Bridgehead Lithiation–Substitution of Bridged Ketones, Lactones, Lactams and Imides: Experimental Observations and Computational Insights

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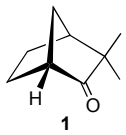
Supporting Information

Computational Methods

Geometry optimisations were performed using either B3LYP/6-31G* or B3LYP/6-31+G* level of theory using Spartan 04 (Windows), and single point B3LYP/6-31+G* energies were also calculated for a range of the B3LYP/6-31G* optimised structures. Zero point vibrational energies were calculated for all structures and the absence of imaginary frequencies was used to characterise the structures as minima on their potential energy surfaces. NBO calculations were performed on all anionic species using the NBO keyword in Spartan 04 (Windows).

Geometry Optimisations using B3LYP/6-31G*



1

H	-0.165006	0.255859	2.042368
C	0.214704	0.159291	1.020274
C	1.973845	-0.554707	-0.507135
C	-0.163668	0.338168	-1.335077
C	1.243307	0.760160	-0.922011
C	-0.917913	-0.047803	-0.035685
C	1.318214	-0.915064	0.864298
H	3.046968	-0.362323	-0.403193
H	1.759854	1.352410	-1.679322
H	0.938727	-1.939019	0.899054
H	1.857820	-1.343369	-1.257809
H	2.044157	-0.817085	1.679054
C	0.962148	1.396205	0.457423
H	1.878734	1.624610	1.012988
H	0.357102	2.306134	0.404876
O	-0.621789	0.288973	-2.456937
C	-2.091153	0.931924	0.188495
H	-1.760278	1.966264	0.325384
H	-2.659176	0.641353	1.080689
H	-2.767117	0.909547	-0.672572
C	-1.493955	-1.468681	-0.150362
H	-1.990807	-1.763024	0.782180
H	-0.731644	-2.219288	-0.379526
H	-2.233076	-1.500535	-0.957457

E = -426.6084402167 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 135.005 kcal/mol

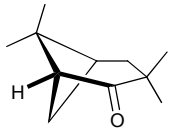
(Single point E = -426.622431 au (B3LYP/6-31+G*)

anion derived from 1

H	-0.003059	0.734511	1.875361
C	0.309175	0.443635	0.855311
C	2.112654	-0.408645	-0.605143
C	-0.062677	-0.125743	-1.420047
C	1.189121	0.625812	-1.294712
C	-0.872059	-0.046913	-0.044191
C	1.493786	-0.567815	0.859293
H	3.157732	-0.062215	-0.518236
H	1.190070	-1.598817	1.082949
H	2.136428	-1.370940	-1.131974
H	2.210109	-0.280353	1.646384
C	0.915072	1.527736	-0.069416
H	1.839369	1.958255	0.349488
H	0.235449	2.369185	-0.261209
O	-0.433497	-0.913407	-2.303061
C	-2.053701	0.943375	-0.074716
H	-1.747236	1.965527	-0.318230
H	-2.582769	0.976109	0.892208
H	-2.778508	0.627685	-0.837361
C	-1.449203	-1.431298	0.277563
H	-2.049506	-1.420298	1.201268
H	-0.668898	-2.190477	0.390879
H	-2.087852	-1.754911	-0.552410

E = -425.9420581751 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 124.610 kcal/mol

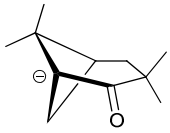
(Single point E = -425.9775964 au (B3LYP/6-31+G*)



13

C	-0.657472	-0.111225	1.280414
C	0.756513	-0.662996	1.017807
H	1.268846	-0.888056	1.961319
C	0.689611	-1.774963	-0.061806
H	1.585341	-2.397425	-0.092247
H	-0.181776	-2.432376	-0.072259
C	-1.519383	0.061690	-0.016915
C	0.754981	-0.625264	-1.109538
C	-0.628845	-0.026032	-1.287646
C	1.544895	0.208501	-0.023599
O	-1.036715	0.352335	-2.370639
C	-2.590372	-1.055770	-0.140025
H	-3.296848	-0.980638	0.695331
H	-2.164824	-2.062833	-0.123079
H	-3.148690	-0.939223	-1.074335
H	-1.178089	-0.786389	1.971589
H	-0.577139	0.851345	1.800395
C	-2.286726	1.399790	-0.014863
H	-2.850322	1.514740	-0.944717
H	-1.621334	2.263934	0.080302
H	-2.988044	1.427364	0.827646
H	1.220644	-0.791788	-2.085257
C	1.399950	1.732863	-0.015723
H	1.888445	2.160045	0.869652
H	0.363939	2.075539	-0.017372
H	1.886340	2.164938	-0.899082
C	3.046865	-0.118426	-0.038360
H	3.262771	-1.190557	-0.043063
H	3.531216	0.310602	0.847967
H	3.526219	0.320278	-0.921898

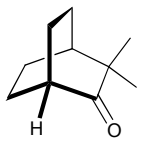
E = -505.2099980 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 169.381 kcal/mol



anion derived from 13

C	-0.636116	-0.222922	1.184767
C	0.785992	-0.758120	0.870736
H	1.273448	-1.072164	1.822538
C	0.605954	-1.754018	-0.282714
H	1.457135	-2.442280	-0.399888
H	-0.292080	-2.382203	-0.254462
C	-1.523542	0.050009	-0.099551
C	0.711467	-0.545886	-1.259757
C	-0.483053	0.275899	-1.276463
C	1.612028	0.141513	-0.124135
O	-0.629059	1.304324	-1.970364
C	-2.549338	-1.068989	-0.381585
H	-3.213749	-1.226304	0.485139
H	-2.094722	-2.030526	-0.627007
H	-3.183730	-0.784022	-1.232183
H	-1.134922	-0.960337	1.833938
H	-0.573484	0.703626	1.773569
C	-2.342776	1.335927	0.113129
H	-2.895804	1.592085	-0.795865
H	-1.697763	2.189943	0.342760
H	-3.056848	1.209998	0.943272
C	1.582503	1.663890	0.047910
H	2.317373	1.993557	0.799430
H	0.604014	2.048782	0.344495
H	1.822220	2.143944	-0.908990
C	3.095065	-0.276865	-0.211865
H	3.214642	-1.353940	-0.365118
H	3.659753	-0.000877	0.695409
H	3.565391	0.225956	-1.067146

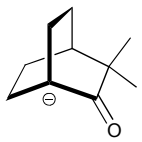
E = -504.5414560 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 159.165 kcal/mol



14

C	-0.021862	-0.035514	1.080542
C	1.646120	-1.238394	-0.406866
C	-0.273027	-0.020398	-1.401721
C	1.234579	0.022236	-1.207587
C	-1.065160	-0.007917	-0.077042
C	0.890197	-1.276757	0.955149
H	2.731495	-1.212640	-0.251898
H	0.309130	-2.198990	1.050493
H	1.437221	-2.137253	-0.998237
H	1.602479	-1.279031	1.788810
C	1.579785	1.282679	-0.378836
H	2.669812	1.351467	-0.280703
H	1.260290	2.179619	-0.922301
O	-0.817400	-0.060671	-2.489691
H	-0.552053	-0.057811	2.041995
C	0.899366	1.204496	1.019813
H	1.655753	1.113556	1.808333
H	0.344805	2.122431	1.236150
C	-1.941036	1.265828	-0.050406
H	-2.641776	1.248726	-0.890457
H	-1.354020	2.185974	-0.130689
H	-2.516642	1.312854	0.882248
C	-2.013305	-1.225972	-0.049529
H	-1.480859	-2.180173	-0.107128
H	-2.694159	-1.178172	-0.903978
H	-2.607340	-1.225508	0.872599
H	1.717608	0.045333	-2.189062

