Supporting Information

Title: **Density Functional Theoretical Investigation on Influence of Hetero-Substitution and Benzannelation on the Thermal 6π Electrocyclization of cis Cyclononatetraene**

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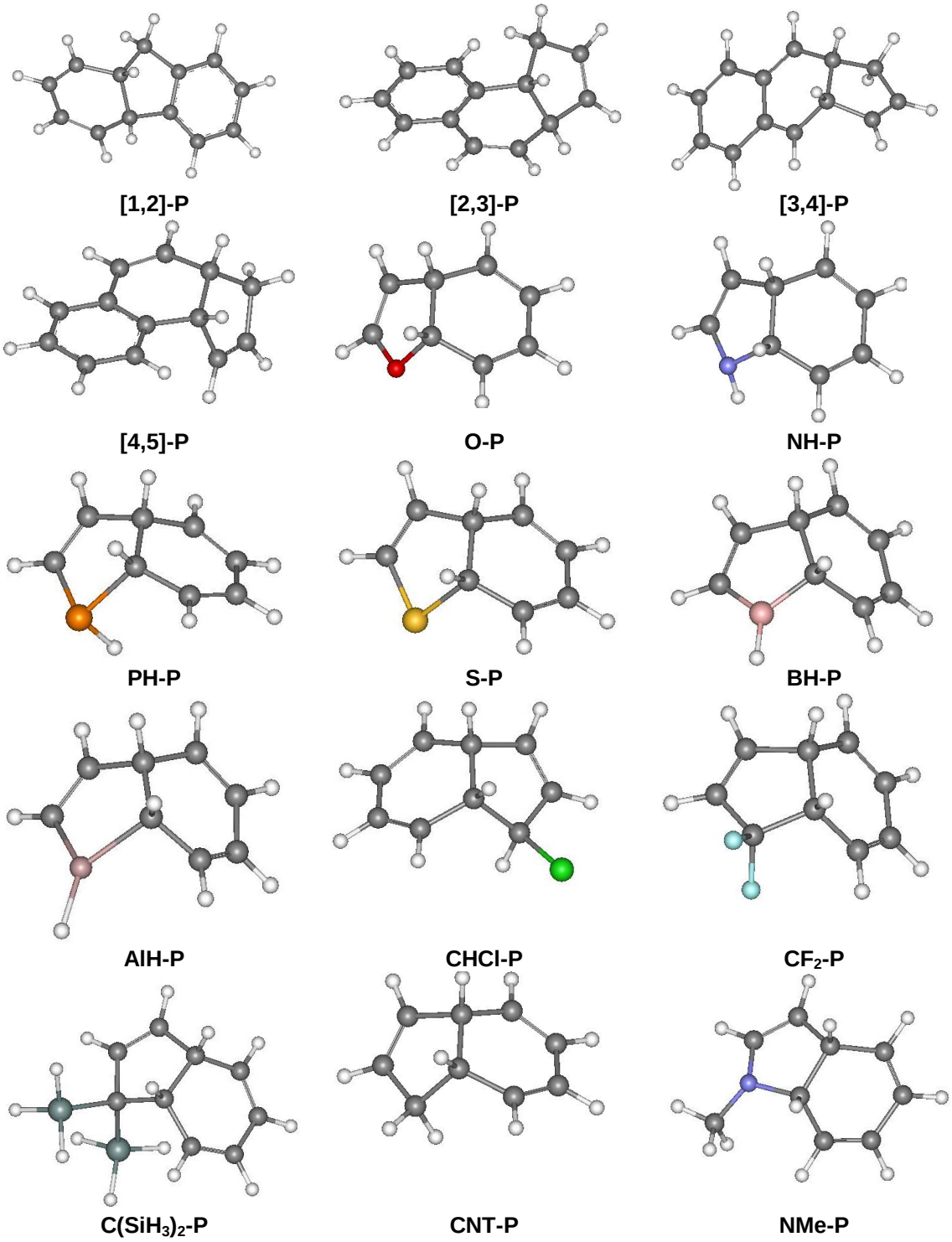
Figure S1.


[1,2]-P
[2,3]-P
[3,4]-P
[4,5]-P
O-P
NH-P
PH-P
S-P
BH-P
AlH-P
CHCl-P
CF_2-P
$C(SiH_3)_2$-P
CNT-P
NMe-P

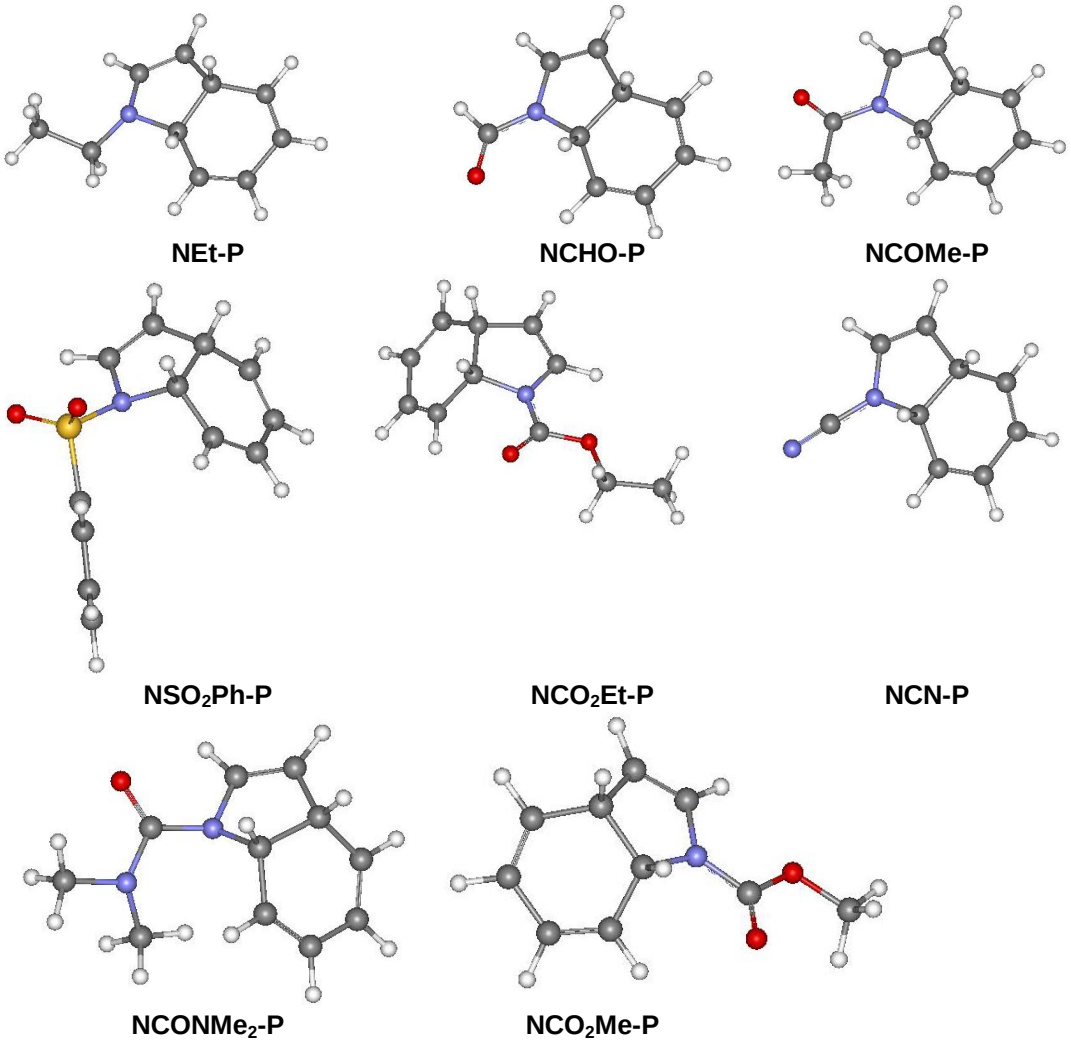

NEt-P
NCHO-P
NCOMe-P
NSO2Ph-P
NCO2Et-P
NCN-P
NCONMe2-P
NCO2Me-P

Figure S2

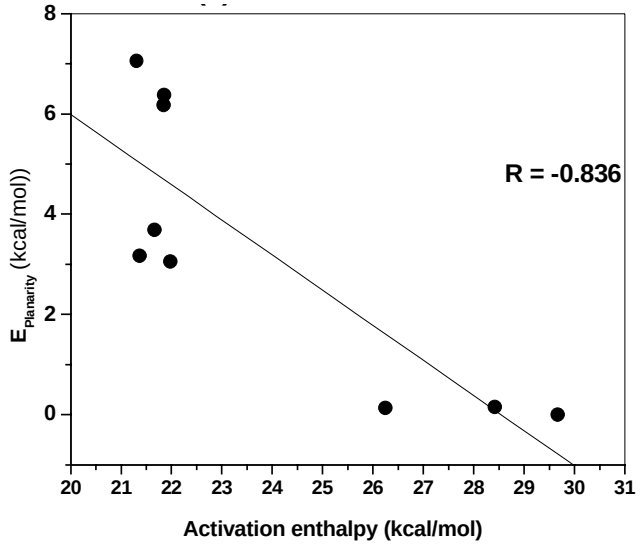

R = -0.836
E Planarity (kcal/mol))
Activation enthalpy (kcal/mol)
8
6
4
2
0
20
21
22
23
24
25
26
27
28
29
30
31

Table S1

[1,2]-R

Electronic energy = -502.5411549
Sum of electronic and zero-point energies = -502.332092
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-0.782886	0.701523	0.530545
6	0.277231	1.556898	1.128891
6	-0.645438	-0.697916	0.493259
6	-1.928832	1.297987	-0.016264
6	1.449044	1.818566	0.533976
6	0.510364	-1.405891	1.178582
6	-1.645226	-1.458100	-0.128582
6	-2.916625	0.529408	-0.628030
1	0.067177	2.017964	2.095278
1	-2.031407	2.379597	0.027290
6	1.837075	1.398029	-0.828383
6	1.734789	-1.754671	0.355181
1	0.124843	-2.347526	1.589158
1	0.834182	-0.819896	2.048104
1	2.137047	2.504394	1.033035
6	-2.768511	-0.857193	-0.692727
1	-1.540958	-2.540629	-0.160248
1	-3.794224	1.009282	-1.053160
6	2.174247	0.186387	-1.304188
6	2.371594	-1.107246	-0.635528
1	2.174237	-2.712529	0.634618
1	1.885190	2.223896	-1.542359
1	-3.530741	-1.468926	-1.168295
1	2.462840	0.164270	-2.356382
1	3.210859	-1.656576	-1.067429

