
C	-2.791291	0.215237	-0.643701
O	-1.372859	0.27997	-0.366594
H	-3.150531	-0.439054	1.397632
H	-3.353605	-1.734946	0.180419
H	-3.132204	1.242409	-0.471675
C	-3.07426	-0.172129	-2.09216
H	-4.15186	-0.154357	-2.276522
H	-2.595243	0.540375	-2.770767
H	-2.690283	-1.173075	-2.294312
C	-0.54819	-0.965342	-0.419211
O	-1.147037	-2.017287	-0.60647
O	0.652526	-0.671594	-0.250755

cp7-6

C	1.610945	-1.341995	1.545354
H	1.033077	-0.433995	1.755548
H	2.344098	-1.51044	2.343195
C	0.680375	-2.560136	1.491604
H	1.241058	-3.452512	1.19538
H	0.290297	-2.729301	2.498869
N	-0.453455	-2.407885	0.59667
H	-1.298646	-1.987516	0.979193
C	-0.308672	-2.586882	-0.741115
O	-1.372058	-2.283356	-1.508291
O	0.726368	-3.012892	-1.259886
C	2.770198	0.01517	-0.189402

N	3.432847	0.846379	0.656818
N	2.691397	0.32775	-1.498604
C	3.228264	2.297516	0.598228
H	3.059023	2.660071	1.616288
H	4.098541	2.81752	0.18008
H	2.319896	2.509753	0.032111
C	4.178398	0.341834	1.803074
H	5.110103	0.910245	1.894064
H	3.618375	0.448673	2.740009
H	4.428584	-0.708478	1.650761
C	3.707401	1.137468	-2.162083
H	3.95931	0.670747	-3.119368
H	3.354153	2.157141	-2.354676
H	4.609194	1.182031	-1.551426
C	1.54317	-0.100904	-2.313572
H	1.635265	-1.135003	-2.656755
H	0.635882	0.032157	-1.718334
H	1.486492	0.562883	-3.17849
N	2.288175	-1.160852	0.244948
H	2.001657	-1.838153	-0.468738
H	-2.034302	-1.758396	-1.019819
Br	-0.223169	1.48968	0.334871
C	-3.673625	1.855184	0.389403
C	-3.376669	0.998903	-0.863102
O	-3.1285	-0.316525	-0.286085
H	-2.909602	2.620442	0.533947
H	-4.680139	2.282575	0.39222
H	-2.428095	1.314917	-1.303652
C	-4.503363	0.907219	-1.873902
H	-4.681069	1.893518	-2.315503
H	-4.246184	0.217488	-2.682364
H	-5.431154	0.565657	-1.404076
C	-3.147169	-0.252118	1.068925
O	-3.580735	0.933737	1.495481
O	-2.854221	-1.18798	1.774

ts1-1

Br	-0.29886	-2.46611	-0.3842
C	1.720776	-1.30926	0.956576
C	2.742662	-1.00602	-0.02844
O	3.142355	-0.33005	1.202117

H	0.909047	-0.62811	1.122407
H	2.470043	-0.29914	-0.81088
H	2.683247	0.716384	1.125949
C	-1.7545	0.834774	0.139676
N	-2.49741	0.53186	-0.94959
N	-2.19253	0.489502	1.376348
C	-3.95118	0.414692	-0.88156
H	-4.37906	0.887476	-1.77118
H	-4.27731	-0.63113	-0.85456
H	-4.32818	0.932892	0.000304
C	-1.87322	0.102671	-2.20821
H	-2.46681	-0.72061	-2.61258
H	-1.84156	0.913425	-2.94464
H	-0.88335	-0.30647	-2.00298
C	-2.80909	-0.82456	1.619653
H	-2.36932	-1.24292	2.528639
H	-3.89233	-0.74299	1.760976
H	-2.55419	-1.50604	0.805307
C	-1.74128	1.215927	2.562972
H	-2.54001	1.193222	3.309167
H	-0.84321	0.766478	3.005246
H	-1.52577	2.254336	2.309496
N	-0.62445	1.538528	0.030328
H	0.112725	1.444661	0.742207
C	-0.219	2.431193	-1.06237
H	0.087536	1.858453	-1.94379
H	-1.07099	3.057383	-1.34831
C	0.970584	3.288813	-0.59196
H	1.293182	3.924118	-1.4188
H	0.664349	3.920471	0.248872
C	2.138934	2.378761	-0.17341
O	1.911253	1.750106	0.961088
O	3.113286	2.223792	-0.89672
H	1.826416	-2.16795	1.602831
C	3.690475	-2.08091	-0.48674
H	3.177785	-2.71137	-1.21926
H	4.576846	-1.63973	-0.95018
H	4.005546	-2.70535	0.354059
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ts1-2			
Br	-1.57061	-1.08823	-1.53524
C	-3.05229	0.20341	-1.20142
C	-3.16386	0.601997	0.267527
O	-1.95489	1.162774	0.789626

H	-3.94871	-0.31909	-1.53346
H	-3.34245	-0.30094	0.862681
H	-1.36038	0.431911	1.481333
C	2.569992	0.009367	0.112406
N	3.155786	-0.50274	-1.00713
N	3.025673	1.179887	0.624312
C	4.574107	-0.32236	-1.29582
H	5.01315	-1.29102	-1.56002
H	4.7395	0.365763	-2.13412
H	5.083823	0.065489	-0.41412
C	2.362027	-1.1722	-2.03884
H	2.67748	-0.79702	-3.01816
H	2.499658	-2.25983	-2.02678
H	1.305205	-0.93366	-1.91429
C	3.265557	2.332887	-0.25348
H	2.408795	3.010266	-0.18159
H	4.182388	2.848645	0.047471
H	3.359826	2.010567	-1.28865
C	2.714799	1.543847	2.011562
H	3.481708	2.242338	2.357354
H	1.730123	2.015173	2.079776
H	2.737285	0.653248	2.640646
N	1.595086	-0.63757	0.734555
H	0.879772	-0.10265	1.265558
C	1.296803	-2.07424	0.720453
H	0.725339	-2.34268	-0.17423
H	2.236722	-2.63592	0.706601
C	0.455314	-2.43274	1.962458
H	0.202015	-3.49395	1.923031
H	1.040527	-2.24235	2.869446
C	-0.84469	-1.60851	2.011424
O	-0.60445	-0.31741	2.112082
O	-1.94506	-2.13202	1.926641
C	-4.31778	1.594138	0.446063
H	-4.11965	2.509885	-0.1156
H	-5.2675	1.163137	0.111618
H	-4.41042	1.847765	1.505385
H	-2.8219	1.049481	-1.84207
C	-0.97026	2.216627	-0.11318
O	0.146083	2.122223	0.355565
O	-1.62107	2.784852	-0.95286

ts1-3

Br	5.815913	-0.07384	-0.36212
C	3.397042	-0.79666	-0.77175
C	2.921187	-0.07839	0.481058
O	1.471798	0.144997	0.345686
H	3.834798	-1.77765	-0.71628
H	3.362131	0.915386	0.518513
H	0.417392	1.281831	1.186509
C	-3.63394	-0.42933	-0.08222
N	-4.88902	-0.33055	-0.60964
N	-3.31591	-1.50834	0.66603
C	-6.07309	-0.8112	0.097423
H	-6.8337	-0.0227	0.097754
H	-6.50385	-1.70062	-0.37782
H	-5.81854	-1.04773	1.130227
C	-5.1235	0.222552	-1.94331
H	-5.69618	-0.49962	-2.53617
H	-5.6925	1.158328	-1.90058
H	-4.17326	0.402892	-2.44441
C	-3.80013	-2.84936	0.331652
H	-2.93797	-3.5007	0.156638
H	-4.39674	-3.26989	1.148176
H	-4.39918	-2.8227	-0.57709
C	-2.23057	-1.47664	1.656022
H	-2.54555	-2.06328	2.524298
H	-1.3142	-1.89279	1.231435
H	-2.02783	-0.45059	1.959867
N	-2.72367	0.521676	-0.28778
H	-1.72705	0.203418	-0.29836
C	-3.00006	1.949469	-0.47062
H	-2.6178	2.269902	-1.44541
H	-4.07927	2.107703	-0.45531
C	-2.34084	2.808377	0.629271
H	-2.54978	3.858923	0.411703
H	-2.74973	2.549883	1.609324
C	-0.83734	2.589636	0.592877
O	-0.46196	1.641477	1.467496
O	-0.10333	3.133242	-0.20152
C	3.184372	-0.85172	1.763515
H	2.722173	-1.84377	1.715818
H	4.264568	-0.96143	1.878259
H	2.779858	-0.31643	2.627432
H	3.512283	-0.25112	-1.69388
C	0.882474	-0.71639	-0.55292
O	-0.35509	-0.70443	-0.65771

O	1.703517	-1.45085	-1.18429
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ts2-1			
Br	-0.41104	-2.20119	-0.26484
C	-2.16463	-0.53488	-0.87611
C	-2.8192	-0.04535	0.340002
O	-3.34938	0.921456	-0.52253
H	-1.3744	0.045521	-1.31359
H	-2.11854	0.339797	1.100318
H	-2.29291	1.998844	-0.72231
C	1.681485	0.633032	0.09936
N	2.110485	0.178607	1.302815
N	2.374757	0.305222	-1.02165
C	3.525701	-0.06826	1.565607
H	3.777478	0.345027	2.54782
H	3.763768	-1.13831	1.57117
H	4.137264	0.428173	0.812296
C	1.167267	-0.25929	2.339267
H	1.615325	-1.11082	2.857535
H	0.962898	0.526937	3.074552
H	0.25302	-0.6214	1.864935
C	2.837313	-1.07416	-1.23256
H	2.35384	-1.47305	-2.12863
H	3.92519	-1.10638	-1.35652
H	2.516482	-1.7057	-0.40708
C	2.246061	1.104971	-2.23823
H	3.16031	0.989052	-2.82626
H	1.397797	0.77998	-2.85472
H	2.122081	2.158929	-1.98603
N	0.65286	1.471808	-0.00421
H	0.123036	1.526972	-0.87931
C	-0.02213	2.271891	1.014554
H	-0.59769	1.630626	1.688332
H	0.708083	2.830143	1.6103
C	-0.9792	3.223804	0.23619
H	-1.77247	3.550706	0.922284
H	-0.41688	4.115802	-0.07018
H	-2.73069	-1.17767	-1.53707
C	-3.83875	-0.96195	0.99344
H	-3.3367	-1.81375	1.463155
H	-4.40998	-0.41734	1.752099
H	-4.5414	-1.33376	0.241238
O	-1.47671	2.60917	-0.92032