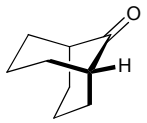
E = -465.9296957 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 153.308 kcal/mol



anion derived from 14

C	0.104655	0.012912	0.985765
C	1.408254	-1.312698	-0.661352
C	-0.218680	0.416797	-1.430240
C	1.178911	-0.005925	-1.427120
C	-1.018556	0.036252	-0.120497
C	0.952615	-1.259433	0.843418
H	2.481289	-1.565757	-0.699083
H	0.390361	-2.155183	1.147664
H	0.899413	-2.149652	-1.164427
H	1.815939	-1.195894	1.524734
C	1.839185	1.100047	-0.588664
H	2.904484	0.871858	-0.403609
H	1.807554	2.077945	-1.087034
O	-0.725574	1.263486	-2.189664
H	-0.369246	0.059593	1.981506
C	1.080277	1.215190	0.809326
H	1.778085	1.225840	1.664673
H	0.521790	2.161026	0.862105
C	-2.052642	1.133858	0.182521
H	-2.738592	1.249556	-0.662161
H	-1.578125	2.108248	0.338851
H	-2.635360	0.889447	1.085755
C	-1.793813	-1.292289	-0.223908
H	-1.167716	-2.133749	-0.533163
H	-2.594421	-1.188708	-0.968741
H	-2.270087	-1.562765	0.733345

E = -465.2568415 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 142.911 kcal/mol

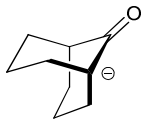


15

H	-1.319291	-2.158947	0.747618
C	-1.314634	-1.283033	0.085219
C	-1.314634	1.283033	0.085219
C	0.000000	0.000000	-1.592184
C	0.000000	1.261676	-0.740406
C	0.000000	-1.261676	-0.740406
C	-1.579595	0.000000	0.897580
H	-2.140493	1.429043	-0.624636
H	-0.974271	0.000000	1.807905
H	-2.140493	-1.429043	-0.624636
H	-1.319291	2.158947	0.747618
H	0.000000	2.123392	-1.417289
H	0.000000	-2.123392	-1.417289
H	-2.623526	0.000000	1.236491
O	0.000000	0.000000	-2.809187
C	1.314634	1.283033	0.085219
H	1.319291	2.158947	0.747618
H	2.140493	1.429043	-0.624636
C	1.579595	0.000000	0.897580
H	0.974271	0.000000	1.807905
H	2.623526	0.000000	1.236491
C	1.314634	-1.283033	0.085219
H	1.319291	-2.158947	0.747618
H	2.140493	-1.429043	-0.624636

E = -426.6184218 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 136.602 kcal/mol

(Single point E = -426.6327234 au (B3LYP/6-31+G*)

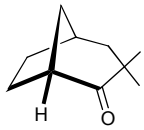


anion derived from 15

H	-1.052239	-1.943790	1.208952
C	-1.146962	-1.272894	0.337759
C	-1.519276	1.248758	-0.288620
C	-0.152372	-0.172669	-1.508206
C	-0.136593	1.150731	-0.930282
C	0.202372	-1.274589	-0.483590
C	-1.629059	0.125982	0.813231
H	-2.299624	1.080826	-1.042251
H	-1.018287	0.427682	1.675911
H	-1.910026	-1.706695	-0.321705
H	-1.744227	2.223014	0.185593
H	0.282346	-2.263820	-0.963179
H	-2.659951	0.029388	1.198838
O	-0.820969	-0.533429	-2.504943
C	1.018329	1.448285	0.032310
H	1.500627	2.420122	-0.202575
C	1.459571	-0.991139	0.374004
H	2.190942	-1.804679	0.251928
H	0.704358	1.558497	1.093049
H	1.205221	-0.973106	1.446439
C	2.092942	0.354397	-0.003087
H	2.490359	0.278769	-1.026522
H	2.942519	0.590359	0.656947

E = -425.9461597 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 126.128 kcal/mol

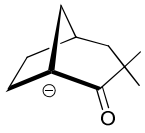
(Single point E = -425.9804511 au (B3LYP/6-31+G*)



16

C	-0.411608	0.641089	1.163198
C	1.120077	0.730908	1.005206
H	1.518049	1.307898	1.848387
C	1.819610	-0.646075	0.890085
H	1.331324	-1.409423	1.504601
H	2.852623	-0.570325	1.247777
C	1.802634	-0.987006	-0.629543
H	2.822762	-1.070933	-1.020262
H	1.304871	-1.935543	-0.855428
C	-1.193501	-0.009603	-0.022754
C	1.102780	0.224504	-1.312658
C	-0.409918	0.036886	-1.361023
C	1.437595	1.382532	-0.351035
H	2.499269	1.648149	-0.434282
H	0.852532	2.290677	-0.542557
O	-0.992392	-0.100106	-2.422052
C	-1.506789	-1.502221	0.262692
H	-2.158267	-1.577357	1.141667
H	-0.608742	-2.094299	0.462531
H	-2.028072	-1.949731	-0.589725
H	-0.659021	0.107062	2.090691
H	-0.782900	1.665842	1.297908
C	-2.537032	0.721760	-0.223004
H	-3.102499	0.272607	-1.043064
H	-2.380747	1.780308	-0.461008
H	-3.134965	0.665606	0.694352
H	1.442325	0.376793	-2.340700

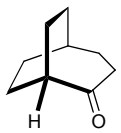
E = -465.9273950 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 153.433 kcal/mol



anion derived from 16

C	-0.344087	0.306006	1.188225
C	1.139011	0.689194	0.901666
H	1.490739	1.334602	1.728072
C	2.128946	-0.510403	0.703311
H	1.766063	-1.413242	1.215144
H	3.109235	-0.268568	1.149908
C	2.197293	-0.744090	-0.862304
H	3.175084	-0.396678	-1.244422
H	2.093028	-1.802404	-1.120939
C	-1.202974	-0.098428	-0.077268
C	1.001412	0.068933	-1.348116
C	-0.191470	-0.677932	-1.141109
C	1.152754	1.325700	-0.499849
H	2.121275	1.816471	-0.701803
H	0.388813	2.100865	-0.618703
O	-0.413363	-1.843791	-1.567544
C	-2.189892	-1.207556	0.327832
H	-2.878261	-0.856261	1.114305
H	-1.654193	-2.087571	0.694054
H	-2.777774	-1.534114	-0.535888
H	-0.369198	-0.529121	1.904902
H	-0.830415	1.154845	1.698866
C	-2.051992	1.073679	-0.618833
H	-2.661311	0.727201	-1.464637
H	-1.455959	1.916756	-0.976190
H	-2.742763	1.455907	0.151320

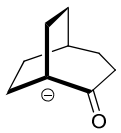
E = -465.2787870 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 143.495 kcal/mol



17

C	-1.476577	-0.977888	0.347334
C	0.482669	-0.905374	-1.330583
H	-0.197007	-1.286860	-2.102660
H	1.451855	-1.384078	-1.519568
C	0.634797	0.639252	-1.455446
H	1.606859	0.873795	-1.905409
H	-0.116734	1.050699	-2.139515
C	-1.893215	0.480343	0.039630
C	0.557546	1.365116	-0.096478
C	-0.861040	1.511409	0.466717
C	1.435780	0.623964	0.937972
H	2.468518	0.644011	0.567733
H	1.429051	1.179736	1.881251
O	-1.126410	2.410674	1.244148
H	-2.128172	-1.640564	-0.236421
H	-1.688291	-1.191203	1.403066
H	0.937661	2.388070	-0.199673
C	-0.000767	-1.353858	0.063946
H	0.035528	-2.451066	0.093744
C	0.975748	-0.841599	1.153138
H	0.500781	-0.950947	2.135878
H	1.856125	-1.495344	1.167191
H	-2.841533	0.723230	0.527134
H	-2.043172	0.588482	-1.043127

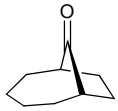
E = -426.6132659 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 136.678 kcal/mol



anion derived from 17

C	1.392033	0.510712	0.827268
C	-0.616463	1.464309	-0.454126
H	0.002272	2.343075	-0.701049
H	-1.640996	1.846445	-0.313731
C	-0.570554	0.376696	-1.586537
H	-1.519203	0.427597	-2.151439
H	0.210977	0.634258	-2.313646
C	1.916477	-0.268859	-0.413954
C	-0.375503	-1.025630	-1.035752
C	0.902311	-1.419814	-0.573655
C	-1.426693	-1.292976	0.024503
H	-2.452660	-1.082406	-0.330357
H	-1.403829	-2.336049	0.357054
O	1.191487	-2.506314	0.006083
H	1.934674	1.467389	0.925372
H	1.636590	-0.080436	1.721323
C	-0.139451	0.832432	0.866660
H	-0.250025	1.580654	1.670214
C	-1.088436	-0.353800	1.242115
H	-0.604424	-0.941732	2.034213
H	-2.003919	0.075138	1.691119
H	2.925360	-0.656248	-0.214109
H	1.979976	0.405560	-1.277572