[2,3]-R

Electronic energy = -502.4987476
Sum of electronic and zero-point energies = -502.289490
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-0.789148	-0.738247	-0.105463
6	-0.848022	0.703483	0.251674
6	0.229282	-1.570195	0.217389
6	-2.000500	-1.323304	-0.686963
6	0.158166	1.642177	0.284141
6	1.460781	-1.243752	1.013969
1	0.125585	-2.615522	-0.074548
6	-3.203265	-0.716615	-0.572347
6	-2.191965	1.209072	0.521463
1	-1.913020	-2.308121	-1.139883
6	1.510613	1.834547	-0.237813
6	2.730422	-1.248599	0.199692
1	1.554633	-1.995888	1.810813
1	1.342414	-0.267317	1.494390
6	-3.306883	0.552579	0.116297
1	-0.214797	2.604542	0.637447
1	-4.101825	-1.188787	-0.960059
1	-2.275509	2.193682	0.976028
6	2.638328	1.159115	-0.604053
6	3.171355	-0.199800	-0.508711
1	3.299516	-2.175648	0.168471
1	1.640259	2.904990	-0.409405
1	-4.287657	0.992754	0.275195
1	3.375344	1.826475	-1.051417
1	4.100065	-0.333933	-1.062674

[3,4]-R

Electronic energy = -502.5408446
Sum of electronic and zero-point energies = -502.331696
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-0.271198	-1.415824	1.184425
6	0.821427	-0.633753	0.544936
6	-1.410466	-1.714190	0.554451
1	-0.127450	-1.733820	2.217518
6	0.686937	0.760226	0.362153
6	-1.699132	-1.375600	-0.888628
6	1.991915	-1.272921	0.110834
1	-2.192505	-2.246866	1.094048
6	-0.445229	1.536102	0.940209
6	-2.535439	-0.136609	-1.131680
6	3.013394	-0.562051	-0.516652
6	1.731008	1.464519	-0.259782
1	-2.223245	-2.224977	-1.346068
1	-0.753250	-1.277624	-1.437666
1	2.089780	-2.345282	0.261170
6	-1.738490	1.632985	0.582595
6	-2.523795	1.061418	-0.520467
6	2.878415	0.813906	-0.708432
1	-0.145378	2.167708	1.779031

[4,5]-R

Electronic energy = -502.4957231
Sum of electronic and zero-point energies = -502.287806
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-1.334019	-1.526532	1.010170
6	-0.212362	-1.648239	0.065769
6	-2.506627	-0.931442	0.777838
1	-1.179818	-2.010867	1.977998
6	0.724858	-0.707584	-0.228995
6	-2.940197	-0.338040	-0.536150
1	-3.240350	-0.904743	1.582189
1	-0.015463	-2.656563	-0.307674
6	0.751258	0.669026	0.330418
6	-2.532689	1.091524	-0.808435
1	-4.035855	-0.381273	-0.590485
1	-2.584747	-0.965534	-1.365303
6	1.948442	-1.146156	-0.908541
6	-0.249336	1.603252	0.371890
6	-1.483261	1.819034	-0.385850
1	-3.230412	1.623246	-1.455873
6	2.073844	1.113231	0.769879
6	3.137881	-0.558479	-0.641437
1	1.889137	-2.027344	-1.542966

1	-3.257718	-0.240653	-1.941335
1	3.908647	-1.078678	-0.852577
1	1.633168	2.539375	-0.390820
1	-2.317330	2.347627	1.170858
1	-3.278000	1.763635	-0.881379
1	3.667190	1.380308	-1.196551

O-R

Electronic energy = -384.7815623
Sum of electronic and zero-point energies = -384.643711
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.925322	-1.578983	-0.516874
6	1.849559	-0.596333	-0.408442
1	1.223633	-2.436303	-1.122642
6	-0.290453	-1.817598	0.242090
6	1.848736	0.599233	0.407800
1	2.789444	-0.774219	-0.933853
1	-0.322685	-2.815161	0.684444
6	-1.420098	-1.137491	0.505946
6	0.922754	1.580137	0.517167
1	2.788507	0.778500	0.932935
1	-2.174165	-1.610438	1.128067
8	-1.967669	-0.001729	-0.000623
6	-1.422079	1.135523	-0.505718
6	-0.293553	1.817358	-0.241435
1	1.219849	2.437527	1.123452
1	-2.176826	1.607644	-1.127657
1	-0.327530	2.815201	-0.682969

PH-R

Electronic energy = -651.5095206
Sum of electronic and zero-point energies = -651.367354
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.013790	-1.605872	-0.681785
6	1.794942	-0.520162	-0.776115
1	1.039367	-2.346354	-1.482741
6	0.188209	-1.906688	0.503826
6	2.008807	0.476918	0.298132
1	2.428615	-0.415451	-1.659286
1	0.553797	-2.712570	1.147516
6	-0.928691	-1.259640	0.865041
6	1.248974	1.527938	0.641779
1	2.942302	0.344196	0.850766
1	-1.401796	-1.542884	1.804742
5	-1.958720	-0.116877	-0.147541
6	-1.115069	1.496974	-0.396213
6	0.044441	2.058618	-0.012967
1	1.641324	2.170465	1.432409
1	-1.666781	-0.658784	-1.432323
1	-1.814702	2.172919	-0.893435
1	0.126257	3.133098	-0.204723
1	0.053187	2.521202	0.880416
1	-1.535021	2.866396	-0.695527
6	3.209180	0.547299	0.290863
1	2.124425	1.999426	1.398751
1	4.052571	-0.934429	-1.092246
1	4.180512	0.949121	0.566208

NH-R

Electronic energy = -364.9342766
Sum of electronic and zero-point energies = -364.780517
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-1.057112	1.751256	0.000312
6	-1.963615	0.706016	-0.000103
1	-1.573573	2.710909	0.000733
6	0.340404	1.968864	0.000230
6	-1.963657	-0.705909	-0.000417
1	-2.986225	1.083696	-0.000103
1	0.556568	3.036584	0.000427
6	1.538963	1.294955	-0.000163
6	-1.057214	-1.751200	0.000014
1	-2.986289	-1.083528	-0.000952
1	2.402869	1.953643	-0.000389
7	1.986090	-0.000053	-0.000399
6	1.538886	-1.295041	0.000127
6	0.340291	-1.968879	0.000453
1	-1.573724	-2.710827	-0.000110
1	2.996922	-0.000087	-0.000717
1	2.402759	-1.953773	0.000249
1	0.556396	-3.036611	0.000933

S-R

Electronic energy = -707.7527117
Sum of electronic and zero-point energies = -707.619437
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.194451	-1.576341	-0.628183
6	2.047474	-0.542229	-0.490037
1	1.481188	-2.335763	-1.358167
6	0.069925	-1.975271	0.212281
6	2.047676	0.542019	0.489697
1	2.938362	-0.569136	-1.121436
1	0.189339	-2.980190	0.625764
6	-1.093038	-1.392587	0.550619
6	1.194773	1.576186	0.628187
1	2.938761	0.568815	1.120823
1	-1.751511	-1.953641	1.211938
6	-1.092966	1.392816	-0.550307
6	0.070045	1.975361	-0.211885
1	1.481815	2.335507	1.358156
1	-1.751491	1.954144	-1.211345
1	0.189348	2.980453	-0.624977
16	-2.021615	0.000006	-0.000187

BH-R

Electronic energy = -335.0292297
Sum of electronic and zero-point energies = -334.883807
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.542133	-0.818624	0.686766
6	0.495674	-1.645130	0.548508
1	2.249084	-1.026262	1.492442
6	1.943470	0.247145	-0.243836
6	-0.495749	-1.645200	-0.548267
1	0.405495	-2.471473	1.257161
1	2.963486	0.117632	-0.620706
6	1.268184	1.355441	-0.627044
6	-1.542151	-0.818646	-0.686746
1	-0.405666	-2.471730	-1.256717
1	1.819311	1.996616	-1.319753
5	0.000118	1.982218	0.000101
6	-1.268157	1.355568	0.626916
6	-1.943508	0.247351	0.243549
1	-2.249116	-1.026480	-1.492357
1	0.000517	3.188285	0.000769
1	-1.819394	1.996791	1.319492
1	-2.963679	0.118099	0.620091

AlH-R

Electronic energy = -552.6093118
Sum of electronic and zero-point energies = -552.471173
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-1.617053	-1.073991	-0.771510
6	-0.421646	-1.663028	-0.611960
1	-2.188302	-1.313531	-1.670554
6	-2.246106	-0.122583	0.158676
6	0.421617	-1.662994	0.612035
1	-0.060508	-2.303377	-1.419251
1	-3.286920	-0.348639	0.415437
6	-1.665377	1.003449	0.630918
6	1.617039	-1.073972	0.771530
1	0.060469	-2.303277	1.419375
1	-2.299497	1.605355	1.289816
13	0.000033	1.814059	0.000020
6	1.665370	1.003390	-0.630999
6	2.246088	-0.122639	-0.158739
1	2.188296	-1.313456	1.670584
1	0.000097	3.411868	0.000128
1	2.299469	1.605250	-1.289960
1	3.286879	-0.348749	-0.415547

CHCl-R

Electronic energy = -808.4786287
Sum of electronic and zero-point energies = -808.325943
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.985033	0.072535	-0.128172
6	0.587078	-0.839093	0.997142
6	0.666358	1.526353	0.115651
17	2.800384	-0.107770	-0.413100
1	0.532318	-0.260513	-1.060886
6	-0.425149	-1.710402	0.919431
6	-0.560965	2.061588	0.227623
1	1.186419	-0.767401	1.901257
1	1.520252	2.189119	0.222327
6	-1.288584	-1.866106	-0.263561
6	-1.926417	1.522287	0.160000
1	-0.608046	-2.380743	1.760218
1	-0.564194	3.132679	0.427290
6	-2.095751	-0.929038	-0.791714
6	-2.518618	0.377874	-0.250542
1	-1.275080	-2.846078	-0.743763
1	-2.647198	2.273676	0.482269
1	-2.678682	-1.231964	-1.663947
1	-3.610217	0.427329	-0.217204

CF_2-R

Electronic energy = -547.3569763
Sum of electronic and zero-point energies = -547.211566
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.368103	0.034406	-0.034743
6	0.767257	-0.816748	1.051676
6	0.855508	1.430032	-0.256485
9	2.713374	0.168551	0.275861
9	1.336931	-0.637944	-1.242444
6	-0.288555	-1.614188	0.895476
6	-0.347363	1.989289	-0.051142
1	1.305252	-0.778076	1.994769
1	1.638781	2.068197	-0.661006
6	-1.125206	-1.696864	-0.320669
6	-1.659830	1.521850	0.413616
1	-0.577631	-2.257709	1.728473
1	-0.372256	3.058997	-0.270483
6	-2.037982	-0.775719	-0.660905
6	-2.384311	0.426156	0.114768
1	-1.040629	-2.602092	-0.921828
1	-2.191989	2.289108	0.977528
1	-2.679566	-0.981980	-1.519260
1	-3.420426	0.438807	0.461500

$C(SiH_3)_2$-R

Electronic energy = -930.2638479
Sum of electronic and zero-point energies = -930.072224
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	2.007116	-1.656360	0.128404
6	2.909457	-0.705244	-0.185460

CNT-R

Electronic energy = -348.882889
Sum of electronic and zero-point energies = -348.721088
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.703019	-1.581865	-0.524236
6	-0.275473	-1.652215	0.624634

