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Supplementary Material

Effect of Substitution for Insertion of CO_2 into Epoxides and Aziridines: An Ab Initio Study

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CONTENT

Table S1. Imaginary frequency of transition state structures

	Freq.(i/cm)
B3LYP/6-31++G(d,p)	
O-TS	-699.90
O-methyl-a-TS	-558.75
O-methyl-b-TS	-683.42
O-phenyl-a-TS	-401.06
O-phenyl-b-TS	-666.21
N-TS	-646.02
N-methyl-a-TS	-516.54
N-methyl-b-TS	-635.63
N-phenyl-a-TS	-365.51
N-phenyl-b-TS	-643.07
MP2/6-31++G(d,p)	
O-TS	-894.93
O-methyl-a-TS	-704.36
O-methyl-b-TS	-866.29
O-phenyl-a-TS	-499.36
O-phenyl-b-TS	-863.40
N-TS	-886.28
N-methyl-a-TS	-721.96
N-methyl-b-TS	-863.80
N-phenyl-a-TS	-527.02
N-phenyl-b-TS	-880.07

THE STRUCTURES IN THE GAS PHASE: AT B3LYP/6-31 ++G(d, p) LEVEL

O-Native

O-RC

Sum of electronic and zero-point Energies= -342.324690
Sum of electronic and thermal Energies= -342.317216
Sum of electronic and thermal Enthalpies= -342.316272
Sum of electronic and thermal Free Energies= -342.359753

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.993678	-0.702877	-0.081162
2	8	0	-1.364361	1.228792	0.067416
3	8	0	-2.188894	-0.956885	-0.042857
4	6	0	1.884043	0.236687	-0.707187
5	1	0	2.652525	-0.212332	-1.334064
6	1	0	2.705253	-0.574734	1.190156
7	6	0	1.914473	0.027773	0.746538
8	1	0	1.401757	1.126386	-1.108652
9	1	0	1.455094	0.765822	1.402144
10	6	0	-1.754851	0.125976	0.011189

O-TS

Sum of electronic and zero-point Energies= -342.232062
Sum of electronic and thermal Energies= -342.226405
Sum of electronic and thermal Enthalpies= -342.225461
Sum of electronic and thermal Free Energies= -342.261501

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.253935	-0.894832	-0.283207
2	8	0	-0.544766	1.242529	0.233065
3	8	0	-2.059237	-0.466587	-0.079178
4	6	0	1.596132	0.588515	-0.375673
5	1	0	1.797566	0.406806	-1.426362
6	1	0	2.170118	-1.385972	0.324717
7	6	0	1.432132	-0.591400	0.465147
8	1	0	1.553585	1.611050	-0.030228
9	1	0	1.249173	-0.391627	1.523159
10	6	0	-1.023248	0.121363	0.017739

O-PC

Sum of electronic and zero-point Energies= -342.343477
Sum of electronic and thermal Energies= -342.338616
Sum of electronic and thermal Enthalpies= -342.337672
Sum of electronic and thermal Free Energies= -342.371925

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.071748	1.112695	0.106019
2	8	0	-0.071683	-1.112701	-0.106040
3	8	0	-2.048597	-0.000032	-0.000002
4	6	0	1.304203	-0.757543	0.118197
5	1	0	1.573068	-1.025156	1.145341
6	1	0	1.926422	1.313806	0.584286
7	6	0	1.304184	0.757559	-0.118195
8	1	0	1.926546	-1.313737	-0.584243
9	1	0	1.573046	1.025228	-1.145322
10	6	0	-0.852197	0.000011	0.000017

O-methyl-a

O-methyl-a-RC

Sum of electronic and zero-point Energies= -381.622438
Sum of electronic and thermal Energies= -381.614489
Sum of electronic and thermal Enthalpies= -381.613545
Sum of electronic and thermal Free Energies= -381.657540

