10.1071/CH19361_AC

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Supplementary Material

What are the potential sites of DNA attack by N-acetyl-p-benzoquinone imine (NAPQI)?

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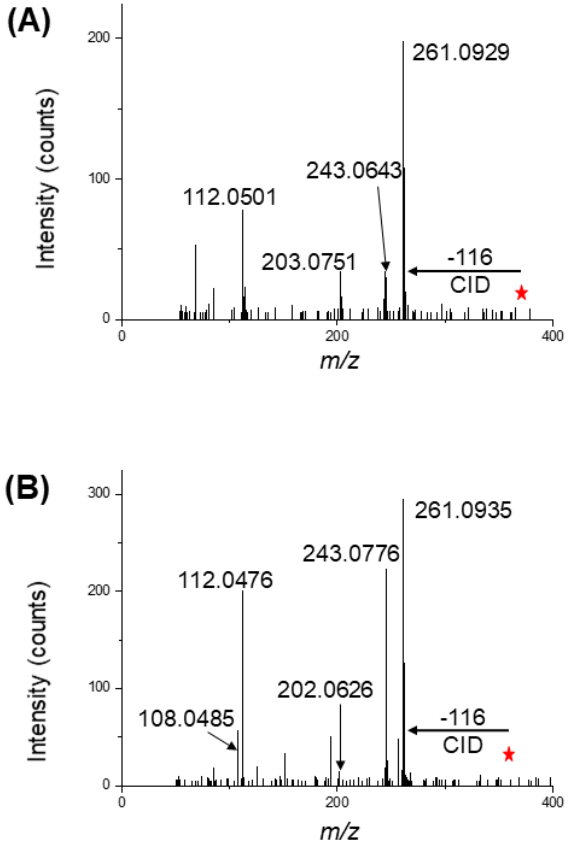


Figure S1. LC-MS/MS data of isomeric dC-NAPQI adducts: (A) shorter retention time isomer (16.6 mins); (B) longer retention time isomer (16.9 mins). The collision gas was helium and a collision energy of 25V was used. A * represents the mass selected precursor ion.

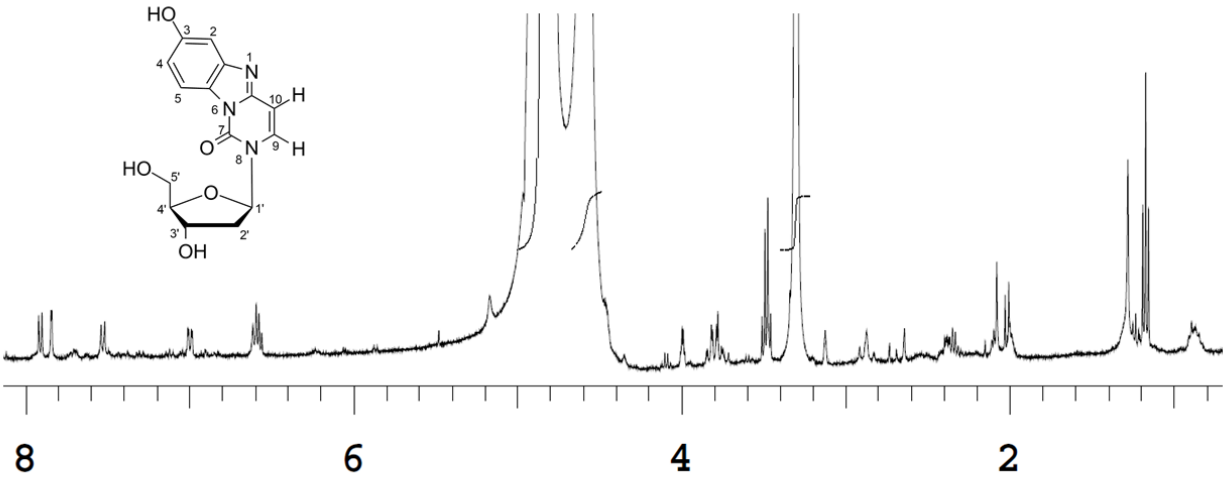


Figure S2. ^{1}H NMR (400 MHz, Methanol-d_4) of dC-BQ adduct: δ 7.91 (d, J = 7.9 Hz, 1H, H-5), 7.84 (d, J = 2.4 Hz, 1H, OH-3), 7.53 (d, J = 8.8 Hz, 1H, H-9), 7.00 (dd, J = 8.7, 2.4 Hz, 1H, H-2), 6.59 (q, J = 7.4, 6.7 Hz, 2H, H-10 and H-4), 3.79 (td, J = 12.3, 3.6 Hz, 2H, H-1'), 3.49 (q, J = 7.0 Hz, 3H, H-5' and OH-5'), 2.90 (d, J = 16.5 Hz, 1H, H-3'), 2.34 (q, J = 6.8 Hz, 1H, H-2'). Inset shows structure of dC-BQ adduct together with numbering system for the protons.

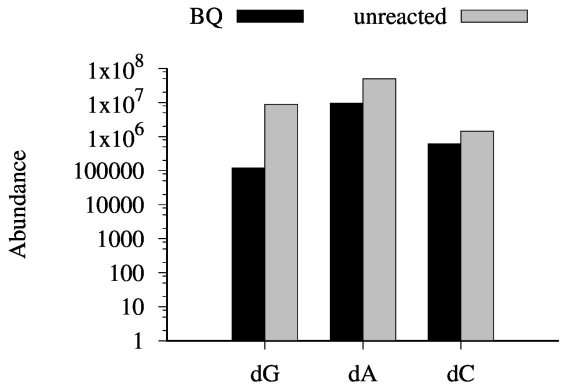
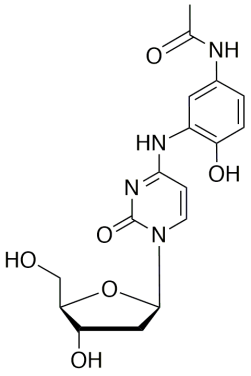


Figure S3. Absolute abundances (integrated EIC peak area) of unreacted nucleoside and nucleoside-BQ adducts formed via reaction of BQ with nucleosides at pH 4.5.

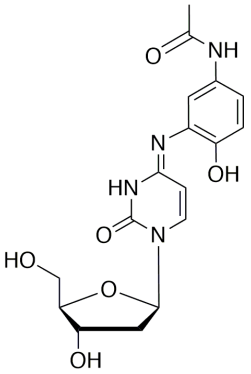
Procedure for searching for conformations and tautomers in the reactions of NAPQI and the nucleosides.

For each of the regioisomeric Michael adducts **4** and **5** formed between NAPQI and the nucleobases there are a number of tautomeric structures for both the nucleobase moiety (which

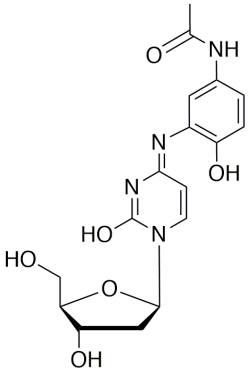
we designate as **a1**, **a2** and **a3**) as well as the modified APAP ring (which we designate as **b1** and **b2**). The naming of these tautomeric adducts is given in Schemes S1 – S5. Full conformational searches were done for both dC and dG adducts. In the case of the dA and dT adducts, we only calculated the amide forms of the modified APAP ring since the results for the dC and dG showed that these are always more stable.



