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SUPPLEMENTARY MATERIAL

Asymmetric Michael Addition Using Bifunctional Bicyclic Guanidine Organocatalyst: A Theoretical Perspective

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Table S1. Structural parameters of optimized C_S, C_2 and C_{2v} structures of unsubstituted [5,5]-bicyclic guanidinium ion[A]

parameter	C_S	C_2	C_{2v}
$r(C_1–N_1)$	1.342	1.325	1.326
$r(C_1–N_2)$	1.326	1.328	1.326
$r(N_1–C_2)$	1.466	1.460	1.458
$r(N_2–C_3)$	1.480	1.480	1.478
$r(C_2–H_a)$	1.097	1.092	1.093
$r(C_2–H_e)$	1.090	1.094	1.093
$r(N_1–H)$	1.011	1.010	1.009
$\tau(N_2'C_1N_1N_2)$	175.3	180.0	180.0
$\tau(N_1C_2C_3N_2)$	-25.8	10.4	0.0
$\tau(HN_2C_1N_1)$	-166.5	-169.6	180.0
$\tau(H_aC_2N_1C_1)$	-144.6	-126.4	-119.3
$\tau(H_eC_2N_1C_1)$	93.2	112.1	119.3

[A] M06-2X/6-31G* optimized geometries. Bond length in Å and torsional angle in degrees. Atom labelling is given in Fig. 1.

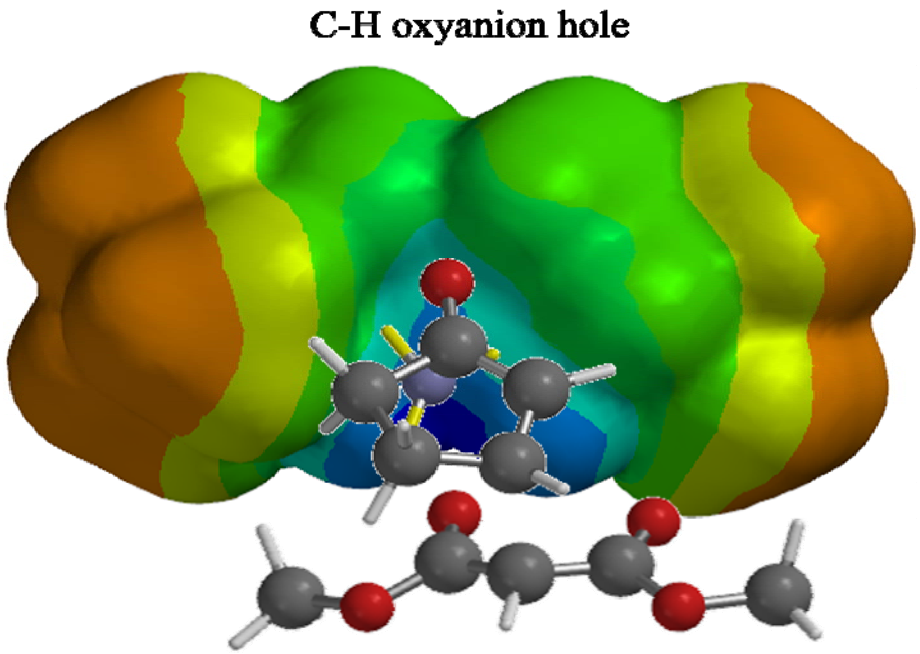

Fig. S1. Electrostatic potential map of the guanidinium catalyst in transition state of ***R*-TS-FO1**. Red indicates electron-rich region while blue represents electron-poor region.

Table S2. Cartesian coordinates, total energies (in Hartrees) and number of imaginary frequencies[A] of the M06-2X/6-31G* optimized geometries of all calculated structures.

***R*-TS-FO1**, E = -1439.69762578 (1)			
N	-0.091781	0.515168	-2.719621
C	0.144440	0.800916	-1.412835
N	1.434793	0.958440	-1.154977
N	-0.946908	0.885435	-0.687795
C	2.203060	0.663820	-2.379527
H	1.768000	0.935357	-0.194777
C	1.144456	-0.060375	-3.249042
C	-1.420762	-0.093970	-2.782456
H	-0.954737	0.890670	0.342361
C	-2.104129	0.481926	-1.508261
C	3.519554	-0.086923	-2.130794
H	-1.938734	0.193073	-3.699991
H	2.449459	1.621308	-2.863309
C	-3.081273	1.652280	-1.754733
H	1.147385	-1.144787	-3.079043
H	1.270069	0.165482	-4.309802
H	-1.324779	-1.181645	-2.710669
H	-2.643109	-0.311624	-0.981417
C	-2.408860	2.772585	-2.553844

***R*-PTSC-FO1**, E = -1439.71469515 (0)			
N	-0.083654	0.609890	-2.751030
C	0.088039	0.860222	-1.424787
N	1.356130	1.076920	-1.106237
N	-1.020024	0.820955	-0.728474
C	2.190240	0.822703	-2.296047
H	1.633777	0.937677	-0.129233
C	1.195963	0.104215	-3.246312
C	-1.385581	-0.035892	-2.902941
H	-1.067701	0.849831	0.316674
C	-2.128286	0.390739	-1.600313
C	3.494756	0.076818	-1.974897
H	-1.892358	0.314884	-3.804640
H	2.456808	1.791763	-2.742316
C	-3.194743	1.493235	-1.779101
H	1.235251	-0.988506	-3.132225
H	1.362088	0.377265	-4.290224
H	-1.258742	-1.122235	-2.941264
H	-2.610634	-0.484126	-1.149951
C	-2.594741	2.727534	-2.458816

C	-4.300583	1.120252	-2.516389
C	-3.541895	2.199392	-0.399263
C	4.090777	-0.501821	-3.491689
C	4.502103	0.869238	-1.441154
C	3.308851	-1.313191	-1.243460
H	-3.108793	3.603412	-2.694574
H	-1.531069	3.157790	-2.024767
H	-2.088487	2.433312	-3.545096
H	-5.034117	1.921296	-2.655780
H	-4.037486	0.739801	-3.509261
H	-4.789476	0.311567	-1.960773
H	-4.286891	2.988844	-0.547762
H	-3.990506	1.410152	0.214711
H	-2.705304	2.614113	0.169899
H	2.532741	-1.986561	-1.617410
H	4.250878	-1.863560	-1.141436
H	2.988629	-1.000856	-0.245408
H	4.702319	1.751185	-2.059897
H	4.115003	1.214397	-0.474546
H	5.454342	0.362427	-1.252496
H	4.193067	0.361126	-4.160769
H	5.082695	-0.946741	-3.363064
H	3.454531	-1.246206	-3.982557
O	0.943425	0.568571	1.508266
C	0.857523	0.056758	2.620027
H	3.409113	-0.472408	1.869425
C	-0.350885	-0.383755	3.276031
O	1.966028	-0.231371	3.347722
C	-1.578975	0.327058	2.985478
C	-0.818592	-2.093734	2.338283
H	-0.226405	-0.683103	4.311135
H	3.200989	1.190870	2.474765
O	-1.864293	0.928081	1.958865
O	-2.493228	0.158350	3.969310
C	-3.774415	0.714467	3.701305
H	-4.228600	0.236613	2.828883
H	-4.372789	0.523863	4.591618
H	-3.699104	1.788032	3.512244
C	3.202443	0.134604	2.757524
H	3.962388	-0.053587	3.515325
H	-1.612441	-2.301674	3.054996
C	-1.107306	-1.872340	0.978651
C	0.444861	-2.943525	2.422622
C	0.019109	-2.131604	0.164401
H	-2.044794	-1.475522	0.611111

C	-4.346465	0.931982	-2.620497
C	-3.732250	1.882177	-0.397091
C	4.169931	-0.300058	-3.297707
C	4.409617	1.027350	-1.191701
C	3.228643	-1.174103	-1.134259
H	-3.355310	3.510286	-2.549380
H	-1.764649	3.131581	-1.870428
H	-2.224574	2.504136	-3.465834
H	-5.138745	1.681751	-2.715112
H	-4.029823	0.659025	-3.632952
H	-4.781809	0.043511	-2.148285
H	-4.535019	2.620080	-0.503978
H	-4.136488	1.009239	0.129280
H	-2.949030	2.303724	0.238319
H	2.545719	-1.872724	-1.627957
H	4.173483	-1.694266	-0.937734
H	2.775739	-0.904668	-0.174127
H	4.657932	1.915522	-1.783631
H	3.937024	1.362887	-0.261474
H	5.344670	0.523058	-0.926194
H	4.314818	0.580059	-3.935723
H	5.153469	-0.740825	-3.105168
H	3.579766	-1.036713	-3.853926
O	1.112510	0.122270	1.388005
C	1.043701	0.128790	2.633939
H	3.253014	-1.373064	2.050463
C	-0.055615	0.367275	3.467734
O	2.170258	-0.176313	3.364323
C	-1.336286	0.721583	2.997073
C	-0.897901	-2.396998	2.230463
H	0.089535	0.292136	4.535626
H	3.577564	0.370218	1.933093
O	-1.735969	0.917585	1.837304
O	-2.238684	0.839536	4.017009
C	-3.549338	1.203715	3.625748
H	-3.996690	0.441140	2.979925
H	-4.122350	1.292529	4.549676
H	-3.553199	2.155059	3.085842
C	3.341261	-0.444029	2.625848
H	4.142225	-0.547598	3.359481
H	-1.540206	-2.265831	3.095484
C	-1.186970	-1.978476	0.991845
C	0.453757	-3.054701	2.335342
C	-0.067195	-2.285366	0.085852
H	-2.077566	-1.441676	0.692445