E = -425.9679636 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 126.683 kcal/mol

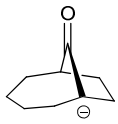


20

C	-0.391552	0.100733	-1.362750
C	-0.760504	-1.142982	-0.562454
C	-2.047096	-0.648176	0.129172
C	-1.767581	0.859007	0.462541
C	-0.546525	1.283421	-0.403221
H	-0.913703	-1.992687	-1.233175
H	-2.897147	-0.731359	-0.558351
H	-2.294802	-1.232296	1.022108
H	-1.559415	0.996827	1.528757
H	-2.646875	1.469592	0.234694
H	-0.743983	2.190567	-0.980345
C	0.357757	-1.450053	0.483202
H	0.376950	-2.532839	0.656479
H	0.075936	-1.002118	1.443799
C	1.777917	-0.976303	0.120957
H	2.113624	-1.494585	-0.785777
H	2.444422	-1.314275	0.924395
C	1.960803	0.564742	-0.078198
H	2.867427	0.882821	0.450647
H	2.144143	0.775534	-1.137074
C	0.796155	1.458188	0.396924
H	0.606953	1.283879	1.463561
H	1.116847	2.502876	0.314995
O	-0.069752	0.149486	-2.530887

E = -426.5994729 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 136.418 kcal/mol

(Single point E = -426.6133318 au (B3LYP/6-31+G*)



anion derived from 20

C	-0.279632	0.068347	-1.401481
C	-1.114671	-0.944015	-0.596035
C	-2.225186	-0.063330	-0.018198
C	-1.448504	1.246597	0.326871
C	-0.252223	1.244346	-0.612530
H	-1.476289	-1.815919	-1.163095
H	-2.993437	0.121008	-0.782958
H	-2.733288	-0.491776	0.860461
H	-1.156233	1.236084	1.398934
H	-2.121604	2.122142	0.234098
C	-0.122371	-1.365139	0.550438
H	-0.246954	-2.437661	0.779943
H	-0.423680	-0.839469	1.466938
C	1.412886	-1.131329	0.362758
H	1.765070	-1.844847	-0.392898
H	1.864746	-1.453862	1.315137
C	2.024159	0.270583	-0.030389
H	2.918308	0.448586	0.591250
H	2.369747	0.166932	-1.061114
C	1.113414	1.538610	-0.015565
H	0.966509	1.871196	1.027668
H	1.708003	2.351245	-0.482340
O	0.451232	-0.298329	-2.357892

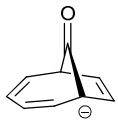
E = -425.9542503 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 126.376 kcal/mol

(Single point E = -425.9875031 au (B3LYP/6-31+G*)

21

C	-1.288869	0.788266	0.000000
C	-0.369357	0.745547	1.228026
C	0.879325	1.401929	0.671276
C	0.879325	1.401929	-0.671276
C	-0.369357	0.745547	-1.228026
H	-0.826242	1.265840	2.075448
H	1.691182	1.755032	1.300175
H	1.691182	1.755032	-1.300175
C	-0.056514	-0.698657	1.597315
H	0.038325	-0.906905	2.660995
C	0.151800	-1.713280	0.733236
H	0.382477	-2.681145	1.175331
C	0.151800	-1.713280	-0.733236
H	0.382477	-2.681145	-1.175331
C	-0.056514	-0.698657	-1.597315
H	0.038325	-0.906905	-2.660995
O	-2.493126	0.875010	0.000000
H	-0.826242	1.265840	-2.075448

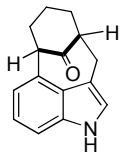
E = -422.9214332 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 90.921 kcal/mol



anion derived from 21

C	0.464385	0.152996	1.392823
C	1.308853	-0.618069	0.346557
C	1.739851	0.495893	-0.601426
C	0.937120	1.565949	-0.388451
C	-0.031103	1.345234	0.711212
H	2.132325	-1.219233	0.759231
H	2.549380	0.415011	-1.325774
H	0.971914	2.479706	-0.987486
C	0.233102	-1.536119	-0.255062
H	0.575734	-2.509278	-0.612998
C	-1.091338	-1.259653	-0.397758
H	-1.684798	-2.072707	-0.828556
C	-1.881407	-0.040597	-0.169167
H	-2.937771	-0.130876	-0.444296
C	-1.407964	1.179539	0.231349
H	-2.064919	2.047466	0.063151
O	0.186635	-0.295263	2.506652

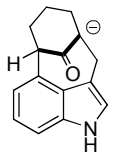
E = -422.2868618 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 80.711 kcal/mol



42

C	-0.754160	-0.974458	-0.510782
C	-3.445143	-0.264146	0.183679
C	-1.085978	0.373581	-0.241896
C	-1.782502	-1.915408	-0.469882
C	-3.105448	-1.571166	-0.135742
C	-2.426064	0.690619	0.125990
H	-1.550172	-2.955056	-0.688769
H	-3.868112	-2.344869	-0.118367
H	-4.460640	0.007585	0.459373
C	-0.335360	1.611692	-0.214597
C	-1.217734	2.586108	0.180341
H	-1.052948	3.647610	0.309621
N	-2.470814	2.042399	0.384877
H	-3.288276	2.553089	0.678750
C	0.671112	-1.466449	-0.733179
C	2.097318	0.725851	-0.644142
C	2.558925	0.322277	0.777368
C	1.330734	-1.872162	0.616670
C	1.567160	-0.458468	-1.455720
H	2.969624	1.087369	-1.199909
H	0.626702	-2.344795	-1.385988
H	2.710798	1.229095	1.377695
H	0.675105	-2.583173	1.132372
C	1.066593	1.883212	-0.698500
H	1.019729	2.199534	-1.750649
H	1.486486	2.733923	-0.145149
O	1.852160	-0.593503	-2.631544
H	2.271312	-2.400301	0.401433
H	3.545232	-0.154048	0.684722
C	1.621873	-0.655448	1.500442
H	2.088556	-0.981041	2.438813
H	0.683931	-0.159454	1.772672

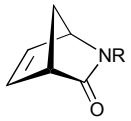
E = -710.6145339 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 169.651 kcal/mol



anion derived from 42

C	-0.424199	-0.988002	-0.542335
C	-3.170105	-0.805748	0.300684
C	-0.996872	0.295389	-0.253367
C	-1.249713	-2.106388	-0.398788
C	-2.592247	-2.033222	0.014310
C	-2.363803	0.329170	0.157664
H	-0.824891	-3.084247	-0.620473
H	-3.178562	-2.946017	0.106199
H	-4.208802	-0.719783	0.615929
C	-0.534141	1.694861	-0.252585
C	-1.601378	2.444493	0.159985
H	-1.667706	3.517981	0.290339
N	-2.726395	1.648110	0.361387
H	-3.526199	1.921286	0.912541
C	1.041397	-1.227271	-0.951287
C	1.846042	1.096930	-0.603821
C	2.428168	0.713233	0.749267
C	1.876985	-1.696393	0.259118
C	1.470098	0.125420	-1.548815
H	1.050783	-2.013492	-1.722445
H	2.239229	1.519621	1.476653
H	1.467355	-2.635500	0.665699
C	0.846326	2.232061	-0.654256
H	0.776689	2.620652	-1.678037
H	1.099126	3.088040	-0.005126
O	1.079021	0.339995	-2.731736
H	2.898452	-1.922067	-0.087056
H	3.535262	0.641854	0.700190
C	1.926814	-0.618002	1.345424
H	2.567266	-0.948102	2.181552
H	0.916000	-0.484862	1.753187

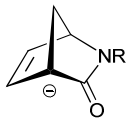
E = -709.9695470 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 159.350 kcal/mol