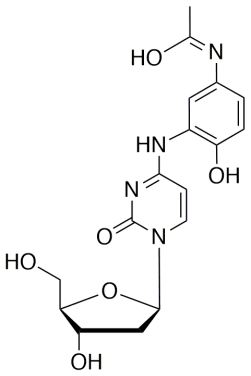
4dCa1b1
0, *0*, 0



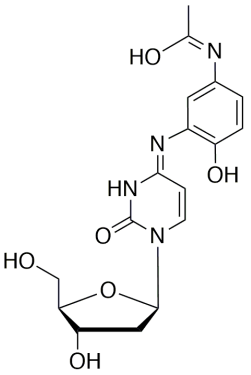
4dCa2b1
21, *18*, 9



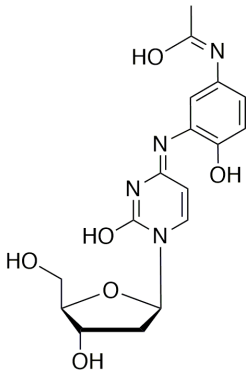
4dCa3b1
58, –, –



4dCa1b2
51, *77*, –

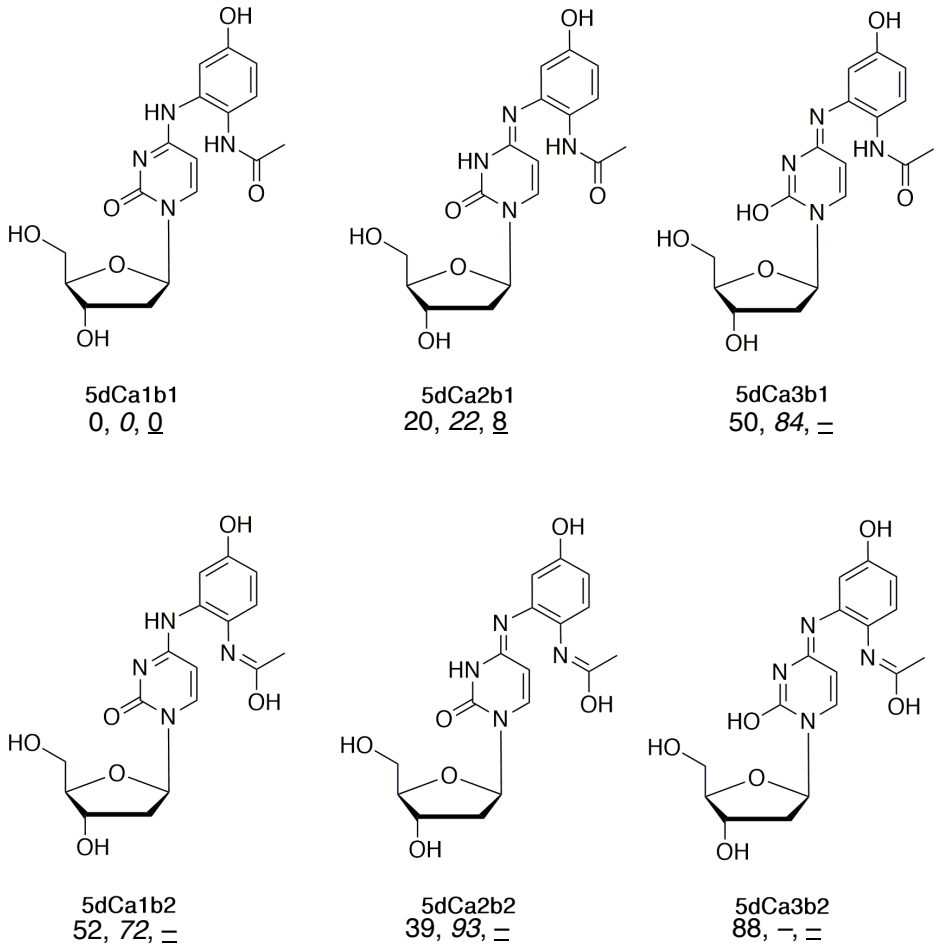


4dCa2b2
41, *91*, –

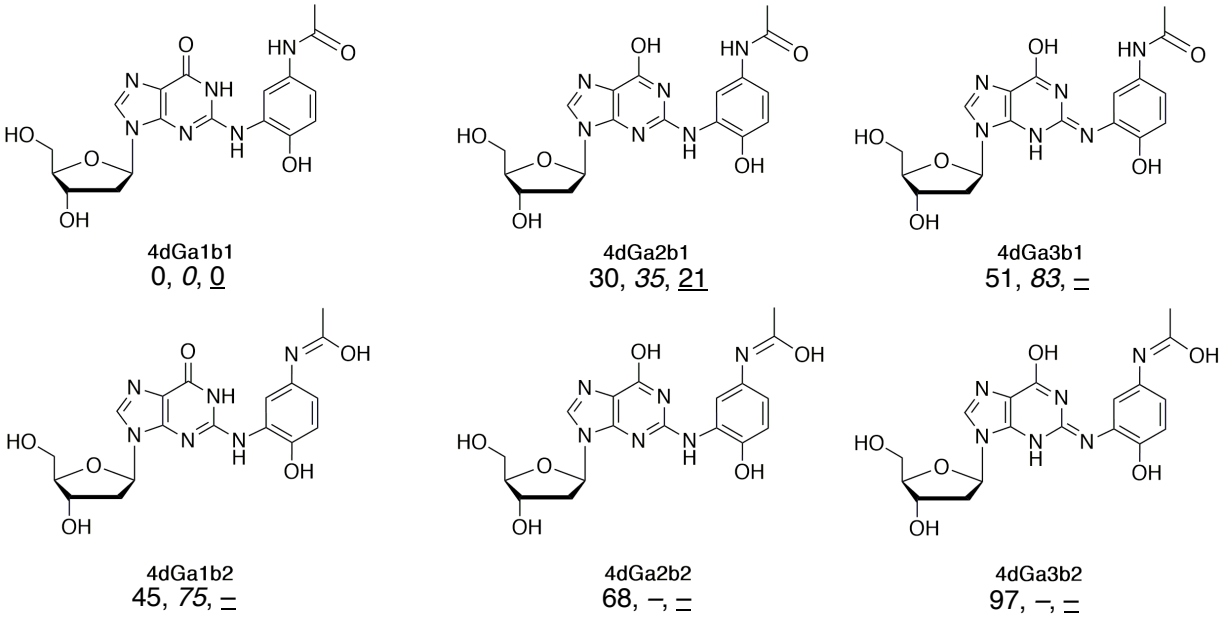


4dCa3b2
95, –, –

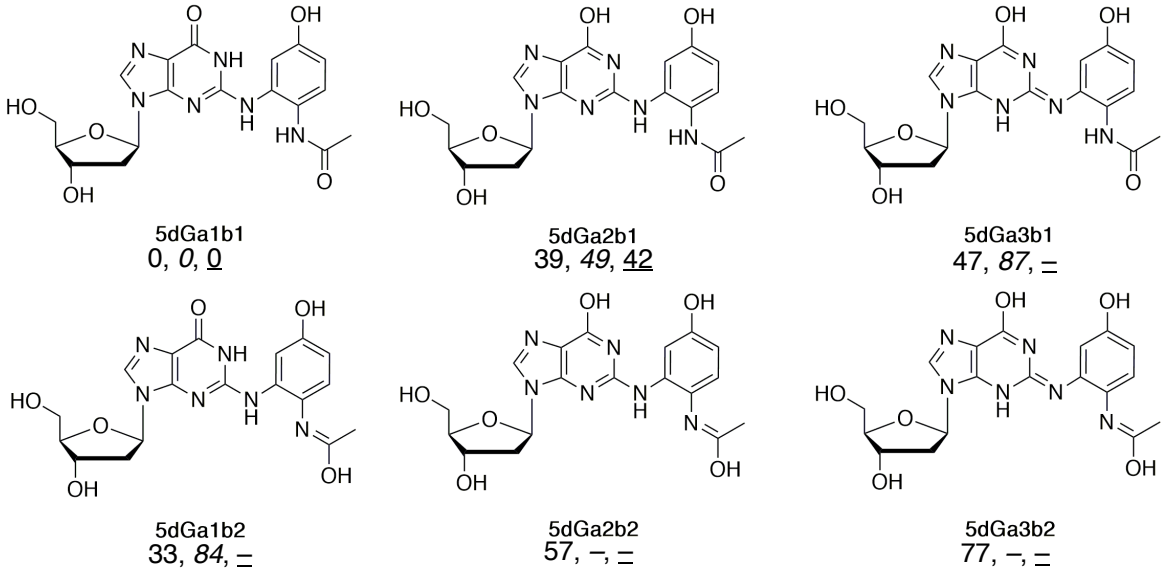
Scheme S1: Tautomers of **4dC** subjected to sequential conformational searches at the AM1 (relative energies in kJ mol^{-1} in normal font), N12/6-31+G(d) (*italics*) and MN15/6-311+G(2df,p) (underlined) levels. N12 and MN15 computations were only carried out for selected low-energy isomers found at the preceding lower-level (AM1 for N12 and N12 for MN15), as described in the computational details in the main text.