H	1.943240	-1.995912	1.152279
O	0.169709	-1.960076	-1.062495
H	0.139160	-3.990358	2.532786
C	1.122840	-2.715632	1.066191
H	1.080597	-2.692498	3.276220
H	1.539972	-3.622883	0.618209
***R*-TS-FO2**, E = -1439.69046767 (1)			
N	-2.217423	1.773145	-0.062512
C	-1.290917	0.889213	-0.495904
N	-0.054955	1.338083	-0.404740
N	-1.849736	-0.172349	-1.059931
C	-0.091662	2.593909	0.378349
H	0.760799	0.710605	-0.459029
C	-1.556186	3.050262	0.143975
C	-3.482534	1.467798	-0.710889
H	-1.300080	-1.003646	-1.264279
C	-3.315380	-0.044698	-1.043180
C	0.979305	3.624672	-0.021461
H	-4.330073	1.658242	-0.049326
H	0.013892	2.318522	1.436639
C	-4.018373	-1.015888	-0.068949
H	-1.651203	3.685733	-0.750662
H	-1.960420	3.580130	1.007924
H	-3.604360	2.065229	-1.626079
H	-3.693012	-0.248982	-2.052515
C	-3.723280	-0.675984	1.394684
C	-5.525984	-0.945751	-0.338033
C	-3.523286	-2.434799	-0.370990
C	0.593711	4.976493	0.594613
C	2.332784	3.190506	0.552783
C	1.097871	3.747358	-1.543552
H	-4.157465	-1.448735	2.039563
H	-2.649297	-0.607618	1.606282
H	-4.177788	0.278185	1.685686
H	-6.057525	-1.633146	0.327622
H	-5.925111	0.058898	-0.156784
H	-5.763745	-1.225517	-1.371427
H	-4.083514	-3.164681	0.222025
H	-3.650236	-2.690959	-1.431096
H	-2.465092	-2.539783	-0.109157
H	0.143695	4.012303	-2.013563
H	1.819494	4.532278	-1.794722
H	1.446054	2.806486	-1.980382
H	2.288630	3.120573	1.645879

H	1.948449	-2.614486	0.766512
O	0.029180	-2.008511	-1.099774
H	0.377032	-4.056000	2.773334
C	0.965894	-3.072925	0.888063
H	1.099636	-2.466189	2.998190
H	1.021709	-4.085834	0.474881
***R*-PTSC-FO2**, E = -1439.71155617 (0)			
N	-2.196433	1.791048	-0.102461
C	-1.239066	0.909551	-0.493562
N	-0.018467	1.339234	-0.285280
N	-1.751739	-0.144446	-1.110983
C	-0.096897	2.627166	0.433392
H	0.838825	0.760855	-0.427144
C	-1.542608	3.077847	0.090144
C	-3.415813	1.474385	-0.833161
H	-1.177323	-0.987243	-1.216255
C	-3.216752	-0.038157	-1.148220
C	1.013615	3.626309	0.061584
H	-4.306565	1.662423	-0.229585
H	-0.052358	2.410514	1.509919
C	-3.929924	-1.015504	-0.186241
H	-1.576286	3.673083	-0.836618
H	-1.998074	3.647271	0.901841
H	-3.480396	2.065395	-1.758377
H	-3.559536	-0.256560	-2.166534
C	-3.675456	-0.660187	1.281210
C	-5.432129	-0.973411	-0.486804
C	-3.400089	-2.427290	-0.464153
C	0.606429	5.009050	0.587120
C	2.318004	3.199123	0.746854
C	1.236383	3.673656	-1.452970
H	-4.133929	-1.419504	1.924664
H	-2.608141	-0.608779	1.520220
H	-4.119586	0.305586	1.547528
H	-5.965179	-1.670040	0.168201
H	-5.854284	0.023747	-0.317887
H	-5.640233	-1.260514	-1.524258
H	-3.944892	-3.161442	0.138435
H	-3.521877	-2.701591	-1.520021
H	-2.337496	-2.505041	-0.208618
H	0.315800	3.913560	-1.997781
H	1.974032	4.447144	-1.693282
H	1.614636	2.713136	-1.817047
H	2.196215	3.178112	1.836656

H	2.633074	2.219915	0.148128
H	3.104004	3.923914	0.289667
H	0.441253	4.888724	1.676972
H	1.395107	5.703485	0.427166
H	-0.320634	5.385335	0.149703
O	0.465710	-1.515022	-1.091414
C	1.388338	-2.297983	-0.893509
H	-0.767258	-3.933658	-0.597368
C	2.696284	-1.961176	-0.384084
O	1.232547	-3.634320	-1.059895
C	3.241723	-0.670748	-0.757048
C	2.366091	-1.597834	1.541556
H	3.408621	-2.779292	-0.379054
H	-0.431752	-3.522575	-2.300468
O	2.610503	0.337676	-1.039130
O	4.590591	-0.653264	-0.649716
C	5.198486	0.613859	-0.865496
H	4.897460	1.324389	-0.090229
H	6.273055	0.439477	-0.818061
H	4.918690	1.018403	-1.841090
C	-0.065924	-4.069178	-1.427346
H	0.028399	-5.129911	-1.658292
H	3.432735	-1.638520	1.760946
C	1.634380	-0.409540	1.747282
C	1.509416	-2.765894	2.034307
C	0.266744	-0.676095	1.990574
H	2.048227	0.591264	1.701738
H	-0.497160	-2.517936	1.165014
O	-0.675966	0.120884	2.145855
H	1.827772	-3.005710	3.055232
C	0.080628	-2.201975	2.042592
H	1.625274	-3.673233	1.435037
H	-0.497261	-2.482545	2.928093
***R*-TS-SO1**, E = -1439.69652666 (1)			
N	-2.666785	1.332554	0.101652
C	-1.664054	0.587734	-0.447332
N	-0.510299	1.228826	-0.465228
N	-2.087443	-0.570491	-0.908997
C	-0.677896	2.521881	0.224650
H	0.410848	0.760995	-0.522493
C	-2.214958	2.714685	0.152959
C	-3.929965	0.793324	-0.378473
H	-1.463682	-1.339440	-1.318452
C	-3.539331	-0.681513	-0.688591

H	2.633568	2.210826	0.398549
H	3.115354	3.913556	0.511277
H	0.381051	4.974196	1.659880
H	1.426667	5.719154	0.440877
H	-0.271024	5.406045	0.063652
O	0.363117	-1.661181	-0.667466
C	1.347666	-2.344609	-1.015184
H	-0.515472	-4.058931	-0.076809
C	2.680530	-1.955042	-1.194087
O	1.177068	-3.692469	-1.231949
C	3.110244	-0.619468	-1.076806
C	2.319593	-1.683724	1.983123
H	3.406348	-2.706659	-1.467563
H	-0.828305	-3.672053	-1.784400
O	2.450772	0.403320	-0.823044
O	4.455983	-0.490732	-1.274816
C	4.964474	0.823719	-1.149739
H	4.850665	1.196941	-0.126221
H	6.023219	0.759580	-1.404018
H	4.454074	1.515350	-1.826442
C	-0.140058	-4.179859	-1.099787
H	-0.093707	-5.241338	-1.347002
H	3.383083	-1.826423	1.820713
C	1.701860	-0.497672	2.041216
C	1.380885	-2.852986	2.149997
C	0.257012	-0.699022	2.244927
H	2.151195	0.482325	1.933446
H	-0.713528	-2.480632	1.570361
O	-0.599523	0.162609	2.339235
H	1.679279	-3.470686	3.005083
C	0.004130	-2.201032	2.346132
H	1.424984	-3.497951	1.264955
H	-0.444584	-2.423166	3.319306
***R*-PTSC-SO1**, E = -1439.70601163 (0)			
N	-2.678294	1.318707	0.126265
C	-1.666242	0.585286	-0.420978
N	-0.507135	1.187137	-0.371648
N	-2.104090	-0.548310	-0.950140
C	-0.665232	2.467817	0.339666
H	0.424586	0.719827	-0.501388
C	-2.199033	2.691591	0.242429
C	-3.930441	0.826895	-0.429920
H	-1.489888	-1.288593	-1.332875
C	-3.563476	-0.643561	-0.787535

C	0.161245	3.657227	-0.388453
H	-4.711509	0.872505	0.380595
H	-0.376096	2.388927	1.271871
C	-3.897477	-1.705815	0.412089
H	-2.517836	3.258155	-0.755376
H	-2.606813	3.237083	1.027801
H	-4.260543	1.319332	-1.285898
H	-4.011173	-1.011036	-1.621251
C	-3.362973	-1.269681	1.779611
C	-5.422615	-1.850324	0.467639
C	-3.280747	-3.057385	0.030427
C	-0.291006	4.976612	0.249370
C	1.638472	3.416574	-0.054024
C	-0.001931	3.721266	-1.910020
H	-3.583064	-2.041754	2.524635
H	-2.277447	-1.127822	1.756224
H	-3.821071	-0.334973	2.121170
H	-5.700641	-2.605063	1.210425
H	-5.917894	-0.914720	0.750387
H	-5.824821	-2.170559	-0.500408
H	-3.597287	-3.826351	0.743054
H	-3.600709	-3.370683	-0.970356
H	-2.186999	-3.019879	0.033070
H	-1.041887	3.887841	-2.213234
H	0.592067	4.551451	-2.307030
H	0.347656	2.795861	-2.377512
H	1.791674	3.364723	1.028982
H	1.994191	2.476209	-0.484582
H	2.246662	4.236025	-0.453766
H	-0.224726	4.929281	1.342919
H	0.351631	5.795724	-0.089156
H	-1.322204	5.231936	-0.022260
O	2.002929	0.239830	-1.229429
C	2.984669	-0.265360	-0.685057
H	3.129547	-0.773162	-3.287849
C	3.128309	-0.630037	0.690799
O	4.063717	-0.629282	-1.430689
C	2.340831	0.031607	1.697967
C	1.929697	-2.429816	0.705840
H	4.098267	-0.999322	1.000356
H	3.884339	0.791101	-2.933721
O	1.317138	0.683123	1.546923
O	2.818367	-0.238978	2.945788
C	2.049356	0.303700	4.007668
H	1.027463	-0.085069	3.987840