ts2-2			
C	2.404383	-0.41779	0.26481
N	2.211708	-1.66524	-0.24431
N	3.492792	0.298171	-0.14653
C	3.31543	-2.57567	-0.52351
H	3.13189	-3.53177	-0.01942
H	3.421139	-2.77428	-1.59743
H	4.248964	-2.15729	-0.14712
C	0.863215	-2.15881	-0.53029
H	0.874019	-2.64417	-1.51229
H	0.525542	-2.89043	0.212209
H	0.152829	-1.33382	-0.56211
C	3.885606	0.31708	-1.55764
H	3.609792	1.279138	-2.00331
H	4.966409	0.172047	-1.6557
H	3.36774	-0.46739	-2.10531
C	3.920116	1.472923	0.611769
H	4.981734	1.645534	0.413796
H	3.358068	2.369551	0.322155
H	3.781371	1.297983	1.678999
N	1.597565	0.1061	1.166112
H	1.402232	1.130333	1.19743
C	0.623306	-0.51906	2.063695
H	-0.21135	-0.94433	1.50402
H	1.100995	-1.29935	2.666528
C	0.098848	0.684511	2.909365
H	-0.86789	0.384124	3.347023
H	0.791071	0.86399	3.749304
O	0.023746	1.817409	2.104692
Br	-2.70508	-1.77323	-0.12465
C	-3.22804	0.094261	-0.6088
C	-2.56601	1.118753	0.310447
O	-1.1873	1.126587	0.130749
H	-4.316	0.091507	-0.54031
H	-2.82655	0.83441	1.348193
H	-0.62142	1.542118	1.149864
C	-3.1997	2.50223	0.046206
H	-3.02984	2.816846	-0.98752
H	-4.27785	2.511102	0.247082
H	-2.72241	3.231852	0.707008
H	-2.90351	0.213599	-1.64143
C	-0.13329	1.877224	-1.85067

O	0.954907	1.831216	-1.4025
O	-1.07596	1.99661	-2.53895
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ts2-3			
C	-3.52856	0.013941	0.241596
N	-4.59537	-0.77916	0.554137
N	-3.74902	1.212678	-0.34285
C	-5.78423	-0.85511	-0.2909
H	-5.99109	-1.90491	-0.52768
H	-6.66698	-0.43662	0.206859
H	-5.61326	-0.31928	-1.2239
C	-4.59121	-1.65009	1.725552
H	-5.52767	-1.51109	2.277101
H	-4.51336	-2.70875	1.44897
H	-3.75947	-1.38662	2.378279
C	-4.88791	2.058376	0.013808
H	-5.45472	1.608791	0.828275
H	-4.51496	3.032082	0.348141
H	-5.55108	2.218146	-0.84344
C	-2.71976	1.851155	-1.17974
H	-3.22925	2.395357	-1.98024
H	-2.10374	2.540771	-0.59593
H	-2.07644	1.083481	-1.61249
N	-2.28316	-0.36297	0.52375
H	-1.54631	0.386853	0.580281
C	-1.72218	-1.70639	0.346691
H	-0.78439	-1.70848	0.907623
H	-2.36521	-2.48071	0.772219
C	-1.4409	-2.01487	-1.13581
H	-0.86477	-2.95343	-1.1802
H	-2.3862	-2.19138	-1.66375
O	-0.79816	-0.95695	-1.80972
Br	5.532615	-0.45186	0.280463
C	3.357689	0.862742	0.566414
C	2.603066	-0.11076	-0.32395
O	1.170154	-0.00196	0.005364
H	3.944751	1.659801	0.144918
H	2.879321	-1.13004	-0.06181
H	-0.02933	-0.67117	-1.27801
C	2.798167	0.150973	-1.80903
H	2.51627	1.179465	-2.05835
H	3.853338	-0.00106	-2.04495

H	2.190532	-0.53459	-2.40725
H	3.498542	0.640995	1.611568
C	0.85925	1.216418	0.579657
O	-0.33871	1.465345	0.794267
O	1.86502	1.945479	0.83591

ts3-1			
C	-1.22502	1.01912	-0.14021
N	-1.95724	1.947437	0.546554
N	-0.12485	1.439832	-0.8131
C	-2.12424	3.316646	0.070522
H	-3.18712	3.581185	0.105142
H	-1.57096	4.036255	0.685834
H	-1.78013	3.396132	-0.96018
C	-2.56551	1.647383	1.840336
H	-2.28852	2.430255	2.555376
I	-3.65943	1.607479	1.780001
H	-2.19216	0.69513	2.2143
C	0.790801	2.453045	-0.26742
H	1.791623	2.004481	-0.20241
H	0.822566	3.341367	-0.90911
H	0.470658	2.742978	0.732721
C	0.295448	0.878081	-2.10291
H	0.190758	1.648949	-2.87729
H	1.34808	0.579389	-2.05428
H	-0.32584	0.021535	-2.35954
N	-1.57795	-0.26664	-0.14617
H	-0.83878	-1.06028	-0.01986
C	-2.95301	-0.75327	-0.00583
H	-3.13977	-1.08276	1.025164
H	-3.64901	0.065063	-0.21898
C	-3.19731	-1.93149	-0.95595
H	-3.04438	-1.59359	-1.98828
I	-2.43828	-2.69595	-0.7566
Br	3.647906	-0.10239	-0.2036
C	1.124228	-2.03004	1.139773
C	1.557029	-1.62557	-0.19284
O	-0.03363	-2.31641	0.367786
H	1.606073	-2.94507	1.50709
H	1.980441	-2.34509	-0.87682
H	1.192213	-0.70103	-0.57787
C	1.028057	-0.99307	2.241345

H	0.449636	-1.37801	3.088218
H	2.034656	-0.73027	2.578082
H	0.554656	-0.07411	1.881973
C	-4.60084	-2.52118	-0.79576
H	-4.74996	-3.36188	-1.47922
H	-4.7639	-2.8909	0.222644
H	-5.37833	-1.77857	-1.00962

ts3-2			
C	-1.94777	-1.05538	0.218081
N	-2.71858	-1.9565	-0.48225
N	-1.59003	-1.391	1.487968
C	-3.79446	-2.71259	0.145937
H	-4.72441	-2.56323	-0.41636
H	-3.58243	-3.78948	0.170587
H	-3.94842	-2.36062	1.165795
C	-2.5109	-2.20745	-1.9027
H	-2.37588	-3.28396	-2.06717
H	-3.36332	-1.87665	-2.50936
H	-1.61367	-1.69131	-2.24321
C	-1.24661	-2.76224	1.85627
H	-0.21049	-2.79363	2.21247
H	-1.89506	-3.13279	2.658692
H	-1.33371	-3.42246	0.994466
C	-1.21704	-0.37521	2.47744
H	-1.60593	-0.68781	3.452244
H	-0.13163	-0.25608	2.531478
H	-1.63094	0.593654	2.204999
N	-1.55074	0.092593	-0.29561
H	-0.56527	0.556822	0.065749
C	-2.28641	0.861931	-1.30128
H	-1.57698	1.159124	-2.0826
H	-3.05548	0.247412	-1.77676
C	-2.9345	2.113121	-0.68998
H	-3.68369	1.794948	0.046545
H	-2.17693	2.67227	-0.13337
Br	4.148488	-0.94982	-0.50996
C	1.819107	0.86104	-0.26039
C	2.375864	-0.46684	0.263232
N	0.638651	1.096764	0.465293
H	2.539377	1.653288	-0.0152
H	2.539412	-0.4154	1.338348

H	1.722551	-1.30666	0.019122
C	1.586032	0.86252	-1.77451
H	1.160774	1.82442	-2.07613
H	2.519112	0.706287	-2.32266
H	0.88593	0.068193	-2.06399
C	0.504187	2.775258	1.369505
O	1.572146	3.293574	1.269628
O	-0.63037	2.77159	1.757588
C	-3.58842	2.997031	-1.75554
H	-4.05683	3.874188	-1.29984
H	-2.85072	3.357185	-2.48128
H	-4.36494	2.457748	-2.31138

ts3-3

C	-2.84305	-0.43879	-0.31907
N	-3.9186	-0.22553	-1.13396
N	-2.80095	-1.56745	0.422624
C	-5.28026	-0.56542	-0.72682
H	-5.92476	0.309282	-0.86736
H	-5.69148	-1.39245	-1.31769
H	-5.29716	-0.83762	0.328006
C	-3.77947	0.387113	-2.45387
H	-4.34891	-0.20415	-3.1791
H	-4.15769	1.415519	-2.4743
H	-2.73304	0.384692	-2.75694
C	-3.37118	-2.82531	-0.06149
H	-2.60361	-3.60341	-0.00169
H	-4.22511	-3.13907	0.549121
H	-3.68636	-2.72966	-1.09962
C	-2.02729	-1.68158	1.666539
H	-2.66252	-2.1562	2.421665
H	-1.14288	-2.30616	1.50703
H	-1.68786	-0.70895	2.027378
N	-1.85843	0.457283	-0.26214
H	-0.94132	0.1585	0.10924
C	-2.02848	1.905507	-0.48247
H	-1.85515	2.151491	-1.53764
H	-3.06901	2.162615	-0.2555
C	-1.07324	2.722106	0.391552
H	-1.18311	2.419948	1.436929
H	-0.04296	2.476354	0.1123
Br	4.586585	-0.15752	-1.26691