Scheme S2: Tautomers of **5dC** subjected to sequential conformational searches at the AM1 (relative energies in kJ mol^{-1} in normal font), N12/6-31+G(d) (*italics*) and MN15/6-311+G(2df,p) (underlined) levels. N12 and MN15 computations were only carried out for selected low-energy isomers found at the preceding lower-level (AM1 for N12 and N12 for MN15), as described in the computational details in the main text.



Scheme S3: Tautomers of **4dG** subjected to sequential conformational searches at the AM1 (relative energies in kJ mol^{-1} in normal font), N12/6-31+G(d) (*italics*) and MN15/6-311+G(2df,p) (underlined) levels. N12 and MN15 computations were only carried out for selected low-energy isomers found at the preceding lower-level (AM1 for N12 and N12 for MN15), as described in the computational details in the main text.



Scheme S4: Tautomers of **5dG** subjected to sequential conformational searches at the AM1 (relative energies in kJ mol^{-1} in normal font), N12/6-31+G(d) (*italics*) and MN15/6-311+G(2df,p) (underlined) levels. N12 and MN15 computations were only carried out for selected low-energy isomers found at the preceding lower-level (AM1 for N12 and N12 for MN15), as described in the computational details in the main text.

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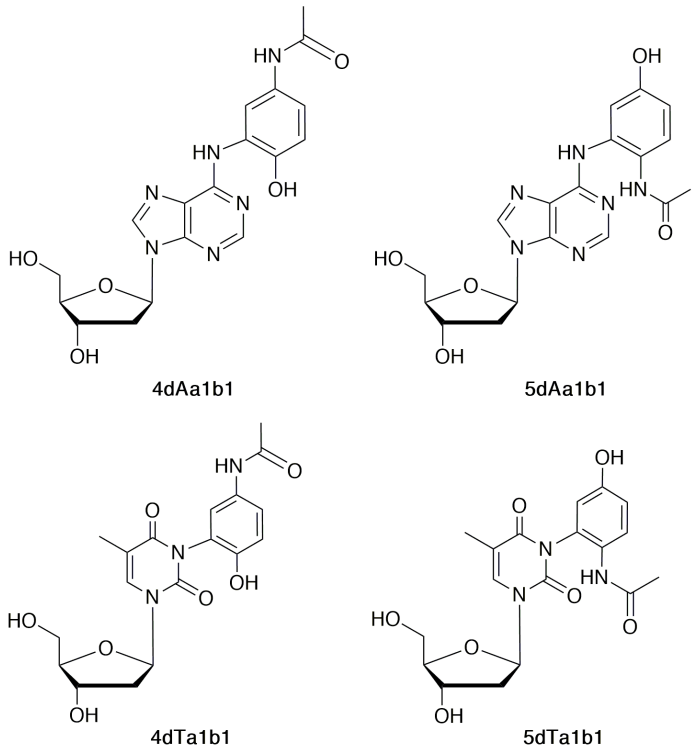

Scheme S5: Limited tautomers of **4dA** and **5dA** subjected to conformational searches followed by DFT optimization.

Table S1: Gibbs free energies of dX-NAPQI adducts. Energies are relative to reactants. Tautomer numbering is as shown in Schemes S1-S5. Only the most stable conformation of each tautomer is given.

Tautomer	X = C	X = G	X = A	X = T
4dXa1b1	-31.8	-28.4	-27.2	25.5
4dXa2b1	-28.0	-23.4	not calculated	not calculated
4dXa3b1	-12.2	not calculated	not calculated	not calculated
4dXa1b2	not calculated	not calculated	Not calculated	not calculated
4dXa2b2	-11.3	-6.9	not calculated	not calculated
4dXa3b2	not calculated	not calculated	not calculated	not calculated
5dXa1b1	-32.2	-27.7	-29.7	27.1
5dXa2b1	-27.9	not calculated	not calculated	not calculated
5dXa3b1	-11.8	not calculated	not calculated	not calculated
5dXa1b2	not calculated	not calculated	not calculated	not calculated
5dXa2b2	-11.7	-8.4	not calculated	not calculated
5dXa3b2	not calculated	not calculated	not calculated	not calculated

Cartesian coordinates of all species used to calculate overall reaction energies.

4dCa1b1

Sum of electronic and zero-point Energies = -834429.2 kcal/mol

O	3.829151	1.894988	2.782596
C	4.189955	2.130047	1.434035
H	4.903866	2.951311	1.441703
H	3.315433	2.439022	0.855608
C	4.842857	0.916349	0.799897
H	5.764820	0.680634	1.332192
O	3.978933	-0.224537	0.919894
C	3.539402	-0.662713	-0.353936
H	4.044570	-1.584566	-0.619893
N	2.122864	-1.003688	-0.283837
C	1.239083	-0.109459	0.219479
H	1.656103	0.811391	0.594259
C	-0.091401	-0.368197	0.265337
H	-0.767610	0.347163	0.696607
C	-0.511056	-1.624928	-0.239188
N	-1.807551	-2.017328	-0.259280
H	-1.936898	-2.996575	-0.463826
N	0.359661	-2.525269	-0.695618
C	1.678551	-2.261528	-0.738652
O	2.507961	-3.079205	-1.173238
C	5.106832	1.089363	-0.699005
H	5.218792	2.141188	-0.964353
C	3.869561	0.468783	-1.317381
H	3.064061	1.200314	-1.334746
H	4.040619	0.114148	-2.329895
O	6.243252	0.357781	-1.129404
H	3.191003	1.174248	2.796249
H	7.026201	0.734060	-0.715662
C	-2.969920	-1.306017	0.046870
C	-3.139980	0.041783	-0.267561
C	-4.023977	-2.023229	0.633624
C	-4.334277	0.691630	0.046516
H	-2.361881	0.578203	-0.778262
C	-5.218904	-1.377059	0.922895
C	-5.373506	-0.028603	0.643439
H	-6.025209	-1.934303	1.379422
H	-6.305633	0.463934	0.882890
O	-3.811081	-3.342465	0.887979
H	-4.605200	-3.746122	1.252835
N	-4.570116	2.046053	-0.224430
C	-3.738480	2.993830	-0.722204
H	-5.494618	2.364319	0.016320
O	-2.567280	2.762466	-1.051575
C	-4.325630	4.368277	-0.846541
H	-4.200649	4.714629	-1.871431
H	-5.378479	4.420115	-0.580683
H	-3.765439	5.046330	-0.202940

4dCa2b1

Sum of electronic and zero-point Energies = -834425.4 kcal/mol

O	5.535229	-0.501813	-2.029393
C	6.202879	0.358444	-1.130415
H	6.110704	1.400619	-1.451526
H	7.259369	0.094413	-1.159363
C	5.718938	0.255529	0.301637
H	6.386246	0.855722	0.923688
O	4.397961	0.812320	0.411317
C	3.505047	-0.128538	0.965659
H	3.376968	0.074967	2.027002
N	2.173678	0.054579	0.394236
C	1.133931	0.371450	1.239426
H	1.409046	0.483456	2.276351
C	-0.138700	0.527092	0.824446
H	-0.912294	0.766764	1.533087
C	-0.457589	0.362195	-0.561743
N	-1.602001	0.422851	-1.155632
N	0.645037	0.061835	-1.351675
C	1.940420	-0.091075	-0.960795
O	2.819155	-0.340919	-1.787521
C	5.626888	-1.171284	0.868825
H	6.243420	-1.863815	0.296833
C	4.148125	-1.494728	0.766727
H	3.917476	-1.893382	-0.216266
H	3.830011	-2.206876	1.522952
O	5.994316	-1.218773	2.240395
H	4.574601	-0.374145	-1.933661
H	6.920492	-0.971439	2.321369
C	-2.749952	0.801724	-0.466203
C	-3.822605	-0.092162	-0.388464
C	-2.915853	2.103014	0.042559

C	-5.027550	0.275740	0.210767
H	-3.699916	-1.077807	-0.801094
C	-4.120946	2.470617	0.632372
C	-5.170394	1.569122	0.723147
H	-4.235190	3.473962	1.020990
H	-6.100085	1.870288	1.186403
O	-1.873410	2.973776	-0.082124
H	-2.118546	3.831670	0.279343
N	-6.132275	-0.581147	0.329293
C	-6.279755	-1.878083	-0.031624
H	-6.936419	-0.160391	0.764974
O	-5.383086	-2.540303	-0.573157
C	-7.620804	-2.482205	0.265401
H	-7.483486	-3.338817	0.924403
H	-8.317375	-1.788519	0.729783
H	-8.055116	-2.851026	-0.662996
H	0.485214	-0.047893	-2.342301