C	0.211928	3.588690	-0.246473
H	-4.742986	0.891518	0.297003
H	-0.378341	2.305714	1.386610
C	-3.983409	-1.704254	0.255190
H	-2.472236	3.274102	-0.651086
H	-2.601592	3.186717	1.127858
H	-4.210532	1.396110	-1.328194
H	-4.008924	-0.920551	-1.749984
C	-3.484466	-1.341128	1.656722
C	-5.512347	-1.814291	0.253588
C	-3.388253	-3.053688	-0.166002
C	-0.226963	4.914720	0.386009
C	1.675998	3.312850	0.117814
C	0.085464	3.657725	-1.771488
H	-3.766362	-2.127934	2.364315
H	-2.393758	-1.245760	1.680062
H	-3.913717	-0.398953	2.013869
H	-5.831583	-2.603158	0.942102
H	-5.995492	-0.884901	0.574347
H	-5.889789	-2.068686	-0.743684
H	-3.728379	-3.842384	0.513033
H	-3.700191	-3.325726	-1.181424
H	-2.293788	-3.039522	-0.144557
H	-0.946132	3.829688	-2.100610
H	0.694194	4.484894	-2.151865
H	0.443921	2.730503	-2.229460
H	1.805651	3.251225	1.203359
H	2.024560	2.367953	-0.309701
H	2.310094	4.121056	-0.263819
H	-0.186691	4.862164	1.480549
H	0.440427	5.721315	0.066145
H	-1.246057	5.193701	0.091791
O	1.767195	0.089709	-1.257812
C	2.899987	-0.142203	-0.782621
H	2.665435	-0.958208	-3.306916
C	3.350352	-0.056616	0.539007
O	3.877432	-0.572342	-1.650802
C	2.488392	0.271987	1.615782
C	1.814260	-2.634577	0.915252
H	4.388989	-0.268571	0.749075
H	3.420742	0.642257	-3.272492
O	1.291313	0.567663	1.593729
O	3.142554	0.205324	2.823896
C	2.354385	0.560185	3.942712
H	1.483623	-0.095320	4.041745

H	2.552686	0.001569	4.926185
H	2.006901	1.394291	3.940592
C	3.985262	-0.290319	-2.807571
H	4.916804	-0.639149	-3.252750
H	2.171121	-2.525655	1.761252
C	0.642668	-2.148396	0.252618
C	2.645638	-3.314112	-0.303049
C	0.503371	-2.527261	-1.107837
H	-0.126913	-1.654381	0.834509
H	2.275053	-2.488843	-2.301596
O	-0.486288	-2.414642	-1.865235
H	2.616465	-4.347281	0.063807
C	1.805929	-3.163597	-1.577573
H	3.694515	-3.041966	-0.441968
H	1.603936	-4.105285	-2.095304
***R*-TS-SO2**, E = -1439.69738105 (1)			
N	1.795336	1.966438	-1.500494
C	1.022872	1.366810	-0.538668
N	1.558623	1.439722	0.661066
N	-0.041629	0.782352	-1.039469
C	2.864965	2.111709	0.566638
H	1.164630	0.994193	1.544894
C	3.145832	2.053850	-0.957574
C	1.417032	1.377796	-2.781483
H	-0.752708	0.250292	-0.511241
C	-0.030448	0.874590	-2.509712
C	3.933491	1.480441	1.478571
H	1.464644	2.115557	-3.585243
H	2.746485	3.165493	0.859298
C	-1.160231	1.775118	-3.052636
H	3.728605	1.158942	-1.229086
H	3.671924	2.940932	-1.315159
H	2.087347	0.541654	-3.028859
H	-0.174206	-0.134163	-2.905035
C	-1.012005	3.215665	-2.555152
C	-1.119919	1.739116	-4.584547
C	-2.500030	1.198728	-2.577243
C	5.293162	2.083430	1.106670
C	3.603184	1.831705	2.935662
C	3.964365	-0.044286	1.331687
H	-1.838010	3.826583	-2.934729
H	-1.039598	3.257733	-1.461406
H	-0.075597	3.674450	-2.892601
H	-1.957101	2.313968	-4.993572

H	3.003339	0.457476	4.813629
H	1.995509	1.591492	3.864179
C	3.571267	-0.413640	-3.024933
H	4.432117	-0.803842	-3.569803
H	2.125198	-2.437356	1.936781
C	0.647723	-2.242116	0.381512
C	2.690479	-3.389084	-0.050595
C	0.595016	-2.647351	-1.026674
H	-0.117912	-1.656029	0.875897
H	2.416909	-2.749465	-2.126184
O	-0.328132	-2.488702	-1.818423
H	2.867027	-4.412249	0.301298
C	1.902962	-3.345618	-1.367183
H	3.664179	-2.897397	-0.136047
H	1.695378	-4.327799	-1.800677
***R*-PTSC-SO2**, E = -1439.70742726 (0)			
N	2.288895	1.993638	-0.099163
C	1.441868	0.958472	0.191212
N	2.094650	-0.164042	0.449668
N	0.182308	1.269771	0.055276
C	3.540093	0.061751	0.287492
H	1.647351	-1.070800	0.655657
C	3.561290	1.402131	-0.494842
C	1.507146	2.979931	-0.844469
H	-0.620772	0.640822	0.284752
C	0.049624	2.662370	-0.393629
C	4.270659	-1.120561	-0.373731
H	1.816258	3.997567	-0.597297
H	3.989954	0.229194	1.277072
C	-0.521274	3.575678	0.714203
H	3.588645	1.235532	-1.583543
H	4.408970	2.028128	-0.210513
H	1.630623	2.823313	-1.925865
H	-0.642181	2.672084	-1.240912
C	0.408682	3.622157	1.930807
C	-0.706151	4.984755	0.139815
C	-1.889740	3.024807	1.137115
C	5.696682	-0.668730	-0.710215
C	4.329354	-2.280281	0.629697
C	3.549058	-1.594342	-1.639348
H	-0.026604	4.264790	2.703533
H	0.539422	2.624570	2.363137
H	1.398017	4.023506	1.682104
H	-1.178602	5.632586	0.885379

H	-0.197961	2.172151	-4.988673
H	-1.206209	0.711461	-4.955707
H	-3.326137	1.783424	-2.996854
H	-2.610581	0.156283	-2.894624
H	-2.581765	1.217553	-1.485937
H	4.131291	-0.360335	0.295585
H	4.780702	-0.453145	1.936381
H	3.027654	-0.488674	1.683515
H	3.583012	2.917929	3.081647
H	2.636455	1.416024	3.237656
H	4.369450	1.417846	3.600288
H	5.267879	3.178681	1.157381
H	6.060493	1.734962	1.805204
H	5.607472	1.792933	0.097472
O	-2.178409	-0.004010	0.610055
C	-2.761416	-1.051739	0.882935
H	-3.166680	0.676667	2.826111
C	-2.468952	-2.360622	0.385890
O	-3.736437	-1.062898	1.832767
C	-1.828304	-2.508476	-0.892736
C	-0.664374	-2.750239	1.540616
H	-3.125154	-3.164990	0.694202
H	-4.440121	0.877511	1.608859
O	-1.216553	-1.663067	-1.531766
O	-1.886415	-3.799416	-1.324903
C	-1.221394	-4.047387	-2.553533
H	-0.155006	-3.818649	-2.474038
H	-1.367373	-5.106926	-2.763432
H	-1.647986	-3.440247	-3.356599
C	-4.049948	0.209170	2.381526
H	-4.809294	0.026389	3.141886
H	-0.542763	-3.661306	0.960682
C	0.205117	-1.666949	1.436515
C	-1.205203	-2.842222	2.958723
C	0.086302	-0.831846	2.576797
H	0.830059	-1.446009	0.578017
H	-1.782373	-0.832102	3.620286
O	0.656868	0.252764	2.833055
H	-0.659651	-3.634076	3.486136
C	-0.891685	-1.466048	3.557988
H	-2.267315	-3.093981	2.994576
H	-0.450102	-1.502374	4.557817
***S*-TS-FO1**, E = -1439.69276476 (1)			
N	2.425360	0.093444	-1.361321
H	0.246183	5.449905	-0.139907
H	-1.352060	4.967165	-0.745371
H	-2.328301	3.675514	1.901756
H	-2.572737	2.974897	0.283556
H	-1.808739	2.013261	1.549193
H	3.420258	-0.791532	-2.373845
H	4.132318	-2.387779	-2.118356
H	2.562786	-2.002221	-1.395911
H	4.857413	-1.982165	1.542725
H	3.327772	-2.629451	0.901217
H	4.868668	-3.126497	0.190731
H	6.207465	-0.273914	0.176267
H	6.280188	-1.517029	-1.081914
H	5.706501	0.105167	-1.486441
O	-1.298911	-0.531504	1.315843
C	-2.454328	-0.997286	1.230871
H	-0.936852	-2.508085	2.821866
C	-3.453347	-0.726092	0.287856
O	-2.831948	-1.937687	2.160004
C	-3.231667	0.146759	-0.803256
C	-1.650675	-2.382193	-1.655926
H	-4.418787	-1.199499	0.394813
H	-1.717118	-1.226977	3.764724
O	-2.215823	0.787415	-1.096165
O	-4.330232	0.223604	-1.626037
C	-4.183727	1.091253	-2.732049
H	-3.347702	0.787542	-3.370109
H	-5.120949	1.032061	-3.287745
H	-4.005874	2.122242	-2.408896
C	-1.898177	-2.149859	3.205750
H	-2.348352	-2.900029	3.858025
H	-2.210489	-1.885922	-2.443179
C	-0.485726	-1.941722	-1.160142
C	-2.144609	-3.644178	-1.000170
C	-0.063210	-2.817376	-0.060964
H	0.037894	-1.038934	-1.453030
H	-1.540939	-3.840890	1.094640
O	0.942734	-2.717743	0.633784
H	-2.218274	-4.460819	-1.727871
C	-1.104387	-3.917055	0.094677
H	-3.143757	-3.479192	-0.586126
H	-0.618450	-4.893977	0.017315
***S*-PTSC-FO1**, E = -1439.71567562 (0)			
N	-0.078546	0.618007	-2.766349