1	2.262949	-2.677025	-0.162542
6	0.865337	-1.567700	1.038566
6	2.909542	0.705224	0.185400
1	3.812247	-1.040795	-0.699800
1	0.957734	-2.260235	1.879489
6	-0.270022	-0.841832	1.040688
6	2.007237	1.656424	-0.128317
1	3.812433	1.040690	0.699618
1	-0.909519	-1.033672	1.904349
6	-0.962191	0.000026	0.000015
6	-0.270038	0.842082	-1.040496
6	0.865335	1.567932	-1.038333
1	2.263213	2.677056	0.162621
14	-2.083075	-1.278714	-0.893179
14	-2.083566	1.278489	0.892994
1	-0.909587	1.034082	-1.904085
1	0.957643	2.260625	-1.879136
1	-2.907933	-2.019018	0.097341
1	-2.996577	-0.591782	-1.851948
1	-1.236945	-2.240657	-1.644439
1	-2.908382	2.018633	-0.097681
1	-2.997110	0.591322	1.851552
1	-1.237818	2.240606	1.644465

NMe-R

Electronic energy = -404.2356873

Sum of electronic and zero-point energies = -404.054850

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-1.481530	1.688174	-0.232918
6	-2.394905	0.659491	-0.154025
1	-1.965530	2.634204	-0.477343
6	-0.114126	1.913141	0.072444
6	-2.371212	-0.708608	0.202944
1	-3.412557	1.005280	-0.337806
1	0.059165	2.978321	0.228392
6	1.092749	1.270632	0.216412
6	-1.432079	-1.715956	0.235555
1	-3.371940	-1.078941	0.427598
1	1.878860	1.949650	0.525259
7	1.633689	0.028706	-0.024266
6	1.115537	-1.223051	-0.275291
6	-0.070405	-1.899143	-0.120598
1	-1.882657	-2.677470	0.483369
1	1.918894	-1.877905	-0.596797
1	0.122036	-2.954595	-0.315934
6	3.113663	-0.006329	0.058543
1	3.516396	-0.567395	-0.788718
1	3.516982	1.004611	0.015487
1	3.438380	-0.486812	0.987952

NCHO-R

Electronic energy = -478.2616347

Sum of electronic and zero-point energies = -478.100994

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-1.773415	1.431343	-0.612497
6	-2.586838	0.358110	-0.509681
6	1.878405	-0.641517	-0.355007
1	1.104156	-2.590129	-0.689674
1	0.167068	-1.312971	-1.442070
6	-1.464465	-1.041296	0.659841
6	1.909570	0.641084	0.046744
1	0.007992	-2.298176	1.454755
1	2.843706	-1.072673	-0.618789
6	-1.941690	-0.108939	-0.378635
6	0.893313	1.618598	0.462905
1	-2.141856	-1.243064	1.491553
1	2.911089	1.071624	0.097300
6	-1.414175	1.101237	-0.629064
6	-0.404614	1.829264	0.163161
1	-2.813563	-0.415087	-0.960340
1	1.331941	2.405825	1.077995
1	-1.901525	1.706847	-1.396363
1	-0.812352	2.761690	0.563575

NEt-R

Electronic energy = -443.5530176

Sum of electronic and zero-point energies = -443.343155

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-1.708446	-1.764638	0.244116
6	-2.681264	-0.796610	0.371387
1	-2.089146	-2.751048	0.510662
6	-0.394377	-1.882695	-0.277412
6	-2.806307	0.579631	0.074555
1	-3.628306	-1.217266	0.710758
1	-0.184128	-2.925877	-0.515337
6	0.738231	-1.155705	-0.558302
6	-1.955359	1.648646	-0.107955
1	-3.852107	0.887745	0.055358
1	1.522265	-1.775252	-0.980656
7	1.229554	0.116003	-0.363368
6	0.671994	1.332717	-0.046853
6	-0.567830	1.926958	-0.010740
1	-2.507974	2.577675	-0.250412
1	1.466555	2.045947	0.143942
1	-0.415411	2.998404	0.121787
6	2.719837	0.166099	-0.432246
1	3.009242	1.158721	-0.784914
1	3.044161	-0.544379	-1.196951
6	3.380081	-0.150457	0.908432
1	3.098059	-1.149788	1.254934
1	4.471078	-0.113097	0.810399
1	3.079473	0.572515	1.674113

NCOMe-R

Electronic energy = -517.5814951

Sum of electronic and zero-point energies = -517.393506

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.328471	-1.686346	-0.675631
6	2.375829	-0.880131	-0.916364
1	1.108137	-2.482674	-1.387696
6	0.544354	-1.688826	0.569542
6	2.914640	0.140918	-0.015032

1	-2.111494	2.221703	-1.284856
6	-0.657994	1.838170	0.230774
6	-2.494889	-0.777952	0.387872
1	-3.497251	0.387552	-1.110607
1	-0.815120	2.822633	0.676418
6	0.537817	1.321971	0.567472
6	-1.471731	-1.641216	0.568544
1	-3.423260	-1.018220	0.908625
1	1.137861	1.920831	1.246919
7	1.276882	0.219839	0.097400
6	0.851122	-1.017136	-0.420434
6	-0.226676	-1.783158	-0.173021
1	-1.681078	-2.493258	1.217787
1	1.648565	-1.455999	-1.007960
1	-0.121054	-2.779421	-0.607552
6	2.671206	0.395865	0.119919
1	2.955611	1.374478	0.541940
8	3.484681	-0.409394	-0.277026
1	2.960604	-1.072870	-1.817560
1	0.753570	-2.504155	1.265035
6	-0.392356	-0.821181	0.961006
6	2.313251	1.235123	0.495181
1	3.969677	0.007490	0.231672
1	-0.873337	-0.960576	1.927603
7	-0.913659	0.263142	0.192711
6	-0.242760	1.478353	-0.019475
6	1.032582	1.866037	0.176090
1	2.952624	1.869263	1.111688
6	-2.270867	0.224857	-0.190260
1	-0.948595	2.225017	-0.363813
1	1.146494	2.942614	0.039774
6	-3.029297	-1.050364	0.128169
8	-2.804306	1.163954	-0.757813
1	-4.017115	-0.966539	-0.326483
1	-2.516245	-1.937156	-0.255935
1	-3.148833	-1.184668	1.209891

NSO_2Ph-R

Electronic energy = -1144.5389266
Sum of electronic and zero-point energies = -1144.297722
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-1.536104	2.009822	0.730038
6	-2.553272	2.209593	-0.128610
1	-0.800701	2.807680	0.842384
6	-1.411438	0.907220	1.686839
6	-3.736122	1.376183	-0.325680
1	-2.569715	3.167109	-0.652747
1	-1.546266	1.184300	2.734612
6	-1.141448	-0.389070	1.482259
6	-3.834600	0.081888	-0.697896
1	-4.678630	1.914148	-0.207485
1	-1.061707	-1.057836	2.333238
7	-0.790336	-1.001988	0.247101
6	-1.587526	-1.240548	-0.877686
6	-2.838175	-0.855793	-1.203821
1	-4.855372	-0.281606	-0.827064
16	0.824283	-1.622235	0.226419
1	-1.097044	-1.936852	-1.547615
1	-3.199230	-1.389507	-2.083800
6	1.832543	-0.177016	-0.103440
8	0.926366	-2.523502	-0.921953
8	1.111227	-2.074164	1.587568
6	2.086853	0.184216	-1.428888
6	2.331424	0.567097	0.967995
6	2.853860	1.320511	-1.681417
1	1.704538	-0.425542	-2.240376
6	3.095934	1.703024	0.699537
1	2.137670	0.246551	1.985358
6	3.353898	2.079843	-0.620278
1	3.065642	1.609079	-2.706884
1	3.496285	2.288191	1.522472
1	3.952660	2.963471	-0.823141

NCO_2Et-R

Electronic energy = -632.1257405
Sum of electronic and zero-point energies = -631.903680
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.804211	-1.803673	0.740599
6	3.011788	-1.226420	0.867636
1	1.499411	-2.527171	1.498325
6	0.923224	-1.703926	-0.430614
6	3.670696	-0.352258	-0.100878
1	3.618238	-1.522185	1.725587
1	0.885505	-2.594493	-1.061267
6	0.136950	-0.701344	-0.830649
6	3.249974	0.825627	-0.605702
1	4.661625	-0.688783	-0.411418
1	-0.474929	-0.830349	-1.717971
7	-0.101236	0.528818	-0.147655
6	0.823474	1.568230	0.045477
6	2.139868	1.690774	-0.210111
1	3.949630	1.319217	-1.282499
6	-1.427326	0.839174	0.182100
1	0.306255	2.443648	0.418699
1	2.473181	2.720250	-0.068661
8	-1.794232	1.883160	0.685847
8	-2.252080	-0.182901	-0.130140
6	-3.647733	0.038488	0.177729
1	-3.992850	0.925619	-0.362359
1	-3.742508	0.243256	1.248489
6	-4.402825	-1.210982	-0.233922
1	-5.468589	-1.087682	-0.013071
1	-4.293201	-1.400336	-1.306608
1	-4.036419	-2.086933	0.310695

NCN-R

Electronic energy = -457.1498698
Sum of electronic and zero-point energies = -457.001119
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.568080	1.566576	0.554053
6	2.484320	0.580698	0.434294
1	1.853690	2.403008	1.193770
6	0.378918	1.837841	-0.239228
6	2.484117	-0.580954	-0.434674
1	3.412395	0.723828	0.990032
1	0.401405	2.827227	-0.699724
6	-0.763978	1.188875	-0.520468
6	1.567727	-1.566731	-0.554106
1	3.412007	-0.724216	-0.990687
1	-1.474814	1.688685	-1.170078
7	-1.332656	0.000088	0.000055
6	-0.764032	-1.188627	0.520835
6	0.378758	-1.837752	0.239550
1	1.853031	-2.403243	-1.193854
1	-1.474819	-1.688213	1.170673
1	0.401293	-2.827020	0.700299
6	-2.684381	0.000024	-0.000111
7	-3.850395	-0.000052	-0.000241

NCO_2Me-R

Electronic energy = -592.8065896
Sum of electronic and zero-point energies = -592.613000
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	2.775008	-0.982532	0.864806
6	1.666719	-1.722068	0.684820
6	3.320577	0.013548	-0.055604
1	3.398957	-1.220108	1.728235
1	1.452110	-2.510162	1.408191
6	0.807720	-1.703601	-0.506942
6	2.744391	1.138070	-0.527011
1	4.354939	-0.166183	-0.354534
1	0.915231	-2.563222	-1.171512
6	-0.105979	-0.809114	-0.892021
6	1.513898	1.818095	-0.125617
1	3.377614	1.753405	-1.168561
1	-0.670974	-0.986844	-1.801768
7	-0.535835	0.344416	-0.169108
6	0.224098	1.497624	0.089549
1	1.692899	2.877490	0.065680
6	-1.897859	0.446371	0.135754
1	-0.421978	2.272902	0.482790
8	-2.426894	1.402456	0.668179
8	-2.559242	-0.671534	-0.237918
6	-3.967797	-0.651918	0.039793
1	-4.455049	0.169716	-0.491480
1	-4.145734	-0.538816	1.112074
1	-4.342742	-1.613326	-0.312600