4dCa2b2

Sum of electronic and zero-point Energies = -834408.7 kcal/mol

O	-4.099109	2.772161	0.004735
C	-5.143904	2.207351	-0.759053
H	-4.921406	2.273651	-1.828552
H	-6.038353	2.799567	-0.568876
C	-5.441752	0.762353	-0.417931
H	-6.321127	0.456184	-0.988911
O	-4.337996	-0.064841	-0.821468
C	-3.878166	-0.839072	0.264330
H	-4.316063	-1.833737	0.209476
N	-2.440492	-1.062423	0.136824
C	-1.976553	-2.360854	0.094462
H	-2.740245	-3.120091	0.147501
C	-0.670823	-2.673566	-0.002691
H	-0.354935	-3.702271	-0.033357
C	0.307733	-1.634898	-0.103389
N	1.572947	-1.871037	-0.217996
N	-0.235369	-0.356639	-0.049147
C	-1.551600	-0.010021	0.073450
O	-1.881026	1.176197	0.114477
C	-5.672312	0.469859	1.074864
H	-5.924654	1.379047	1.619685
C	-4.352223	-0.126624	1.523885
H	-3.661668	0.660114	1.810466
H	-4.473048	-0.814250	2.356521
O	-6.686745	-0.505749	1.270096
H	-3.326922	2.179712	-0.032157
H	-7.521541	-0.152052	0.948571
C	2.486656	-0.843014	-0.445248
C	3.474052	-0.550352	0.497290
C	2.513932	-0.154017	-1.675901
C	4.472110	0.397626	0.254016
H	3.460137	-1.075189	1.441605
C	3.499752	0.791958	-1.926625
C	4.474814	1.070490	-0.974995
H	3.498018	1.314961	-2.874260
H	5.216681	1.830068	-1.177104
O	1.548157	-0.465285	-2.588420
H	1.675791	0.050074	-3.390949
N	5.380521	0.710643	1.277539
C	6.642086	0.590688	1.098364
O	7.231518	0.103987	-0.019711
C	7.640164	0.947389	2.135262
H	7.149116	1.348596	3.015113
H	8.217801	0.066315	2.416853
H	8.343870	1.684109	1.747782
H	6.560178	-0.123705	-0.679169
H	0.392922	0.431558	-0.108998

4dCa3b1

Sum of electronic and zero-point Energies= -834409.6 kcal/mol

O	3.154503	2.307250	1.637229
C	4.318346	1.674683	2.138307
H	4.092927	1.133975	3.060619
H	5.094834	2.412291	2.358350
C	4.872005	0.704525	1.122680
H	5.805771	0.312528	1.529254
O	3.978607	-0.403180	0.932700
C	3.576622	-0.507713	-0.418100
H	4.100956	-1.326613	-0.896787
N	2.156516	-0.855400	-0.446645
C	1.251452	-0.080164	0.238582
H	1.671165	0.769675	0.755129
C	-0.059312	-0.396830	0.269966
H	-0.738045	0.224451	0.829330
C	-0.516753	-1.590608	-0.392305
N	-1.737432	-2.060330	-0.390501
N	0.431725	-2.344592	-1.049789
C	1.669906	-1.971369	-1.059680
O	2.582148	-2.683310	-1.714477
C	5.124473	1.286975	-0.277003

H	5.216976	2.372077	-0.244998
C	3.910813	0.832211	-1.060072
H	3.095113	1.536594	-0.918610
H	4.112301	0.737525	-2.123493
O	6.278774	0.721101	-0.879820
H	2.825260	2.914688	2.304595
H	7.051544	0.978635	-0.367956
C	-2.824128	-1.356968	0.095313
C	-3.137796	-0.024429	-0.198964
C	-3.746878	-2.120242	0.839637
C	-4.330201	0.539569	0.261321
H	-2.467998	0.559116	-0.805471
C	-4.918612	-1.556080	1.317033
C	-5.209259	-0.227002	1.033716
H	-5.602498	-2.155285	1.900900
H	-6.127170	0.212683	1.398860
O	-3.458100	-3.430240	1.081714
H	-2.630598	-3.605299	0.598743
N	-4.711113	1.865735	-0.004538
C	-4.188628	2.764569	-0.871708
H	-5.535556	2.166753	0.488406
O	-3.198865	2.530299	-1.580657
C	-4.894222	4.086770	-0.938719
H	-5.306581	4.215220	-1.939519
H	-5.697947	4.188587	-0.213953
H	-4.169035	4.883482	-0.779861
H	2.147210	-3.451735	-2.106767

5dCa1b1

Sum of electronic and zero-point Energies = -834429.6 kcal/mol

O	-4.444103	2.988724	-0.465031
C	-4.860451	2.058514	0.517873
H	-5.774985	2.454453	0.954587
H	-4.107599	1.979828	1.306687
C	-5.142861	0.693121	-0.079720
H	-5.959252	0.769887	-0.798267
O	-3.989107	0.227609	-0.795524
C	-3.437471	-0.921963	-0.173326
H	-3.656894	-1.801029	-0.769306
N	-1.985003	-0.811283	-0.175771
C	-1.387675	0.276552	0.369466
H	-2.040346	0.997698	0.834771
C	-0.044120	0.451522	0.321262
H	0.408735	1.313740	0.777495
C	0.705843	-0.556159	-0.339539
N	2.052743	-0.512056	-0.454913
H	2.501552	-1.349209	-0.820346
N	0.125007	-1.639233	-0.855792
C	-1.207557	-1.814225	-0.788725
O	-1.769860	-2.823322	-1.248117
C	-5.443052	-0.374054	0.976930
H	-5.851745	0.069485	1.885501
C	-4.080530	-0.997974	1.204523
H	-3.520964	-0.404641	1.924957
H	-4.146985	-2.017930	1.572873
O	-6.321894	-1.376172	0.491430
H	-3.643026	2.644256	-0.873228
H	-7.179254	-0.976025	0.316723
C	2.926909	0.540307	-0.171002
C	2.611261	1.851492	-0.529663
C	4.160513	0.272411	0.451113
C	3.471842	2.896310	-0.218542
H	1.696502	2.060373	-1.061935
C	5.013448	1.336363	0.743783
C	4.679957	2.643202	0.429161
H	5.953701	1.128418	1.234975
H	5.351449	3.455746	0.668904
O	3.091396	4.151228	-0.582356
H	3.766049	4.789958	-0.329631
N	4.556143	-1.016349	0.869865
C	4.581020	-2.152669	0.137319
H	5.060235	-1.044345	1.742149
O	4.117642	-2.207103	-1.014733
C	5.188761	-3.352034	0.792487
H	4.443983	-4.145601	0.837888
H	6.008959	-3.709659	0.171122
H	5.560044	-3.154984	1.794614

5dCa2b1

Sum of electronic and zero-point Energies = -834425.3 kcal/mol

O	-5.087210	0.704138	-1.975455
C	-5.686373	-0.473043	-1.476250
H	-5.469863	-1.323910	-2.129783
H	-6.763724	-0.311786	-1.485126
C	-5.264351	-0.833691	-0.066764
H	-5.875177	-1.678398	0.258822
O	-3.890397	-1.255330	-0.067549
C	-3.134806	-0.496665	0.850816
H	-3.018750	-1.056899	1.776653
N	-1.772732	-0.331512	0.351197

C	-0.733027	-0.849373	1.090691
H	-1.028277	-1.343981	2.002389
C	0.560307	-0.750082	0.725592
H	1.329802	-1.167396	1.350956
C	0.904590	-0.067978	-0.485854
N	2.065721	0.168935	-0.998012
N	-0.196126	0.429394	-1.172513
C	-1.512672	0.320486	-0.839624
O	-2.385340	0.784027	-1.575719
C	-5.362512	0.301750	0.967546
H	-6.029417	1.091221	0.623477
C	-3.928399	0.778527	1.103746
H	-3.711414	1.527365	0.348895
H	-3.725850	1.195142	2.086439
O	-5.797198	-0.174340	2.233647
H	-4.123572	0.647711	-1.846494
H	-6.701126	-0.493760	2.150245
C	3.216775	-0.404823	-0.485724
C	3.359832	-1.795090	-0.388810
C	4.330005	0.405962	-0.183236
C	4.574834	-2.363897	-0.027476
H	2.527114	-2.436495	-0.638314
C	5.540581	-0.181720	0.171586
C	5.681803	-1.560790	0.245014
H	6.384336	0.455855	0.396124
H	6.628643	-2.008234	0.513793
O	4.633795	-3.726264	0.037186
H	5.516219	-4.008924	0.298262
N	4.244680	1.813154	-0.273220
C	3.437921	2.593939	0.481039
H	4.932709	2.278748	-0.842402
O	2.665762	2.127114	1.329616
C	3.525789	4.069046	0.226264
H	2.584955	4.409975	-0.205802
H	3.657657	4.586146	1.174752
H	4.335021	4.339287	-0.447643
H	-0.017172	0.908441	-2.042539