59 R = Me

H	-0.551534	-2.192114	1.277128
C	-0.722094	-1.263726	0.743844
C	-1.300093	0.877648	0.055808
N	0.904528	0.242263	-0.312728
C	0.185013	1.315003	0.183096
C	-0.060348	-0.854684	-0.586260
C	-1.455192	-0.211154	1.128223
H	0.389748	-1.641921	-1.193033
H	-2.003038	-0.079222	2.054429
C	-1.199326	-0.017523	-1.209147
H	-2.110271	-0.592385	-1.394248
H	-0.886492	0.514669	-2.113074
O	0.633326	2.340947	0.662218
C	2.276696	0.001219	0.079372
H	2.719995	0.962908	0.347254
H	2.844305	-0.438315	-0.748297
H	2.340766	-0.670429	0.948900
H	-2.005992	1.706815	0.076515

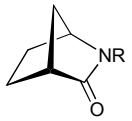
E = -402.1015593 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 95.005 kcal/mol



anion derived from **59** R = Me

H	0.832296	-0.483145	2.315610
C	0.894002	-0.349579	1.235360
C	1.292123	-0.558783	-1.108127
N	-0.803946	0.369736	-0.417165
C	-0.211157	-0.660832	-1.236605
C	0.320129	0.850539	0.441206
C	1.386073	-1.182436	0.292039
H	0.024555	1.739588	1.020470
H	1.729826	-2.202711	0.484296
C	1.380012	0.951576	-0.648125
H	2.376390	1.196206	-0.255987
H	1.110693	1.668112	-1.439182
O	-0.918297	-1.495206	-1.804003
C	-2.090675	0.101956	0.170131
H	-2.658661	-0.501943	-0.544583
H	-2.648565	1.029202	0.380703
H	-2.014799	-0.472279	1.113963

E = -401.4351384 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 84.811 kcal/mol

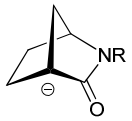


61 R = Me

H	0.004530	-1.634911	1.289283
C	-0.692342	-1.265759	0.529767
C	-1.083486	1.075273	-0.069127
N	1.058255	0.249159	-0.283650
C	0.399954	1.364407	0.199723
C	0.054910	-0.734296	-0.723491
C	-1.481961	0.001165	0.994377
H	0.494787	-1.493525	-1.374470
H	-1.223120	0.318668	2.008679
H	-1.362599	-2.092138	0.267977
H	-2.563508	-0.168968	0.965922
C	-0.992055	0.210838	-1.342507
H	-1.930820	-0.294848	-1.593484
H	-0.612320	0.747651	-2.216766
O	0.904946	2.312492	0.778762
C	2.415211	-0.085365	0.088355
H	2.888682	0.825785	0.460677
H	2.975786	-0.457245	-0.777316
H	2.450381	-0.848816	0.879720
H	-1.705231	1.970434	-0.082431

E = -403.3499205 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 110.430 kcal/mol

(Single point E = -403.3641136 au (B3LYP/6-31+G*)

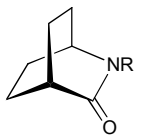


anion derived from 61 R = Me

H	0.060192	-0.739510	1.766189
C	0.792988	-0.167472	1.179600
C	1.079060	-0.378086	-1.311923
N	-1.013355	0.348149	-0.435884
C	-0.386549	-0.647349	-1.274639
C	0.105015	0.938979	0.325455
C	1.504819	-1.029261	0.044767
H	-0.219253	1.827126	0.891817
H	1.224181	-2.088385	0.113855
H	1.501409	0.278529	1.896570
H	2.597100	-0.975711	0.189101
C	1.099331	1.100405	-0.833504
H	2.095617	1.426345	-0.493603
H	0.731385	1.821449	-1.578512
O	-1.054466	-1.585824	-1.722589
C	-2.270998	0.039779	0.192021
H	-2.812714	-0.627328	-0.485770
H	-2.876518	0.942393	0.375655
H	-2.157242	-0.484227	1.161395

E = -402.6784719358 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 99.928 kcal/mol

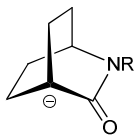
(Single point E = -402.7146914 au (B3LYP/6-31+G*)



64 R = H

C	1.202332	-0.468252	0.000000
C	-0.611301	0.730694	-1.260493
C	-1.051364	-1.378062	0.000000
C	-1.286656	0.133189	0.000000
N	0.297276	-1.623381	0.000000
C	0.903345	0.373517	-1.258593
H	-0.760115	1.817212	-1.262603
H	-2.363838	0.315007	0.000000
H	1.171090	-0.200874	-2.151520
H	-1.100865	0.343545	-2.160353
H	1.527846	1.274648	-1.252396
C	-0.611301	0.730694	1.260493
H	-0.760115	1.817212	1.262603
H	-1.100865	0.343545	2.160353
O	-1.915738	-2.243183	0.000000
H	2.233317	-0.832806	0.000000
C	0.903345	0.373517	1.258593
H	1.527846	1.274648	1.252396
H	1.171090	-0.200874	2.151520
H	0.624673	-2.579995	0.000000

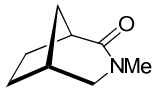
E = -403.3618335 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 111.082 kcal/mol



anion derived from **64** R = H

C	0.094070	-0.656830	0.959136
C	1.274277	0.247445	-1.013079
C	-0.915060	-0.886741	-1.219660
C	-0.200641	0.400883	-1.429333
N	-0.454117	-1.582750	-0.059537
C	1.487390	-0.245830	0.468400
H	1.785772	1.216995	-1.140453
H	2.170957	-1.106978	0.527778
H	1.786921	-0.454234	-1.687955
H	1.896477	0.541162	1.124003
C	-0.853259	1.298803	-0.354160
H	-0.329076	2.269687	-0.308888
H	-1.904750	1.522560	-0.589009
O	-1.888275	-1.352565	-1.826819
H	0.142576	-1.190822	1.918751
C	-0.787984	0.617236	1.074534
H	-0.364866	1.281864	1.847461
H	-1.789657	0.323323	1.427576
H	-1.150754	-2.243208	0.281254

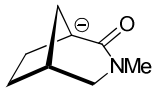
E = -402.6836649 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 100.455 kcal/mol



68

C	0.731560	-1.212319	-0.146425
C	-0.794213	-1.177933	-0.290402
H	-1.129554	-2.182452	-0.570840
C	-1.487736	-0.668928	1.001540
H	-0.915713	-0.940233	1.895762
H	-2.477669	-1.125981	1.107930
C	-1.603468	0.872923	0.821454
H	-2.651785	1.176484	0.719703
H	-1.185085	1.436528	1.661050
N	1.320335	0.120823	-0.004307
C	-0.855679	1.162584	-0.506354
C	0.643074	1.298745	-0.236416
C	-1.147006	-0.101186	-1.331436
H	-2.206433	-0.145147	-1.613275
H	-0.549034	-0.174270	-2.247459
O	1.189074	2.396299	-0.187643
C	2.750973	0.162039	0.249404
H	3.308279	-0.322011	-0.565287
H	2.990008	-0.358991	1.185670
H	3.053996	1.206176	0.322985
H	1.012452	-1.812452	0.731708
H	1.178180	-1.707664	-1.024574
H	-1.174554	2.096966	-0.972787

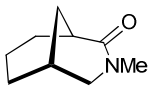
E = -442.6721603867 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 128.859 kcal/mol



anion derived from 68

C	0.709943	-1.064249	0.353750
C	-0.815896	-1.117155	0.088215
H	-1.151268	-2.159889	0.238472
C	-1.679734	-0.142225	0.952610
H	-1.197017	0.067167	1.918189
H	-2.655551	-0.604869	1.182095
C	-1.804420	1.176597	0.080006
H	-2.842387	1.266696	-0.291252
H	-1.588000	2.074393	0.670114
N	1.368991	0.027302	-0.381738
C	-0.771255	0.947616	-1.016050
C	0.540568	1.219752	-0.509360
C	-0.985155	-0.526773	-1.329044
H	-2.001876	-0.715707	-1.716917
H	-0.268348	-0.949990	-2.044082
O	1.013641	2.311579	-0.119283
C	2.735727	0.246705	0.029624
H	3.354675	-0.635870	-0.202602
H	2.840438	0.454626	1.113006
H	3.127366	1.117735	-0.500451
H	0.904735	-0.972245	1.443413
H	1.164823	-2.021198	0.041284

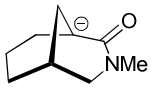
E = -442.0114325588 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 118.401 kcal/mol