C	1.942133	-0.61832	0.08635
C	3.106564	0.102575	0.745321
N	0.707105	-0.17477	0.724472
H	1.866619	-0.29732	-0.95162
H	3.236569	1.163016	0.60707
H	3.885542	-0.43573	1.254798
C	2.060691	-2.13318	0.177492
H	1.193222	-2.61754	-0.28222
H	2.96464	-2.44236	-0.35194
H	2.128359	-2.44789	1.224056
C	0.903356	0.271174	2.052066
O	2.130577	0.326827	2.37426
O	-0.10916	0.547105	2.690768
C	-1.31314	4.224455	0.222607
H	-0.60976	4.794647	0.834944
H	-1.17897	4.542384	-0.81774
H	-2.32591	4.507759	0.531597

ts4-1

C	1.625695	-0.57036	-0.19249
N	2.557595	-1.24237	0.548879
N	0.61859	-1.28261	-0.75596
C	2.994836	-2.59386	0.214417
H	4.090191	-2.62767	0.216947
H	2.62684	-3.33474	0.934283
H	2.641434	-2.86329	-0.78026
C	3.122662	-0.67667	1.771576
H	3.043562	-1.41583	2.576642
H	4.179265	-0.41035	1.651104
H	2.560069	0.208592	2.064185
C	-0.04624	-2.39244	-0.0562
H	-1.11484	-2.14927	0.024115
H	0.08159	-3.33416	-0.60253
H	0.364967	-2.49959	0.94687
C	0.0414	-0.96576	-2.06824
H	0.273411	-1.78187	-2.76456
H	-1.04761	-0.88276	-1.98585
H	0.460501	-0.03566	-2.44893
N	1.700983	0.751048	-0.35559
H	0.816318	1.385217	-0.27264
C	2.948999	1.52152	-0.33435
H	3.112405	1.959758	0.658486

H	3.786991	0.846936	-0.53665
C	2.884593	2.6424	-1.37231
H	2.797954	2.236746	-2.38479
H	2.019241	3.282251	-1.18001
Br	-3.36429	-0.50174	-0.04421
C	-1.25812	2.06109	0.903575
C	-1.65126	1.414146	-0.34305
O	-0.22301	2.485529	0.02826
H	-1.90955	2.893392	1.199144
H	-2.24846	1.939822	-1.07236
H	-1.11157	0.546494	-0.64668
C	-0.89398	1.210726	2.104883
H	-0.37905	1.810352	2.863325
H	-1.80468	0.784726	2.534921
H	-0.24656	0.375621	1.819751
H	3.790167	3.254706	-1.32148

ts4-2

C	-2.23326	-0.58628	0.126825
N	-3.07797	-1.50635	-0.45334
N	-2.00694	-0.6986	1.464375
C	-4.28452	-1.98214	0.211474
H	-5.14771	-1.84154	-0.45063
H	-4.22291	-3.04833	0.465822
H	-4.45427	-1.41153	1.124291
C	-2.82065	-2.06217	-1.77577
H	-2.83355	-3.15793	-1.71959
H	-3.57656	-1.75212	-2.50826
H	-1.83835	-1.74668	-2.12671
C	-1.88104	-1.99818	2.119448
H	-0.8841	-2.08372	2.566833
H	-2.6244	-2.11569	2.916512
H	-2.00314	-2.80369	1.396593
C	-1.55641	0.442737	2.267447
H	-2.04119	0.383969	3.247567
H	-0.46997	0.435929	2.388976
H	-1.81672	1.379737	1.779068
N	-1.64805	0.374993	-0.56064
H	-0.62974	0.772902	-0.21079
C	-2.20763	1.011502	-1.7565
H	-1.42385	1.03371	-2.52155
H	-3.0355	0.420211	-2.15404

C	-2.68422	2.435648	-1.45478
H	-3.53631	2.420695	-0.76739
H	-1.89084	3.023497	-0.98891
Br	3.851183	-1.40731	-0.1086
C	1.788095	0.695653	-0.38549
C	2.116935	-0.57192	0.409438
O	0.614349	1.217602	0.186003
H	2.600035	1.418223	-0.22675
H	2.215868	-0.34365	1.469334
H	1.370767	-1.35439	0.258102
C	1.64633	0.442406	-1.88973
H	1.387487	1.37786	-2.39462
H	2.576587	0.060037	-2.3184
H	0.854537	-0.29075	-2.09108
C	0.664981	3.049734	0.717832
O	1.799447	3.397627	0.610659
O	-0.47983	3.272206	0.997513
H	-3.00034	2.92725	-2.38094

ts4-3

C	2.89205	-0.28233	-0.17936
N	3.949415	-1.14033	-0.07318
N	2.890499	0.632312	-1.17402
C	5.325058	-0.71309	-0.31935
H	5.946758	-0.99537	0.537468
H	5.745709	-1.18149	-1.21699
H	5.365445	0.370041	-0.43027
C	3.7747	-2.5368	0.322416
H	4.351832	-3.17098	-0.35906
H	4.122562	-2.72363	1.344767
H	2.724933	-2.81729	0.243656
C	3.479139	0.343917	-2.48251
H	2.728612	0.539685	-3.25493
H	4.34841	0.981004	-2.67974
H	3.776796	-0.70179	-2.54694
C	2.141782	1.894646	-1.10017
H	2.802413	2.703231	-1.42992
H	1.270143	1.858369	-1.76063
H	1.783401	2.097584	-0.08955
N	1.884303	-0.35089	0.689805
H	0.980458	0.077343	0.427009
C	2.014684	-0.79289	2.091935

H	1.854796	-1.87506	2.162947
H	3.042671	-0.59332	2.41163
C	1.016923	-0.06744	2.990849
H	1.104243	1.016472	2.894463
H	-0.00897	-0.34298	2.733162
Br	-4.47068	-1.26167	-0.31876
C	-1.85023	0.200945	-0.46694
C	-3.03711	0.693235	0.344383
O	-0.63417	0.759606	0.113683
H	-1.76153	-0.87797	-0.3492
H	-3.1808	0.355418	1.357274
H	-3.81827	1.281541	-0.1027
C	-1.94735	0.580314	-1.93796
H	-1.06523	0.234641	-2.4863
H	-2.83763	0.108398	-2.35954
H	-2.02815	1.666847	-2.04622
C	-0.86041	1.977615	0.796595
O	-2.0941	2.26589	0.887202
O	0.136545	2.565733	1.207704
H	1.194047	-0.35873	4.030014

ts5-1

C	-1.23989	1.007921	-0.13667
N	-1.98005	1.927584	0.551215
N	-0.14155	1.438947	-0.80587
C	-2.16222	3.295223	0.075729
H	-3.22916	3.543892	0.100222
H	-1.62544	4.021007	0.698214
H	-1.80914	3.381781	-0.9513
C	-2.6011	1.615782	1.83632
H	-2.34296	2.400661	2.556056
H	-3.69332	1.561187	1.761554
H	-2.21969	0.667722	2.212825
C	0.763009	2.460497	-0.25728
H	1.768121	2.021748	-0.19235
H	0.786578	3.350297	-0.89726
H	0.438504	2.745343	0.742909
C	0.286377	0.884312	-2.09622
H	0.177763	1.656679	-2.86854
H	1.341115	0.593232	-2.0456
H	-0.32806	0.024151	-2.35713
N	-1.58046	-0.28202	-0.14519

H	-0.83444	-1.06618	-0.0155
C	-2.94952	-0.77954	-0.00871
H	-3.12746	-1.14292	1.012657
H	-3.66633	0.021744	-0.20354
C	-3.18972	-1.93352	-0.99011
H	-3.1143	-1.54669	-2.01266
H	-2.38654	-2.67537	-0.86231
N	-4.54641	-2.45284	-0.79094
H	-4.79641	-3.0638	-1.5638
H	-4.57062	-3.03644	0.042868
Br	3.640941	-0.07619	-0.20563
C	1.137482	-2.02622	1.143956
C	1.561267	-1.61553	-0.18945
O	-0.02019	-2.32232	0.374991
H	1.629606	-2.937	1.508303
H	1.989267	-2.32956	-0.87627
H	1.187934	-0.69281	-0.57088
C	1.034396	-0.9916	2.247064
H	0.465498	-1.3842	3.096855
H	2.039533	-0.71652	2.578355
H	0.547207	-0.07848	1.891125

ts5-2

C	-2.32702	-0.85165	0.10219
N	-3.39867	-1.35608	-0.60118
N	-2.02649	-1.45634	1.286375
C	-4.62561	-1.78547	0.058821
H	-5.48151	-1.25429	-0.37543
H	-4.79992	-2.86308	-0.05773
H	-4.57661	-1.5497	1.121654
C	-3.39896	-1.44132	-2.05513
H	-3.7261	-2.44435	-2.35544
H	-4.0768	-0.71121	-2.51569
H	-2.39048	-1.28165	-2.43634
C	-2.12634	-2.90328	1.458344
H	-1.13619	-3.31203	1.691894
H	-2.80457	-3.1604	2.280384
H	-2.48402	-3.37191	0.542435
C	-1.26656	-0.76101	2.329498
H	-1.62919	-1.10674	3.302926
H	-0.19412	-0.9564	2.240173
H	-1.40313	0.315699	2.243598

N	-1.60028	0.163761	-0.32026
H	-0.48818	0.290974	0.029527
C	-2.10486	1.261607	-1.14629
H	-1.2193	1.769896	-1.54265
H	-2.68981	0.927721	-2.00553
C	-2.94601	2.26187	-0.33904
H	-3.83208	1.742558	0.047825
H	-2.35685	2.599161	0.524851
N	-3.40406	3.331537	-1.23405
H	-4.07714	3.917816	-0.74657
H	-2.62043	3.943238	-1.45589
Br	4.669521	-0.66338	-0.4593
C	1.848637	0.187629	-0.43234
C	2.967484	-0.28356	0.502134
O	0.767238	0.522777	0.407122
H	2.216777	1.081824	-0.95794
H	3.215375	0.496279	1.218006
H	2.705793	-1.21126	1.012693
C	1.45733	-0.87526	-1.46238
H	0.681215	-0.49468	-2.13396
H	2.321687	-1.16925	-2.06349
H	1.06771	-1.76857	-0.95912
C	0.834319	2.311026	1.194038
O	1.877097	2.769313	0.849349
O	-0.20975	2.368504	1.774793

ts5-3

C	-2.7442	-0.57246	-0.38169
N	-3.78875	-0.33537	-1.22767
N	-2.8197	-1.61812	0.471837
C	-5.17844	-0.48401	-0.80067
H	-5.71714	0.448569	-1.0026
H	-5.68511	-1.29604	-1.3353
H	-5.22207	-0.68017	0.270116
C	-3.59371	0.157503	-2.5891
H	-4.20865	-0.44062	-3.27054
H	-3.88933	1.208134	-2.69218
H	-2.54934	0.046509	-2.879
C	-3.51554	-2.8553	0.115353
H	-2.82696	-3.69604	0.247691
H	-4.38817	-3.02219	0.756295
H	-3.83331	-2.82906	-0.92608