C	1.405932	-0.397579	-0.612226
N	0.409513	-0.868834	-1.335696
N	1.646913	-0.308609	0.684999
C	0.803337	-0.758991	-2.760709
H	-0.510643	-1.118114	-0.947986
C	1.870642	0.356717	-2.685229
C	3.173739	1.035017	-0.529226
H	0.898713	-0.516490	1.343125
C	2.751308	0.636814	0.918777
C	-0.331907	-0.558824	-3.772862
H	4.248314	0.927429	-0.696711
H	1.320535	-1.693205	-3.030993
C	3.853740	0.018745	1.798178
H	1.421332	1.359481	-2.703755
H	2.624971	0.253457	-3.467133
H	2.852173	2.057258	-0.745104
H	2.345028	1.524753	1.417472
C	4.474435	-1.206790	1.122315
C	4.923666	1.081865	2.065541
C	3.220788	-0.401844	3.130554
C	0.319013	-0.271387	-5.132623
C	-1.149474	-1.853873	-3.865372
C	-1.261052	0.587984	-3.377214
H	5.220967	-1.663912	1.780646
H	3.709198	-1.957495	0.900615
H	4.975703	-0.944989	0.184301
H	5.699710	0.680925	2.725867
H	5.413211	1.409488	1.141943
H	4.490179	1.963968	2.550655
H	3.986466	-0.774466	3.819274
H	2.717846	0.446229	3.612690
H	2.487609	-1.202946	2.983187
H	-0.717394	1.498518	-3.104374
H	-1.934510	0.822417	-4.209879
H	-1.863537	0.287533	-2.518115
H	-0.524296	-2.696185	-4.184098
H	-1.612918	-2.097624	-2.904195
H	-1.952671	-1.733318	-4.601233
H	1.053189	-1.042265	-5.397758
H	-0.446752	-0.255850	-5.914648
H	0.821601	0.702333	-5.141324
O	-2.426041	-1.256271	-0.825663
C	-3.254665	-0.879425	-0.009253
H	-4.275168	-0.360151	-2.385880
C	-3.008151	-0.444824	1.354852

C	0.076474	0.907243	-1.449120
N	1.338587	1.147803	-1.119142
N	-1.036481	0.875234	-0.761269
C	2.193102	0.857009	-2.285583
H	1.601609	1.002965	-0.139695
C	1.212585	0.130451	-3.248282
C	-1.373436	-0.041709	-2.920819
H	-1.085752	0.961499	0.278983
C	-2.123497	0.351839	-1.608170
C	3.478587	0.097897	-1.918817
H	-1.885789	0.318536	-3.815480
H	2.486758	1.813092	-2.742066
C	-3.273054	1.365459	-1.791164
H	1.261137	-0.961697	-3.138083
H	1.386572	0.408961	-4.289504
H	-1.234682	-1.124825	-2.982118
H	-2.525781	-0.549090	-1.129032
C	-2.765380	2.650508	-2.451574
C	-4.365917	0.720971	-2.651627
C	-3.861083	1.696100	-0.414632
C	4.223866	-0.227523	-3.217525
C	4.347399	1.017809	-1.050875
C	3.172715	-1.186116	-1.143254
H	-3.588883	3.363907	-2.562344
H	-1.990466	3.122204	-1.839014
H	-2.349406	2.465081	-3.448311
H	-5.224810	1.395630	-2.729195
H	-4.025335	0.505735	-3.670183
H	-4.717508	-0.216086	-2.204274
H	-4.714276	2.374245	-0.527961
H	-4.212573	0.787404	0.088905
H	-3.124441	2.164854	0.243111
H	2.591336	-1.898672	-1.736164
H	4.113644	-1.668924	-0.852534
H	2.599186	-0.968442	-0.235735
H	4.585225	1.950270	-1.575223
H	3.846145	1.274603	-0.110900
H	5.289747	0.520600	-0.797819
H	4.422436	0.678882	-3.801813
H	5.185664	-0.699497	-2.991932
H	3.652446	-0.922523	-3.843207
O	1.041498	0.128509	1.352099
C	0.941274	-0.012938	2.587482
H	3.023998	-1.636357	1.834596
C	-0.130016	0.313554	3.434402

O	-4.550036	-0.715820	-0.355477
C	-1.805617	-0.937307	1.985313
H	-3.882496	-0.423033	1.996638
H	-4.619740	-2.047953	-1.949328
O	-0.754387	-1.223654	1.422205
O	-1.913335	-0.985668	3.334351
C	-0.722545	-1.318014	4.032376
H	0.030173	-0.530593	3.911054
H	-1.004621	-1.398606	5.081617
H	-0.309451	-2.263555	3.672905
C	-4.850487	-1.005390	-1.716048
H	-5.917434	-0.816703	-1.829977
H	-3.734423	1.672371	0.931959
C	-1.804978	1.698598	-0.068232
C	-1.972501	2.018227	2.278626
C	-0.491836	2.002435	0.341296
H	-2.103021	1.635757	-1.104028
H	0.087176	1.250562	2.302919
O	0.532829	2.195765	-0.345124
H	-2.360138	3.027063	2.460271
C	-0.489715	2.085778	1.882473
H	-2.167870	1.428800	3.178276
H	0.006207	3.006537	2.205989
C	-2.666864	1.476301	1.027929
***S*-TS-FO2**, E = -1439.68829264 (1)			
N	-2.739719	0.770005	-0.086524
C	-1.546725	0.282530	-0.493201
N	-0.598663	1.195219	-0.543231
N	-1.630000	-0.980067	-0.878920
C	-1.125616	2.427376	0.088427
H	0.399462	0.937736	-0.579539
C	-2.654223	2.221262	-0.080097
C	-3.785512	-0.109769	-0.581503
H	-0.800935	-1.517581	-1.133174
C	-3.017596	-1.455467	-0.747000
C	-0.563448	3.727371	-0.509431
H	-4.611954	-0.187407	0.127659
H	-0.889031	2.369396	1.159210
C	-3.214510	-2.462386	0.407189
H	-3.027074	2.636629	-1.029906
H	-3.215503	2.654984	0.749053
H	-4.174552	0.249225	-1.545513
H	-3.311719	-1.944639	-1.683282
C	-2.970318	-1.810325	1.772789

O	1.981558	-0.572028	3.284566
C	-1.327789	0.895129	2.979929
C	0.619931	-3.408395	1.959519
H	-0.006008	0.164265	4.497092
H	3.501361	0.066059	2.016521
O	-1.700405	1.138824	1.816198
O	-2.177375	1.200932	4.002845
C	-3.408637	1.781962	3.614710
H	-3.980942	1.105441	2.972392
H	-3.953161	1.969980	4.540867
H	-3.251726	2.719302	3.073313
C	3.163645	-0.825206	2.555980
H	3.913276	-1.114103	3.294712
H	1.199029	-3.955483	2.698166
C	1.042675	-3.110795	0.724812
C	-0.771419	-2.911058	2.250831
C	-0.002306	-2.342876	0.013465
H	1.992467	-3.374974	0.274380
H	-2.086422	-2.526823	0.512263
O	0.041681	-1.952679	-1.140915
H	-0.773258	-2.259333	3.130256
C	-1.167528	-2.152590	0.974924
H	-1.437429	-3.755603	2.465259
H	-1.292194	-1.080444	1.164292
***S*-PTSC-FO2**, E = -1439.70944560 (0)			
N	-0.078546	0.618007	-2.766349
C	0.076474	0.907243	-1.449120
N	1.338587	1.147803	-1.119142
N	-1.036481	0.875234	-0.761269
C	2.193102	0.857009	-2.285583
H	1.601609	1.002965	-0.139695
C	1.212585	0.130451	-3.248282
C	-1.373436	-0.041709	-2.920819
H	-1.085752	0.961499	0.278983
C	-2.123497	0.351839	-1.608170
C	3.478587	0.097897	-1.918817
H	-1.885789	0.318536	-3.815480
H	2.486758	1.813092	-2.742066
C	-3.273054	1.365459	-1.791164
H	1.261137	-0.961697	-3.138083
H	1.386572	0.408961	-4.289504
H	-1.234682	-1.124825	-2.982118
H	-2.525781	-0.549090	-1.129032
C	-2.765380	2.650508	-2.451574

C	-4.645462	-3.008282	0.328835
C	-2.236702	-3.624775	0.199450
C	-1.415624	4.894011	0.006666
C	0.879145	3.910349	-0.021185
C	-0.577602	3.697905	-2.040222
H	-2.991616	-2.580195	2.552066
H	-2.011390	-1.281663	1.834647
H	-3.755895	-1.084265	2.012376
H	-4.811115	-3.734993	1.130545
H	-5.393939	-2.216874	0.447391
H	-4.831543	-3.513077	-0.626801
H	-2.413286	-4.404654	0.946943
H	-2.357643	-4.076074	-0.794052
H	-1.199094	-3.293677	0.307577
H	-1.584089	3.531058	-2.440620
H	-0.220490	4.656035	-2.433062
H	0.074574	2.905739	-2.420365
H	0.914503	3.961169	1.073479
H	1.515112	3.083142	-0.350942
H	1.294986	4.843502	-0.418466
H	-1.471567	4.887793	1.101623
H	-0.971923	5.846301	-0.301514
H	-2.436903	4.861353	-0.390102
O	0.997289	-1.538390	-1.545381
C	2.083769	-1.938087	-1.149679
H	0.553887	-4.135667	-1.184255
C	3.085650	-1.172729	-0.436633
O	2.429565	-3.243715	-1.234226
C	3.113917	0.261369	-0.637161
H	4.067018	-1.633700	-0.397137
H	1.170741	-3.748755	-2.807568
O	2.158088	1.001362	-0.834886
O	4.360088	0.767767	-0.492916
C	4.438172	2.187664	-0.480621
H	3.895542	2.593234	0.379711
H	5.498516	2.425898	-0.403188
H	4.015520	2.608728	-1.396054
C	1.450838	-4.096413	-1.810141
H	1.909571	-5.083092	-1.865095
C	2.392539	-1.416746	1.389448
H	2.835043	-2.411062	1.450944
C	0.990848	-1.260118	1.478190
C	3.030940	-0.322903	2.251222
C	0.628439	-0.022786	2.055409
H	0.265691	-2.000369	1.160905