69

C	0.990841	-1.222067	-0.192179
C	-0.503387	-1.298350	-0.546342
H	-0.660384	-2.280810	-1.010538
C	-1.447887	-1.194714	0.671513
H	-1.205920	-1.981703	1.398231
C	-1.565181	1.323335	0.331330
H	-2.588350	1.332531	-0.070984
H	-1.398587	2.294021	0.811713
N	1.512349	0.135960	-0.014804
C	-0.584370	1.158083	-0.854093
C	0.853215	1.296625	-0.350890
C	-0.817459	-0.186127	-1.555033
H	-1.856973	-0.257246	-1.901425
H	-0.175918	-0.277228	-2.441633
O	1.366369	2.405011	-0.219707
H	1.186804	-1.788087	0.730907
H	1.574924	-1.714001	-0.986952
H	-0.727789	1.992752	-1.547257
H	-2.468948	-1.401940	0.319323
C	-1.420127	0.183665	1.352340
H	-0.479282	0.305557	1.904315
H	-2.221305	0.243605	2.099871
C	2.894381	0.216258	0.432589
H	3.564026	-0.282684	-0.281949
H	3.012206	-0.270213	1.409521
H	3.166752	1.267765	0.512132

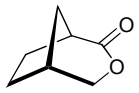
E = -481.9921978 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 147.229 kcal/mol



anion derived from **69**

C	1.025551	1.068648	-0.288624
C	-0.416558	1.352497	0.223595
H	-0.507854	2.444661	0.384214
C	-1.566663	0.948984	-0.738937
H	-1.431057	1.442181	-1.715875
C	-1.681249	-1.388059	0.366852
H	-2.607328	-1.245712	0.955399
H	-1.619817	-2.455079	0.116921
N	1.664746	-0.078395	0.381103
C	-0.451451	-0.919039	1.117038
C	0.765964	-1.234914	0.479224
C	-0.581878	0.535115	1.518417
H	-1.567461	0.742270	1.970533
H	0.181258	0.842095	2.248560
O	1.133388	-2.320575	-0.042471
H	1.018917	0.922519	-1.390245
H	1.655393	1.956230	-0.109422
H	-2.495007	1.373081	-0.317606
C	-1.768961	-0.570290	-0.952942
H	-0.971101	-0.947992	-1.606530
H	-2.721160	-0.725253	-1.496156
C	2.969340	-0.371885	-0.168109
H	3.662573	0.461475	0.033818
H	2.959851	-0.547047	-1.262460
H	3.350565	-1.285515	0.293699

E = -481.3416305 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 136.890 kcal/mol

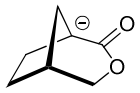


70

C	1.692816	-0.389346	-0.394923
C	0.896186	0.660984	0.377764
H	1.612563	1.337909	0.856819
C	-0.111650	1.413440	-0.527911
H	0.274195	1.539532	-1.545373
H	-0.300368	2.416776	-0.131520
C	-1.407351	0.551031	-0.491004
H	-2.229047	1.095065	-0.012578
H	-1.754331	0.254453	-1.485389
O	0.897546	-1.478931	-0.918147
C	-1.032117	-0.676546	0.386855
C	-0.372172	-1.732936	-0.490673
C	-0.010560	-0.083533	1.371447
H	-0.502865	0.605353	2.068059
H	0.520057	-0.840041	1.961701
O	-0.925596	-2.738085	-0.865435
H	2.196697	0.050300	-1.262259
H	2.457392	-0.840060	0.250491
H	-1.901395	-1.145365	0.852075

E = -423.2183962 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 103.189 kcal/mol

(Single point E = -423.2339195 au (B3LYP/6-31+G*)

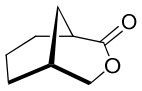


anion derived from 70

C	1.646685	0.031952	-0.502848
C	0.472476	0.951751	-0.061542
H	0.811639	2.001359	-0.145547
C	-0.871327	0.751728	-0.833329
H	-0.691423	0.423976	-1.868156
H	-1.418716	1.708247	-0.897112
C	-1.649792	-0.356027	-0.008524
H	-2.520120	0.106985	0.491942
H	-2.031309	-1.152924	-0.656939
O	1.653848	-1.249055	0.127520
C	-0.577248	-0.861654	0.951387
C	0.291208	-1.765363	0.277300
C	0.118869	0.433968	1.345379
H	-0.567260	1.122245	1.868271
H	1.005254	0.299262	1.977727
O	0.079425	-2.866788	-0.234003
H	1.648061	-0.091255	-1.602752
H	2.599731	0.511594	-0.228771

E = -422.5700735 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 93.064 kcal/mol

(Single point E = -422.6062407 au (B3LYP/6-31+G*)

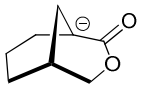


71

C	-1.771288	-0.399572	0.683386
C	-1.181988	0.390503	-0.487308
H	-2.039047	0.754228	-1.070043
C	-0.330704	1.606700	-0.066025
H	-0.928540	2.282384	0.559808
C	1.731602	0.112067	-0.082537
H	2.150347	0.512689	-1.016633
H	2.572678	-0.247089	0.520495
O	-0.843934	-1.257972	1.388125
C	0.808367	-1.077857	-0.450245
C	0.311618	-1.724270	0.839723
C	-0.350505	-0.585887	-1.328669
H	0.043128	-0.097359	-2.229170
H	-0.971037	-1.427966	-1.662553
O	0.937187	-2.569872	1.434173
H	-2.183429	0.263373	1.451096
H	-2.582746	-1.045888	0.325217
H	1.400248	-1.843129	-0.961032
H	-0.076111	2.168147	-0.976501
C	0.966562	1.216029	0.665041
H	0.731067	0.871690	1.680114
H	1.606527	2.099050	0.783537

E = -462.5389116816 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 121.836 kcal/mol

(Single point E = -462.554523 au (B3LYP/6-31+G*)

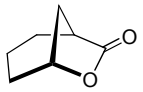


anion derived from 71

C	1.807394	0.109404	-0.672283
C	0.904960	0.844660	0.368628
H	1.488445	1.691123	0.782803
C	-0.423316	1.441624	-0.169638
H	-0.213815	2.144343	-0.993133
C	-1.633597	-0.787172	0.343118
H	-2.177353	-0.469471	1.251759
H	-2.241618	-1.563722	-0.139351
O	1.813623	-1.310511	-0.548480
C	-0.235461	-1.277814	0.660162
C	0.442095	-1.823469	-0.441304
C	0.553995	-0.226417	1.413208
H	-0.041120	0.211988	2.232419
H	1.473328	-0.626307	1.865446
O	0.079852	-2.603571	-1.334704
H	1.523924	0.399118	-1.701955
H	2.852283	0.424469	-0.530278
H	-0.852359	2.053739	0.642719
C	-1.489779	0.417482	-0.630309
H	-1.187727	-0.001875	-1.599147
H	-2.443754	0.952378	-0.799680

E = -461.9013261 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 111.766 kcal/mol

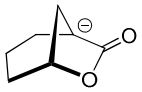
(Single point E = -461.9365242 au (B3LYP/6-31+G*)



72

C	-0.088106	1.384201	-0.263420
H	-0.200226	2.466614	-0.357974
C	-1.437223	0.671257	-0.098362
H	-1.851819	0.954213	0.878592
C	-0.010068	-1.385707	0.524695
H	-0.186781	-1.442625	1.606721
O	0.553356	0.924636	-1.489907
C	1.212652	-0.462482	0.290319
C	1.329914	-0.169479	-1.208645
C	0.897919	0.940159	0.826100
H	0.457618	0.942875	1.828382
H	1.787764	1.579581	0.831589
O	1.943627	-0.763104	-2.056208
H	2.133573	-0.910941	0.668607
H	-2.143853	1.021142	-0.859516
H	0.215980	-2.401717	0.182163
C	-1.265109	-0.859161	-0.205875
H	-2.161066	-1.366059	0.170051
H	-1.188150	-1.123402	-1.267312