C	-2.03555	-1.68549	1.713873
H	-2.68722	-2.06438	2.507422
H	-1.18975	-2.37109	1.595874
H	-1.64252	-0.70611	1.997088
N	-1.65421	0.195734	-0.40999
H	-0.80047	-0.16462	0.039471
C	-1.62441	1.646691	-0.65871
H	-0.56529	1.904317	-0.73979
H	-2.08842	1.905064	-1.61094
C	-2.27678	2.464075	0.466024
H	-3.33607	2.18444	0.535636
H	-1.79336	2.199563	1.41554
N	-2.20691	3.883284	0.100724
H	-2.79689	4.425279	0.726736
H	-1.25993	4.224438	0.255793
Br	4.688482	-0.09088	-1.25317
C	2.159315	-0.67126	0.271431
C	3.123044	0.44033	0.652079
O	0.835509	-0.31749	0.779205
H	2.057572	-0.70152	-0.81216
H	3.041241	1.411002	0.191883
H	3.984912	0.250554	1.266635
C	2.578471	-2.02862	0.815811
H	1.843049	-2.79468	0.55201
H	3.543903	-2.29178	0.377821
H	2.672648	-1.99057	1.905799
C	0.892464	0.542231	1.892378
O	2.0715	0.93559	2.156893
O	-0.17966	0.809509	2.434252

ts6-1

C	1.656129	-0.76719	0.110776
N	1.83422	-2.06857	-0.27171
N	2.739879	-0.0421	0.486824
C	2.844417	-2.92827	0.335942
H	2.380463	-3.8753	0.634216
H	3.664226	-3.15486	-0.3571
H	3.254816	-2.44675	1.223277
C	1.049011	-2.66324	-1.35269
H	1.72717	-3.18324	-2.03827
H	0.312778	-3.38569	-0.98219
H	0.533198	-1.88338	-1.91128

C	4.002912	-0.12048	-0.24774
H	4.211778	0.850672	-0.70941
H	4.832024	-0.37514	0.421578
H	3.937688	-0.86752	-1.03752
C	2.599776	1.131071	1.363224
H	3.552382	1.276287	1.880517
H	2.317082	2.028165	0.800833
H	1.818662	0.939666	2.100155
N	0.455482	-0.20803	0.147833
H	0.378152	0.857668	-0.05903
C	-0.81399	-0.91377	0.303384
H	-1.23323	-1.22639	-0.65682
H	-0.65408	-1.81797	0.90425
C	-1.82093	0.025272	0.990157
H	-1.45323	0.331798	1.974207
H	-1.93723	0.937447	0.396346
N	-3.14092	-0.61464	1.165089
H	-3.08464	-1.41541	1.797109
H	-4.27399	-0.0139	1.135483
Br	0.052592	2.770312	-0.50289
C	-3.95974	-1.00848	-0.12342
O	-5.01243	-0.31755	0.129016
O	-3.57393	-1.7491	-0.99017

ts7-1

C	-2.24399	-0.04482	-0.77739
H	-1.99095	0.400923	-1.74167
H	-2.11316	-1.12974	-0.85462
C	-1.31598	0.525653	0.300202
H	-1.47625	1.603012	0.414179
H	-1.51141	0.03652	1.259381
N	0.082546	0.264172	-0.06023
H	0.686171	0.348209	0.778687
C	0.662626	1.117222	-1.15849
O	1.805919	0.700759	-1.52638
O	-0.01422	2.054167	-1.58155
C	3.66224	-2.26307	-0.16353
H	4.225902	-2.9373	0.494876
H	3.991995	-2.45334	-1.18662
C	2.172119	-2.58123	0.012305
H	1.875026	-2.31891	1.033068
H	2.013003	-3.65177	-0.13525

N	1.306049	-1.82024	-0.92914
H	0.884999	-2.40266	-1.64879
H	0.521308	-1.07868	-0.42954
H	1.784619	-0.97943	-1.35833
C	-4.3333	1.191113	-0.13528
N	-3.98672	2.429766	-0.5898
N	-5.41992	1.083796	0.679718
C	-4.07878	3.61417	0.259147
H	-3.09324	4.088968	0.328977
H	-4.7857	4.348068	-0.14705
H	-4.39926	3.330502	1.261226
C	-3.31344	2.620359	-1.878
H	-3.67523	3.558397	-2.31159
H	-2.22226	2.66236	-1.77975
H	-3.58714	1.808831	-2.55365
C	-6.63278	1.862353	0.439771
H	-7.4633	1.184331	0.211468
H	-6.90383	2.456224	1.320368
H	-6.49039	2.529867	-0.40934
C	-5.57969	-0.07659	1.56708
H	-6.22607	0.222821	2.397047
H	-5.99692	-0.9463	1.047294
H	-4.607	-0.37449	1.95942
N	-3.66325	0.095652	-0.45553
H	-4.14287	-0.86413	-0.40308
Br	-4.50438	-2.86047	-0.44968
C	4.851114	-0.05189	-0.29171
N	5.330111	-0.17159	-1.56507
N	5.354039	0.932259	0.49044
C	6.73999	0.069399	-1.86231
H	7.122556	-0.75703	-2.47163
H	6.890229	1.001998	-2.42
H	7.315586	0.113086	-0.93776
C	4.47118	-0.44186	-2.72095
H	4.82043	0.180056	-3.55159
H	4.526196	-1.48912	-3.04583
H	3.445244	-0.14379	-2.50102
C	5.61782	2.266143	-0.05363
H	5.033423	2.999266	0.511145
H	6.679197	2.52641	0.02676
H	5.306657	2.316274	-1.09588
C	5.344809	0.844074	1.956914

H	6.191941	1.425027	2.332346
H	4.405533	1.211431	2.382461
H	5.461486	-0.19581	2.263563
N	3.93939	-0.87643	0.217725
H	3.377024	-0.53583	1.044804
Br	2.020191	-0.15671	2.65819
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ts7-2			
C	-0.8804	1.573	1.505014
H	-0.52557	0.583967	1.820744
H	-1.6846	1.880809	2.183011
C	0.230186	2.634947	1.597981
H	-0.15274	3.586481	1.213941
H	0.468685	2.777823	2.655604
N	1.460008	2.311448	0.899051
H	2.237001	1.922151	1.412842
C	1.586055	2.430902	-0.47151
O	2.709359	2.010193	-0.99124
O	0.650859	2.900529	-1.14396
C	-2.11947	0.466859	-0.35273
N	-3.11189	-0.06301	0.411831
N	-1.9443	0.039165	-1.61836
C	-3.37117	-1.50534	0.45199
H	-3.41164	-1.81754	1.49995
H	-4.32308	-1.76153	-0.02798
H	-2.53984	-2.04137	-0.00575
C	-3.86603	0.748068	1.360514
H	-4.92858	0.497238	1.270705
H	-3.55972	0.562838	2.397411
H	-3.74096	1.806114	1.129266
C	-3.02873	-0.57312	-2.38245
H	-3.01489	-0.16386	-3.39653
H	-2.92173	-1.66185	-2.44403
H	-3.98874	-0.33329	-1.92644
C	-0.60504	0.028465	-2.24246
H	0.030017	-0.66015	-1.67535
H	-0.71738	-0.34326	-3.26113
H	-0.15937	1.024748	-2.28399
N	-1.36936	1.476943	0.117688
H	-0.81129	2.029394	-0.55099
Br	0.132808	-2.22103	0.587273
C	2.247105	-0.81081	0.759165

C	3.154766	-0.9567	-0.37745
O	3.74773	0.165323	0.271598
H	1.521786	-0.02428	0.745071
H	2.52612	-1.245	1.708744
H	2.708889	-0.70733	-1.34804
C	4.028915	-2.18876	-0.45335
H	3.426955	-3.05434	-0.74706
H	4.828646	-2.04552	-1.18615
H	4.485964	-2.39004	0.520135
H	3.235829	1.268529	-0.38948

ts7-3			
C	2.811553	-1.45416	1.375552
H	2.394823	-0.59639	1.911998
H	3.692562	-1.81388	1.921272
C	1.776966	-2.59188	1.304707
H	2.216328	-3.45408	0.795687
H	1.543867	-2.89388	2.331041
N	0.555631	-2.23935	0.620249
H	-0.10816	-1.62212	1.084122
C	0.545162	-2.16529	-0.76282
O	-0.47472	-1.54642	-1.28951
O	1.490248	-2.64119	-1.42701
C	3.536754	0.233652	-0.29371
N	4.205704	1.004073	0.61116
N	3.262476	0.752325	-1.50824
C	3.872785	2.418129	0.789576
H	3.756537	2.617883	1.859624
H	4.653391	3.080875	0.397018
H	2.9209	2.632689	0.305127
C	5.192152	0.445472	1.530002
H	6.066113	1.105539	1.554882
H	4.803101	0.352096	2.550803
H	5.51408	-0.53488	1.178623
C	4.167541	1.701278	-2.15558
H	4.394682	1.341657	-3.16417
H	3.715374	2.695982	-2.23657
H	5.100369	1.776799	-1.59795
C	2.125728	0.288637	-2.32071
H	1.246938	0.148206	-1.69486
H	1.9088	1.067864	-3.0538
H	2.338405	-0.64941	-2.8408

N	3.182797	-1.01598	0.015326
H	2.797331	-1.62539	-0.72971
Br	-5.49132	0.334236	-0.44983
C	-3.52109	0.598251	-0.37051
C	-2.85385	-0.33422	0.647434
O	-1.44888	-0.22078	0.488239
H	-3.16858	0.384418	-1.37874
H	-3.3712	1.64763	-0.12603
H	-3.14607	-1.36434	0.387266
C	-3.26947	-0.05889	2.091924
H	-4.35076	-0.16588	2.21303
H	-2.77118	-0.76857	2.759668
H	-2.98149	0.95397	2.385893
H	-0.99997	-0.91123	-0.50239
C	-0.44229	1.481908	0.79266
O	-1.25315	2.31133	1.037875
O	0.678025	1.09846	0.62695

ts7-4

C	2.791365	1.096324	-1.6074
H	2.105694	0.304511	-1.91957
H	3.587661	1.192644	-2.35524
C	2.043589	2.435089	-1.52735
H	2.719532	3.230444	-1.20479
H	1.693965	2.684646	-2.53375
N	0.908733	2.426329	-0.6239
H	0.112288	1.855768	-0.88715
C	1.135734	2.568998	0.72112
O	0.103216	2.267171	1.52243
O	2.209523	2.948704	1.183692
C	3.43836	-0.55819	0.118503
N	3.682105	-1.55124	-0.7764
N	3.324171	-0.86207	1.423802
C	2.938517	-2.815	-0.70814
H	2.621097	-3.07834	-1.72141
H	3.547847	-3.63542	-0.31219
H	2.038854	-2.66873	-0.11087
C	4.559083	-1.36356	-1.9286
H	5.209267	-2.23964	-2.02284
H	3.997647	-1.25136	-2.86354
H	5.188144	-0.48553	-1.77981
C	4.024589	-2.00475	2.009822