C	-4.365917	0.720971	-2.651627
C	-3.861083	1.696100	-0.414632
C	4.223866	-0.227523	-3.217525
C	4.347399	1.017809	-1.050875
C	3.172715	-1.186116	-1.143254
H	-3.588883	3.363907	-2.562344
H	-1.990466	3.122204	-1.839014
H	-2.349406	2.465081	-3.448311
H	-5.224810	1.395630	-2.729195
H	-4.025335	0.505735	-3.670183
H	-4.717508	-0.216086	-2.204274
H	-4.714276	2.374245	-0.527961
H	-4.212573	0.787404	0.088905
H	-3.124441	2.164854	0.243111
H	2.591336	-1.898672	-1.736164
H	4.113644	-1.668924	-0.852534
H	2.599186	-0.968442	-0.235735
H	4.585225	1.950270	-1.575223
H	3.846145	1.274603	-0.110900
H	5.289747	0.520600	-0.797819
H	4.422436	0.678882	-3.801813
H	5.185664	-0.699497	-2.991932
H	3.652446	-0.922523	-3.843207
O	1.041498	0.128509	1.352099
C	0.941274	-0.012938	2.587482
H	3.023998	-1.636357	1.834596
C	-0.130016	0.313554	3.434402
O	1.981558	-0.572028	3.284566
C	-1.327789	0.895129	2.979929
C	0.619931	-3.408395	1.959519
H	-0.006008	0.164265	4.497092
H	3.501361	0.066059	2.016521
O	-1.700405	1.138824	1.816198
O	-2.177375	1.200932	4.002845
C	-3.408637	1.781962	3.614710
H	-3.980942	1.105441	2.972392
H	-3.953161	1.969980	4.540867
H	-3.251726	2.719302	3.073313
C	3.163645	-0.825206	2.555980
H	3.913276	-1.114103	3.294712
H	1.199029	-3.955483	2.698166
C	1.042675	-3.110795	0.724812
C	-0.771419	-2.911058	2.250831
C	-0.002306	-2.342876	0.013465
H	1.992467	-3.374974	0.274380

H	3.273152	-0.768042	3.223057
C	1.922089	0.728112	2.416049
H	3.963268	0.069344	1.835256
O	-0.505469	0.444741	2.267884
H	2.043454	1.578319	1.733024
H	1.852723	1.132618	3.429923
***S*-TS-SO1**, E = -1439.69179380 (1)			
N	1.410729	-0.523509	-2.737325
C	0.528132	-0.523025	-1.703462
N	1.121483	-0.328165	-0.542516
N	-0.711590	-0.809004	-2.080278
C	2.556859	-0.071240	-0.774613
H	0.646044	-0.114801	0.348499
C	2.750748	-0.664281	-2.194319
C	0.789698	-1.198442	-3.862878
H	-1.528346	-0.365095	-1.567372
C	-0.725998	-1.022683	-3.546218
C	3.496877	-0.636120	0.304648
H	1.083580	-0.741889	-4.809513
H	2.708893	1.017154	-0.825033
C	-1.454574	0.099880	-4.322478
H	3.049615	-1.722651	-2.156455
H	3.485349	-0.105612	-2.776920
H	1.069086	-2.261544	-3.880444
H	-1.250127	-1.962264	-3.755781
C	-0.916816	1.479116	-3.930650
C	-1.279210	-0.134154	-5.828989
C	-2.953442	0.018700	-3.998147
C	4.935449	-0.467201	-0.202199
C	3.320445	0.179369	1.590965
C	3.210152	-2.112769	0.594979
H	-1.398881	2.250544	-4.540822
H	-1.136644	1.696351	-2.880059
H	0.165684	1.552384	-4.089795
H	-1.948266	0.531963	-6.382944
H	-0.260573	0.073012	-6.172503
H	-1.533463	-1.164716	-6.106470
H	-3.492437	0.792947	-4.554964
H	-3.362986	-0.953427	-4.298907
H	-3.151970	0.176592	-2.934840
H	3.342493	-2.742394	-0.292471
H	3.912602	-2.472840	1.354897
H	2.194412	-2.243294	0.977295
H	3.522274	1.242112	1.411824

H	-2.086422	-2.526823	0.512263
O	0.041681	-1.952679	-1.140915
H	-0.773258	-2.259333	3.130256
C	-1.167528	-2.152590	0.974924
H	-1.437429	-3.755603	2.465259
H	-1.292194	-1.080444	1.164292
***S*-PTSC-SO1**, E = -1439.70141004 (0)			
N	1.444007	-0.523190	-2.740262
C	0.570793	-0.439871	-1.699421
N	1.160926	-0.186657	-0.557381
N	-0.675306	-0.723066	-2.067865
C	2.606499	-0.003530	-0.798651
H	0.677848	0.098018	0.323089
C	2.782414	-0.670687	-2.187921
C	0.800685	-1.267643	-3.809577
H	-1.488191	-0.381147	-1.528445
C	-0.705770	-1.008011	-3.517320
C	3.508738	-0.549438	0.319973
H	1.109710	-0.901223	-4.790092
H	2.802125	1.074289	-0.898849
C	-1.362907	0.111862	-4.357084
H	3.052689	-1.732899	-2.098677
H	3.529543	-0.160397	-2.798437
H	1.038949	-2.338556	-3.738413
H	-1.278166	-1.928190	-3.680806
C	-0.653174	1.452584	-4.149353
C	-1.316013	-0.289326	-5.837255
C	-2.833399	0.240517	-3.937587
C	4.962554	-0.384122	-0.140695
C	3.273994	0.286414	1.583472
C	3.216429	-2.021721	0.627388
H	-1.130727	2.223089	-4.763821
H	-0.717693	1.772854	-3.103937
H	0.404037	1.404151	-4.432860
H	-1.897218	0.423939	-6.430179
H	-0.298169	-0.292946	-6.240577
H	-1.751012	-1.283729	-5.994047
H	-3.330970	0.987118	-4.565745
H	-3.363026	-0.710852	-4.068923
H	-2.938379	0.559113	-2.897075
H	3.412371	-2.673067	-0.232490
H	3.874642	-2.353974	1.438037
H	2.180445	-2.150622	0.954174
H	3.455319	1.350998	1.391830

H	2.304825	0.083155	1.981239
H	4.021029	-0.176621	2.354289
H	5.147165	0.577481	-0.461016
H	5.641067	-0.766956	0.579063
H	5.136934	-1.087909	-1.083468
O	0.419616	-1.324344	2.070129
C	-0.080242	-0.942274	3.122060
H	-0.442369	-3.556531	3.019458
C	-0.595898	0.366040	3.413007
O	-0.310332	-1.812506	4.141546
C	-0.183547	1.475729	2.600829
H	-0.848561	0.577967	4.444647
H	1.163607	-3.205969	3.689091
O	0.230682	1.441166	1.446147
O	-0.377059	2.668684	3.230123
C	0.017187	3.810793	2.485886
H	-0.582515	3.920280	1.577440
H	-0.139389	4.664467	3.145191
H	1.069172	3.740095	2.196673
C	0.089020	-3.150844	3.884631
H	-0.161024	-3.714545	4.783312
C	-2.511806	-0.058236	2.538435
H	-2.671323	-0.783750	3.332055
C	-2.341810	-0.431952	1.205502
C	-3.228704	1.281954	2.602811
C	-2.600013	0.663427	0.351780
H	-1.988043	-1.396145	0.860987
H	-2.286778	2.626217	1.139895
O	-2.508633	0.723695	-0.896428
H	-4.286656	1.094139	2.822449
C	-3.059875	1.852083	1.187677
H	-2.842078	1.939054	3.385297
H	-3.974485	2.280595	0.768188
***S*-TS-SO2**, E = -1439.69278728 (1)			
N	2.189487	0.617682	-2.031399
C	1.424768	0.268833	-0.952521
N	1.860592	0.789068	0.177293
N	0.472350	-0.586033	-1.259632
C	3.107447	1.528637	-0.089949
H	1.603857	0.387747	1.130182
C	3.482126	1.057954	-1.522356
C	1.960778	-0.383178	-3.065240
H	-0.330199	-0.805790	-0.644934
C	0.563433	-0.956744	-2.684345

H	2.251938	0.171319	1.953380
H	3.958855	-0.037023	2.374695
H	5.186320	0.659639	-0.392898
H	5.642856	-0.686890	0.661503
H	5.188427	-1.005842	-1.015844
O	0.339864	-1.352411	1.937217
C	0.158716	-0.921952	3.081775
H	-0.521915	-3.482120	3.026552
C	0.023974	0.420522	3.503640
O	0.040592	-1.808154	4.125114
C	-0.040035	1.466696	2.571655
H	-0.074876	0.641496	4.556591
H	1.212921	-3.346497	3.361649
O	0.043030	1.423955	1.329738
O	-0.255404	2.690841	3.167409
C	-0.068875	3.810417	2.323246
H	-0.761745	3.807539	1.477011
H	-0.244629	4.688168	2.946976
H	0.950034	3.835011	1.923112
C	0.214262	-3.166957	3.772455
H	0.081900	-3.735660	4.694010
C	-2.784198	-0.239028	2.669504
H	-2.661121	-0.909984	3.514440
C	-2.504470	-0.553666	1.394943
C	-3.289799	1.170314	2.840782
C	-2.737854	0.612917	0.546522
H	-2.090149	-1.484891	1.030474
H	-2.522769	2.576294	1.334597
O	-2.585083	0.690031	-0.668511
H	-4.303797	1.170581	3.257611
C	-3.235734	1.752507	1.420755
H	-2.649135	1.720159	3.537349
H	-4.201444	2.107189	1.048866
***S*-PTSC-SO2**, E = -1439.70968934 (0)			
N	2.201664	0.119074	-2.124331
C	1.257887	0.073477	-1.138380
N	1.572948	0.850426	-0.113255
N	0.316073	-0.804791	-1.379275
C	2.824960	1.564449	-0.419935
H	0.880779	1.111516	0.595577
C	3.415723	0.665448	-1.535767
C	2.036616	-1.077795	-2.940777
H	-0.557812	-0.920605	-0.820307
C	0.537234	-1.415810	-2.696165