$NCONMe_2$-R

Electronic energy = -612.2422988
Sum of electronic and zero-point energies = -612.007767
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	2.063639	-1.823032	-0.285370
6	3.185372	-1.096062	-0.487788
1	2.037794	-2.803959	-0.764594
6	0.993620	-1.622810	0.681314
6	3.609129	0.131615	0.151859
1	3.942837	-1.560164	-1.121814
1	0.906495	-2.443309	1.397306
6	0.036161	-0.691039	0.850602
6	2.965189	1.312693	0.304936
1	4.644905	0.111784	0.495106
1	-0.672118	-0.865760	1.654782
7	-0.343514	0.418273	0.066475
6	0.451144	1.458706	-0.430689
6	1.738935	1.832190	-0.273093
1	3.564824	2.098730	0.767381
6	-1.750303	0.710266	0.019948
1	-0.174538	2.152553	-0.976855
1	1.901968	2.823827	-0.699343
8	-2.165523	1.859335	-0.003753
7	-2.590113	-0.385870	0.054921
6	-4.006201	-0.082413	0.242160
6	-2.341108	-1.601548	-0.721069
1	-4.486938	0.222575	-0.698174
1	-4.507642	-0.978976	0.620710
1	-4.115895	0.729521	0.960738
1	-2.635369	-2.485619	-0.143688
1	-2.931530	-1.582559	-1.648831
1	-1.288676	-1.691552	-0.979328

Table S2

1,2]-TS

Electronic energy = -502.5078968
Sum of electronic and zero-point energies = -502.299820
Value of imaginary frequencies = -506.7

Atom number	X	Y	Z
6	0.500820	1.171357	0.639182
6	1.492597	1.639299	-0.247173
1	0.334723	1.888976	1.451898
6	-0.814382	0.546209	0.283521
6	2.483304	0.958832	-0.971744
1	1.677476	2.718320	-0.202221
6	-0.924249	-0.786036	-0.116812
6	-1.975696	1.329159	0.362954
6	3.130555	-0.206766	-0.531022
1	3.034088	1.554321	-1.699095
6	0.371194	-1.542349	-0.127971
1	-1.904497	2.364875	0.686924
6	-2.164508	-1.324018	-0.459174
6	-3.218791	0.792554	0.023327
6	1.354169	-1.035868	0.920278
6	2.703111	-0.925615	0.589505
1	4.139705	-0.365230	-0.908918
1	0.839687	-1.477201	-1.116555
1	0.193207	-2.611657	0.060075
1	-2.234146	-2.367823	-0.757977
1	-4.110137	1.410687	0.092509
6	-3.315462	-0.535550	-0.394192
1	1.111897	-1.351192	1.936501
1	3.464471	-1.290049	1.281453
1	-4.282442	-0.961277	-0.648669

[2,3]-TS

Electronic energy = -502.4868945
Sum of electronic and zero-point energies = -502.279606
Value of imaginary frequencies = -351.9

Atom number	X	Y	Z
6	-2.152464	0.800581	0.968427
6	-1.208110	1.748910	0.590281
1	-2.605471	1.017654	1.941135
6	-3.101947	0.083802	0.087401
6	-0.113444	1.702148	-0.299763
1	-1.227464	2.677762	1.172230
1	-4.125020	0.458085	0.165947
6	-2.838387	-0.895762	-0.772184
6	0.839073	0.669699	-0.405351
1	0.252403	2.675498	-0.629682
1	-3.607432	-1.284126	-1.436955
6	-1.446310	-1.444140	-0.870285
6	-0.583189	-1.223531	0.354570
6	0.659024	-0.595122	0.281342
1	-0.947826	-1.008387	-1.746726
1	-1.488639	-2.528611	-1.058937
6	2.164777	1.003968	-0.844860
1	-0.685168	-1.999131	1.115607
6	1.822655	-1.197960	0.863491
1	2.299963	1.891700	-1.458822
6	3.250730	0.290034	-0.410600
1	1.685449	-2.070087	1.499086
6	3.081496	-0.791100	0.503743
1	4.251533	0.576302	-0.723057
1	3.954252	-1.315820	0.882906

[3,4]-TS

Electronic energy = -502.4867659
Sum of electronic and zero-point energies = -502.279508
Value of imaginary frequencies = -598.6

Atom number	X	Y	Z
6	1.689688	1.017864	-0.840648
6	0.345735	1.433598	-0.745356
1	2.183141	1.407303	-1.741028
6	2.627735	1.096213	0.330084
6	-0.734275	0.729231	-0.153270
1	0.038970	2.270519	-1.377485
1	3.098899	2.068020	0.478745
6	2.855078	0.068305	1.135722
6	-0.835188	-0.723002	-0.262236
1	3.502533	0.124517	2.007310
6	2.104400	-1.180457	0.804606
6	-1.915830	1.444036	0.228481
6	1.562728	-1.149579	-0.634651
6	0.217405	-1.474094	-0.836722
1	1.272506	-1.319356	1.506935
1	2.737740	-2.073951	0.909822
6	-2.110381	-1.324101	-0.023627
1	-1.849746	2.526644	0.303045
6	-3.094779	0.810703	0.527040

[4,5]-TS

Electronic energy = -502.4846078
Sum of electronic and zero-point energies = -502.277732
Value of imaginary frequencies = -344.9

Atom number	X	Y	Z
6	0.523050	-1.305120	0.553955
6	-0.660984	-0.581502	0.338728
1	0.419563	-2.081593	1.319347
6	1.452046	-1.708992	-0.519700
6	-0.765249	0.712786	-0.322124
1	1.200619	-2.675213	-0.966813
6	2.521048	-1.062080	-0.969726
6	-1.892436	-1.166532	0.791825
6	0.140170	1.760108	-0.066588
1	3.100672	-1.457818	-1.802505
6	2.977924	0.221375	-0.352239
6	-2.046640	1.068054	-0.876154
1	-1.829713	-2.053195	1.418991
6	-3.108802	-0.742122	0.324745
6	2.219737	0.721829	0.866476
6	1.245169	1.696025	0.806572
1	-0.255543	2.754171	-0.278820
1	2.953351	1.006854	-1.120597
1	4.037856	0.121566	-0.074510

1	2.268798	-1.569863	-1.353334
1	-0.055331	-2.220349	-1.584226
1	-2.188607	-2.402566	-0.138753
6	-3.197882	-0.598849	0.391783
1	-3.957147	1.387364	0.851303
1	-4.138369	-1.097470	0.610425
1	-2.109527	1.972971	-1.476179
6	-3.177750	0.359592	-0.576289
1	-4.016693	-1.267201	0.608766
1	2.803700	0.693511	1.786924
1	1.270475	2.479802	1.570628
1	-4.138444	0.665624	-0.982125

O-TS

Electronic energy = -384.7458527
Sum of electronic and zero-point energies = -384.609926
Value of imaginary frequencies = -536.9

Atom number	X	Y	Z
6	-0.353347	1.218472	0.735350
6	0.915774	1.536693	0.222014
1	-0.585986	1.726370	1.677670
6	-1.551331	1.074870	-0.134631
6	1.711312	0.742660	-0.610644
1	1.422081	2.410535	0.641955
1	-2.108828	1.976353	-0.375638
6	-1.933195	-0.097205	-0.623174
6	1.793565	-0.657613	-0.509839
1	2.562453	1.223958	-1.090850
1	-2.762655	-0.285600	-1.295508
8	-1.254985	-1.227713	-0.301171
6	-0.294635	-1.142952	0.719279
6	1.035498	-1.412020	0.388963
1	2.705865	-1.103295	-0.904682
1	-0.700886	-1.546856	1.647568
1	1.565984	-2.157184	0.984941

NH-TS

Electronic energy = -364.8813307
Sum of electronic and zero-point energies = -364.732764
Value of imaginary frequencies = -522.4

Atom number	X	Y	Z
6	-0.388470	1.216013	0.726434
6	0.846280	1.581735	0.172714
1	-0.612765	1.700689	1.682849
6	-1.618656	1.020468	-0.101930
6	1.660741	0.786938	-0.651458
1	1.342075	2.472897	0.570838
1	-2.213067	1.910212	-0.301597
6	-1.981509	-0.157943	-0.598457
6	1.818245	-0.602178	-0.490995
1	2.481164	1.286449	-1.166103
1	-2.834884	-0.315578	-1.252233
7	-1.207007	-1.290011	-0.281941
6	-0.236756	-1.127952	0.759470
6	1.109085	-1.359728	0.453412
1	2.749173	-1.013102	-0.881826
1	-0.781658	-1.699226	-1.109920
1	-0.622881	-1.413401	1.738728
1	1.688125	-2.042976	1.077708

PH-TS

Electronic energy = -651.4784699
Sum of electronic and zero-point energies = -651.337003
Value of imaginary frequencies = -466.8

Atom number	X	Y	Z
6	0.375761	1.372164	0.754439
6	1.659213	1.227890	0.225194
1	0.341154	1.907024	1.710084
6	-0.797095	1.724858	-0.097651
6	2.088247	0.240773	-0.678753
1	2.463962	1.815101	0.676581
1	-0.825759	2.793085	-0.332459
6	-1.771042	0.946132	-0.561328
6	1.696890	-1.104354	-0.624491
1	3.023661	0.426777	-1.206872
1	-2.574139	1.360462	-1.168025
15	-1.806500	-0.815700	-0.115627
6	-0.274767	-0.977165	0.905701
6	0.845502	-1.618169	0.368158
1	2.360683	-1.804736	-1.130197
1	-1.302520	-1.327860	-1.345881
1	-0.538243	-1.284614	1.920504
1	1.212443	-2.522516	0.863063

S-TS

Electronic energy = -707.7175138
Sum of electronic and zero-point energies = -707.584956
Value of imaginary frequencies = -497.9

Atom number	X	Y	Z
6	0.263569	1.408289	0.736345
6	1.531841	1.339062	0.143203
1	0.260777	1.965893	1.680237
6	-0.984905	1.666576	-0.031379
6	2.038258	0.349403	-0.710667
1	2.289633	2.032863	0.519415
1	-1.183997	2.726718	-0.195752
6	-1.855698	0.780015	-0.502826
6	1.791731	-1.025354	-0.566751
1	2.947062	0.597006	-1.259017
1	-2.734987	1.056692	-1.077637
6	-0.222551	-0.971380	0.888606
6	0.967144	-1.550893	0.432983
1	2.532854	-1.684878	-1.015865
1	-0.550112	-1.264584	1.886024
1	1.378312	-2.389088	1.001765
16	-1.632242	-0.938433	-0.242266

BH-TS

Electronic energy = -335.0044074
Sum of electronic and zero-point energies = -334.859687
Value of imaginary frequencies = -362.2

Atom number	X	Y	Z
6	0.041966	-1.114965	0.716630
6	-1.356939	-1.127547	0.632045
1	0.511543	-1.470789	1.633372
6	0.842635	-1.293231	-0.516850
6	-1.975332	-0.309046	-0.300226
1	-1.961306	-1.676263	1.354073
1	0.508014	-2.092445	-1.181864
6	1.945305	-0.549945	-0.746272
6	-1.427093	0.928769	-0.723609
1	-3.027377	-0.466696	-0.537675
1	2.622358	-0.794553	-1.562824
5	2.019574	0.624854	0.222894
6	0.678812	1.197062	0.747061
6	-0.410859	1.619709	-0.068322
1	-2.067441	1.528598	-1.368438
1	3.033389	1.153449	0.591578
1	0.813349	1.885236	1.593453
1	-0.561373	2.704359	-0.078887