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.517188	0.141311	-0.640784
2	8	0	-1.934652	0.138058	1.215236
3	8	0	-2.591089	-0.442577	-0.952995
4	6	0	1.496498	-0.023239	0.406070
5	1	0	1.044080	-0.164063	1.389323
6	6	0	1.295901	1.283744	-0.237219
7	6	0	-2.239558	-0.150616	0.122000
8	6	0	2.672996	-0.910846	0.091816
9	1	0	3.063374	-0.699716	-0.908055
10	1	0	2.380862	-1.965807	0.131289
11	1	0	3.474953	-0.753894	0.822457
12	1	0	0.737076	2.064181	0.277734
13	1	0	2.013048	1.630710	-0.980402

O-methyl-a-TS

Sum of electronic and zero-point Energies= -381.538953
Sum of electronic and thermal Energies= -381.531789
Sum of electronic and thermal Enthalpies= -381.530845
Sum of electronic and thermal Free Energies= -381.570518

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.183673	0.867536	-0.413665
2	8	0	-0.924365	-0.960142	0.858409
3	8	0	-2.334862	0.008809	-0.681378
4	6	0	1.358225	-0.220080	0.447832
5	1	0	1.214714	-0.971613	1.215241
6	6	0	0.776220	1.118293	0.609646
7	6	0	-1.359972	-0.195892	-0.011536
8	6	0	2.138716	-0.602277	-0.738738
9	1	0	2.203571	0.185727	-1.488785
10	1	0	1.736954	-1.518171	-1.188552
11	1	0	3.144419	-0.873925	-0.374877
12	1	0	0.335866	1.308315	1.590887
13	1	0	1.428538	1.939777	0.295925

O-methyl-a-PC

Sum of electronic and zero-point Energies= -381.640260
Sum of electronic and thermal Energies= -381.634000
Sum of electronic and thermal Enthalpies= -381.633056
Sum of electronic and thermal Free Energies= -381.670748
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.750119	1.077522	-0.350206
2	8	0	-0.134723	-0.864389	0.565215
3	8	0	-2.249622	-0.620863	-0.222591
4	6	0	1.091073	-0.096723	0.495251
5	1	0	1.547835	-0.143634	1.487091
6	6	0	0.565972	1.316980	0.174975
7	6	0	-1.154263	-0.181258	-0.021225
8	6	0	2.018761	-0.685600	-0.556808
9	1	0	1.569331	-0.625033	-1.553417
10	1	0	2.230079	-1.734768	-0.334340
11	1	0	2.966694	-0.136359	-0.568987
12	1	0	0.479076	1.948692	1.064699
13	1	0	1.153436	1.832549	-0.587549

O-methyl-b

O-methyl-b-RC

Sum of electronic and zero-point Energies= -381.622376
Sum of electronic and thermal Energies= -381.613560
Sum of electronic and thermal Enthalpies= -381.612616
Sum of electronic and thermal Free Energies= -381.659843

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.524779	-0.190705	0.572640
2	8	0	2.059368	0.950894	-0.620434
3	8	0	2.507038	-1.133257	0.341433
4	6	0	-1.186393	1.088231	0.629230
5	1	0	-1.851848	1.217261	1.482215
6	6	0	-1.531865	0.112197	-0.414581
7	1	0	-0.554452	1.941892	0.388508
8	1	0	-1.113325	0.283947	-1.408175
9	6	0	2.259665	-0.094178	-0.131378
10	6	0	-2.788824	-0.717554	-0.370356
11	1	0	-3.579714	-0.243401	-0.963007
12	1	0	-2.606419	-1.715025	-0.784475
13	1	0	-3.142759	-0.832300	0.658337

O-methyl-b-TS

Sum of electronic and zero-point Energies= -381.530504
Sum of electronic and thermal Energies= -381.523465
Sum of electronic and thermal Enthalpies= -381.522521
Sum of electronic and thermal Free Energies= -381.561846

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.073240	-0.583109	0.387130
2	8	0	1.399131	1.086233	-0.295811
3	8	0	2.212558	-1.039779	0.052002
4	6	0	-0.806664	1.265326	0.360776
5	1	0	-1.016825	1.257610	1.426112
6	6	0	-1.124491	0.041307	-0.369659
7	1	0	-0.430184	2.176463	-0.080338
8	1	0	-0.883061	0.100660	-1.434823
9	6	0	1.445076	-0.124823	-0.030733
10	6	0	-2.454158	-0.643617	-0.110640
11	1	0	-3.266666	-0.118112	-0.623071
12	1	0	-2.399768	-1.666746	-0.493295
13	1	0	-2.669669	-0.685796	0.960370