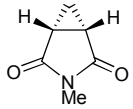
E = -423.2292434 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 103.502 kcal/mol



anion derived from **72**

C	1.299302	0.442493	-0.308202
H	2.228003	1.025783	-0.430413
C	0.071955	1.388410	-0.294594
H	0.197686	2.065091	0.566929
C	-1.248849	-0.647179	0.685334
H	-1.364103	-0.379370	1.750139
O	1.251457	-0.498326	-1.400122
C	0.074135	-1.394433	0.466493
C	0.291099	-1.512443	-0.958974
C	1.213595	-0.463788	0.911896
H	0.997818	0.084357	1.841865
H	2.169427	-0.995935	1.061122
O	-0.199602	-2.209262	-1.839122
H	0.076096	2.024808	-1.192826
H	-2.128269	-1.258477	0.428615
C	-1.291784	0.644852	-0.196008
H	-2.076145	1.358892	0.118660
H	-1.561819	0.324526	-1.210794

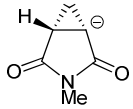
E = -422.5750309 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 93.091 kcal/mol



73

C	-0.610378	0.429788	0.758212
C	-0.610378	0.429788	-0.758212
C	0.802800	0.122607	-1.178885
N	1.508227	-0.151963	0.000000
C	0.802800	0.122607	1.178885
H	2.489767	-0.401219	0.000000
O	1.271578	0.113362	2.295155
O	1.271578	0.113362	-2.295155
C	-1.302918	-0.680496	0.000000
H	-2.388765	-0.663717	0.000000
H	-0.865495	-1.675109	0.000000
H	-1.184408	1.120495	1.364653
H	-1.184408	1.120495	-1.364653

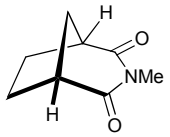
E = -398.7354465 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 61.615 kcal/mol



anion derived from 73

H	-1.336736	-1.407295	0.915258
C	-0.715940	-0.679205	0.391470
C	-0.556469	0.782473	0.849478
C	0.793770	1.128304	0.400250
N	1.443334	-0.075774	-0.035535
C	0.599321	-1.178901	-0.083410
H	2.382473	-0.091037	-0.416027
O	0.962700	-2.329132	-0.346065
O	1.379816	2.211597	0.325500
C	-1.398228	0.473223	-0.350078
H	-2.492578	0.492701	-0.274898
H	-1.061464	0.673045	-1.375943

E = -398.1065432 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 52.230 kcal/mol

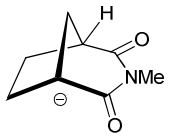


75

C	0.704115	-1.255991	-0.157353
C	-0.795716	-1.175187	-0.403388
H	-1.105393	-2.156180	-0.768752
C	-1.527864	-0.761953	0.907832
H	-1.043259	-1.180387	1.795122
H	-2.550405	-1.152791	0.887864
C	-1.525742	0.794118	0.890793
H	-1.052754	1.231492	1.775213
N	1.369092	-0.020264	-0.052619
C	-0.776656	1.174617	-0.419302
C	0.722638	1.220856	-0.165792
C	-1.101863	-0.003908	-1.350773
H	-2.161088	0.002374	-1.633552
H	-0.503683	-0.015227	-2.268174
O	1.297392	-2.312623	-0.034466
O	1.349954	2.258000	-0.042726
C	2.813222	-0.002063	0.201498
H	3.325450	0.532857	-0.601999
H	3.152835	-1.034691	0.250566
H	3.019699	0.513628	1.142913
H	-1.062753	2.157354	-0.799236
H	-2.547223	1.185968	0.846329

E = -516.7081326 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 116.957 kcal/mol

(Single point E = -516.7269199 au (B3LYP/6-31+G*)

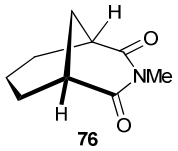


anion derived from 75

C	0.746202	-1.103425	0.319528
C	-0.766382	-1.163185	0.056724
H	-1.052687	-2.218612	0.169797
C	-1.648609	-0.234679	0.963958
H	-1.181442	-0.066448	1.942808
H	-2.614947	-0.728037	1.157743
C	-1.793301	1.116774	0.148701
H	-2.826050	1.201332	-0.233335
H	-1.601862	1.992124	0.778601
N	1.379788	0.013523	-0.185562
C	-0.744703	0.954143	-0.951226
C	0.542133	1.230737	-0.412363
C	-0.937761	-0.508831	-1.328381
H	-1.950344	-0.683522	-1.729094
H	-0.220572	-0.891676	-2.065527
O	1.361808	-2.011279	0.886790
O	1.020719	2.301167	0.000465
C	2.800512	0.166004	0.069688
H	3.397316	-0.467921	-0.601170
H	3.049864	-0.117400	1.099294
H	3.040317	1.219212	-0.087439

E = -516.0687622924 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 107.248 kcal/mol

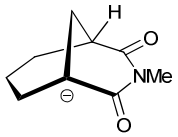
(Single point E = -516.1074375 au (B3LYP/6-31+G*)



76

C	0.931675	-1.264925	-0.242134
C	-0.520009	-1.237557	-0.709731
H	-0.652646	-2.163343	-1.278193
C	-1.477881	-1.261524	0.508577
H	-1.268359	-2.144380	1.122992
C	-1.451769	1.291273	0.491764
H	-2.471436	1.421398	0.103547
H	-1.224969	2.177360	1.095396
N	1.580056	-0.024465	-0.096488
C	-0.494075	1.231729	-0.725110
C	0.956619	1.223790	-0.257229
C	-0.791025	-0.005239	-1.576719
H	-1.836355	0.002981	-1.909468
H	-0.164677	-0.017436	-2.477107
O	1.567893	2.248770	-0.008555
H	-0.604480	2.153952	-1.304043
H	-2.499962	-1.376002	0.121943
C	-1.382971	0.019450	1.355210
H	-0.445556	0.013496	1.926995
H	-2.187416	0.032190	2.100679
C	2.977860	-0.007835	0.352775
H	3.345164	-1.031428	0.335803
H	3.044587	0.398160	1.366034
H	3.565362	0.629532	-0.310368
O	1.504372	-2.309947	0.013431

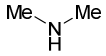
E = -556.0289648 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 135.696 kcal/mol



anion derived from 76

C	1.103426	1.133151	-0.198630
C	-0.352219	1.374569	0.245316
H	-0.409620	2.464106	0.401887
C	-1.459602	1.001552	-0.783930
H	-1.240042	1.476056	-1.751592
C	-1.683092	-1.344327	0.321308
H	-2.604419	-1.176191	0.907742
H	-1.657045	-2.410521	0.062919
N	1.661793	-0.056723	0.206440
C	-0.443710	-0.911619	1.083668
C	0.746374	-1.234494	0.421872
C	-0.566924	0.538753	1.511032
H	-1.562959	0.735974	1.939840
H	0.169279	0.821816	2.278603
O	1.119024	-2.305111	-0.105854
H	-2.385767	1.474770	-0.417491
C	-1.723305	-0.511491	-0.993243
H	-0.937029	-0.919977	-1.641553
H	-2.675057	-0.626464	-1.544188
C	3.029656	-0.323846	-0.202219
H	3.188964	-0.061510	-1.255376
H	3.198440	-1.392846	-0.065733
H	3.740718	0.262363	0.395670
O	1.743115	1.992010	-0.816487

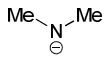
E = -555.4006076 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 125.857 kcal/mol



104

N	0.399765	0.596177	0.000000
H	-0.041662	1.513447	0.000000
C	0.018224	-0.115559	-1.212769
H	0.590808	-1.048992	-1.280553
H	0.267378	0.491401	-2.089700
H	-1.055461	-0.381662	-1.268314
C	0.018224	-0.115559	1.212769
H	0.590808	-1.048992	1.280553
H	-1.055461	-0.381662	1.268314
H	0.267378	0.491401	2.089700

E = -135.1628700 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 58.282 kcal/mol

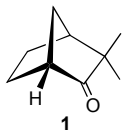


100

N	0.000000	0.000000	0.917780
C	-1.141530	0.000000	0.094066
H	-1.251505	0.886679	-0.622800
H	-2.076990	0.000000	0.692645
H	-1.251505	-0.886679	-0.622800
C	1.141530	0.000000	0.094066
H	1.251505	0.886679	-0.622800
H	1.251505	-0.886679	-0.622800
H	2.076990	0.000000	0.692645

E = -134.4979818 au (B3LYP/6-31G*//B3LYP/6-31G*)
This Molecule has 0 Imaginary Frequencies
Zero point vibrational energy: 46.710 kcal/mol