AlH-TS

Electronic energy = -552.5735722
Sum of electronic and zero-point energies = -552.435983
Value of imaginary frequencies = -400.6

Atom number	X	Y	Z
6	-0.215459	-1.017848	0.780922
6	-1.623208	-0.991998	0.806781
1	0.284728	-1.336362	1.696285
6	0.470702	-1.450777	-0.476254
6	-2.304807	-0.294808	-0.174809
1	-2.168203	-1.446689	1.633254
1	-0.128752	-2.138093	-1.079983
6	1.733522	-1.114179	-0.823594
6	-1.764551	0.853073	-0.804026
1	-3.370025	-0.470902	-0.323815
1	2.179684	-1.599786	-1.688703
13	2.077493	0.491310	0.152768
6	0.355097	1.277075	0.581122
6	-0.720241	1.615881	-0.270423
1	-2.417358	1.366071	-1.508176
1	3.406436	1.220718	0.634884
1	0.491366	2.067393	1.341481
1	-0.871617	2.692111	-0.409524

CHCl-TS

Electronic energy = -808.4476017
Sum of electronic and zero-point energies = -808.296331
Value of imaginary frequencies = -489.3

Atom number	X	Y	Z
6	0.988970	0.019723	-0.346983
6	0.181434	-0.556877	0.799472
6	0.856484	1.489394	-0.506805
17	2.789807	-0.410429	-0.057899
1	0.766757	-0.508559	-1.274562
6	-0.615311	-1.678404	0.569503
6	-0.235203	2.036274	0.016794
1	0.692122	-0.479239	1.757655
1	1.594861	2.046299	-1.074449
6	-1.330679	1.286065	0.687549
6	-1.605152	-1.688497	-0.416155
1	-0.573781	-2.523218	1.258514
1	-0.405493	3.111406	-0.059467
6	-2.383372	0.633842	0.019866
1	-1.677395	1.832028	1.572829
6	-2.381365	-0.556340	-0.723732
1	-2.009550	-2.643784	-0.747948
1	-3.390558	0.986432	0.263818
1	-3.278516	-0.755154	-1.309156

CF_2-TS

Electronic energy = -547.3253533
Sum of electronic and zero-point energies = -547.181000
Value of imaginary frequencies = -496.3

Atom number	X	Y	Z
6	0.959780	1.473371	0.622813
6	2.077955	0.903483	-0.006797
1	1.236026	2.151467	1.438780
6	-0.226838	2.003050	-0.103034
6	2.191983	-0.333303	-0.661945
1	3.040553	1.383474	0.193427
1	-0.168277	3.066380	-0.342146
6	-1.287413	1.293454	-0.465279
6	1.547143	-1.509083	-0.252353
1	3.088386	-0.479832	-1.263528
1	-2.116951	1.678535	-1.049777
6	-1.288501	-0.137001	-0.076135
6	-0.288527	-0.507475	1.016751
6	0.618675	-1.535055	0.795877
1	2.025867	-2.441140	-0.548722
9	-2.543057	-0.481189	0.404824
9	-1.112759	-0.908722	-1.203323
1	-0.756075	-0.434282	1.997186
1	0.727270	-2.324049	1.541884

$C(SiH_3)_2$-TS

Electronic energy = -930.2281807
Sum of electronic and zero-point energies = -930.038330
Value of imaginary frequencies = -507.3

Atom number	X	Y	Z
6	1.515477	-1.531556	-0.117984
6	2.769941	-0.904325	-0.065933

CNT-TS

Electronic energy = -348.8485018
Sum of electronic and zero-point energies = -348.688146
Value of imaginary frequencies = -510.3

Atom number	X	Y	Z
6	-0.401390	1.219882	0.726057
6	0.819298	1.583725	0.133708

1	1.514346	-2.483537	-0.660067
6	0.639095	-1.566531	1.083535
6	2.988613	0.442564	0.219610
1	3.641608	-1.474639	-0.395022
1	0.958875	-2.247274	1.873410
6	-0.489432	-0.874942	1.216381
6	2.133298	1.471654	-0.211841
1	4.000968	0.751089	0.477348
1	-1.102789	-0.957005	2.112377
6	-0.966062	-0.041243	0.068647
6	0.101944	0.190641	-1.020096
6	1.014135	1.267356	-1.022599
1	2.573989	2.468034	-0.227166
14	-2.428343	-1.017981	-0.694478
14	-1.614839	1.648645	0.689327
1	-0.307347	0.016632	-2.021286
1	0.955926	1.945774	-1.879670
1	-1.904495	-2.243849	-1.354090
1	-3.388913	-1.411066	0.370304
1	-3.153871	-0.205861	-1.713103
1	-2.050942	2.489944	-0.456761
1	-2.793441	1.425347	1.578881
1	-0.581423	2.375395	1.468640

NMe-TS

Electronic energy = -404.1887018

Sum of electronic and zero-point energies = -404.012068

Value of imaginary frequencies = -538.6

Atom number	X	Y	Z
6	0.717278	1.499550	0.475349
6	1.798760	0.975117	-0.249724
1	1.020501	2.193657	1.267901
6	-0.582439	1.914705	-0.139151
6	1.887414	-0.298399	-0.836383
1	2.759760	1.493371	-0.168127
1	-0.653259	2.947295	-0.475270
6	-1.611470	1.081996	-0.277006
6	1.332334	-1.459693	-0.268558
1	2.721019	-0.469735	-1.517021
1	-2.543318	1.334290	-0.776863
7	-1.493499	-0.219988	0.216979
6	-0.403624	-0.427579	1.130075
6	0.528294	-1.440629	0.879739
1	1.814028	-2.396231	-0.549526
1	-0.691958	-0.213954	2.161153
1	0.760340	-2.158742	1.668286
6	-1.824461	-1.271402	-0.741942
1	-1.908472	-2.228977	-0.221504
1	-2.793163	-1.027219	-1.192910
1	-1.083500	-1.375829	-1.549370

NCHO-TS

Electronic energy = -478.224311

Sum of electronic and zero-point energies = -478.065697

Value of imaginary frequencies = -507.6

Atom number	X	Y	Z
6	1.470518	1.067277	0.721876
6	2.438052	0.203989	0.180982
1	-0.596734	1.761917	1.659677
6	-1.667404	1.025965	-0.038387
6	1.669326	0.803523	-0.665168
1	1.279740	2.511986	0.487036
1	-2.263781	1.932617	-0.155619
6	-2.073684	-0.122848	-0.562591
6	1.895652	-0.569342	-0.468945
1	2.462710	1.333506	-1.192060
1	-2.983856	-0.203058	-1.153207
6	-1.193933	-1.317734	-0.372827
6	-0.165029	-1.150950	0.744249
6	1.192038	-1.328982	0.473025
1	2.854028	-0.943790	-0.827813
1	-0.671591	-1.539952	-1.312168
1	-1.797122	-2.210571	-0.147697
1	-0.517624	-1.520642	1.708704
1	1.784983	-1.981446	1.118416

NEt-TS

Electronic energy = -443.5024542

Sum of electronic and zero-point energies = -443.297312

Value of imaginary frequencies = -538.9

Atom number	X	Y	Z
6	1.540961	1.289071	0.313415
6	2.315817	0.472887	-0.524876
1	2.137764	1.899304	1.001570
6	0.312095	2.017246	-0.128197
6	1.970006	-0.793541	-1.025161
1	3.379392	0.713792	-0.622504
1	0.459505	3.019097	-0.527333
6	-0.910680	1.497006	-0.044417
6	1.228645	-1.741920	-0.297631
1	2.607012	-1.205259	-1.807590
1	-1.802876	1.997998	-0.404907
7	-1.067497	0.228163	0.521909
6	0.071379	-0.238202	1.266848
6	0.655427	-1.470548	0.952699
1	1.396064	-2.782283	-0.576588
1	0.027792	0.075183	2.311884
1	0.820479	-2.199425	1.748522
6	-1.835204	-0.747885	-0.270710
1	-1.875069	-1.668208	0.318159
1	-1.318949	-0.996349	-1.212358
6	-3.260395	-0.275128	-0.566537
1	-3.289848	0.569930	-1.262130
1	-3.823774	-1.093719	-1.028268
1	-3.773313	0.018886	0.355591

NCOMe-TS

Electronic energy = -517.5452012

Sum of electronic and zero-point energies = -517.358697

Value of imaginary frequencies = -515.6

Atom number	X	Y	Z
6	1.388222	-1.699988	-0.693601
6	2.432315	-0.777703	-0.884825
1	1.509607	-2.658177	-1.196969
6	0.507962	-1.637021	0.388989
6	2.725213	0.262880	0.000971

1	1.794595	1.564181	1.642855
6	0.644968	1.958544	-0.133770
6	2.219301	-0.879681	-0.672185
1	3.453559	0.284176	0.577085
1	1.089689	2.905642	-0.430700
6	-0.585424	1.647159	-0.526100
6	1.114377	-1.745017	-0.579504
1	3.087988	-1.291060	-1.184878
1	-1.206142	2.260301	-1.171262
7	-1.152100	0.464548	-0.064015
6	-0.422720	-0.396639	0.846179
6	0.107872	-1.605144	0.376180
1	1.249379	-2.728437	-1.027354
1	-0.935460	-0.443483	1.806688
1	-0.180553	-2.510519	0.913459
6	-2.470725	0.150756	-0.316841
1	-2.952715	0.902356	-0.971386
8	-3.054120	-0.825307	0.114086
1	3.239533	-1.120401	-1.531020
1	0.355756	-2.566795	0.942784
6	-0.011169	-0.458571	0.941951
6	1.812319	1.046707	0.726927
1	3.781738	0.353462	0.267092
1	-0.358903	-0.517246	1.975103
7	-0.857441	0.402833	0.137485
6	-0.385000	1.657548	-0.244208
6	0.865273	1.981425	0.064694
1	2.235073	1.466578	1.646757
6	-2.182788	0.072086	-0.158358
1	-1.099180	2.283656	-0.760947
1	1.247742	2.972219	-0.170243
6	-2.698129	-1.264469	0.341874
8	-2.892024	0.832869	-0.802642
1	-3.766948	-1.303690	0.127617
1	-2.196005	-2.094928	-0.165295
1	-2.535435	-1.394826	1.417369

NSO_2Ph-TS

Electronic energy = -1144.5014343

Sum of electronic and zero-point energies = -1144.261867

Value of imaginary frequencies = -513.1

Atom number	X	Y	Z
6	-1.382351	2.298272	0.274451
6	-2.601241	2.316143	-0.430366
1	-0.859033	3.251338	0.335401
6	-1.057590	1.312806	1.203062
6	-3.634010	1.398566	-0.235224
1	-2.876489	3.282061	-0.852487
1	-0.650807	1.652403	2.157919
6	-1.403484	-0.044393	1.091363
6	-3.537163	0.022607	0.052298
1	-4.626595	1.847595	-0.140265
1	-1.399818	-0.626086	2.012242
7	-0.879716	-0.810881	-0.022939
6	-1.752302	-1.353766	-0.971996
6	-3.024530	-0.975041	-0.920888
1	-4.405835	-0.356894	0.602630
16	0.627863	-1.578058	0.240614
1	-1.325079	-2.049071	-1.681588
1	-3.747095	-1.395201	-1.616525
6	1.816917	-0.263844	-0.043787
8	0.776503	-2.565146	-0.832366
8	0.724384	-1.961657	1.652171
6	2.112378	0.109470	-1.357164
6	2.445061	0.339345	1.045787
6	3.049125	1.117116	-1.577098
1	1.625704	-0.391033	-2.187625
6	3.382935	1.346668	0.811857
1	2.210234	0.008807	2.051496
6	3.681675	1.736103	-0.494702
1	3.290711	1.414915	-2.593378
1	3.882781	1.821450	1.651364
1	4.413918	2.518926	-0.672429