H	4.508848	-1.68137	2.935825
H	3.334562	-2.82264	2.243871
H	4.791411	-2.36719	1.326126
C	2.518968	-0.04588	2.345244
H	1.581764	0.224354	1.863908
H	2.293512	-0.65875	3.219253
H	3.042704	0.857314	2.672102
N	3.352343	0.715291	-0.29801
H	3.32097	1.450627	0.410705
H	-0.58068	1.759703	1.03311
Br	-5.63028	-0.46191	0.291039
C	-3.16797	-1.09773	-0.04482
C	-2.80153	0.344871	-0.35413
O	-1.35321	0.497248	-0.10479
H	-3.24149	-1.42531	0.979382
H	-3.5943	-1.73516	-0.79934
H	-3.2888	1.005058	0.360261
C	-3.10704	0.756393	-1.78484
H	-4.18696	0.691183	-1.93234
H	-2.77929	1.783543	-1.97007
H	-2.60445	0.089619	-2.49385
C	-0.67351	-0.72145	-0.18651
O	-1.44676	-1.72389	-0.30691
O	0.558171	-0.687	-0.13442

ts8-2

C	2.326887	1.691201	-1.40417
H	1.941548	0.788608	-1.88843
H	2.934119	2.245231	-2.13055
C	1.162757	2.589127	-0.94863
H	1.560735	3.496057	-0.48521
H	0.604186	2.889032	-1.84124
N	0.263039	1.96003	-0.01047
H	-0.3894	1.256243	-0.34956
C	0.654451	1.799398	1.308795
O	-0.04043	0.945658	2.006051
O	1.641503	2.424018	1.752931
C	3.813206	0.131415	-0.16898
N	4.347347	-0.42959	-1.29161
N	3.994644	-0.49063	1.014335
C	4.278583	-1.87329	-1.51921
H	3.904122	-2.05122	-2.53255

H	5.258904	-2.35545	-1.42384
H	3.573891	-2.31955	-0.81861
C	4.908678	0.375022	-2.37159
H	5.860536	-0.0676	-2.68509
H	4.246574	0.418984	-3.24444
H	5.1025	1.387617	-2.01784
C	5.22235	-1.22981	1.307507
H	5.637704	-0.86482	2.25226
H	5.030273	-2.30395	1.406335
H	5.959545	-1.06898	0.521681
C	3.056586	-0.33147	2.137607
H	2.029859	-0.34568	1.778021
H	3.201249	-1.18226	2.806429
H	3.221465	0.597303	2.690663
N	3.143025	1.283427	-0.243
H	2.867939	1.759158	0.637076
H	-0.6337	0.258839	1.311761
C	-2.5744	-0.66703	0.727274
C	-3.29709	-1.01317	-0.57065
O	-1.21297	-0.44703	0.408227
H	-3.00827	0.27851	1.090701
H	-3.16069	-0.23158	-1.32019
H	-2.99142	-1.98302	-0.96491
C	-2.77054	-1.73196	1.808325
H	-2.27661	-1.41783	2.732747
H	-3.83506	-1.87505	2.018914
H	-2.3423	-2.68683	1.491208
F	-4.70438	-1.10775	-0.32373
C	-0.00549	-1.89947	-0.33998
O	1.033096	-1.31242	-0.36047
O	-0.7091	-2.83374	-0.52781
B	-5.90325	0.603244	-0.56297
F	-5.49714	1.205785	0.549138
F	-7.04058	-0.07548	-0.56295
F	-5.35462	0.960507	-1.72186

ts9-2

C	-3.13234	-0.07162	2.16542
H	-2.49673	-0.88994	1.81252
H	-3.66393	-0.40649	3.064487
C	-2.27195	1.152232	2.528421
H	-2.91614	1.953161	2.902031

H	-1.60119	0.85793	3.34205
N	-1.49184	1.6723	1.43057
H	-0.65538	1.173143	1.132949
C	-2.11253	2.409381	0.436364
O	-1.43021	2.567525	-0.66304
O	-3.27119	2.846472	0.606307
C	-4.54598	-0.59332	0.190521
N	-4.72714	-1.90351	0.523889
N	-4.85975	-0.19352	-1.05933
C	-4.36313	-2.97647	-0.4023
H	-3.75416	-3.71167	0.133814
H	-5.24314	-3.48824	-0.80995
H	-3.76043	-2.56957	-1.21335
C	-5.18265	-2.31348	1.848402
H	-5.95459	-3.08247	1.734706
H	-4.37095	-2.72966	2.456767
H	-5.62192	-1.46341	2.370468
C	-5.97053	-0.79498	-1.79699
H	-6.63673	0.000857	-2.14486
H	-5.61593	-1.35531	-2.66907
H	-6.53855	-1.46218	-1.14982
C	-4.22632	0.974995	-1.692
H	-3.16032	0.991553	-1.47521
H	-4.35952	0.874371	-2.77092
H	-4.66465	1.91946	-1.3582
N	-4.08552	0.275817	1.092771
H	-4.08781	1.28798	0.861345
H	-0.56186	1.825723	-0.70045
C	1.609504	1.200536	-1.00029
C	2.522104	0.351166	-0.1253
O	0.30116	0.87663	-0.59225
H	2.430848	0.615107	0.929702
H	2.35575	-0.7139	-0.27868
C	-0.51275	-0.89458	-1.41106
O	-1.55873	-0.91498	-0.84459
O	0.346561	-1.254	-2.13545
P	5.552433	-0.67949	0.277186
F	4.660817	-1.80976	-0.41744
F	6.140853	-0.31004	-1.15494
F	3.900451	0.600358	-0.4871
F	4.586324	-0.77342	1.552205
F	6.056151	0.732026	0.816977

F	6.721867	-1.58346	0.803594
H	1.772594	0.89534	-2.04659
C	1.90826	2.694305	-0.86033
H	2.942695	2.910407	-1.14319
H	1.241725	3.278104	-1.50062
H	1.754431	3.020885	0.174218

ts10-2			
C	3.229335	1.272556	-1.53045
H	2.829422	0.366306	-1.99529
H	4.122923	1.584558	-2.08527
C	2.190514	2.406604	-1.59409
H	2.610525	3.312372	-1.1486
H	1.991726	2.616059	-2.6504
N	0.94583	2.112859	-0.9221
H	0.310815	1.449848	-1.35593
C	0.893708	2.148162	0.466983
O	-0.13526	1.573503	1.010404
O	1.823569	2.685228	1.108604
C	3.918037	-0.251	0.301529
N	4.616265	-1.09404	-0.51248
N	3.613342	-0.66182	1.549134
C	4.284304	-2.51789	-0.58298
H	4.199389	-2.80572	-1.63588
H	5.050591	-3.14673	-0.11396
H	3.317198	-2.69021	-0.11182
C	5.627745	-0.61184	-1.44683
H	6.503642	-1.26737	-1.38969
H	5.26931	-0.60787	-2.48311
H	5.936835	0.396629	-1.17143
C	4.500864	-1.55022	2.298419
H	4.692299	-1.11059	3.282336
H	4.051495	-2.53909	2.442812
H	5.452127	-1.66217	1.779191
C	2.450977	-0.13869	2.285535
H	1.592229	-0.05655	1.622616
H	2.214184	-0.85602	3.073717
H	2.646112	0.840039	2.732288
N	3.567283	0.963855	-0.12706
H	3.152351	1.633736	0.548268
C	-3.43335	1.839162	1.175376
C	-4.01135	1.961795	-0.24025
C	-3.10502	1.283306	-1.28671
C	-2.48654	-0.0706	-0.8318

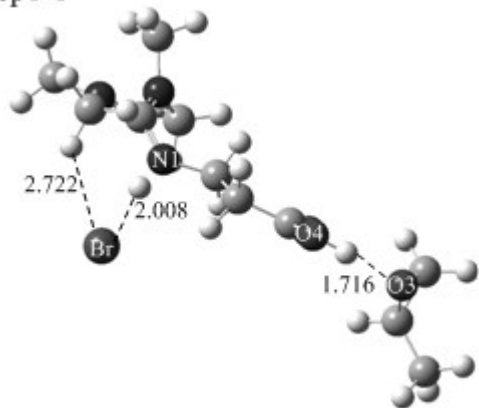
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H	-5.00764	1.510643	-0.27074
H	-4.13507	3.019468	-0.50127
H	-2.47236	2.362247	1.213065
H	-4.09162	2.338702	1.894443
H	-2.60588	-0.82038	-1.61887
H	-3.99176	0.032375	2.299282
H	-2.26294	0.292665	2.149252
H	-2.2677	1.944875	-1.53406
O	-1.08589	0.051333	-0.59884
H	-2.64783	-1.55284	0.726549
Br	-4.98845	-1.28687	-0.04836
H	-0.68705	0.826529	0.247729
C	-0.01894	-1.57451	-0.81551
O	1.087095	-1.19604	-0.54976
O	-0.79179	-2.41026	-1.15074

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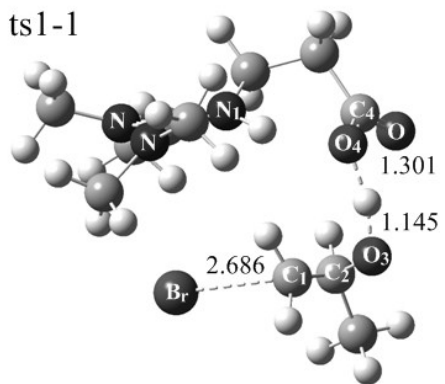
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H	-1.17752	-0.06827	1.514921
H	-0.77261	2.118283	0.598791
H	-0.81852	1.511322	-1.08099
C	-2.29253	-0.56262	-0.26992
H	-2.56151	-1.56194	0.080618
H	-3.12935	0.110924	-0.05734
H	-2.1407	-0.6026	-1.35244
C	1.208859	-0.21942	-0.0197
O	0.918281	1.113171	-0.02682
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(a) route 1