Geometry Optimisations using B3LYP/6-31+G*



1

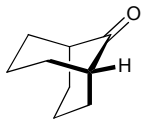
H	-0.175134	0.247619	2.039225
C	0.210914	0.155661	1.018410
C	1.975401	-0.554133	-0.505348
C	-0.157778	0.346460	-1.336453
C	1.246822	0.763953	-0.917994
C	-0.919123	-0.046099	-0.044050
C	1.314732	-0.919622	0.863001
H	3.048492	-0.360317	-0.397601
H	1.766867	1.359087	-1.671239
H	0.934222	-1.943872	0.892205
H	1.862369	-1.340518	-1.259525
H	2.037287	-0.825145	1.681936
C	0.961860	1.394633	0.464168
H	1.878368	1.619044	1.022703
H	0.358607	2.306366	0.414347
O	-0.607782	0.306619	-2.464990
C	-2.093748	0.931726	0.187791
H	-1.765785	1.968634	0.313462
H	-2.645341	0.642638	1.091515
H	-2.784957	0.900727	-0.661347
C	-1.493372	-1.468980	-0.158924
H	-1.956123	-1.772834	0.788841
H	-0.735530	-2.213878	-0.420834
H	-2.261271	-1.497769	-0.939299

E = -426.6224928 au (B3LYP/6-31+G*//B3LYP/6-31+G*)

anion derived from 1

H	-0.018689	0.703187	1.876635
C	0.304443	0.428612	0.855677
C	2.118223	-0.405928	-0.604017
C	-0.065572	-0.094115	-1.431571
C	1.195980	0.644518	-1.277546
C	-0.870489	-0.048757	-0.060620
C	1.486365	-0.589551	0.850930
H	3.156443	-0.048150	-0.510671
H	1.174655	-1.623456	1.048275
H	2.150918	-1.355146	-1.153410
H	2.201660	-0.319854	1.645414
C	0.919554	1.530427	-0.038443
H	1.847355	1.944726	0.387452
H	0.248380	2.376862	-0.229415
O	-0.439005	-0.842761	-2.348428
C	-2.053767	0.943269	-0.070357
H	-1.746291	1.972686	-0.279456
H	-2.579858	0.938912	0.899142
H	-2.776383	0.650527	-0.844293
C	-1.446051	-1.435665	0.262717
H	-1.915245	-1.440879	1.259763
H	-0.684660	-2.221609	0.240012
H	-2.207966	-1.707853	-0.477789

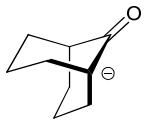
E = -425.9779401 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



15

H	-1.315726	-2.159575	0.748449
C	-1.315568	-1.283621	0.085174
C	-1.315568	1.283621	0.085174
C	0.000000	0.000000	-1.588508
C	0.000000	1.261968	-0.741103
C	0.000000	-1.261968	-0.741103
C	-1.583244	0.000000	0.896855
H	-2.141755	1.433870	-0.624151
H	-0.981503	0.000000	1.810005
H	-2.141755	-1.433870	-0.624151
H	-1.315726	2.159575	0.748449
H	0.000000	2.124982	-1.417082
H	0.000000	-2.124982	-1.417082
H	-2.629265	0.000000	1.231126
O	0.000000	0.000000	-2.808982
C	1.315568	1.283621	0.085174
H	1.315726	2.159575	0.748449
H	2.141755	1.433870	-0.624151
C	1.583244	0.000000	0.896855
H	0.981503	0.000000	1.810005
H	2.629265	0.000000	1.231126
C	1.315568	-1.283621	0.085174
H	1.315726	-2.159575	0.748449
H	2.141755	-1.433870	-0.624151

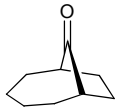
E = -426.632755 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



anion derived from 15

H	-1.050935	-1.928020	1.217583
C	-1.157692	-1.264997	0.342596
C	-1.513680	1.258640	-0.291641
C	-0.145273	-0.181584	-1.514125
C	-0.130746	1.145073	-0.935489
C	0.189897	-1.277601	-0.483448
C	-1.632225	0.138827	0.811397
H	-2.300923	1.106677	-1.041382
H	-1.029984	0.439101	1.681138
H	-1.929233	-1.706103	-0.303361
H	-1.712258	2.238144	0.181010
H	0.263494	-2.266455	-0.963664
H	-2.670971	0.055335	1.178832
O	-0.785442	-0.537910	-2.534367
C	1.028691	1.442276	0.028471
H	1.510960	2.405592	-0.222727
C	1.450327	-1.003132	0.375367
H	2.175289	-1.821277	0.246358
H	0.701071	1.565619	1.083222
H	1.191863	-0.990477	1.447492
C	2.096828	0.340231	0.009541
H	2.520687	0.267843	-1.004422
H	2.930256	0.574198	0.691618

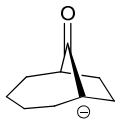
E = -425.980718 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



20

C	-0.397010	0.102666	-1.360504
C	-0.759369	-1.142862	-0.564132
C	-2.048266	-0.648914	0.126751
C	-1.767171	0.857161	0.465397
C	-0.547128	1.284263	-0.403033
H	-0.912233	-1.992210	-1.236083
H	-2.897300	-0.729968	-0.563167
H	-2.297254	-1.236603	1.017786
H	-1.556215	0.990962	1.532083
H	-2.646571	1.469957	0.241264
H	-0.749437	2.191539	-0.979159
C	0.357699	-1.451157	0.482831
H	0.375683	-2.535123	0.651824
H	0.074112	-1.005937	1.444652
C	1.779763	-0.977674	0.124970
H	2.120184	-1.498483	-0.779313
H	2.442642	-1.313803	0.933007
C	1.964161	0.563516	-0.076323
H	2.867607	0.881665	0.459156
H	2.157737	0.773050	-1.134346
C	0.798847	1.461565	0.392113
H	0.611019	1.296499	1.460937
H	1.120930	2.505419	0.299778
O	-0.092431	0.154473	-2.536488

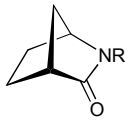
E = -426.613376 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



anion derived from 20

C	0.300410	0.086761	1.406196
C	1.133373	-0.924428	0.605545
C	2.226449	-0.037557	-0.000898
C	1.429109	1.256461	-0.357735
C	0.245265	1.251945	0.602739
H	1.513651	-1.777928	1.187960
H	3.002322	0.170618	0.750467
H	2.724497	-0.478571	-0.879553
H	1.111243	1.225188	-1.422949
H	2.082776	2.144430	-0.283403
C	0.140881	-1.383551	-0.526612
H	0.271357	-2.462652	-0.716594
H	0.441882	-0.886414	-1.459700
C	-1.397649	-1.153324	-0.352854
H	-1.753251	-1.858166	0.410039
H	-1.838139	-1.492169	-1.305095
C	-2.027887	0.250760	0.011907
H	-2.888941	0.426970	-0.655620
H	-2.433950	0.148226	1.022277
C	-1.134523	1.536393	0.033120
H	-1.003730	1.911604	-0.997634
H	-1.729082	2.317064	0.545420
O	-0.416065	-0.271659	2.382977

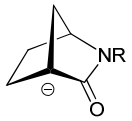
E = -425.987849 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



61 R = Me

H	0.005030	-1.638788	1.288905
C	-0.691313	-1.269773	0.528263
C	-1.086864	1.073404	-0.062973
N	1.058168	0.255435	-0.274331
C	0.394146	1.363946	0.207695
C	0.057534	-0.731072	-0.721951
C	-1.486765	-0.006660	0.995393
H	0.504171	-1.485815	-1.373928
H	-1.233612	0.306755	2.012849
H	-1.357339	-2.098146	0.260024
H	-2.568392	-0.178184	0.960058
C	-0.991086	0.212849	-1.339862
H	-1.929125	-0.294272	-1.592743
H	-0.612054	0.754093	-2.212474
O	0.892517	2.319974	0.789120
C	2.420866	-0.080195	0.082246
H	2.915188	0.831503	0.425938
H	2.958135	-0.476099	-0.787458
H	2.460951	-0.826752	0.889628
H	-1.710157	1.967797	-0.074401