NCO_2Et-TS

Electronic energy = -632.088505

Sum of electronic and zero-point energies = -631.868117

Value of imaginary frequencies = -505.9

Atom number	X	Y	Z
6	3.428090	0.704814	0.159744
6	2.454685	1.214542	-0.715242
6	3.251404	-0.266352	1.148030
1	4.467563	0.978327	-0.039192
1	2.875497	1.640911	-1.632764
6	1.278984	1.979946	-0.228993
6	2.410663	-1.384678	1.009816
1	4.042650	-0.369871	1.889744
1	1.429913	3.041349	-0.044156
6	0.083090	1.437788	-0.024793
6	1.649080	-1.635051	-0.131851
1	2.645576	-2.231187	1.653679
1	-0.782264	1.962273	0.353961
7	-0.097777	0.094470	-0.348003
6	0.990052	-0.679808	-0.915918
1	1.702962	-2.647637	-0.536815
6	-1.332820	-0.529157	-0.354601
1	0.747411	-0.986526	-1.932664
8	-1.523956	-1.668120	-0.739157
8	-2.306209	0.286400	0.125892
6	-3.626229	-0.297231	0.164597
1	-3.596813	-1.200767	0.781608
1	-3.911854	-0.597309	-0.848541
6	-4.565425	0.749870	0.733486
1	-5.583263	0.347687	0.781203
1	-4.262132	1.040238	1.744593
1	-4.578935	1.646890	0.105835

NCN-TS

Electronic energy = -457.1131208
Sum of electronic and zero-point energies = -456.966245
Value of imaginary frequencies = -517.1

Atom number	X	Y	Z
6	1.377911	1.172421	0.625833
6	2.358603	0.371816	0.016701
1	1.742917	1.714546	1.504778
6	0.402272	1.976411	-0.158065
6	2.163849	-0.773956	-0.759969
1	3.396863	0.557886	0.303779
1	0.726017	2.962633	-0.480594
6	-0.812044	1.537638	-0.465546
6	1.176093	-1.741543	-0.505306
1	3.014355	-1.125248	-1.342789
1	-1.549868	2.062519	-1.060648
7	-1.191669	0.286309	0.027901
6	-0.341767	-0.444149	0.964639
6	0.256441	-1.635748	0.539969
1	1.369875	-2.731998	-0.913515
1	-0.768249	-0.429567	1.968041
1	0.122927	-2.519506	1.166684
6	-2.434278	-0.177814	-0.142546
7	-3.513661	-0.600839	-0.290758

NCO_2Me-TS

Electronic energy = -592.7694223
Sum of electronic and zero-point energies = -592.57746
Value of imaginary frequencies = -506.9

Atom number	X	Y	Z
6	-3.100145	0.469645	-0.048990
6	-2.120710	1.150639	0.692136
6	-2.900173	-0.572622	-0.956975
1	-4.144195	0.663533	0.210236
1	-2.512476	1.624392	1.599161
6	-1.066502	1.970005	0.042772
6	-1.942928	-1.588590	-0.788519
1	-3.729173	-0.821384	-1.618590
1	-1.336318	2.989329	-0.225012
6	0.159846	1.524579	-0.208249
6	-1.079038	-1.654764	0.304973
1	-2.137842	-2.511944	-1.332334
1	0.938418	2.087228	-0.702959
7	0.497206	0.241801	0.220609
6	-0.463796	-0.570655	0.943470
1	-1.002231	-2.623758	0.802382
6	1.784297	-0.260690	0.183961
1	-0.118584	-0.752264	1.960556
8	2.119979	-1.331420	0.654786
8	2.634615	0.589709	-0.449598
6	3.987369	0.121145	-0.531546
1	4.036740	-0.825395	-1.076022
1	4.409035	-0.021163	0.466965
1	4.530121	0.900361	-1.068348

$NCONMe_2$-TS

Electronic energy = -612.202231
Sum of electronic and zero-point energies = -611.969658
Value of imaginary frequencies = -515.3

Atom number	X	Y	Z
6	-2.172387	1.751849	-0.496167
6	-3.288665	0.892739	-0.421920
1	-2.379675	2.749965	-0.881041
6	-1.017906	1.598111	0.258023
6	-3.344719	-0.202593	0.428054
1	-4.230155	1.313676	-0.771103
1	-0.650094	2.513644	0.730573
6	-0.385509	0.402619	0.681182
6	-2.273893	-1.052424	0.780242
1	-4.290017	-0.348881	0.956025
1	0.204545	0.525418	1.589207
7	0.303069	-0.500834	-0.211845
6	-0.386370	-1.607381	-0.720410
6	-1.595434	-1.881131	-0.244557
1	-2.454041	-1.608542	1.707761
6	1.704465	-0.661878	-0.115510
1	0.152565	-2.211811	-1.436997
1	-2.113867	-2.779537	-0.572778
8	2.233588	-1.753831	-0.283800
7	2.428962	0.479838	0.211912
6	3.830031	0.238175	0.544841
6	2.213829	1.735959	-0.507076
1	4.446923	0.080026	-0.351771
1	4.212902	1.108677	1.087805
1	3.911499	-0.648248	1.174041
1	2.412178	2.586675	0.155533
1	2.893952	1.807444	-1.369991
1	1.189712	1.804845	-0.867563

Table S3

[1,2]-P

Electronic energy = -502.5806291
Sum of electronic and zero-point energies = -502.369401
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.794289	-0.444895	0.347493
6	-0.675073	-0.652846	0.687061
6	1.020411	0.853339	-0.126651
6	1.843435	-1.356378	0.447458
6	-1.396545	-1.494078	-0.347775
6	-1.219091	0.811901	0.765022
6	-0.269871	1.640923	-0.162574
6	2.302782	1.251294	-0.500667
6	3.129809	-0.957931	0.070077
1	-0.774803	-1.158800	1.660989
1	1.670685	-2.362976	0.822491
6	-2.614172	-1.164900	-0.807116
6	-2.676298	0.955139	0.411514
1	-1.055311	1.168967	1.789581
1	-0.673642	1.678092	-1.183598
1	-0.159270	2.677342	0.177157
1	-0.900638	-2.402245	-0.684848
6	3.357512	0.338247	-0.400977
1	2.485551	2.260139	-0.863894
1	3.957923	-1.657299	0.150949
6	-3.306284	0.040842	-0.343427
1	-3.192197	1.855950	0.738389
1	-3.119988	-1.806040	-1.525702
1	4.361769	0.640486	-0.686711
1	-4.345511	0.182442	-0.631428

[2,3]-P

Electronic energy = -502.5818512
Sum of electronic and zero-point energies = -502.370602
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.614939	-0.432186	0.280787
6	1.021850	0.857220	-0.126404
6	-0.855761	-0.731651	0.477033
6	1.577664	-1.430764	0.437235
6	0.025330	1.926075	-0.240653
6	-1.758301	0.501679	0.793345
6	-1.529831	-1.399035	-0.766202
1	-0.963477	-1.437246	1.309521
6	2.928710	-1.178381	0.184436
6	2.378829	1.099893	-0.384680
1	1.266124	-2.422384	0.760154
6	-1.237556	1.786882	0.188069
6	-3.089549	0.096441	0.178258
6	-2.960553	-0.927508	-0.667122
1	-1.857014	0.649243	1.881047
1	-1.423786	-2.490873	-0.748793
1	-1.069174	-1.054049	-1.703236
6	3.329232	0.091372	-0.233179
1	0.359951	2.875662	-0.654902
1	3.662129	-1.969851	0.313967
1	2.687395	2.094775	-0.698950
1	-4.010454	0.636109	0.383417
1	-3.766651	-1.361263	-1.252917
1	-1.932271	2.622292	0.119382
1	4.377209	0.297357	-0.434225

[3,4]-P

Electronic energy = -502.5428573
Sum of electronic and zero-point energies = -502.332648
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-0.172088	1.484337	-0.464588
6	0.938151	0.742391	-0.231184
6	-1.547798	0.891349	-0.535846
1	-0.085773	2.567842	-0.535483
6	0.839551	-0.737286	-0.116715
6	-1.582403	-0.648280	-0.812153
6	-2.385446	1.088699	0.776785
6	2.252059	1.345975	-0.066433
1	-2.110425	1.383491	-1.338734
6	-0.329075	-1.369925	-0.381742
6	-2.804529	-1.096874	-0.022780
6	-3.232820	-0.160229	0.823933
6	3.340360	0.600548	0.237974
6	2.047159	-1.468728	0.239216
1	-1.731499	-0.848024	-1.887357
1	-2.974793	2.014171	0.751512
1	-1.734624	1.152381	1.660292
1	2.330173	2.425104	-0.178825
6	3.233521	-0.838107	0.404142

[4,5]-P

Electronic energy = -502.5811309
Sum of electronic and zero-point energies = -502.369995
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.257275	1.730407	0.204681
6	-0.002753	1.907007	-0.215222
6	1.774570	0.441498	0.795459
1	1.965280	2.556349	0.148916
6	-1.019503	0.857808	-0.118984
6	0.830217	-0.769587	0.501608
6	3.138274	0.036732	0.151372
1	1.900858	0.587693	1.878016
1	-0.316764	2.871188	-0.611036
6	-0.637187	-0.437589	0.285840
6	1.492566	-1.413510	-0.711773
6	2.739923	-0.978786	-0.892093
1	0.888737	-1.481812	1.339610
1	3.813118	-0.412578	0.896022
1	3.670795	0.900805	-0.266609
6	-2.369856	1.124113	-0.387107
1	0.984939	-2.163127	-1.312206
1	3.419960	-1.327768	-1.664413
6	-1.615601	-1.422342	0.428069

1	-0.375233	-2.456757	-0.322952
1	-3.229480	-2.091060	-0.133845
1	-4.074015	-0.271078	1.503075
1	4.310276	1.073062	0.368824
1	1.969882	-2.547828	0.351970
1	4.125657	-1.404529	0.657864

O-P

Electronic energy = -384.8178245
Sum of electronic and zero-point energies = -384.678319
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-0.315027	0.787831	0.679424
6	0.871208	1.473173	0.041170
1	-0.364486	1.116356	1.728934
6	-1.628688	1.074300	-0.036495
6	-0.285376	-0.775287	0.627750
6	1.947474	0.799133	-0.388831
1	0.816519	2.555926	-0.054405
1	-2.066256	2.056811	-0.153213
6	-2.091114	-0.063081	-0.555786
8	-1.352915	-1.181400	-0.304634
6	1.007924	-1.396011	0.189739
1	-0.590745	-1.183499	1.598842
6	2.026225	-0.659261	-0.279782
1	2.787607	1.326768	-0.833712
1	-2.975396	-0.240220	-1.157267
1	1.075407	-2.479531	0.244104
1	2.944916	-1.146191	-0.599353