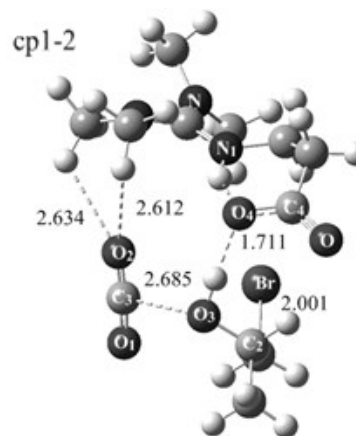
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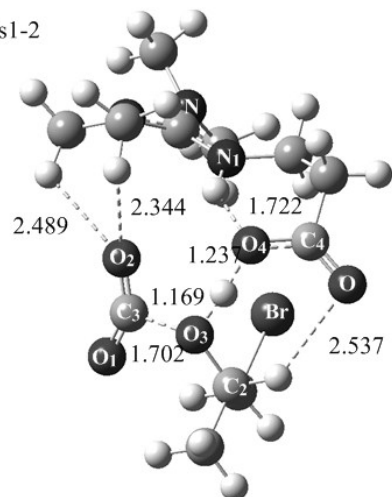
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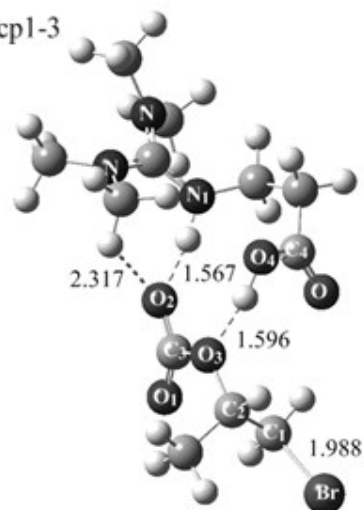
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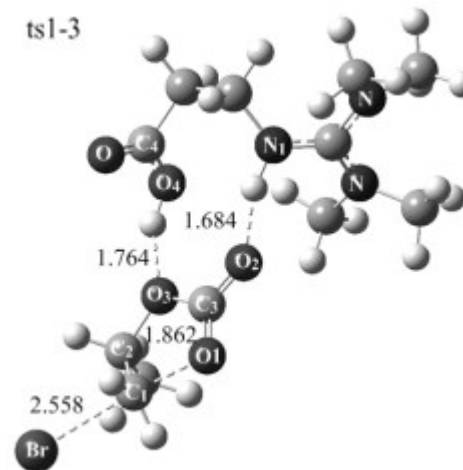
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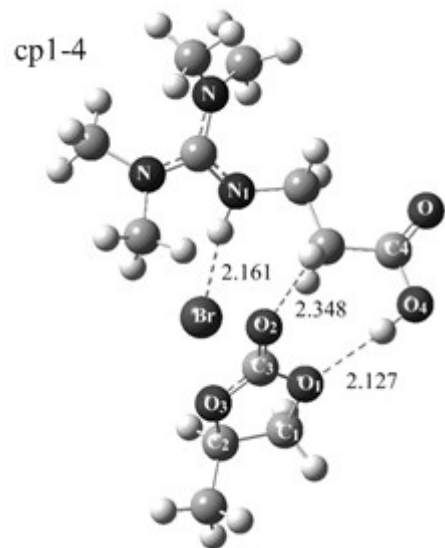


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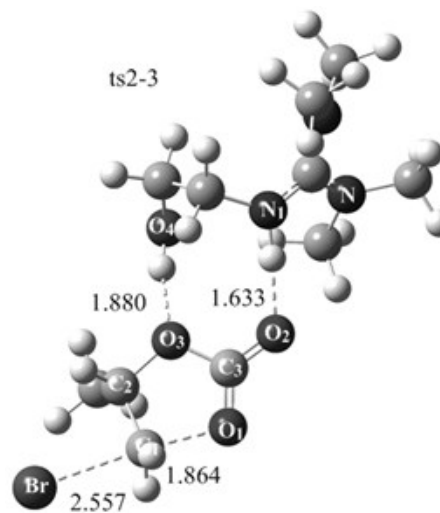
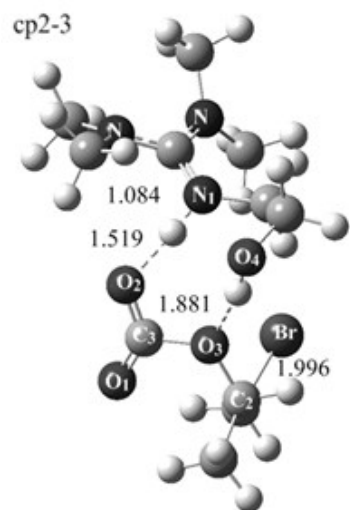
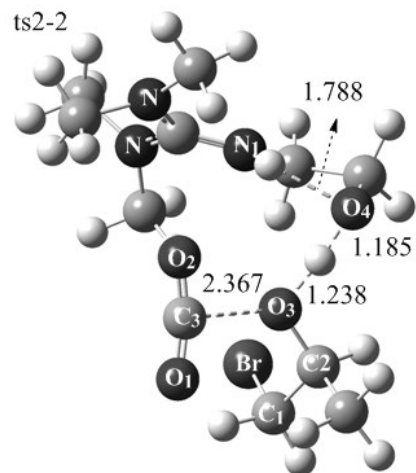
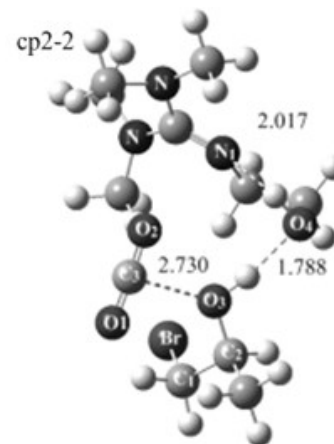
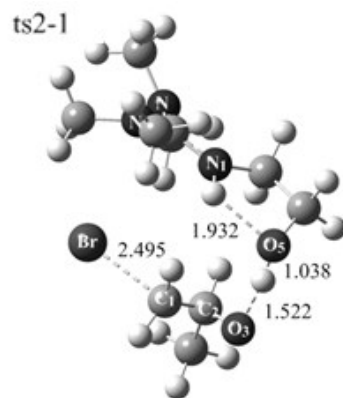
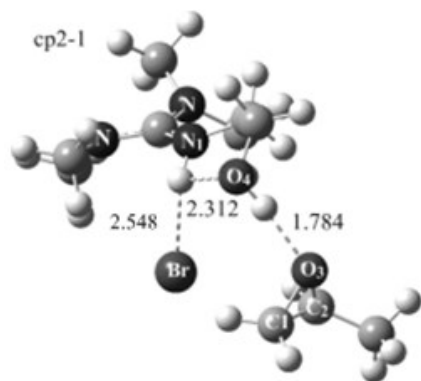


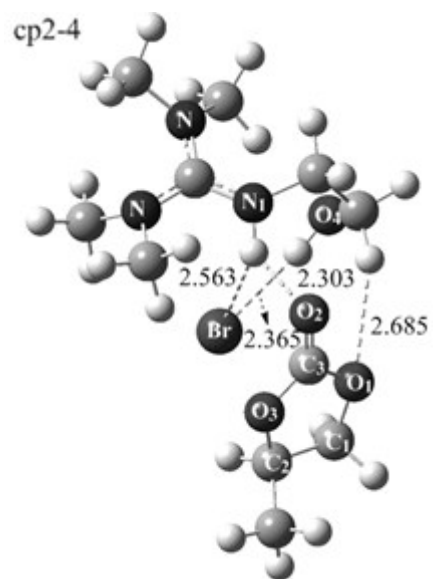
ts1-3



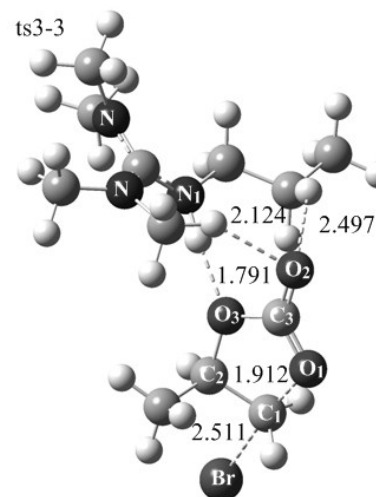
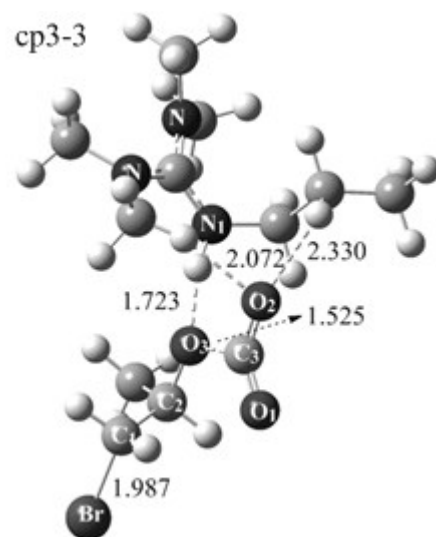
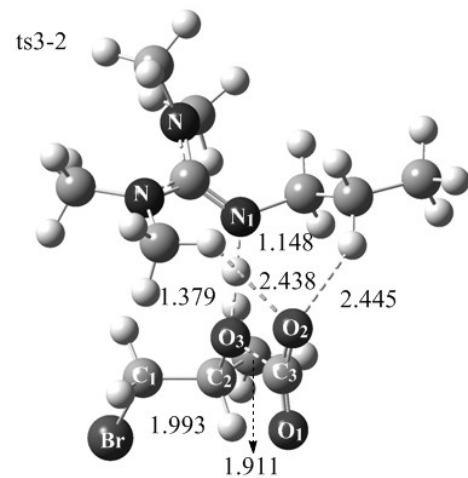
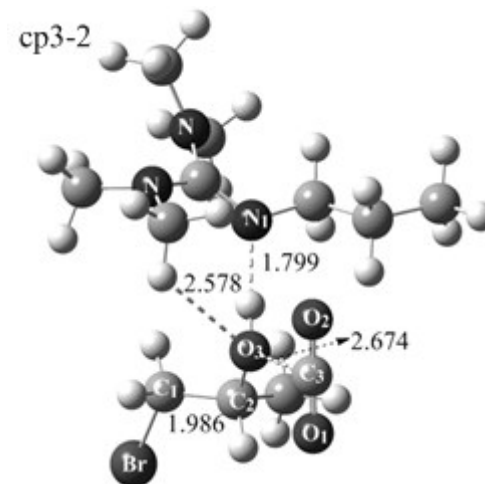
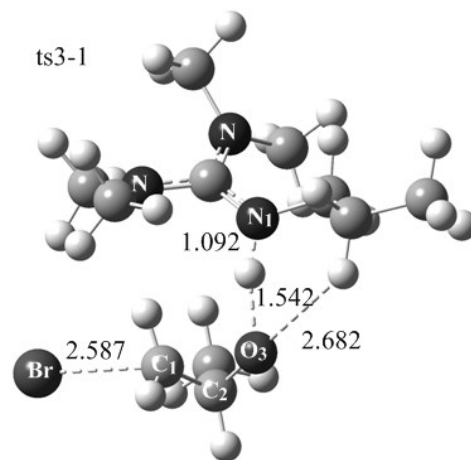
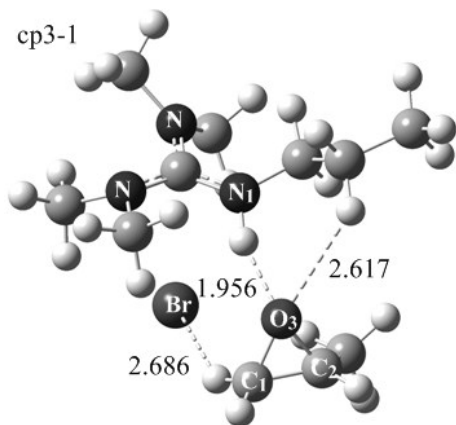