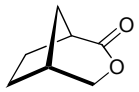
E = -403.364187 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



anion derived from 61 R = Me

H	0.072562	-0.737083	1.776125
C	0.799741	-0.161498	1.185992
C	1.081616	-0.382357	-1.298460
N	-1.010759	0.317135	-0.431574
C	-0.388852	-0.660794	-1.270789
C	0.101588	0.932726	0.323370
C	1.519108	-1.026918	0.060664
H	-0.233856	1.822560	0.879067
H	1.249720	-2.088420	0.129019
H	1.508576	0.296237	1.895038
H	2.610404	-0.958573	0.189189
C	1.094438	1.101036	-0.835969
H	2.090488	1.429786	-0.500764
H	0.721875	1.807681	-1.590905
O	-1.046690	-1.603103	-1.733826
C	-2.283149	0.039375	0.188377
H	-2.884811	-0.535610	-0.521808
H	-2.813516	0.969334	0.442970
H	-2.188484	-0.561514	1.114283

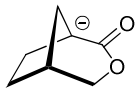
E = -402.71508 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



70

C	1.698166	-0.380405	-0.394372
C	0.894451	0.664929	0.377523
H	1.608071	1.344546	0.858054
C	-0.117310	1.415403	-0.526341
H	0.267576	1.545478	-1.544118
H	-0.309727	2.417239	-0.126706
C	-1.409788	0.547024	-0.491842
H	-2.234817	1.085610	-0.012007
H	-1.754408	0.251247	-1.487717
O	0.906191	-1.484196	-0.908853
C	-1.030198	-0.680442	0.385675
C	-0.366103	-1.734671	-0.489949
C	-0.009423	-0.084969	1.370253
H	-0.506156	0.601268	2.067157
H	0.523935	-0.840180	1.960537
O	-0.919122	-2.742805	-0.867005
H	2.190890	0.054539	-1.269822
H	2.466173	-0.828832	0.247490
H	-1.898399	-1.150785	0.852043

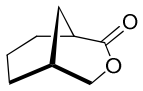
E = -423.2339629 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



anion derived from **70**

C	1.650723	0.039226	-0.504061
C	0.474405	0.952639	-0.066365
H	0.811579	2.003025	-0.145272
C	-0.867693	0.746765	-0.842315
H	-0.686207	0.408607	-1.873677
H	-1.416312	1.702364	-0.910209
C	-1.654287	-0.352240	-0.011302
H	-2.513507	0.116560	0.498973
H	-2.045218	-1.149937	-0.652766
O	1.643888	-1.258874	0.115082
C	-0.577530	-0.854126	0.947904
C	0.295862	-1.765902	0.283512
C	0.117860	0.441904	1.343333
H	-0.574899	1.127288	1.859808
H	0.999861	0.307041	1.981877
O	0.074182	-2.876079	-0.216146
H	1.664074	-0.090136	-1.600842
H	2.603218	0.501877	-0.207535

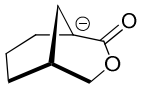
E = -422.6064868 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



71

C	-1.792248	-0.345452	0.670999
C	-1.166698	0.438015	-0.484691
H	-2.007799	0.840045	-1.066680
C	-0.274141	1.618712	-0.044715
H	-0.850228	2.305201	0.590607
C	1.736497	0.053357	-0.076263
H	2.169039	0.448478	-1.007070
H	2.565910	-0.339396	0.522585
O	-0.900146	-1.258879	1.362255
C	0.772499	-1.099874	-0.459757
C	0.246645	-1.745608	0.818440
C	-0.366747	-0.556974	-1.335132
H	0.048290	-0.071189	-2.228009
H	-1.014564	-1.373076	-1.683178
O	0.842363	-2.621748	1.405930
H	-2.174793	0.316769	1.454250
H	-2.625711	-0.956956	0.303664
H	1.339238	-1.878509	-0.979563
H	-0.000188	2.184033	-0.947820
C	1.009512	1.175842	0.681821
H	0.763311	0.831471	1.694991
H	1.679961	2.035738	0.807335

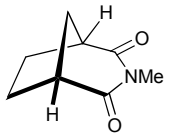
E = -462.554576 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



anion derived from **71**

C	1.818006	-0.107703	-0.645993
C	0.966305	0.811165	0.282673
H	1.612414	1.648241	0.615814
C	-0.302066	1.445441	-0.351326
H	-0.026181	2.020733	-1.250550
C	-1.696186	-0.611934	0.392239
H	-2.218189	-0.156901	1.254310
H	-2.358989	-1.388633	-0.010797
O	1.710377	-1.507920	-0.351684
C	-0.342100	-1.164338	0.791690
C	0.318956	-1.905073	-0.202763
C	0.513649	-0.094808	1.439931
H	-0.062889	0.483643	2.181831
H	1.388420	-0.508940	1.962432
O	-0.087533	-2.778965	-0.992609
H	1.562814	0.059513	-1.707887
H	2.883657	0.129632	-0.523151
H	-0.681321	2.187135	0.374586
C	-1.448787	0.464767	-0.704291
H	-1.189975	-0.076119	-1.625332
H	-2.360383	1.051065	-0.929122

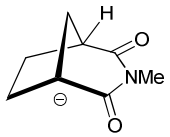
E = -461.9368094 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



75

C	0.701747	-1.253643	-0.153783
C	-0.796343	-1.174223	-0.404614
H	-1.105793	-2.154477	-0.773086
C	-1.534828	-0.762978	0.904159
H	-1.057253	-1.185575	1.793840
H	-2.558416	-1.151824	0.874632
C	-1.528036	0.793470	0.891540
H	-1.055412	1.226821	1.778681
N	1.373020	-0.021111	-0.051930
C	-0.775226	1.175533	-0.416886
C	0.722743	1.218223	-0.161775
C	-1.099442	-0.001380	-1.350898
H	-2.158939	0.006238	-1.634635
H	-0.500098	-0.011878	-2.268151
O	1.293432	-2.314002	-0.026451
O	1.349835	2.258935	-0.036456
C	2.819764	-0.003979	0.200471
H	3.327371	0.544922	-0.596769
H	3.165190	-1.035735	0.234085
H	3.025612	0.497882	1.149868
H	-1.060817	2.158855	-0.796546
H	-2.548113	1.189927	0.844702

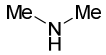
E = -516.72697 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



anion derived from 75

C	0.744137	-1.101485	0.315508
C	-0.764312	-1.163742	0.048689
H	-1.052636	-2.219686	0.144716
C	-1.651685	-0.244609	0.963162
H	-1.185470	-0.079263	1.943203
H	-2.616755	-0.743557	1.148103
C	-1.805440	1.112933	0.159151
H	-2.830241	1.189993	-0.241091
H	-1.630887	1.985403	0.797724
N	1.376414	0.027354	-0.159454
C	-0.743795	0.963417	-0.931705
C	0.542169	1.236131	-0.384131
C	-0.931713	-0.496677	-1.330807
H	-1.943149	-0.665096	-1.735140
H	-0.210672	-0.863488	-2.072301
O	1.367390	-2.022830	0.862584
O	1.014159	2.306893	0.047044
C	2.807218	0.164446	0.063062
H	3.357954	-0.597591	-0.503186
H	3.062827	0.044560	1.123859
H	3.094486	1.166895	-0.258990

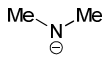
E = -516.107766 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



104

N	0.386605	0.596093	0.000000
H	-0.038272	1.520549	0.000000
C	0.017166	-0.117532	-1.217379
H	0.592902	-1.049361	-1.278016
H	0.272495	0.490458	-2.091919
H	-1.056730	-0.381887	-1.275299
C	0.017166	-0.117532	1.217379
H	0.592902	-1.049361	1.278016
H	-1.056730	-0.381887	1.275299
H	0.272495	0.490458	2.091919

E = -135.170317 au (B3LYP/6-31+G*//B3LYP/6-31+G*)



100

N	0.000000	0.000000	0.907818
C	-1.151958	0.000000	0.087533
H	-1.237983	0.892468	-0.616656
H	-2.077475	0.000000	0.691869
H	-1.237983	-0.892468	-0.616656
C	1.151958	0.000000	0.087533
H	1.237983	0.892468	-0.616656
H	1.237983	-0.892468	-0.616656
H	2.077475	0.000000	0.691869

E = -134.530123 au (B3LYP/6-31+G*//B3LYP/6-31+G*)