PH-P

Electronic energy = -651.5553593
Sum of electronic and zero-point energies = -651.410293
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.027884	0.958905	0.708608
6	1.114681	1.457623	-0.226861
1	0.241124	1.363234	1.713283
6	-1.338739	1.443727	0.257455
6	-0.046047	-0.596469	0.782694
6	2.130870	0.674016	-0.621077
1	1.056786	2.495587	-0.548643
1	-1.601234	2.494141	0.383157
6	-2.146290	0.552230	-0.324234
6	1.241293	-1.310105	0.494513
1	-0.404610	-0.876110	1.780464
15	-1.474680	-1.163419	-0.367595
6	2.242090	-0.716365	-0.177322
1	2.907212	1.073063	-1.270022
1	-3.136622	0.797561	-0.698155
1	1.322348	-2.348758	0.807591
1	-0.771692	-1.064817	-1.608249
1	3.152427	-1.263983	-0.408162

6	-3.337276	0.129494	-0.251147
1	-2.659434	2.125754	-0.697927
6	-2.960299	-1.148511	0.162577
1	-1.322984	-2.420083	0.750470
1	-4.379962	0.352817	-0.460934
1	-3.706642	-1.929643	0.280410

NH-P

Electronic energy = -364.9493288
Sum of electronic and zero-point energies = -364.797414
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-0.277826	0.821784	0.662277
6	0.975327	1.446299	0.090436
1	-0.384939	1.186792	1.695133
6	-1.525305	1.163499	-0.142526
6	-0.306352	-0.756382	0.675845
6	2.007559	0.724009	-0.366772
1	0.999624	2.534026	0.047966
1	-1.866891	2.174863	-0.324976
6	-2.114627	0.043794	-0.571473
6	0.934923	-1.425595	0.141528
1	-0.466298	-1.102118	1.705189
7	-1.528603	-1.145562	-0.101808
6	1.985120	-0.740961	-0.334562
1	2.887268	1.215364	-0.775529
1	-3.007534	-0.034971	-1.184177
1	0.946972	-2.514603	0.162571
1	-1.338063	-1.824690	-0.835253
1	2.857159	-1.274414	-0.706790

S-P

Electronic energy = -707.7967199
Sum of electronic and zero-point energies = -707.660353
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.023928	0.948328	0.703665
6	1.101569	1.456470	-0.233839
1	0.257144	1.323299	1.714373
6	-1.356574	1.422931	0.282674
6	-0.046282	-0.602914	0.770709
6	2.125406	0.681908	-0.625524
1	1.029360	2.492702	-0.557205
1	-1.656742	2.459613	0.405563
6	-2.120466	0.502359	-0.311661
6	1.240069	-1.312655	0.483128
1	-0.437970	-0.898053	1.748154
6	2.239936	-0.705777	-0.178161
1	2.900728	1.081630	-1.274667
1	-3.112165	0.666878	-0.719838
1	1.323537	-2.351466	0.792613
1	3.156439	-1.247136	-0.399979
16	-1.419115	-1.116960	-0.440935

BH-P

Electronic energy = -335.0637156

Sum of electronic and zero-point energies = -334.916030

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.336672	-0.753492	0.727749
6	-0.912206	-1.426024	0.191395
1	0.545470	-1.159143	1.730712
6	1.505727	-1.088565	-0.179882
6	0.296520	0.813987	0.764976
6	-1.907842	-0.738974	-0.391267
1	-0.958679	-2.511284	0.263166
1	1.739927	-2.133808	-0.390584
6	2.173718	-0.026334	-0.688458
6	-0.913912	1.436338	0.114363
1	0.380446	1.199300	1.792900
5	1.549454	1.253928	-0.121129
6	-1.898217	0.719839	-0.457298
1	-2.770089	-1.267421	-0.792166
1	3.024562	-0.150885	-1.354142
1	-0.950699	2.523993	0.098197
1	1.893794	2.386000	-0.295887
1	-2.734761	1.222960	-0.936026

AlH-P

Electronic energy = -552.6367803

Sum of electronic and zero-point energies = -552.495978

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.126954	0.901056	0.795645
6	1.471701	1.255037	0.181794
1	0.065194	1.370643	1.789831
6	-0.931247	1.581649	-0.083081
6	-0.109592	-0.642531	0.942926
6	2.206886	0.369759	-0.513274
1	1.802084	2.287809	0.279164
1	-0.791434	2.660776	-0.204374
6	-1.930875	0.913969	-0.698692
6	0.831153	-1.516194	0.180665
1	-0.171758	-0.959760	1.990569
13	-1.774856	-0.914008	-0.124139
6	1.849221	-1.040927	-0.572793
1	3.132621	0.687360	-0.988467
1	-2.624695	1.473546	-1.321983
1	0.670065	-2.593116	0.243039
1	-2.569316	-2.256425	-0.427084
1	2.475157	-1.719643	-1.146038

CHCl-P

Electronic energy = -808.5183338

Sum of electronic and zero-point energies = -808.363716

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.076080	0.025023	-0.456370
6	-0.014968	-0.335386	0.600483
6	1.054378	1.522479	-0.516679
17	2.735162	-0.631776	0.007962
1	0.885355	-0.436635	-1.428374
6	-0.754724	-1.605062	0.273540
6	-0.016085	2.023168	0.101098
6	-0.907211	0.950489	0.702459
1	0.510648	-0.453253	1.553759
1	1.815831	2.087749	-1.043427
6	-1.998770	-1.591159	-0.229777
6	-2.232779	0.839596	-0.022414
1	-0.220973	-2.541916	0.416625
1	-0.274344	3.077934	0.145480
1	-1.122862	1.187532	1.756959
6	-2.724435	-0.336033	-0.441666
1	-2.495027	-2.522513	-0.492050
1	-2.794118	1.760355	-0.170324
1	-3.691177	-0.377747	-0.938046

CF_2-P

Electronic energy = -547.3976233

Sum of electronic and zero-point energies = -547.249938

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.635265	1.081899	0.602099
6	2.050435	1.045024	0.069344
1	0.662820	1.585713	1.581169
6	-0.291108	1.868052	-0.309865
6	-0.076382	-0.310408	0.746093
6	2.660949	-0.092474	-0.288368
1	2.559387	2.002871	-0.021358
1	-0.054489	2.882705	-0.619301
6	-1.383742	1.195418	-0.665763
6	0.737484	-1.496238	0.291713
1	-0.373084	-0.469475	1.789635
6	-1.409771	-0.167190	-0.051747
6	1.988972	-1.388130	-0.174502
1	3.679069	-0.070695	-0.669449
1	-2.193859	1.544070	-1.296925
1	0.256002	-2.467659	0.361671
9	-2.497057	-0.312097	0.785754
9	-1.563203	-1.148440	-1.003635
1	2.533878	-2.278414	-0.478524

$C(SiH_3)_2$-P

Electronic energy = -930.3006251

Sum of electronic and zero-point energies = -930.107303

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-1.216606	1.302492	-0.424329
6	-2.481845	0.808240	0.245523

CNT-P

Electronic energy = -348.9197571

Sum of electronic and zero-point energies = -348.756092

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-0.320557	0.754859	0.697197
6	0.776121	1.485517	-0.049915

1	-1.528950	1.928793	-1.276480
6	-0.326437	2.107937	0.503407
6	-0.259421	0.165384	-0.931888
6	-2.904359	-0.459410	0.129151
1	-3.061527	1.537543	0.808734
1	-0.635290	3.062561	0.920227
6	0.829694	1.493089	0.766141
6	-0.926160	-1.171506	-1.134516
1	0.132305	0.497095	-1.903606
6	0.970463	0.147410	0.083542
6	-2.140682	-1.450569	-0.632794
1	-3.832782	-0.775184	0.599036
1	1.599049	1.886518	1.426528
1	-0.373759	-1.926154	-1.691020
14	2.618373	0.008779	-0.858200
14	0.889657	-1.201797	1.440974
1	-2.579193	-2.434870	-0.780595
1	2.744307	1.138688	-1.820796
1	3.778631	0.046326	0.074610
1	2.675983	-1.265929	-1.626763
1	1.209267	-2.556623	0.910711
1	1.923504	-0.865684	2.461076
1	-0.431854	-1.229218	2.114089

NMe-P

Electronic energy = -404.2577694

Sum of electronic and zero-point energies = -404.077862

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.535502	1.029299	0.597819
6	1.973135	0.872719	0.162747
1	0.526298	1.565866	1.560250
6	-0.318803	1.797820	-0.406259
6	2.466279	-0.278948	-0.312498
1	2.592907	1.766550	0.204254
1	-0.034096	2.740862	-0.853716
6	-1.497218	1.177441	-0.534294
6	1.627221	-1.475765	-0.400511
1	3.497972	-0.343950	-0.649626
1	-2.350261	1.490906	-1.128175
7	-1.629559	0.036826	0.261378
6	-0.267934	-0.311758	0.764218
6	0.368105	-1.495226	0.060476
1	2.056949	-2.371527	-0.844311
1	-0.368058	-0.576441	1.827171
1	-0.214565	-2.411885	0.007676
6	-2.537267	-1.019561	-0.140185
1	-2.668346	-1.728402	0.685464
1	-3.517397	-0.582222	-0.358020
1	-2.208610	-1.583676	-1.029696

NCHO-P

Electronic energy = -478.2971777

Sum of electronic and zero-point energies = -478.135165

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.951855	0.916533	0.683365
6	2.318759	0.513213	0.176882
1	-0.278023	1.082396	1.749392
6	-1.698871	1.033797	0.118658
6	-0.222295	-0.807301	0.605747
6	1.895395	0.869785	-0.460637
1	0.634604	2.551001	-0.223916
1	-2.162551	2.015099	0.180612
6	-2.220075	-0.030389	-0.492839
6	1.154443	-1.336303	0.300960
1	-0.554518	-1.213514	1.569263
6	-1.298897	-1.226065	-0.452632
6	2.118406	-0.557837	-0.215357
1	2.672479	1.431435	-0.974523
1	-3.182458	-0.050369	-0.997566
1	1.331683	-2.397721	0.466098
1	-1.809653	-2.156567	-0.172911
1	-0.843859	-1.400751	-1.438033
1	3.090279	-0.977390	-0.465512

NEt-P

Electronic energy = -443.5726063

Sum of electronic and zero-point energies = -443.364096

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.023790	1.003619	0.595265
6	2.465085	0.745042	0.226378
1	1.004630	1.558870	1.547118
6	0.253217	1.797799	-0.456228
6	2.882489	-0.429435	-0.265977
1	3.153978	1.581509	0.327612
1	0.622719	2.691182	-0.942050
6	-0.973982	1.276261	-0.572291
6	1.948275	-1.544075	-0.437161
1	3.919838	-0.572261	-0.558963
1	-1.786830	1.642755	-1.189357
7	-1.203663	0.181953	0.269687
6	0.133283	-0.277458	0.746951
6	0.679959	-1.477021	-0.006473
1	2.311572	-2.449033	-0.919983
1	0.028537	-0.563828	1.803676
1	0.020235	-2.333209	-0.125515
6	-2.220413	-0.810344	-0.058743
1	-2.145352	-1.606592	0.691539
1	-2.041569	-1.284409	-1.040402
6	-3.636002	-0.230520	-0.015835
1	-3.783257	0.545326	-0.775134
1	-4.372534	-1.019382	-0.205989
1	-3.840535	0.212207	0.964326