5dCa2b2

Sum of electronic and zero-point Energies = -834409.0 kcal/mol

O	-5.017474	0.963801	1.779068
C	-5.518174	1.324424	0.508791
H	-5.200886	2.337169	0.241463
H	-6.605115	1.325148	0.582090
C	-5.110618	0.381742	-0.604366
H	-5.648649	0.676097	-1.508079
O	-3.703305	0.515997	-0.864532
C	-3.057713	-0.734200	-0.760218
H	-2.926865	-1.159218	-1.753676
N	-1.698634	-0.547031	-0.259832
C	-0.646250	-0.966900	-1.041335
H	-0.929450	-1.397061	-1.988815
C	0.644037	-0.863468	-0.667039
H	1.425050	-1.217587	-1.316938
C	0.970275	-0.287507	0.603228
N	2.125146	-0.121716	1.153757
N	-0.143499	0.112812	1.331655
C	-1.455262	0.020011	0.977354
O	-2.338921	0.427581	1.733591
C	-5.350195	-1.111369	-0.322920
H	-6.087757	-1.250441	0.466673
C	-3.976035	-1.617778	0.072856
H	-3.809873	-1.460495	1.134055
H	-3.842486	-2.671610	-0.155629
O	-5.759623	-1.807135	-1.491837
H	-4.055944	0.825328	1.710025
H	-6.607641	-1.454246	-1.778293
C	3.293952	-0.402071	0.448919
C	4.114868	-1.444406	0.895159
C	3.728363	0.399578	-0.635713
C	5.326127	-1.720978	0.273099
H	3.793609	-2.042241	1.737834
C	4.942479	0.084965	-1.251869
C	5.748423	-0.955682	-0.810296
H	5.261311	0.682106	-2.094800
H	6.690606	-1.170756	-1.293070
O	6.136111	-2.742048	0.694583
H	5.744288	-3.178294	1.458013
N	2.939335	1.427736	-1.165736
C	2.744832	2.520111	-0.534825
O	1.923901	3.444783	-1.080584
C	3.322780	2.983251	0.752385
H	2.534462	3.118684	1.492517
H	4.049349	2.274199	1.134067
H	3.804327	3.950479	0.610672
H	1.576030	3.094694	-1.912474
H	0.022351	0.533263	2.233882

5dCa3b1

Sum of electronic and zero-point Energies = -834409.1 kcal/mol

O	3.642707	1.939301	1.951757
C	4.865732	1.240082	2.090866
H	4.930937	0.773641	3.076643
H	5.715641	1.918922	1.983741
C	4.991029	0.175854	1.034464
H	5.966595	-0.300744	1.167952
O	3.966271	-0.811489	1.207903
C	3.561156	-1.348987	-0.024254
H	3.688762	-2.425655	-0.006093
N	2.104334	-1.119434	-0.184758
C	1.476624	-0.027465	0.357294
H	2.091975	0.600631	0.981732
C	0.167104	0.210432	0.125908
H	-0.300193	1.066499	0.582659
C	-0.591872	-0.701664	-0.688530
N	-1.872741	-0.632590	-0.946342
N	0.086150	-1.783132	-1.210857
C	1.347422	-1.935352	-0.967550
O	2.022777	-2.951107	-1.498492
C	4.864202	0.617181	-0.419834
H	4.106614	1.395189	-0.512208
C	4.404535	-0.670297	-1.097544
H	3.858713	-0.510982	-2.022793
H	5.274729	-1.290753	-1.306729
O	6.108953	1.105085	-0.872375
H	3.598907	2.616079	2.632191
H	5.976922	1.547183	-1.715683
C	-2.643465	0.469660	-0.635041
C	-2.304420	1.777797	-0.998854
C	-3.906248	0.242145	-0.025616
C	-3.175314	2.832996	-0.752874
H	-1.364147	1.969366	-1.494776
C	-4.767775	1.310327	0.210211
C	-4.407928	2.606094	-0.148400
H	-5.722437	1.131600	0.673636
H	-5.084186	3.429812	0.035232
O	-2.773739	4.085038	-1.135022
H	-3.452130	4.728643	-0.906911
N	-4.187001	-1.091221	0.288521
C	-5.216843	-1.634305	0.972749
H	-3.473954	-1.721069	-0.052215
O	-6.137338	-0.961730	1.465256
C	-5.190098	-3.128373	1.110765
H	-4.309205	-3.590331	0.672318
H	-5.237380	-3.386247	2.168067
H	-6.078394	-3.543230	0.634757
H	1.416929	-3.481448	-2.032243

4dGa1b1

Sum of electronic and zero-point Energies = -927056.6 kcal/mol

H	7.495213	-2.096532	-0.558439
O	6.827864	-1.418996	-0.424016
C	6.581321	-0.777047	-1.661824
H	6.246026	-1.500976	-2.408114
H	7.488319	-0.296161	-2.037116
C	5.525097	0.286417	-1.499077
H	5.434772	0.806037	-2.455058
O	4.266119	-0.322257	-1.185862
C	3.625536	0.405038	-0.153309
H	2.988256	1.179486	-0.576307
N	2.751787	-0.486643	0.564876
C	3.119590	-1.609664	1.268576
H	4.150257	-1.901689	1.357542
N	2.103899	-2.256554	1.780763
C	1.004607	-1.526231	1.395960
C	-0.371264	-1.716120	1.667795
O	-0.921744	-2.610330	2.326382
N	-1.151765	-0.707822	1.085947
H	-2.142090	-0.773124	1.272425
C	-0.685063	0.330154	0.335996
N	-1.569417	1.233399	-0.159290
H	-1.134091	2.090120	-0.462916
N	0.597236	0.507795	0.081074
C	1.383324	-0.424575	0.630824
C	5.794820	1.329811	-0.402080
H	6.809043	1.252921	-0.013204
C	4.758595	1.003963	0.663365
H	5.154876	0.263982	1.355834
H	4.449554	1.880569	1.227189
O	5.602009	2.615020	-0.977023
H	5.794318	3.277830	-0.306317
C	-2.957891	1.276211	0.038524
C	-3.519874	2.456524	0.547810
C	-3.784627	0.203102	-0.287929
C	-4.893386	2.532467	0.750575
C	-5.162288	0.288274	-0.096282
H	-3.349492	-0.693113	-0.700701
C	-5.709922	1.455864	0.436499
H	-5.318659	3.438575	1.159264
H	-6.776041	1.526311	0.597464
O	-2.669131	3.475827	0.825386

H	-3.155685	4.252494	1.120745
N	-6.018761	-0.790244	-0.393222
H	-6.766157	-0.953796	0.265780
C	-6.077997	-1.581044	-1.494277
C	-5.149474	-1.326605	-2.639053
H	-4.899717	-0.274669	-2.751920
H	-4.221135	-1.881568	-2.503680
H	-5.624333	-1.689024	-3.546387
O	-6.917707	-2.495066	-1.536077