C	4.179989	1.312493	0.992719
H	1.974539	0.064351	-4.060798
H	2.876172	2.602686	-0.126203
C	-0.614195	-0.447905	-3.542845
H	4.196327	0.220427	-1.505917
H	3.899818	1.867024	-2.124687
H	2.735363	-1.162395	-3.017248
H	0.578471	-2.050802	-2.755073
C	-0.721741	1.078594	-3.486877
C	-0.399466	-0.916486	-4.988105
C	-1.908053	-1.078002	-3.012807
C	5.460554	2.018873	0.532466
C	3.685592	1.948368	2.299094
C	4.452222	-0.176073	1.238254
H	-1.540484	1.411981	-4.134648
H	-0.938230	1.413520	-2.467940
H	0.196742	1.564502	-3.837004
H	-1.280112	-0.668640	-5.589268
H	0.463279	-0.437010	-5.463235
H	-0.258418	-2.003024	-5.038090
H	-2.750989	-0.780776	-3.646310
H	-1.846449	-2.173114	-3.023467
H	-2.116065	-0.751490	-1.991454
H	4.802089	-0.688772	0.335138
H	5.238242	-0.278471	1.994064
H	3.559399	-0.686490	1.611933
H	3.461772	3.012394	2.159068
H	2.789249	1.440906	2.670368
H	4.459530	1.865081	3.069568
H	5.277102	3.079921	0.324419
H	6.223488	1.958669	1.315109
H	5.878240	1.559152	-0.371312
O	-1.855627	0.921620	-0.390059
C	-2.867868	0.762575	0.278318
H	-2.509672	3.375095	0.087411
C	-3.202044	-0.378277	1.090118
O	-3.778742	1.763443	0.422113
C	-2.559012	-1.634759	0.831899
H	-4.209776	-0.423974	1.484766
H	-3.372347	2.779152	-1.344378
O	-1.484575	-1.834389	0.268318
O	-3.247262	-2.677039	1.371658
C	-2.653435	-3.953520	1.188781
H	-1.675851	-4.007795	1.676773
H	-3.340763	-4.667903	1.641633

C	3.731468	1.802964	0.801046
H	2.260934	-0.878199	-3.990739
H	2.580637	2.541853	-0.863420
C	-0.450855	-0.879378	-3.758961
H	4.044716	-0.136518	-1.117838
H	3.999064	1.237675	-2.259304
H	2.690617	-1.885651	-2.581790
H	0.393037	-2.498250	-2.609281
C	-0.248003	0.618607	-4.010694
C	-0.246008	-1.668956	-5.056089
C	-1.880576	-1.103254	-3.248394
C	5.111725	2.236243	0.290586
C	3.133749	2.936142	1.644889
C	3.848316	0.541401	1.660643
H	-0.997220	0.972494	-4.726926
H	-0.377162	1.190101	-3.085025
H	0.741505	0.841837	-4.425284
H	-0.959446	-1.332931	-5.815337
H	0.760065	-1.535869	-5.470285
H	-0.409889	-2.740636	-4.894288
H	-2.597018	-0.839078	-4.033845
H	-2.047362	-2.148060	-2.963794
H	-2.091217	-0.487569	-2.368269
H	4.208211	-0.319565	1.085696
H	4.558663	0.716526	2.475602
H	2.877893	0.287718	2.097480
H	3.068138	3.862800	1.062747
H	2.138307	2.678162	2.016389
H	3.773163	3.130503	2.512802
H	5.033130	3.099403	-0.381832
H	5.746394	2.527678	1.133349
H	5.623938	1.428621	-0.244887
O	-1.158175	0.888093	0.118125
C	-2.233845	0.871126	0.741013
H	-0.867597	3.003564	1.637134
C	-3.100705	-0.216929	0.958091
O	-2.674297	2.021684	1.337443
C	-2.806365	-1.503193	0.481462
H	-4.006269	-0.062442	1.526369
H	-1.680749	3.359818	0.094547
O	-1.821103	-1.900911	-0.172098
O	-3.751197	-2.428361	0.852312
C	-3.510033	-3.748442	0.403728
H	-2.567106	-4.137238	0.800728
H	-4.346328	-4.345387	0.770634

H	-2.521697	-4.171186	0.125756
C	-3.456780	2.961029	-0.269309
H	-4.274196	3.652793	-0.065973
C	-2.095220	0.322392	2.782635
H	-2.868483	1.072621	2.927065
C	-0.799694	0.655052	2.384498
C	-2.041934	-0.876641	3.717028
C	0.095816	-0.387317	2.700507
H	-0.519507	1.543696	1.832714
H	-0.695387	-2.367769	2.820804
O	1.320907	-0.467223	2.435579
H	-2.119824	-0.507844	4.746833
C	-0.651825	-1.478365	3.458473
H	-2.860318	-1.582420	3.557394
H	-0.110551	-1.753798	4.368063
guanidine-malonate neutral complex, E = -1170.46974877 (0)			
N	0.112273	-1.916442	-0.833297
C	0.575816	-1.055754	0.162058
N	-0.072010	-1.320869	1.326713
N	1.540460	-0.263755	-0.133606
C	-1.029772	-2.412374	1.157969
H	-0.152405	-0.596986	2.032317
C	-0.528040	-3.041695	-0.175518
C	1.208603	-1.987465	-1.789608
C	1.910284	-0.619248	-1.516998
C	-2.512044	-1.967767	1.180043
H	1.869522	-2.841021	-1.563817
H	-0.901193	-3.139238	1.971423
C	3.437636	-0.608931	-1.722006
H	-1.341361	-3.454119	-0.778013
H	0.196296	-3.845602	0.030448
H	0.851286	-2.085324	-2.818065
H	1.495852	0.133778	-2.207189
C	4.142947	-1.509969	-0.704197
C	3.751941	-1.077959	-3.146286
C	3.928862	0.830953	-1.538277
C	-3.409581	-3.201443	1.034309
C	-2.799201	-1.315898	2.539731
C	-2.801811	-0.957803	0.069035
H	5.229295	-1.437012	-0.828545
H	3.885400	-1.205535	0.314226
H	3.870433	-2.564594	-0.825583
H	4.827736	-1.010559	-3.342717

H	-3.466873	-3.795528	-0.688518
C	-1.840012	3.152481	1.156842
H	-2.365157	3.986479	1.625510
C	-2.031268	-0.469235	4.254889
H	-2.896641	-0.560835	4.904719
C	-1.399169	0.678222	3.983381
C	-1.443190	-1.661691	3.546447
C	-0.289229	0.414300	3.050706
H	-1.639513	1.670227	4.344643
H	-0.464569	-1.182427	1.635372
O	0.507291	1.234880	2.621713
H	-1.094720	-2.406832	4.271791
C	-0.297370	-1.068090	2.712889
H	-2.207784	-2.144364	2.927508
H	0.681122	-1.498093	2.949938
gaunidinium-malonate ion-pair complex, E = -1170.45743790 (0)			
N	-0.284995	-0.041098	-2.510107
C	-0.092241	-0.215567	-1.169568
N	0.037813	0.911537	-0.514798
N	0.003262	-1.492016	-0.837268
C	-0.060845	2.028022	-1.478120
H	0.190232	0.985288	0.526037
C	0.188590	1.301102	-2.826694
C	0.038997	-1.303324	-3.163494
H	-0.081384	-1.749979	0.159983
C	-0.226468	-2.327894	-2.022593
C	0.874390	3.212565	-1.173117
H	-0.591433	-1.474381	-4.038812
H	-1.096204	2.400023	-1.476643
C	-1.625433	-2.986962	-2.027462
H	1.258566	1.285011	-3.086786
H	-0.374474	1.749487	-3.646825
H	1.093849	-1.323434	-3.472897
H	0.524748	-3.125304	-2.049250
C	-2.742872	-1.943121	-2.119224
C	-1.707333	-3.954168	-3.212827
C	-1.783427	-3.772647	-0.719346
C	0.904374	4.122865	-2.407544
C	0.302500	3.998847	0.013981
C	2.287437	2.731487	-0.828874
H	-3.716158	-2.442621	-2.068208
H	-2.689893	-1.231392	-1.288688
H	-2.704697	-1.379866	-3.057775

H	3.452312	-2.121147	-3.304436
H	3.235089	-0.457148	-3.887954
H	5.014610	0.885524	-1.679972
H	3.448967	1.505434	-2.255106
H	3.687797	1.189205	-0.533002
H	-2.627463	-1.385095	-0.925170
H	-3.847223	-0.630924	0.120237
H	-2.159357	-0.077581	0.180492
H	-2.567195	-2.001330	3.363946
H	-2.219723	-0.397376	2.679915
H	-3.860853	-1.054007	2.613772
H	-3.178253	-3.950374	1.801423
H	-4.460618	-2.917481	1.152138
H	-3.306517	-3.676433	0.053280
C	0.753417	2.574480	0.891926
H	1.566385	1.881808	1.120625
H	1.094476	3.609104	0.971210
C	0.383491	2.305496	-0.555454
C	-0.396922	2.315709	1.829344
O	1.090924	2.576074	-1.489151
O	-0.535084	1.324475	2.512233
O	-0.829086	1.736387	-0.658578
O	-1.281388	3.315313	1.814000
C	-1.214636	1.302274	-1.964211
H	-2.303464	1.253524	-1.957709
H	-0.858481	2.005774	-2.717747
C	-2.464372	3.087112	2.579676
H	-3.068123	3.985746	2.466544
H	-2.995294	2.213354	2.192515
H	-2.213586	2.918103	3.628881
H	-0.799260	0.306068	-2.143588
guanidinium ion, E = -674.800380017 (0)			
N	-0.768375	-0.011050	0.156162
C	0.545844	-0.255576	0.096196
N	1.055833	-0.004979	-1.103001
N	1.014773	-0.775456	1.220326
C	-0.004659	0.566318	-1.977033
H	2.043365	0.098459	-1.291795
C	-1.288867	0.172979	-1.197063
C	-1.330341	-0.691312	1.321054
H	1.991631	-0.922256	1.429824
C	-0.076000	-0.869406	2.227983
C	0.079410	0.079606	-3.433107
H	-2.102088	-0.083645	1.795394