O-methyl-b-PC

Sum of electronic and zero-point Energies= -381.640927
Sum of electronic and thermal Energies= -381.634672
Sum of electronic and thermal Enthalpies= -381.633728
Sum of electronic and thermal Free Energies= -381.671275

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.071749	-0.949029	0.126433
2	8	0	-0.919527	1.112851	-0.023355
3	8	0	-2.311722	-0.676977	-0.129374
4	6	0	0.507234	1.286345	-0.058179
5	1	0	0.811379	1.508522	-1.087765
6	6	0	1.041155	-0.070059	0.423386
7	1	0	0.773006	2.119752	0.594139
8	1	0	1.168843	-0.071660	1.513080
9	6	0	-1.211058	-0.219220	-0.019622
10	6	0	2.298562	-0.563129	-0.263722
11	1	0	3.132979	0.112445	-0.045030
12	1	0	2.565692	-1.561351	0.092659
13	1	0	2.156726	-0.606101	-1.347896

O-phenyl-a

O-phenyl-a-RC

Sum of electronic and zero-point Energies= -573.316667
Sum of electronic and thermal Energies= -573.304904
Sum of electronic and thermal Enthalpies= -573.303960
Sum of electronic and thermal Free Energies= -573.360650

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.224275	-0.631507	0.537718
2	8	0	3.582039	1.174593	-0.265347
3	8	0	3.984196	-0.980040	-1.080909
4	6	0	0.295493	0.467790	0.612648
5	1	0	0.719454	1.415922	0.280180
6	6	0	0.876512	-0.123890	1.835274
7	6	0	3.763905	0.089019	-0.665396
8	1	0	1.676860	0.398069	2.358656
9	1	0	0.265252	-0.792404	2.439919
10	6	0	-1.111002	0.216070	0.181736
11	6	0	-1.624628	-1.085015	0.087630
12	6	0	-1.940047	1.302730	-0.128077
13	6	0	-2.950852	-1.291256	-0.296197
14	1	0	-0.973809	-1.928558	0.296266
15	6	0	-3.268280	1.095796	-0.507628
16	1	0	-1.544461	2.314126	-0.073295
17	6	0	-3.777828	-0.202672	-0.591025
18	1	0	-3.337644	-2.303490	-0.371744
19	1	0	-3.900742	1.946553	-0.744085
20	1	0	-4.808630	-0.366010	-0.891372

O-phenyl-a-TS

Sum of electronic and zero-point Energies= -573.246269
Sum of electronic and thermal Energies= -573.236180
Sum of electronic and thermal Enthalpies= -573.235236
Sum of electronic and thermal Free Energies= -573.283169

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.782724	-0.943214	0.108883
2	8	0	2.636348	1.239170	0.024689
3	8	0	3.190191	-0.299831	-1.590680
4	6	0	0.380098	0.423098	1.056546
5	1	0	0.685705	1.457267	1.176615
6	6	0	1.365979	-0.620764	1.427810
7	6	0	2.687745	0.172339	-0.597366
8	1	0	2.173578	-0.221820	2.045931
9	1	0	0.929345	-1.509731	1.893163
10	6	0	-0.880555	0.188804	0.449668
11	6	0	-1.380114	-1.115060	0.178229
12	6	0	-1.693057	1.314559	0.149439
13	6	0	-2.652067	-1.274269	-0.345330
14	1	0	-0.745136	-1.976320	0.350771
15	6	0	-2.971294	1.144842	-0.366522
16	1	0	-1.300296	2.310747	0.330282
17	6	0	-3.448737	-0.147862	-0.613031
18	1	0	-3.030811	-2.268016	-0.560733
19	1	0	-3.590700	2.007448	-0.588750
20	1	0	-4.443783	-0.282691	-1.027077