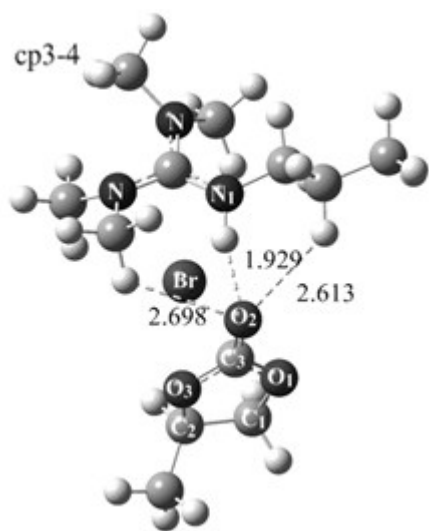
(b) route 2





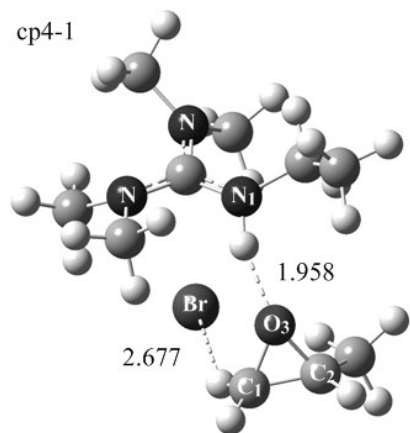
(c) route3



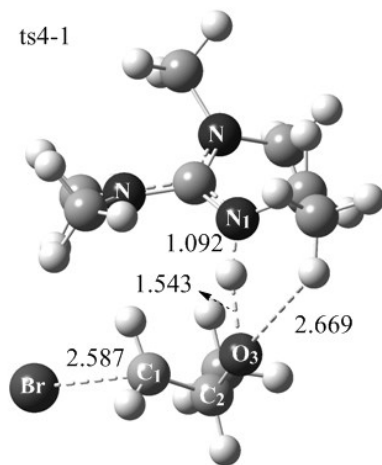


(d) route 4

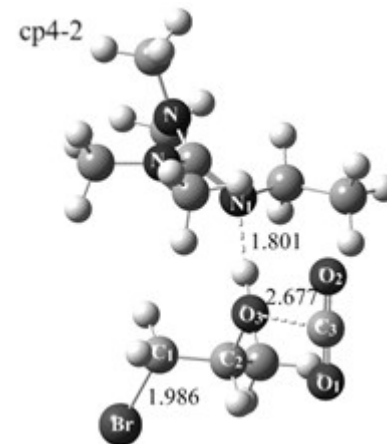
cp4-1



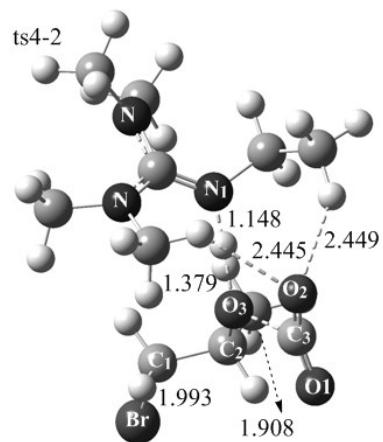
ts4-1



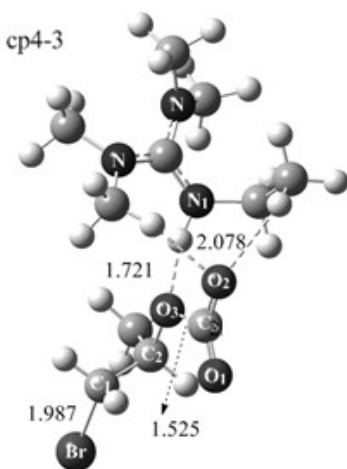
cp4-2



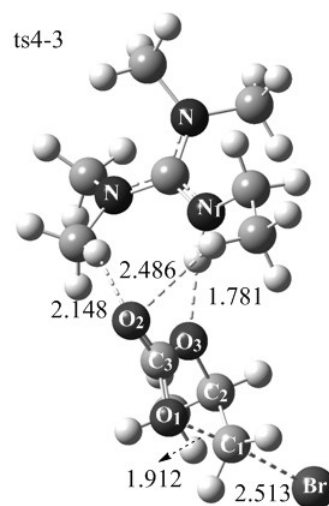
ts4-2



cp4-3



ts4-3



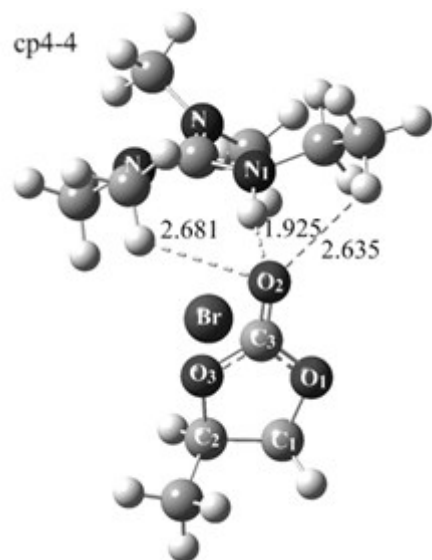
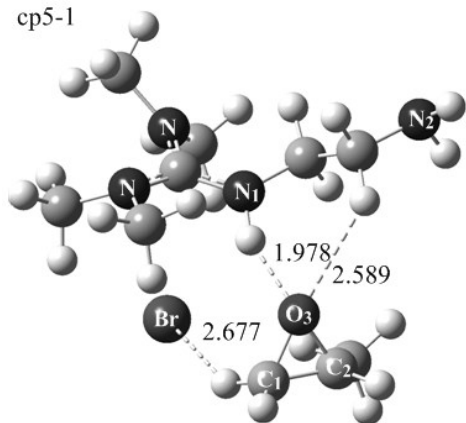
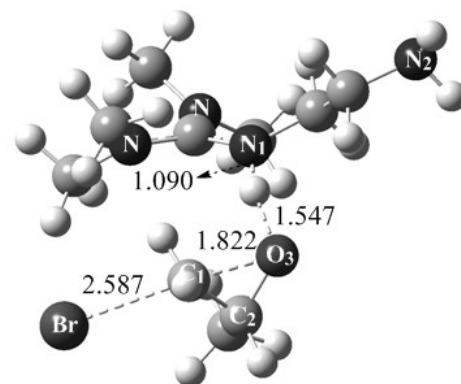


Figure S1 Optimized geometries for the intermediates and transition states involved in routes 1-4. Distances are in angstroms.