H	-2.673963	-4.467875	-3.211381
H	-1.612096	-3.437219	-4.174159
H	-0.922319	-4.717166	-3.156518
H	-2.728051	-4.326271	-0.722708
H	-0.970006	-4.497567	-0.589750
H	-1.790387	-3.100894	0.146010
H	2.723911	2.122262	-1.629330
H	2.941530	3.597888	-0.681818
H	2.278765	2.145643	0.095487
H	-0.692000	4.394120	-0.224888
H	0.236197	3.370739	0.906964
H	0.954710	4.849224	0.243374
H	-0.107526	4.425285	-2.704223
H	1.470880	5.032268	-2.183392
H	1.384993	3.637744	-3.265096
H	1.145158	3.701684	3.292807
C	2.031546	3.108686	3.540981
O	1.676777	1.815322	3.987929
H	2.566722	3.573112	4.370498
H	2.675610	3.065614	2.656773
C	0.691777	-0.226209	3.598129
C	1.020389	1.034865	3.079171
O	0.804945	1.514276	1.946871
C	0.000391	-1.201000	2.867061
H	0.974600	-0.449848	4.615958
O	-0.443970	-1.143264	1.701587
O	-0.191179	-2.346922	3.593225
C	-0.902351	-3.377788	2.945435
H	-0.356402	-3.758845	2.073945
H	-1.889276	-3.037950	2.615565
H	-1.011353	-4.175896	3.681341
guanidine, E = -674.391281807 (0)			
N	-0.813170	0.061490	0.177983
C	0.533816	-0.288581	0.167668
N	1.029599	-0.116741	-1.106864
N	1.048754	-0.763790	1.233684
C	-0.011208	0.490357	-1.943516
H	1.990690	0.182011	-1.198963
C	-1.291710	0.058954	-1.188825
C	-1.366248	-0.644917	1.321039
C	-0.076778	-0.836717	2.190176
C	0.075587	0.077140	-3.423976
H	-2.149197	-0.064306	1.816281
H	0.049737	1.590991	-1.897957

H	0.099049	1.659487	-1.966016
C	0.071696	0.159561	3.369041
H	-1.724123	-0.763176	-1.568278
H	-2.042627	0.960435	-1.229817
H	-1.761229	-1.656492	1.028490
H	-0.057158	-1.876436	2.656028
C	-0.021588	1.595592	2.844222
C	-1.038207	-0.106520	4.393702
C	1.431345	-0.054103	4.047668
C	-1.101911	0.699663	-4.189951
C	1.395086	0.588358	-4.037781
C	0.032816	-1.447941	-3.534740
H	0.117460	2.299768	3.669641
H	0.756416	1.805223	2.101115
H	-0.996294	1.808259	2.392241
H	-0.936273	0.584434	5.235312
H	-2.038329	0.040061	3.973064
H	-0.978262	-1.126048	4.789977
H	1.512274	0.587041	4.929990
H	1.557632	-1.091207	4.379476
H	2.266098	0.208865	3.387689
H	-0.920436	-1.863349	-3.192171
H	0.153239	-1.745294	-4.580625
H	0.838863	-1.915853	-2.960316
H	1.489456	1.675676	-3.940888
H	2.269332	0.117753	-3.571334
H	1.436796	0.343717	-5.102867
H	-1.092278	1.793308	-4.121169
H	-1.048165	0.431762	-5.248942
H	-2.063710	0.337592	-3.809215
dimethyl malonate, E = -496.045317978 (0)			
H	3.728209	0.881774	-0.374596
C	3.569624	-0.000724	0.257031
O	2.297949	-0.000601	0.849170
H	4.294477	-0.001025	1.077935
H	3.727858	-0.883043	-0.374937
C	0.000000	0.000000	0.581716
C	1.241073	-0.000309	-0.088760
O	1.528426	-0.000287	-1.279941
C	-1.241073	0.000309	-0.088760
H	0.000000	0.000000	1.662356
O	-1.528426	0.000287	-1.279941
O	-2.297949	0.000601	0.849170
C	-3.569624	0.000724	0.257031

C	0.077262	0.174971	3.351825
H	-1.624094	-0.943734	-1.504231
H	-2.110416	0.766653	-1.341540
H	-1.786950	-1.616461	1.017487
H	-0.081607	-1.837654	2.641641
C	0.026330	1.617006	2.839326
C	-1.035379	-0.052935	4.380870
C	1.431894	-0.074236	4.024285
C	-1.105480	0.708178	-4.169090
C	1.387630	0.625209	-4.000448
C	0.055328	-1.444316	-3.599262
H	0.179911	2.317078	3.668483
H	0.813507	1.788885	2.098469
H	-0.937616	1.851973	2.374578
H	-0.894498	0.607972	5.243344
H	-2.029549	0.153072	3.969178
H	-1.026308	-1.086808	4.745979
H	1.569134	0.609508	4.869789
H	1.495659	-1.100881	4.403938
H	2.246812	0.071747	3.311436
H	-0.907945	-1.878147	-3.312336
H	0.228200	-1.698561	-4.650695
H	0.835426	-1.915110	-2.994392
H	1.464170	1.709143	-3.854236
H	2.256986	0.149483	-3.532465
H	1.445918	0.425349	-5.075519
H	-1.119972	1.797107	-4.041052
H	-1.036706	0.496395	-5.241246
H	-2.061657	0.309302	-3.812187

dimethyl malonate ion, E = -495.475763273 (0)			
H	3.729569	0.887654	-0.442578
C	3.608902	-0.000759	0.181467
O	2.324909	-0.000332	0.804024
H	4.333165	-0.001254	0.994596
H	3.728799	-0.889000	-0.442967
C	0.000000	0.000000	0.744445
C	1.285801	0.000184	-0.055127
O	1.411445	-0.000122	-1.247868
C	-1.285801	-0.000184	-0.055127
H	0.000067	-0.868847	1.410894
O	-1.411445	0.000122	-1.247868
O	-2.324909	0.000332	0.804024
C	-3.608902	0.000759	0.181467
H	-3.729569	-0.887654	-0.442578

H	-3.728209	-0.881774	-0.374596
H	-3.727858	0.883043	-0.374937
H	-4.294477	0.001025	1.077935
cyclopentenone-guanidinium hydrogen-bond complex, E = -944.062459123 (0)			
H	0.177939	-1.573458	6.282675
C	0.262310	-0.910983	5.426568
C	0.195072	-1.304815	4.146331
C	0.470451	0.570810	5.586274
H	0.051689	-2.312915	3.776962
C	0.348494	-0.138103	3.271151
O	0.332249	-0.135498	2.045084
C	0.534067	1.093078	4.143036
H	1.492037	1.563019	3.899853
H	1.387670	0.771598	6.149639
H	-0.350100	1.014070	6.160163
H	-0.250731	1.820003	3.913048
N	-0.240713	-0.159381	-2.251064
C	0.111420	-0.170375	-0.955197
N	0.475706	1.021171	-0.509994
N	0.098029	-1.382295	-0.429465
C	0.300280	2.016060	-1.592571
H	0.532169	1.204354	0.487854
C	0.206494	1.098269	-2.845506
C	-0.222420	-1.532257	-2.749798
H	0.167660	-1.515050	0.575509
C	-0.390532	-2.353393	-1.433783
C	1.403940	3.086095	-1.617837
H	-1.035756	-1.706137	-3.456250
H	-0.666924	2.518319	-1.451100
C	-1.821640	-2.849642	-1.132853
H	1.181303	0.967757	-3.333489
H	-0.512343	1.475888	-3.573616
H	0.733475	-1.751977	-3.241185
H	0.282977	-3.216355	-1.441720
C	-2.837060	-1.703999	-1.188000
C	-2.183400	-3.930043	-2.158881
C	-1.831619	-3.472526	0.269860
C	1.150182	3.990710	-2.829642
C	1.296767	3.916257	-0.331612
C	2.802627	2.467517	-1.703085
H	-3.834288	-2.083849	-0.946144
H	-2.597383	-0.920363	-0.460461
H	-2.890534	-1.246887	-2.181840

H	-3.728799	0.889000	-0.442967
H	-4.333165	0.001254	0.994596
H	-0.000067	0.868847	1.410894
cyclopentenone-guanidinium Lewis-acid complex, E = -944.052345005 (0)			
N	2.369991	0.195462	-1.304568
C	1.609117	-0.775544	-0.795872
N	0.855967	-1.372562	-1.711006
N	1.749214	-0.911345	0.514931
C	1.168069	-0.797632	-3.044310
H	0.435129	-2.282266	-1.586119
C	1.889178	0.517279	-2.645949
C	2.805178	1.085486	-0.232598
H	1.090639	-1.425147	1.081524
C	2.536807	0.232930	1.049050
C	-0.067322	-0.648676	-3.946084
H	3.861353	1.336054	-0.346277
H	1.886568	-1.462046	-3.543933
C	3.791802	-0.234891	1.808521
H	1.193837	1.363005	-2.587726
H	2.712346	0.750384	-3.322300
H	2.205070	1.999476	-0.240473
H	1.890047	0.795339	1.731587
C	4.730666	-1.019801	0.888022
C	4.500869	1.002125	2.372247
C	3.349583	-1.131050	2.971937
C	0.387063	0.031999	-5.243202
C	-0.605251	-2.048850	-4.268511
C	-1.169177	0.176951	-3.274831
H	5.601818	-1.364458	1.453271
H	4.231921	-1.902143	0.473759
H	5.101917	-0.411119	0.056541
H	5.368972	0.696477	2.963454
H	4.863061	1.668012	1.581908
H	3.836770	1.577453	3.027305
H	4.213919	-1.415353	3.578984
H	2.639389	-0.613140	3.627682
H	2.886644	-2.057201	2.613665
H	-0.852796	1.206302	-3.080393
H	-2.044515	0.214449	-3.931143
H	-1.471799	-0.263994	-2.319344
H	0.166941	-2.681923	-4.719559
H	-0.992175	-2.553927	-3.375075
H	-1.435515	-1.979436	-4.977344