4dGa2b1

Sum of electronic and zero-point Energies = -927051.5 kcal/mol

H	7.508323	-1.868628	-0.939522
O	6.829446	-1.299222	-0.568215
C	6.781323	-0.100967	-1.321807
H	6.557966	-0.315842	-2.369620
H	7.740504	0.421813	-1.279800
C	5.724567	0.824008	-0.771303
H	5.789125	1.759377	-1.331943
O	4.422962	0.259676	-0.973678
C	3.664413	0.346247	0.220575
H	3.071688	1.259280	0.222334
N	2.718549	-0.737587	0.250623
C	2.994618	-2.085157	0.284626
H	4.005911	-2.446936	0.333353
N	1.928603	-2.843427	0.239143
C	0.882402	-1.950586	0.167439
C	-0.502723	-2.071792	0.095182
O	-1.083406	-3.274639	0.088292
N	-1.271078	-0.995778	0.030636
C	-0.696282	0.217012	0.038815
N	-1.485356	1.329122	-0.029731
H	-0.961543	2.188720	-0.041396
N	0.620996	0.471956	0.109875
C	1.351371	-0.630179	0.166972
C	5.834708	1.139485	0.735511
H	6.802262	0.837917	1.134454
C	4.692052	0.350421	1.341833
H	5.016446	-0.664217	1.558474
H	4.311445	0.802259	2.253609
O	5.617984	2.517967	0.999358
H	6.324550	3.024611	0.587615
C	-2.862042	1.499853	-0.072601
C	-3.804974	0.471174	-0.048338
C	-3.307488	2.834495	-0.139025
C	-5.169886	0.764790	-0.086123
H	-3.474334	-0.546026	0.000351
C	-4.662916	3.117325	-0.175312
C	-5.599044	2.092086	-0.149364
H	-4.983739	4.149068	-0.225916
H	-6.654577	2.323870	-0.178416
O	-2.342249	3.799286	-0.163997
H	-2.738047	4.675211	-0.211165
N	-6.161695	-0.228137	-0.059165
C	-6.050477	-1.577891	-0.012734
H	-7.103440	0.126664	-0.082844
O	-4.964191	-2.173754	0.007938
C	-7.348455	-2.330291	-0.000824
H	-7.452040	-2.868663	-0.943347
H	-7.319855	-3.070229	0.796870
H	-8.219559	-1.694018	0.133969
H	-2.042594	-3.161985	0.034561

4dGa2b2

Sum of electronic and zero-point Energies = -927035.1 kcal/mol

H	-7.558949	-1.741983	1.173684
O	-6.891834	-1.173172	0.780821
C	-6.796046	0.010644	1.552073
H	-6.528697	-0.225802	2.584844
H	-7.750060	0.544699	1.563298
C	-5.753995	0.935052	0.971639
H	-5.770467	1.851243	1.565955
O	-4.452059	0.345681	1.081001
C	-3.785505	0.386598	-0.169925
H	-3.136968	1.259712	-0.215748
N	-2.911466	-0.751594	-0.277068
C	-3.263309	-2.079495	-0.352810
H	-4.294501	-2.383502	-0.356030
N	-2.240356	-2.894672	-0.403720
C	-1.143552	-2.062693	-0.355277
C	0.234705	-2.259407	-0.377317
O	0.739576	-3.493397	-0.458490
N	1.067301	-1.230263	-0.319585
C	0.558425	0.010214	-0.236978
N	1.402319	1.081110	-0.173986
H	0.918506	1.961001	-0.100032
N	-0.745314	0.335030	-0.208430
C	-1.538060	-0.721889	-0.268093
C	-5.943014	1.297210	-0.514819
H	-6.951512	1.065050	-0.854926

C	-4.891318	0.459031	-1.211649
H	-5.286559	-0.532918	-1.415098
H	-4.554124	0.903737	-2.143756
O	-5.657440	2.666227	-0.762984
H	-6.303200	3.206955	-0.297966
C	2.784076	1.200594	-0.182649
C	3.701580	0.155440	-0.276586
C	3.272790	2.522191	-0.093833
C	5.079778	0.402378	-0.267604
H	3.346009	-0.856184	-0.354644
C	4.632996	2.771497	-0.106458
C	5.542830	1.720030	-0.189946
H	4.981017	3.794441	-0.052068
H	6.602681	1.928489	-0.226473
O	2.331714	3.507797	-0.003920
H	2.749522	4.372195	0.056859
N	5.954836	-0.684514	-0.427717
C	6.867457	-0.922859	0.437725
O	7.050394	-0.236353	1.591375
C	7.849738	-2.024473	0.295171
H	7.751098	-2.728491	1.121929
H	7.703114	-2.550792	-0.641546
H	8.864259	-1.626885	0.329729
H	6.402493	0.480677	1.657334
H	1.704837	-3.441973	-0.460207

5dGa1b1

Sum of electronic and zero-point Energies = -927055.9 kcal/mol

H	7.682333	-1.152488	0.013495
O	6.857712	-0.660054	0.021970
C	6.665295	-0.077645	-1.254225
H	6.592549	-0.852032	-2.021573
H	7.500379	0.578836	-1.511843
C	5.404190	0.748990	-1.268207
H	5.342685	1.234828	-2.243823
O	4.261639	-0.100752	-1.106885
C	3.367739	0.464971	-0.165851
H	2.636863	1.094444	-0.670594
N	2.617499	-0.595655	0.457251
C	3.117735	-1.634225	1.206548
H	4.172627	-1.740000	1.384218
N	2.192522	-2.451216	1.642744
C	1.017755	-1.925391	1.161024
C	-0.320654	-2.359708	1.316496
O	-0.755488	-3.336534	1.943050
N	-1.214755	-1.510399	0.651313
H	-2.190466	-1.751914	0.751691
C	-0.875147	-0.413128	-0.084115
N	-1.861539	0.319411	-0.660770
H	-1.549693	1.210965	-1.011003
N	0.370713	-0.005478	-0.226624
C	1.258992	-0.775098	0.413161
C	5.303768	1.827383	-0.178179
H	6.257641	1.983790	0.323450
C	4.248538	1.276855	0.769507
H	4.713116	0.625265	1.507057
H	3.701325	2.061140	1.286579
O	4.893468	3.033215	-0.808544
H	4.830842	3.719122	-0.136691
C	-3.214538	-0.017666	-0.809473
C	-4.203604	0.949263	-0.552414
C	-3.584029	-1.292049	-1.235460
C	-5.541553	0.607023	-0.731475
C	-4.929540	-1.625309	-1.358850
H	-2.833901	-2.024981	-1.491480
C	-5.916466	-0.674044	-1.107589
H	-6.299161	1.357888	-0.563962
H	-6.960227	-0.929164	-1.226962
O	-5.219745	-2.891978	-1.754459
H	-6.172587	-3.016663	-1.813036
N	-3.837663	2.249995	-0.147890
H	-3.227887	2.779832	-0.754723
C	-4.243239	2.926268	0.955693
C	-5.090312	2.220689	1.967089
H	-4.919286	1.147988	1.987226
H	-4.882963	2.647251	2.944553
H	-6.144478	2.390705	1.746751
O	-3.900927	4.109295	1.108172

5dGa2b2

Sum of electronic and zero-point Energies = -927036.5 kcal/mol

H	-7.500844	-0.776266	0.875321
O	-6.714565	-0.384122	0.487638
C	-6.461226	0.849950	1.134610
H	-6.336572	0.698619	2.209374
H	-7.290768	1.545948	0.982355
C	-5.211238	1.487743	0.579339
H	-5.113425	2.469527	1.047336
O	-4.060560	0.706494	0.926557
C	-3.265113	0.457681	-0.218855

H	-2.456848	1.184196	-0.279696
N	-2.632987	-0.829075	-0.076836
C	-3.259614	-2.048518	0.035990
H	-4.331820	-2.127252	0.038020
N	-2.434150	-3.057946	0.150550
C	-1.186732	-2.476777	0.111648
C	0.115644	-2.962924	0.173804
O	0.339867	-4.273881	0.301341
N	1.149078	-2.138102	0.109924
C	0.921476	-0.820524	-0.026935
N	1.979546	0.037985	-0.097211
H	1.712431	1.007435	-0.185456
N	-0.282260	-0.225095	-0.098971
C	-1.284744	-1.085735	-0.022578
C	-5.176789	1.657223	-0.952739
H	-6.167622	1.533294	-1.387692
C	-4.216082	0.574826	-1.400393
H	-4.751787	-0.360704	-1.540337
H	-3.702980	0.828178	-2.324014
O	-4.643534	2.918387	-1.329791
H	-5.248266	3.607498	-1.037633
C	3.350766	-0.153374	-0.154998
C	3.983137	-1.396142	-0.143229
C	4.127889	1.033453	-0.232760
C	5.369918	-1.471568	-0.232908
H	3.403788	-2.298516	-0.067516
C	5.512555	0.916080	-0.340340
C	6.145545	-0.322121	-0.341113
H	6.103471	1.813390	-0.452119
H	7.220545	-0.393283	-0.433094
O	5.920632	-2.724575	-0.219090
H	6.879074	-2.665177	-0.283690
N	3.448690	2.246774	-0.322391
C	3.781910	3.288081	0.342277
O	3.119749	4.439213	0.100982
C	4.806254	3.450923	1.405973
H	5.107082	2.490785	1.812977
H	5.691078	3.950230	1.009835
H	4.406631	4.078152	2.200770
H	2.474651	4.284943	-0.603288
H	1.292706	-4.434572	0.321226