NCOMe-P

Electronic energy = -517.6149883

Sum of electronic and zero-point energies = -517.425141

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.960520	-1.591015	-0.642207
6	2.986299	-0.596816	-0.320841
1	2.252097	-2.458936	-1.229100
6	0.690393	-1.457966	-0.236169
6	2.668853	0.536667	0.317671

1	1.073957	1.264395	1.720878
6	0.327068	2.034562	-0.143211
6	2.580718	-0.698651	-0.329337
1	3.093666	1.275512	0.228727
1	0.826029	2.968962	-0.366014
6	-0.896519	1.692224	-0.549039
6	1.542573	-1.728338	-0.420529
1	3.578598	-0.939398	-0.687561
1	-1.601917	2.266308	-1.138509
7	-1.267238	0.412006	-0.114443
6	-0.141460	-0.216636	0.642094
6	0.291310	-1.518644	0.010006
1	1.811986	-2.690134	-0.850679
1	-0.523099	-0.430126	1.647212
1	-0.475092	-2.283716	-0.058289
6	-2.503728	-0.148884	-0.218211
1	-3.211434	0.492292	-0.779429
8	-2.815685	-1.235050	0.246582
1	4.011286	-0.792588	-0.625120
1	-0.049504	-2.212578	-0.488220
6	0.218844	-0.298978	0.616039
6	1.256570	0.876893	0.733064
1	3.426834	1.287755	0.530326
1	-0.044022	-0.672950	1.612799
7	-0.985314	0.364628	0.031556
6	-0.622602	1.633614	-0.454313
6	0.622756	1.971367	-0.117907
1	1.290828	1.219483	1.779331
6	-2.280672	-0.102265	-0.049771
1	-1.367713	2.186170	-1.008701
1	1.120721	2.896527	-0.377890
6	-2.573398	-1.476642	0.531739
8	-3.162686	0.562699	-0.582142
1	-3.623017	-1.490254	0.831487
1	-2.437927	-2.243865	-0.239936
1	-1.946279	-1.741902	1.387447

NSO_2Ph-P

Electronic energy = -1144.5719081

Sum of electronic and zero-point energies = -1144.32884

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.618889	2.460434	-0.638689
6	2.809662	2.439998	0.212855
1	1.172859	3.424139	-0.873846
6	1.080001	1.334378	-1.129836
6	3.498861	1.307873	0.415585
1	3.135916	3.372600	0.666732
1	0.197256	1.366042	-1.762213
6	1.655888	-0.020019	-0.814330
6	3.101638	-0.007978	-0.218756
1	4.392984	1.301527	1.035676
1	1.645232	-0.645961	-1.713086
7	0.856866	-0.763953	0.240379
6	1.786496	-1.518781	1.006583
6	3.047130	-1.143253	0.790423
1	3.827327	-0.227007	-1.017461
16	-0.596656	-1.517427	-0.228688
1	1.398736	-2.268887	1.681571
1	3.911641	-1.518431	1.323844
6	-1.812904	-0.228136	0.060310
8	-0.823504	-2.599156	0.735631
8	-0.580676	-1.787201	-1.673219
6	-1.911490	0.360262	1.323493
6	-2.691200	0.104636	-0.970797
6	-2.904724	1.310720	1.548648
1	-1.216277	0.084904	2.109404
6	-3.683814	1.057338	-0.731650
1	-2.589587	-0.376019	-1.937726
6	-3.789381	1.658703	0.523062
1	-2.989018	1.780273	2.524489
1	-4.373202	1.326762	-1.526681
1	-4.562305	2.400361	0.704957

NCO_2Et-P

Electronic energy = -632.1626127

Sum of electronic and zero-point energies = -631.938822

No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-2.091743	0.943680	0.674594
6	-3.393637	0.734851	-0.066206
1	-2.344629	1.236919	1.705635
6	-1.226469	2.030531	0.048062
6	-1.132120	-0.304621	0.713533
6	-3.694009	-0.400223	-0.710117
1	-4.083838	1.576331	-0.068391
1	-1.584949	3.025391	-0.183251
6	0.008529	1.579886	-0.178273
7	0.163965	0.239866	0.209643
6	-1.585738	-1.497314	-0.095637
1	-0.960314	-0.632896	1.745016
6	-2.764120	-1.531931	-0.732204
1	-4.640299	-0.499274	-1.236405
1	0.860083	2.097892	-0.595845
6	1.326416	-0.468692	0.317486
1	-0.901374	-2.339447	-0.113298
1	-3.054538	-2.422568	-1.284851
8	1.400194	-1.602986	0.764219
8	2.387846	0.246856	-0.139572
6	3.657759	-0.436492	-0.078361
1	3.593133	-1.360732	-0.661386
1	3.863234	-0.714313	0.960345
6	4.706893	0.510659	-0.630272
1	5.691049	0.030265	-0.603456
1	4.483753	0.780924	-1.667517
1	4.756038	1.429483	-0.036893

NCN-P

Electronic energy = -457.1854343
Sum of electronic and zero-point energies = -457.035205
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	0.944503	0.969544	0.628590
6	2.160514	0.625398	-0.203316
1	1.296769	1.275517	1.625167
6	0.108655	2.078037	-0.000294
6	2.446670	-0.628917	-0.579460
1	2.812561	1.452575	-0.475930
1	0.469258	3.085217	-0.162689
6	-1.073352	1.606223	-0.398800
6	1.582103	-1.751682	-0.210743
1	3.339596	-0.837444	-1.163155
1	-1.882760	2.114112	-0.907670
7	-1.227541	0.237813	-0.096660
6	-0.084573	-0.200880	0.787902
6	0.416329	-1.572870	0.427542
1	1.908838	-2.756009	-0.469274
1	-0.472213	-0.205354	1.814380
1	-0.220065	-2.415499	0.684674
6	-2.369116	-0.438994	-0.182574
7	-3.349942	-1.070423	-0.268852

NCO_2Me-P

Electronic energy = -592.8435883
Sum of electronic and zero-point energies = -592.648234
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	-3.029326	0.578981	0.022795
6	-1.705648	0.914001	0.672797
6	-3.285344	-0.606539	-0.544751
1	-3.775504	1.371184	0.020111
1	-1.919115	1.243496	1.701716
6	-0.957577	2.022622	-0.057680
6	-2.281864	-1.673597	-0.564403
1	-4.250360	-0.796824	-1.008139
1	-1.398339	2.977911	-0.312423
6	0.290019	1.645301	-0.340786
6	-1.074758	-1.526204	-0.002113
1	-2.540888	-2.610958	-1.051444
1	1.075987	2.196957	-0.836554
7	0.562449	0.340371	0.100591
6	-0.659104	-0.262238	0.713893
1	-0.336266	-2.321311	-0.016814
6	1.774652	-0.282703	0.165022
1	-0.402262	-0.519661	1.747803
8	1.959609	-1.383188	0.660367
8	2.753396	0.476574	-0.398134
6	4.054987	-0.124280	-0.380714
1	4.052537	-1.071255	-0.927022
1	4.384515	-0.307732	0.645493
1	4.712286	0.596435	-0.869091

$NCONMe_2$-P

Electronic energy = -612.2714008
Sum of electronic and zero-point energies = -612.035469
No. of imaginary frequencies = nil

Atom number	X	Y	Z
6	1.878637	-2.028466	0.162173
6	2.974796	-1.269984	-0.442298
1	1.933669	-3.114930	0.141630
6	0.827086	-1.421909	0.736155
6	3.064736	0.057317	-0.273392
1	3.725781	-1.809795	-1.013984
1	0.027672	-2.001369	1.187993
6	0.709877	0.078313	0.791488
6	2.056336	0.834609	0.544852
1	3.888625	0.622152	-0.704939
1	0.334419	0.367804	1.782187
7	-0.240024	0.713231	-0.211529
6	0.320751	1.966175	-0.538634
6	1.589785	2.100271	-0.151011
1	2.523132	1.064259	1.516058
6	-1.638667	0.676610	-0.025105
1	-0.303615	2.675186	-1.064792
1	2.232065	2.944311	-0.368500
8	-2.307166	1.696419	0.103235
7	-2.198041	-0.593456	0.014586
6	-3.612336	-0.638921	0.371156
6	-1.802881	-1.613006	-0.957585
1	-4.260288	-0.385325	-0.480810
1	-3.856513	-1.651362	0.709576
1	-3.811682	0.072313	1.172719
1	-1.857066	-2.610122	-0.506279
1	-2.476699	-1.593749	-1.828727
1	-0.784444	-1.435197	-1.296194

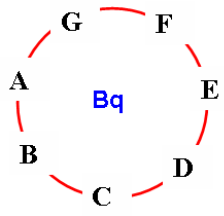
TABLE S4

molecules	Activation enthalpy (kcal/mol)	Group electronegativity	Barriers to planarity ($E_{Planarity}$) (kcal/mol)
NMe	26.25	2.32	0.13
NEt	28.42	2.35	0.15
NCN	21.37	3.46	3.17
NCOMe	21.31	2.93	7.05
NCO_2Me	21.85	3.16	6.17
NCHO	21.67	2.89	3.68
NH	29.67	2.1	0.00
NSO_2PH	21.98		3.05
NCO_2ET	21.86		6.37

TABLE S5

Reaction	*NICS(0) for annelated benzene (ppm)*		
	R	TS	P
[1,2]	-9.3	-8.6	-9.3
[2,3]	4.2	-7.5	-8.5
[3,4]	-9.0	-7.5	3.9
[4,5]	1.2	-7.2	-8.5

Nucleus Independent Chemical Shift (NICS) value for any ring is calculated at the centre using the keyword NMR available in the Gaussian package. The coordinates of the centre of the ring is computed from the coordinates of atoms constituting the ring. A fictitious atom Bq is fixed at the centre. The magnetic effect felt by Bq is taken as the NICS value for that ring. It is also possible to get NICS values away from the centre of the ring, in a direction perpendicular to the plane of the ring. Such values are denoted as NICS(X) values where X is the distance of the Bq from the centre of the ring, in a direction perpendicular to the plane of the ring.



Input for the calculation of NICS(0) for benzene molecule is given below.

Atom	X	Y	Z
C	-1.2093439174	0.0005557203	-0.6983867908
C	-1.2093178982	0.0010665293	0.6982167713
C	-0.0001083292	0.0003918184	1.3965483145
C	1.209401743	-0.000543076	0.698284854
C	1.2093738466	-0.0009363881	-0.6981139488
C	-0.0000044376	-0.0005043946	-1.3965507398
H	-2.150508181	0.000913535	-1.241630982
H	-2.1505449498	0.0018530758	1.2413965682
H	-0.0000764509	0.0006406077	2.4832359683
H	2.1504229948	-0.000973468	1.2417625604
H	2.1504690037	-0.0017558201	-1.2415086837
H	0.0002315403	-0.0008591853	-2.483246194
Bq	0.0	0.0	0.0