H	-3.174354	-4.336766	-1.937179
H	-2.214438	-3.537497	-3.180642
H	-1.468188	-4.759677	-2.132329
H	-2.807743	-3.922699	0.472856
H	-1.074941	-4.260248	0.363627
H	-1.655286	-2.720554	1.048185
H	2.962856	1.921839	-2.638522
H	3.554483	3.261458	-1.662113
H	2.990147	1.782789	-0.869921
H	0.299286	4.355878	-0.221033
H	1.512541	3.314091	0.559334
H	2.023270	4.733905	-0.349785
H	0.148211	4.433526	-2.796470
H	1.876559	4.808567	-2.845445
H	1.253526	3.442229	-3.772777
parent guanidinium C_S, E = -360.430012568 (0)			
C	0.091654	-0.658571	0.000000
N	0.294439	-1.126721	-1.224069
C	-0.104453	-0.089022	-2.200781
C	-0.080207	1.188450	-1.329546
N	-0.317197	0.619285	0.000000
H	0.604821	-0.049292	-3.026989
H	-1.107505	-0.298765	-2.582331
H	-0.862443	1.895050	-1.606398
H	0.896930	1.685737	-1.362449
C	-0.080207	1.188450	1.329546
H	0.896930	1.685737	1.362449
H	-0.862443	1.895050	1.606398
N	0.294439	-1.126721	1.224069
C	-0.104453	-0.089022	2.200781
H	0.604821	-0.049292	3.026989
H	-1.107505	-0.298765	2.582331
H	0.413465	-2.103476	1.455629
H	0.413465	-2.103476	-1.455629
parent guanidinium C_2, E = -360.427109841 (1)			
C	0.000000	0.000000	-0.787311
N	-1.222710	-0.087316	-1.298077
C	-2.217963	0.019237	-0.207871
C	-1.350423	-0.102857	1.082077
N	0.000000	0.000000	0.537859
H	-2.728533	0.983454	-0.263006
H	-2.950837	-0.783622	-0.287964

H	1.190122	-0.531318	-5.731751
H	-0.450022	0.096115	-5.944525
H	0.742479	1.052430	-5.060850
C	-2.576301	2.767927	1.622660
H	-3.085470	2.998699	2.553564
C	-1.494226	1.985909	1.514266
C	-3.040721	3.328910	0.304165
C	-1.075286	1.912746	0.103460
H	-0.970511	1.479250	2.316159
H	-2.571018	2.052103	-1.427256
O	-0.105415	1.317693	-0.339562
H	-3.000412	4.423465	0.322654
C	-2.070335	2.722083	-0.720488
H	-4.084776	3.060565	0.113446
H	-1.534552	3.470493	-1.311370
proton transfer TS, E = -1170.44286932 (1)			
N	0.158808	-2.202791	-0.227600
C	0.012771	-0.860549	-0.433380
N	1.080166	-0.334827	-1.023564
N	-1.148321	-0.368871	-0.083767
C	2.105110	-1.367380	-1.213620
H	1.215030	0.684941	-1.072899
C	1.256592	-2.666842	-1.062731
C	-1.179791	-2.746002	-0.040437
C	-1.927075	-1.485336	0.487541
C	3.283980	-1.226019	-0.223409
H	-1.596989	-3.102583	-0.994556
H	2.505080	-1.294037	-2.231621
C	-3.424561	-1.396294	0.152282
H	1.812313	-3.476091	-0.583459
H	0.890904	-3.015734	-2.039245
H	-1.187891	-3.566281	0.680177
H	-1.827694	-1.461011	1.583760
C	-3.666271	-1.326377	-1.358438
C	-4.125489	-2.624423	0.742757
C	-3.978429	-0.123394	0.804182
C	4.371197	-2.236216	-0.602779
C	3.846941	0.195835	-0.355453
C	2.823564	-1.458903	1.218512
H	-4.733248	-1.176493	-1.554116
H	-3.115244	-0.491246	-1.800606
H	-3.367499	-2.247129	-1.870941
H	-5.205939	-2.560983	0.577804

H	-1.489052	-1.065189	1.582529
H	-1.555104	0.702521	1.790512
C	1.350423	0.102857	1.082077
H	1.489052	1.065189	1.582529
H	1.555104	-0.702521	1.790512
N	1.222710	0.087316	-1.298077
C	2.217963	-0.019237	-0.207871
H	2.950837	0.783622	-0.287964
H	2.728533	-0.983454	-0.263006
H	1.447231	-0.047659	-2.273475
H	-1.447231	0.047659	-2.273475
parent guanidinium C_{2v}, E =-360.427009497 (2)			
C	0.000000	0.000000	-0.014008
N	0.000000	0.000000	1.312227
N	1.224307	0.000000	-0.522404
N	-1.224307	0.000000	-0.522404
C	1.350760	0.000000	1.862010
C	-1.350760	0.000000	1.862010
C	2.224037	0.000000	0.566575
C	-2.224037	0.000000	0.566575
H	1.452610	0.000000	-1.505515
H	-1.452610	0.000000	-1.505515
H	1.523572	0.890173	2.471985
H	1.523572	-0.890173	2.471985
H	-1.523572	-0.890173	2.471985
H	-1.523572	0.890173	2.471985
H	2.851581	-0.889965	0.498761
H	2.851581	0.889965	0.498761
H	-2.851581	0.889965	0.498761
H	-2.851581	-0.889965	0.498761
R-product, E = -764.713542866 (0)			
O	0.768465	1.448034	1.630520
C	0.850281	0.470407	2.330170
H	3.137147	-0.833261	1.113126
C	-0.281410	-0.351888	2.871022
O	2.013382	-0.126088	2.671852
C	-1.499574	0.397642	3.286484
C	-0.686173	-1.413869	1.670444
H	0.081906	-0.949469	3.708283
H	2.989694	0.967304	1.202207
O	-1.908966	1.462070	2.892421
O	-2.221375	-0.357368	4.167555
C	-3.477623	0.196065	4.516944
H	-3.773740	-3.552969	0.277328
H	-3.954209	-2.696505	1.823125
H	-5.060430	-0.057163	0.648162
H	-3.787813	-0.114539	1.883268
H	-3.519196	0.772363	0.373288
H	2.488450	-2.489274	1.379906
H	3.651928	-1.264924	1.909070
H	2.000623	-0.785409	1.476700
H	4.150838	0.406472	-1.388070
H	3.112598	0.951259	-0.053138
H	4.731349	0.308503	0.281319
H	4.726800	-2.070111	-1.626305
H	5.229137	-2.135219	0.069651
H	4.016537	-3.270354	-0.528810
C	-0.915124	2.259894	0.521819
H	-1.184957	0.835635	0.198088
H	-1.854751	2.752033	0.753496
C	-0.108278	2.080113	1.727392
C	-0.316107	2.715835	-0.718041
O	-0.520375	2.190925	2.863285
O	0.774165	2.409215	-1.197785
O	1.177773	1.684444	1.484973
O	-1.160204	3.510464	-1.418178
C	1.981149	1.600623	2.657036
H	2.984340	1.341619	2.315622
H	1.992984	2.558065	3.183255
C	-0.700532	3.894564	-2.706990
H	-1.503559	4.488295	-3.143225
H	0.214142	4.487582	-2.632820
H	-0.495500	3.016443	-3.324820
H	1.602301	0.835094	3.339306
S-product, E = -764.713542909 (0)			
O	-2.942186	-1.864986	-0.533277
C	-3.311855	-1.016084	0.240360
H	-4.741499	-0.692214	-1.930343
C	-2.559668	-0.362331	1.347295
O	-4.541679	-0.432966	0.118456
C	-1.439131	-1.158181	1.947795
H	-3.253505	-0.072928	2.137842
H	-5.498915	-1.946707	-0.933061
O	-0.673522	-1.886396	1.368616
O	-1.350296	-0.848531	3.259905
C	-0.050439	-0.920309	3.848665
H	0.377466	0.089340	3.832384

H	-4.096262	0.348821	3.628104
H	-3.948215	-0.523284	5.188593
H	-3.354909	1.160572	5.018581
C	3.109506	0.043622	1.771187
H	4.014813	0.095325	2.381284
H	-1.659227	-1.058512	1.303559
C	0.358746	-1.577413	0.629289
C	-0.768361	-2.821155	2.295224
C	1.248050	-2.598018	0.948222
H	0.550868	-0.828824	-0.132776
H	1.270210	-3.056746	3.064755
O	2.354090	-2.928373	0.452894
H	-1.429031	-3.434983	1.671981
C	0.670357	-3.336392	2.185801
H	-1.176502	-2.811931	3.314242
H	0.747246	-4.423531	2.073427
Cyclopentenone, E = -269.225418546 (0)			
H	1.678640	2.013062	0.059776
C	0.941319	1.216081	0.033520
C	1.223972	-0.089387	0.043586
C	-0.539560	1.508345	-0.019213
H	2.203325	-0.550722	0.078460
C	-0.032422	-0.879735	-0.001154
O	-0.135557	-2.083625	-0.004827
C	-1.194598	0.118680	-0.042539
H	-1.785984	-0.062664	-0.943995
H	-0.783127	2.104127	-0.905814
H	-0.845573	2.104127	0.847816
H	-1.848606	-0.062664	0.814568

H	-0.187803	-1.263298	4.877247
H	0.573059	-1.628042	3.299437
C	-5.288341	-0.875258	-1.001065
H	-6.218096	-0.304790	-0.988427
H	-1.906372	0.932434	-0.311496
C	-0.535791	1.322930	1.351441
C	-2.725798	2.213401	1.291882
C	-0.623699	2.081210	2.513972
H	0.359699	0.790531	1.047040
H	-2.566451	1.938127	3.460361
O	0.229708	2.373478	3.388113
H	-2.576883	3.061023	0.612863
C	-2.103516	2.528959	2.655862
H	-3.799306	1.985521	1.318532
H	-2.175202	3.583184	2.945492
C	-1.875516	1.032274	0.782520

[A] Number of imaginary frequencies in parenthesis.