4dAa1b1

Sum of electronic and zero-point Energies = -879853.2 kcal/mol

H	7.064462	1.306781	-2.629838
O	6.584425	0.777725	-1.987631
C	6.966189	1.189646	-0.687865
H	6.736754	2.247405	-0.538620
H	8.039458	1.050118	-0.535177
C	6.241782	0.376726	0.355033
H	6.621251	0.687156	1.330931
O	4.837093	0.648257	0.293082
C	4.119884	-0.566021	0.449499
H	3.955396	-0.765986	1.507455
N	2.813311	-0.419612	-0.131070
C	2.476661	-0.390427	-1.459559
H	3.211609	-0.527793	-2.231663
N	1.200603	-0.173565	-1.674647
C	0.663370	-0.041834	-0.415720
C	-0.639918	0.213725	0.045311
N	-1.671835	0.351145	-0.821371
H	-1.499901	0.042131	-1.764130
N	-0.841985	0.308719	1.368290
C	0.202040	0.166657	2.189441
H	-0.016390	0.261938	3.244221
N	1.472605	-0.083218	1.877698
C	1.647472	-0.180296	0.559392
C	6.399536	-1.149511	0.237429
H	7.154618	-1.422272	-0.497879
C	5.012989	-1.621706	-0.177320
H	4.926873	-1.600639	-1.261457
H	4.791499	-2.625500	0.176102
O	6.782489	-1.639135	1.515175
H	6.892866	-2.592751	1.451174
C	-3.008864	0.626284	-0.479980
C	-3.366616	1.851619	0.102952
C	-4.001511	-0.299148	-0.785962
C	-4.704967	2.105758	0.390370
C	-5.342964	-0.033871	-0.514233
H	-3.719138	-1.240188	-1.236521
C	-5.690826	1.182861	0.071739
H	-4.974952	3.056424	0.830121
H	-6.725363	1.424014	0.258537
O	-2.391432	2.763994	0.331607
H	-2.772999	3.572523	0.688776
N	-6.304897	-0.993206	-0.886449
C	-7.386904	-1.452415	-0.210635
O	-8.129965	-2.287916	-0.753073
C	-7.658986	-0.962468	1.176103
H	-6.760557	-0.651620	1.701870
H	-8.345391	-0.115974	1.144092

H	-8.147539	-1.762913	1.725378
H	-6.138262	-1.471592	-1.759784

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Sum of electronic and zero-point Energies = -879855.7 kcal/mol

H	-5.934987	3.160487	-1.193964
O	-5.605773	2.350280	-0.796708
C	-6.260190	1.250406	-1.402813
H	-6.013851	1.195642	-2.466046
H	-7.344850	1.346034	-1.309780
C	-5.848724	-0.036713	-0.732835
H	-6.430607	-0.841559	-1.185579
O	-4.457357	-0.289748	-0.968260
C	-3.816338	-0.647112	0.243417
H	-3.804460	-1.729588	0.358289
N	-2.435477	-0.243385	0.173216
C	-1.950298	1.031682	0.052021
H	-2.606985	1.883133	0.036229
N	-0.642891	1.089732	-0.053582
C	-0.242482	-0.223004	-0.001893
C	1.020443	-0.837970	-0.059245
N	2.132308	-0.066049	-0.179782
H	1.942378	0.924503	-0.210577
N	1.082226	-2.174017	0.011143
C	-0.054923	-2.865696	0.137496
H	0.058660	-3.939567	0.190298
N	-1.300798	-2.402882	0.206805
C	-1.339706	-1.072382	0.129613
C	-6.050112	-0.080960	0.788968
H	-6.678539	0.738194	1.135894
C	-4.634634	0.018674	1.337184
H	-4.349132	1.063271	1.442226
H	-4.523342	-0.474261	2.299653
O	-6.668107	-1.322137	1.101283
H	-6.797066	-1.364085	2.053852
C	3.480877	-0.376862	-0.261311
C	4.371452	0.708350	-0.427487
C	3.995133	-1.671204	-0.177639
C	5.736970	0.472572	-0.505462
C	5.369592	-1.876100	-0.250303
H	3.332848	-2.508486	-0.050293
C	6.254196	-0.812017	-0.412956
H	6.401671	1.313305	-0.641917
H	7.318765	-0.989204	-0.473161
N	3.858732	2.025196	-0.531558
H	3.455360	2.313342	-1.412988
C	3.952176	3.007044	0.401020
O	3.559950	4.152843	0.136177
C	4.545792	2.662905	1.730929
H	4.138046	3.335147	2.480361
H	4.363402	1.630723	2.017252
H	5.625317	2.814248	1.694766
O	5.802594	-3.164104	-0.155269
H	6.762888	-3.198194	-0.218210

4dTa1b1

Sum of electronic and zero-point Energies = -871549.1 kcal/mol

H	-6.274763	2.031916	-0.903949
O	-5.692923	1.318806	-0.629690
C	-5.844852	0.240313	-1.534216
H	-5.583895	0.550074	-2.548970
H	-6.878575	-0.114997	-1.543123
C	-4.962453	-0.914213	-1.130492
H	-5.192255	-1.746621	-1.797719
O	-3.581754	-0.565769	-1.301509
C	-2.841792	-0.914720	-0.149988
H	-2.385731	-1.892438	-0.270847
N	-1.735626	0.027956	-0.016515
C	-1.994883	1.370508	-0.036630
H	-3.030812	1.627459	-0.188981
C	-1.039245	2.316925	0.104261
C	-1.338195	3.776258	0.081229
H	-2.401868	3.946284	-0.067378
H	-1.039606	4.254919	1.014360
H	-0.796690	4.277909	-0.721577
C	0.318459	1.884629	0.299517
O	1.275389	2.643079	0.474296
N	0.529341	0.495647	0.278123
C	-0.459588	-0.466281	0.143333
O	-0.202329	-1.665881	0.169548
C	-5.116636	-1.388822	0.321449
H	-6.008042	-0.971773	0.787595
C	-3.843938	-0.894232	0.992643
H	-3.986331	0.122962	1.353687
H	-3.538820	-1.521769	1.826248
O	-5.207498	-2.806335	0.300110
H	-5.301436	-3.116531	1.205859
C	1.852522	0.020015	0.528406
C	2.228615	-0.281823	1.840448
C	2.754388	-0.115725	-0.513373
C	3.515609	-0.756113	2.078712

C	4.048213	-0.576784	-0.270857
H	2.446791	0.138861	-1.517283
C	4.412562	-0.918245	1.032842
H	3.803867	-1.016821	3.087774
H	5.387874	-1.330538	1.237151
O	1.308400	-0.109508	2.817929
H	1.674748	-0.358216	3.672593
C	6.236348	-0.472386	-1.500897
N	4.911328	-0.735288	-1.370315
H	4.469359	-1.007669	-2.236247
O	6.790527	-0.707618	-2.587354
C	6.999896	0.099764	-0.349633
H	6.389474	0.731377	0.290449
H	7.410375	-0.704473	0.261456
H	7.832357	0.673298	-0.747332