O-phenyl-a-PC

Sum of electronic and zero-point Energies= -573.332293
Sum of electronic and thermal Energies= -573.322974
Sum of electronic and thermal Enthalpies= -573.322029
Sum of electronic and thermal Free Energies= -573.368435

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.659770	-0.531490	0.821849
2	8	0	-1.436657	0.347238	-0.830274
3	8	0	-3.611432	0.958450	-0.602365
4	6	0	-0.598700	-0.691481	-0.263991
5	1	0	-0.674307	-1.564854	-0.922187
6	6	0	-1.311390	-0.961546	1.074331
7	6	0	-2.664528	0.322056	-0.240357
8	1	0	-1.325005	-2.015795	1.354230
9	1	0	-0.893124	-0.363171	1.890293
10	6	0	0.838396	-0.253023	-0.156852
11	6	0	1.174131	1.015692	0.337173
12	6	0	1.859837	-1.137541	-0.522816
13	6	0	2.512560	1.387913	0.465362
14	1	0	0.388932	1.718631	0.599020
15	6	0	3.200865	-0.769011	-0.384161
16	1	0	1.607701	-2.116639	-0.922879
17	6	0	3.529102	0.495047	0.109606
18	1	0	2.762786	2.376359	0.839060
19	1	0	3.984162	-1.464072	-0.671400
20	1	0	4.570098	0.787325	0.210415

O-phenyl-b

O-phenyl-b-RC

Sum of electronic and zero-point Energies= -573.316592
Sum of electronic and thermal Energies= -573.304805
Sum of electronic and thermal Enthalpies= -573.303861
Sum of electronic and thermal Free Energies= -573.360789

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.270327	-0.771505	0.402101
2	8	0	3.202397	1.515566	-0.381124
3	8	0	4.154676	-0.538976	-0.964994
4	6	0	0.798238	-1.079841	1.721674
5	1	0	0.195423	-1.984141	1.794262
6	6	0	0.260898	0.079468	0.978392
7	1	0	1.520687	-0.923482	2.522188
8	1	0	0.634177	1.064205	1.261241
9	6	0	3.660581	0.477127	-0.666787
10	6	0	-1.090828	0.073954	0.345526
11	6	0	-1.501530	-0.975895	-0.488053
12	6	0	-1.972748	1.133955	0.595308
13	6	0	-2.779869	-0.969975	-1.048721
14	1	0	-0.807147	-1.781057	-0.707925
15	6	0	-3.253358	1.137172	0.037358
16	1	0	-1.655560	1.960507	1.226655
17	6	0	-3.661023	0.083617	-0.785079
18	1	0	-3.086578	-1.785463	-1.697509
19	1	0	-3.927872	1.964228	0.239395
20	1	0	-4.654494	0.087031	-1.223878

O-phenyl-b-TS

Sum of electronic and zero-point Energies= -573.222753
Sum of electronic and thermal Energies= -573.212491
Sum of electronic and thermal Enthalpies= -573.211547
Sum of electronic and thermal Free Energies= -573.260237

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.388010	0.582762	0.003799
2	8	0	-3.233178	-0.859192	0.234058
3	8	0	-3.560615	1.201912	-0.744938
4	6	0	-1.105731	-1.060032	1.120635
5	1	0	-0.883622	-0.480111	2.010974
6	6	0	-0.537692	-0.553978	-0.130207
7	1	0	-1.671900	-1.974907	1.227687
8	1	0	-0.792849	-1.172799	-0.996355
9	6	0	-3.026894	0.265749	-0.232422
10	6	0	0.934479	-0.203534	-0.103732
11	6	0	1.368577	1.042063	0.365320
12	6	0	1.872743	-1.150316	-0.538874
13	6	0	2.734496	1.334216	0.399450
14	1	0	0.634971	1.778811	0.674135
15	6	0	3.236456	-0.856788	-0.496481
16	1	0	1.537730	-2.111520	-0.921747
17	6	0	3.669483	0.386769	-0.025723
18	1	0	3.066643	2.305684	0.753298
19	1	0	3.957824	-1.592171	-0.840031
20	1	0	4.730128	0.618265	0.000887