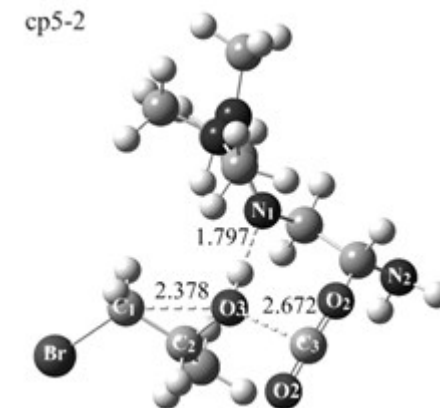
cp5-1



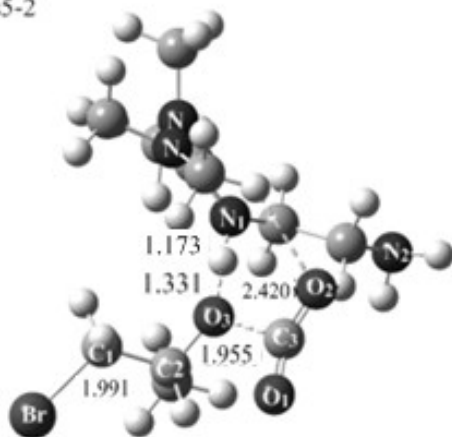
ts5-1



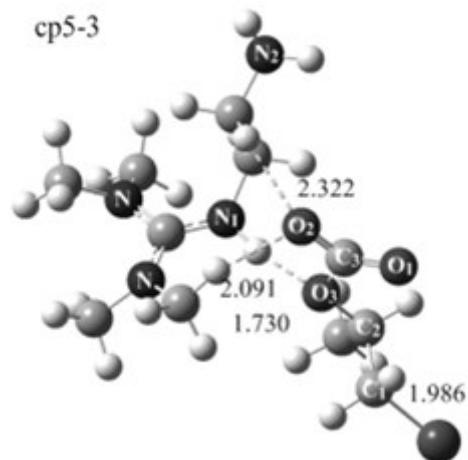
cp5-2



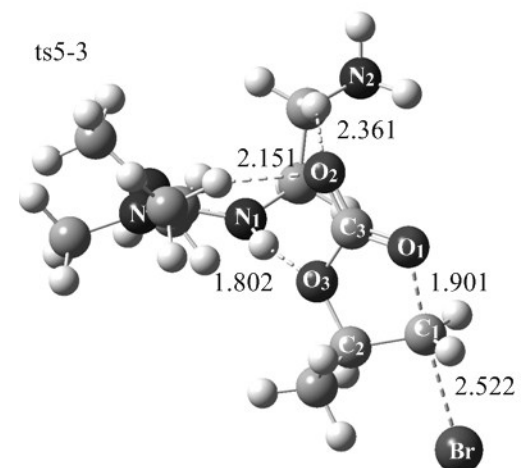
ts5-2



cp5-3



ts5-3



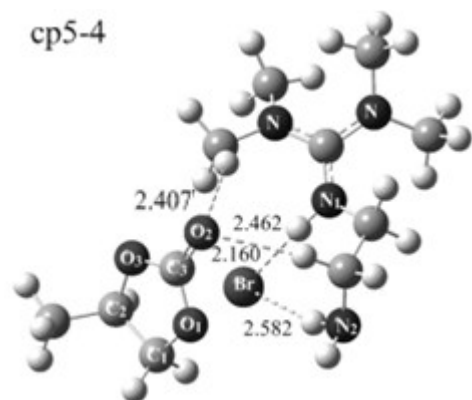
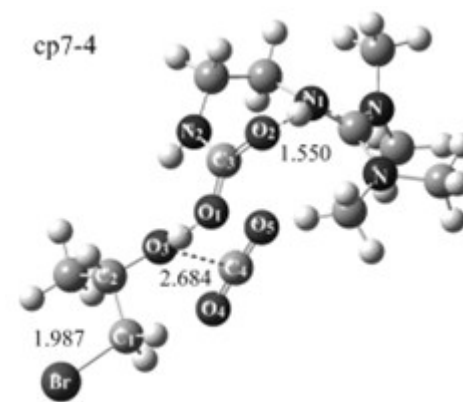
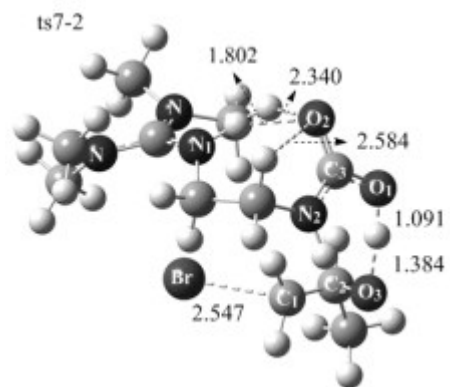
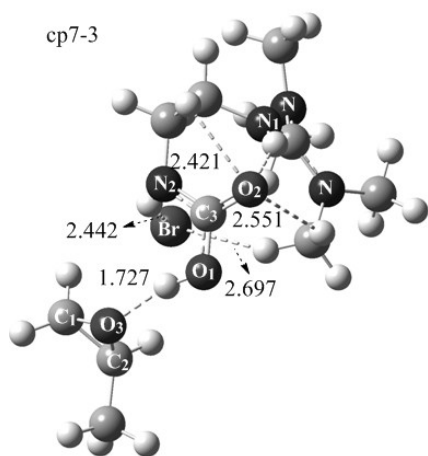
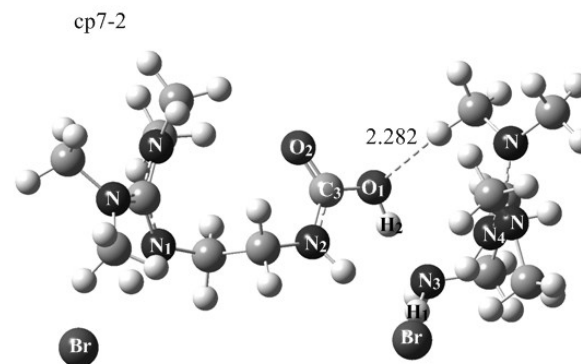
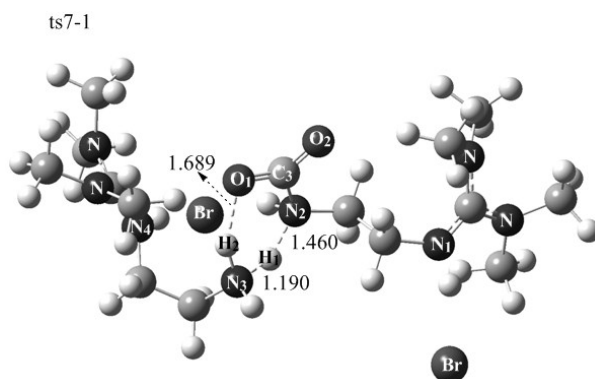
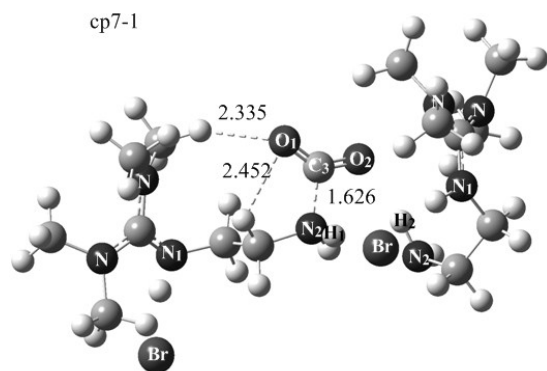
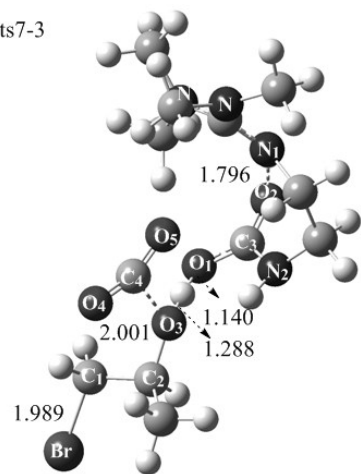


Figure. S2 Optimized geometries for the intermediates and transition states involved in route 5. Distances are in angstroms.

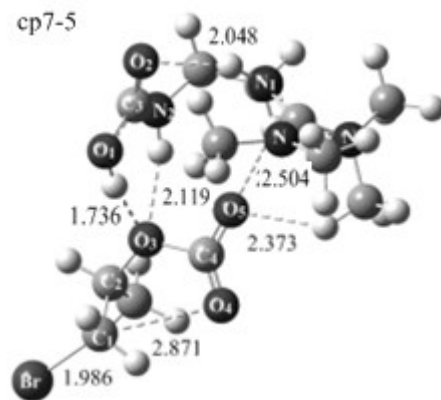
(a) route 7



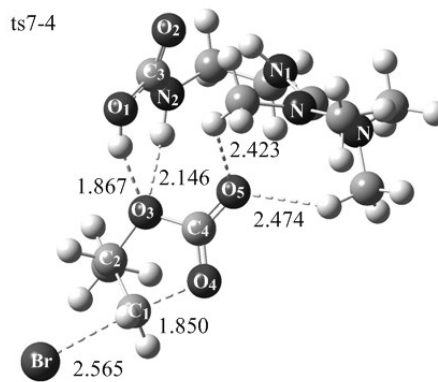
ts7-3



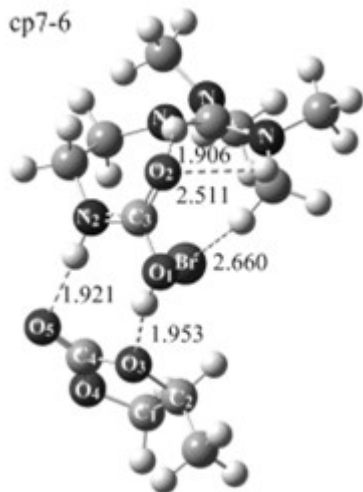
cp7-5



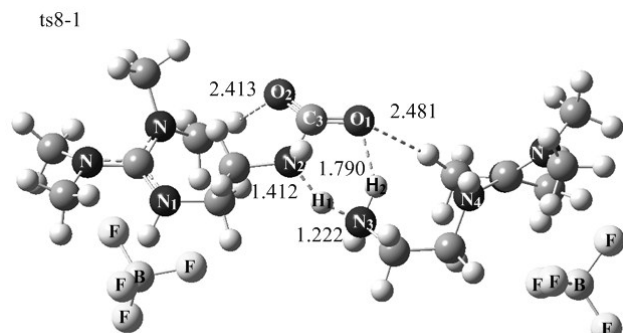
ts7-4



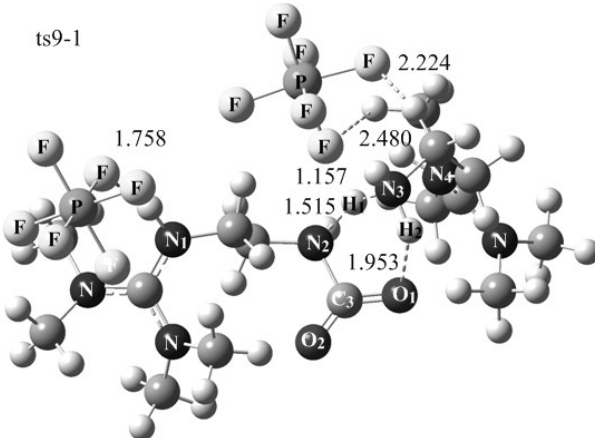
cp7-6



(b) route 8



(c) route 9



(d) route 10

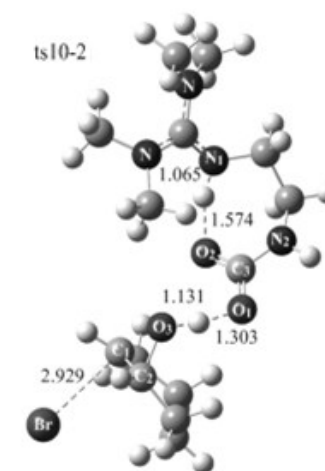


Figure S3 Optimized geometries for the intermediates and transition states involved in routes 6-10. Distances are in angstroms.