5dTa1b1

Sum of electronic and zero-point Energies = -871550.8 kcal/mol

H	5.968320	-0.463290	2.038636
O	5.342783	-0.209736	1.355245
C	5.663830	-0.909980	0.167168
H	5.601094	-1.988527	0.329773
H	6.679888	-0.673927	-0.159196
C	4.718109	-0.524256	-0.942239
H	5.070050	-1.009651	-1.854099
O	3.398574	-1.005134	-0.653309
C	2.448321	0.013333	-0.889427
H	2.046021	-0.064595	-1.894868
N	1.318017	-0.204168	0.007253
C	1.542081	-0.330660	1.350734
H	2.574726	-0.246955	1.648571
C	0.563065	-0.561362	2.254881
C	0.827395	-0.700708	3.714007
H	1.888918	-0.590708	3.922451
H	0.286170	0.053599	4.286220
H	0.503195	-1.674158	4.083384
C	-0.786612	-0.685894	1.775222
O	-1.767418	-0.905854	2.488194
N	-0.960011	-0.539285	0.385067
C	0.056442	-0.315067	-0.534489
O	-0.172159	-0.215689	-1.735072
C	4.588094	0.983441	-1.206524
H	5.361875	1.549124	-0.689860
C	3.198873	1.318314	-0.681100
H	3.252991	1.559896	0.378940
H	2.741900	2.151780	-1.208267
O	4.706914	1.184842	-2.607744
H	4.661109	2.129959	-2.782677
C	-2.280100	-0.713583	-0.143905
C	-3.138739	0.390448	-0.268546
C	-2.674948	-1.988331	-0.512617
C	-4.418351	0.162370	-0.783539
C	-3.952172	-2.193886	-1.021685
H	-1.989081	-2.815180	-0.406072
C	-4.819628	-1.113251	-1.154861
H	-5.098707	0.987768	-0.893969
H	-5.813148	-1.268208	-1.552896
N	-2.662208	1.645438	0.114457
H	-1.698730	1.663866	0.406351
C	-3.310176	2.838768	0.172592
C	-2.479473	4.002141	0.624332
H	-2.949856	4.454204	1.496467
H	-1.454605	3.738188	0.870957
H	-2.471280	4.751933	-0.166110
O	-4.501893	2.976778	-0.125911
O	-4.296005	-3.463744	-1.371717
H	-5.193859	-3.481749	-1.718691

NAPQI

Sum of electronic and zero-point Energies = -322594.4 kcal/mol

N	-1.413439	0.817580	0.076229
C	-2.521529	0.007722	0.156936
C	-3.217730	-0.271747	-1.132116
H	-3.645870	0.651770	-1.524097
H	-2.515006	-0.645197	-1.875766
H	-4.012854	-0.993336	-0.968326
O	-2.950303	-0.339467	1.255829
C	-0.178409	0.446494	0.046342
C	0.236324	-0.950677	0.040300
C	0.849086	1.475979	0.008802
C	1.540631	-1.277182	0.002872
H	-0.529809	-1.712380	0.066572
C	2.154197	1.151416	-0.029577
H	0.519612	2.504809	0.014257
C	2.579885	-0.246636	-0.035261
H	1.868227	-2.306888	-0.004606
H	2.928077	1.904811	-0.057309
O	3.778674	-0.552891	-0.072593

dC

Sum of electronic and zero-point Energies = -511802.9 kcal/mol

C	2.388815	1.449889	0.358680
C	1.119616	0.985661	0.284881
N	0.857915	-0.311188	-0.023017
C	1.911218	-1.213370	-0.270076
N	3.176910	-0.757893	-0.202764
C	3.428068	0.515284	0.096587
O	1.645058	-2.399157	-0.534420
N	4.706471	0.908035	0.147727
H	5.445546	0.255638	-0.045524
H	4.946040	1.860242	0.356697
H	0.261393	1.616266	0.451229
H	2.594824	2.480449	0.597059
C	-0.520352	-0.757544	-0.127172
O	-1.200063	0.102304	-1.024599
C	-1.330935	-0.700784	1.158249
H	-0.473866	-1.766128	-0.526710
C	-2.593911	0.145499	-0.702000
C	-2.757911	-0.578046	0.643511
H	-1.066794	0.185656	1.732858
C	-3.088313	1.569929	-0.736408
H	-3.146800	-0.409106	-1.462835
H	-3.388312	-0.012902	1.328659
O	-3.355433	-1.839991	0.378878
O	-2.484824	2.326244	0.298042
H	-2.859267	2.005461	-1.711834
H	-4.174902	1.550611	-0.618355
H	-3.482849	-2.294927	1.216823
H	-2.832978	3.220891	0.265173
H	-1.186787	-1.579134	1.782417

dG

Sum of electronic and zero-point Energies = -604433.5 kcal/mol

H	-4.380657	-2.616419	0.544073
O	-3.816713	-1.882459	0.287665
C	-4.071879	-0.792975	1.155190
H	-3.842728	-1.063604	2.188743
H	-5.122690	-0.496187	1.106464
C	-3.232915	0.397489	0.762354
H	-3.525903	1.229227	1.405849
O	-1.846746	0.111589	0.984193
C	-1.082063	0.505541	-0.142133
H	-0.712955	1.520948	-0.009460
N	0.084993	-0.333101	-0.225907
C	0.114815	-1.691516	-0.440567
H	-0.788528	-2.255465	-0.586948
N	1.324535	-2.190345	-0.431986
C	2.139812	-1.107650	-0.196257
C	3.547991	-1.018684	-0.079430
O	4.395554	-1.919909	-0.171538
N	3.957912	0.295126	0.175737
H	4.955060	0.427064	0.268722
C	3.136357	1.382765	0.295656
N	3.722268	2.575215	0.499867
H	4.688103	2.629685	0.771898
H	3.132121	3.350817	0.743070
N	1.823922	1.299531	0.184774
C	1.388872	0.057348	-0.057577
C	-3.359898	0.841582	-0.702668
H	-4.209489	0.368772	-1.193274
C	-2.037799	0.411715	-1.320456
H	-2.108312	-0.615745	-1.671457
H	-1.739080	1.046094	-2.151298
O	-3.531142	2.252376	-0.707474
H	-3.607723	2.543378	-1.621219

dA

Sum of electronic and zero-point Energies = -557231.5 kcal/mol

H	3.865965	2.918935	0.253022
O	3.391230	2.103752	0.072103
C	3.786655	1.132538	1.023629
H	3.554788	1.472501	2.035803
H	4.862350	0.947207	0.965152
C	3.075542	-0.172662	0.767540
H	3.467066	-0.902370	1.478924
O	1.668927	-0.017769	0.996390
C	0.937726	-0.599939	-0.069496
H	0.694418	-1.634809	0.164725
N	-0.321975	0.083273	-0.200490
C	-0.520799	1.396970	-0.538581
H	0.302550	2.048495	-0.770380
N	-1.782631	1.755376	-0.533372
C	-2.456705	0.613361	-0.168287
C	-3.821596	0.331303	0.012359
N	-4.782558	1.246564	-0.170322
H	-5.745234	1.005309	-0.017271
H	-4.555134	2.189829	-0.425628
N	-4.168709	-0.916542	0.381217
C	-3.208533	-1.827270	0.556216

H -3.548237 -2.810414 0.851810
N -1.891526 -1.682091 0.413838
C -1.570302 -0.438025 0.051863
C 3.227801 -0.740662 -0.651595
H 4.018679 -0.236414 -1.205065
C 1.860241 -0.507575 -1.273937
H 1.815121 0.488957 -1.708322
H 1.619799 -1.238230 -2.042139
O 3.539240 -2.122043 -0.526645
H 3.624303 -2.494804 -1.409773

dT
Sum of electronic and zero-point Energies=
-548929.2 kcal/mol
H -2.629380 3.324598 -0.228770
O -2.372997 2.412711 -0.069703
C -3.081336 1.581270 -0.970708
H -2.828685 1.832083 -2.003778
H -4.160107 1.703627 -0.845377
C -2.746106 0.132781 -0.718873
H -3.365294 -0.467345 -1.388282
O -1.368739 -0.111386 -1.026058
C -0.775574 -0.888242 -0.002890
H -0.844110 -1.945814 -0.240157
N 0.645790 -0.583206 0.030400
C 1.062559 0.701718 0.267534
H 0.271322 1.409850 0.452480
C 2.360605 1.089454 0.263490
C 2.788601 2.489924 0.534810
H 3.462551 2.535567 1.390983
H 3.326090 2.909742 -0.316140
H 1.928305 3.121775 0.742068
C 3.356712 0.089156 -0.022551
O 4.576733 0.283114 -0.065386
N 2.857071 -1.180316 -0.268390
H 3.532589 -1.901211 -0.478809
C 1.548658 -1.583923 -0.273502
O 1.229211 -2.744116 -0.521943
C -2.968911 -0.358787 0.719520
H -3.529670 0.364637 1.309441
C -1.557081 -0.552320 1.256837
H -1.198258 0.373640 1.701287
H -1.502396 -1.341536 2.002371
O -3.695652 -1.577430 0.646055
H -3.860208 -1.884296 1.542901