O-phenyl-b-PC

Sum of electronic and zero-point Energies= -573.332292
Sum of electronic and thermal Energies= -573.322973
Sum of electronic and thermal Enthalpies= -573.322029
Sum of electronic and thermal Free Energies= -573.368434

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.436635	0.346947	-0.830409
2	8	0	-2.659803	-0.531159	0.822005
3	8	0	-3.611421	0.958236	-0.602808
4	6	0	-1.311435	-0.961126	1.074690
5	1	0	-0.893195	-0.362454	1.890446
6	6	0	-0.598700	-0.691572	-0.263711
7	1	0	-1.325058	-2.015270	1.354985
8	1	0	-0.674306	-1.565190	-0.921580
9	6	0	-2.664526	0.321986	-0.240526
10	6	0	0.838399	-0.253092	-0.156713
11	6	0	1.174158	1.015633	0.337274
12	6	0	1.859824	-1.137577	-0.522795
13	6	0	2.512589	1.387895	0.465308
14	1	0	0.388974	1.718554	0.599214
15	6	0	3.200859	-0.769008	-0.384298
16	1	0	1.607671	-2.116682	-0.922828
17	6	0	3.529116	0.495058	0.109435
18	1	0	2.762829	2.376347	0.838979
19	1	0	3.984143	-1.464046	-0.671625
20	1	0	4.570115	0.787365	0.210127

N-Native

N-RC

Sum of electronic and zero-point Energies= -322.448591
Sum of electronic and thermal Energies= -322.441168
Sum of electronic and thermal Enthalpies= -322.440224
Sum of electronic and thermal Free Energies= -322.482974

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.443529	1.246734	0.021600
2	8	0	-2.154359	-0.981122	-0.011932
3	6	0	1.917157	0.205557	-0.732666
4	1	0	2.721833	-0.278469	-1.281814
5	1	0	2.744744	-0.418686	1.227538
6	6	0	1.930851	0.122942	0.750554
7	1	0	1.489731	1.078035	-1.219441
8	1	0	1.513986	0.935538	1.339377
9	6	0	-1.756568	0.118620	0.003636
10	7	0	0.938227	-0.642589	-0.026966
11	1	0	1.196584	-1.625905	-0.083385

N-TS

Sum of electronic and zero-point Energies= -322.364485
Sum of electronic and thermal Energies= -322.358998
Sum of electronic and thermal Enthalpies= -322.358054
Sum of electronic and thermal Free Energies= -322.393497

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.541293	1.257841	0.273573
2	8	0	-2.068627	-0.407505	-0.134242
3	6	0	1.613541	0.548092	-0.492919
4	1	0	1.808596	0.260450	-1.520650
5	1	0	2.161544	-1.364175	0.353027
6	6	0	1.465408	-0.532529	0.485343
7	1	0	1.549409	1.598498	-0.251748
8	1	0	1.398761	-0.224522	1.528971
9	6	0	-0.960384	0.093510	0.024888
10	7	0	0.177770	-0.849986	-0.118616
11	1	0	0.005268	-1.777472	-0.497816

N-PC

Sum of electronic and zero-point Energies= -322.473647
Sum of electronic and thermal Energies= -322.468621
Sum of electronic and thermal Enthalpies= -322.467677
Sum of electronic and thermal Free Energies= -322.502080

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.081818	-1.130663	0.087176
2	8	0	2.070047	-0.022585	0.031248
3	6	0	-1.300296	-0.772809	-0.112989
4	1	0	-1.575205	-1.013789	-1.145581
5	1	0	-2.061890	1.253124	-0.504232
6	6	0	-1.347310	0.744172	0.148334
7	1	0	-1.910274	-1.357166	0.577143
8	1	0	-1.595817	0.970612	1.194677
9	6	0	0.862752	-0.006356	-0.011833
10	7	0	0.030515	1.084125	-0.175123
11	1	0	0.423788	1.994282	0.015387

N-methyl-a

N-methyl-a-RC

Sum of electronic and zero-point Energies= -361.743407
Sum of electronic and thermal Energies= -361.734656
Sum of electronic and thermal Enthalpies= -361.733712
Sum of electronic and thermal Free Energies= -361.779751

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.049046	1.024897	-0.626295
2	8	0	-2.557413	-1.078167	0.261620
3	6	0	1.529144	0.235448	-0.359327
4	1	0	1.928058	0.674284	1.773988
5	6	0	1.216486	0.830809	0.965165
6	1	0	1.142301	0.751351	-1.237458
7	1	0	0.644346	1.752584	1.031613
8	6	0	-2.259189	-0.033190	-0.171169
9	7	0	0.451718	-0.336505	0.471047
10	1	0	0.766194	-1.191810	0.928692
11	6	0	2.809706	-0.534442	-0.589125
12	1	0	2.664703	-1.328606	-1.330672
13	1	0	3.600489	0.128503	-0.958499
14	1	0	3.166673	-0.996358	0.339143

N-methyl-a-TS

Sum of electronic and zero-point Energies= -361.667986
Sum of electronic and thermal Energies= -361.660951
Sum of electronic and thermal Enthalpies= -361.660007
Sum of electronic and thermal Free Energies= -361.699236

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.971194	-0.953669	0.893949
2	8	0	2.315327	-0.041409	-0.727943
3	6	0	-1.371909	-0.249824	0.424416
4	1	0	-1.447597	1.904699	0.316779
5	6	0	-0.807963	1.089343	0.665521
6	1	0	-1.196344	-1.032183	1.152619
7	1	0	-0.452940	1.267292	1.681577
8	6	0	1.317324	-0.154430	-0.016464
9	7	0	0.262641	0.848466	-0.291628
10	1	0	0.373290	1.456759	-1.096807
11	6	0	-2.172075	-0.591459	-0.768534
12	1	0	-1.755972	-1.466601	-1.281435
13	1	0	-3.167560	-0.902974	-0.412088
14	1	0	-2.275796	0.232590	-1.476926

N-methyl-a-PC

Sum of electronic and zero-point Energies= -361.769794
Sum of electronic and thermal Energies= -361.763327
Sum of electronic and thermal Enthalpies= -361.762382
Sum of electronic and thermal Free Energies= -361.800243

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.132457	-0.902133	0.529169
2	8	0	2.275856	-0.634934	-0.189284
3	6	0	-1.092580	-0.124677	0.495799
4	1	0	-1.273319	1.857080	-0.449693
5	6	0	-0.605995	1.323533	0.234292
6	1	0	-1.547896	-0.221358	1.484692
7	1	0	-0.521218	1.899058	1.166172
8	6	0	1.162486	-0.191369	-0.028602
9	7	0	0.689675	1.058482	-0.367218
10	1	0	1.367695	1.781838	-0.555162
11	6	0	-2.021878	-0.673510	-0.578132
12	1	0	-2.211929	-1.736478	-0.406541
13	1	0	-2.979621	-0.141512	-0.555274
14	1	0	-1.580140	-0.555334	-1.572888

N- methyl-b

N-methyl-b-RC

Sum of electronic and zero-point Energies= -361.743466
Sum of electronic and thermal Energies= -361.734666
Sum of electronic and thermal Enthalpies= -361.733722
Sum of electronic and thermal Free Energies= -361.780477

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.073765	0.989512	-0.663670
2	8	0	2.533336	-1.084631	0.314326
3	6	0	-1.240394	0.921375	0.889839
4	1	0	-1.959373	0.822907	1.701193
5	6	0	-1.527138	0.207897	-0.381208
6	1	0	-0.684445	1.855228	0.881751
7	1	0	-1.138860	0.652791	-1.296754
8	6	0	2.259214	-0.052286	-0.162679
9	7	0	-0.450667	-0.270916	0.507225
10	1	0	-0.758244	-1.088088	1.033856
11	6	0	-2.791298	-0.602442	-0.556743
12	1	0	-3.588747	0.010620	-0.991874
13	1	0	-2.622983	-1.455742	-1.223796
14	1	0	-3.151803	-0.987611	0.404550

N-methyl-b-TS

Sum of electronic and zero-point Energies= -361.659848
Sum of electronic and thermal Energies= -361.652953
Sum of electronic and thermal Enthalpies= -361.652009
Sum of electronic and thermal Free Energies= -361.690706

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.382665	1.096318	-0.364023
2	8	0	2.262548	-0.968271	0.113883
3	6	0	-0.819970	1.232883	0.507172
4	1	0	-1.028516	1.104857	1.565202
5	6	0	-1.143988	0.102978	-0.372380
6	1	0	-0.427263	2.180203	0.169825
7	1	0	-0.984367	0.321873	-1.430022
8	6	0	1.383968	-0.126959	-0.044598
9	7	0	0.001828	-0.598935	0.204772
10	1	0	-0.139386	-1.482257	0.689429
11	6	0	-2.458503	-0.628137	-0.125656
12	1	0	-3.299416	-0.030633	-0.487580
13	1	0	-2.453599	-1.579908	-0.666101
14	1	0	-2.610991	-0.830560	0.939735

N-methyl-b-PC

Sum of electronic and zero-point Energies= -361.768370
Sum of electronic and thermal Energies= -361.761935
Sum of electronic and thermal Enthalpies= -361.760991
Sum of electronic and thermal Free Energies= -361.798698

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.920823	1.127525	-0.013600
2	8	0	-2.381518	-0.615580	-0.097654
3	6	0	0.513071	1.265382	-0.038576
4	1	0	0.824340	1.494266	-1.064951
5	6	0	1.056212	-0.105079	0.415368
6	1	0	0.791769	2.087013	0.623074
7	1	0	1.172581	-0.115606	1.510535
8	6	0	-1.246799	-0.205118	-0.034368
9	7	0	-0.076351	-0.936969	0.015092
10	1	0	-0.156281	-1.904784	0.293385
11	6	0	2.374997	-0.503151	-0.238485
12	1	0	3.165201	0.204347	0.036079
13	1	0	2.693440	-1.497346	0.091018
14	1	0	2.277257	-0.516861	-1.328378

N-phenyl-a

N-phenyl-a-RC

Sum of electronic and zero-point Energies= -553.437468
Sum of electronic and thermal Energies= -553.425825
Sum of electronic and thermal Enthalpies= -553.424881
Sum of electronic and thermal Free Energies= -553.479427

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.732799	0.994432	0.523115
2	8	0	-4.014598	-0.204248	-1.465261
3	6	0	-0.291233	0.088812	0.690788
4	1	0	-0.290171	-1.940724	1.586423
5	6	0	-0.912443	-1.068546	1.398177
6	1	0	-0.679441	1.076124	0.931350
7	1	0	-1.686816	-0.888680	2.139790
8	6	0	-3.836171	0.376680	-0.466390
9	7	0	-1.299304	-0.760168	0.013219
10	1	0	-0.845844	-1.391132	-0.646944
11	6	0	1.141820	0.090571	0.267602
12	6	0	1.822311	-1.078314	-0.112244
13	6	0	1.839916	1.306809	0.232827
14	6	0	3.158979	-1.030984	-0.509805
15	1	0	1.314025	-2.039725	-0.096066
16	6	0	3.179460	1.356749	-0.160469
17	1	0	1.327144	2.222174	0.516857
18	6	0	3.844794	0.187465	-0.534744
19	1	0	3.666126	-1.947109	-0.798805
20	1	0	3.699642	2.310163	-0.178225
21	1	0	4.885043	0.223158	-0.844202

N-phenyl-a-TS

Sum of electronic and zero-point Energies= -553.372613
Sum of electronic and thermal Energies= -553.362467
Sum of electronic and thermal Enthalpies= -553.361523
Sum of electronic and thermal Free Energies= -553.409603

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.593663	-1.171831	-0.473672
2	8	0	-3.083084	-0.423208	1.636130
3	6	0	-0.404339	0.071794	-1.139330
4	1	0	-0.917954	2.187814	-1.113291
5	6	0	-1.374022	1.195359	-1.109060
6	1	0	-0.740295	-0.836980	-1.624228
7	1	0	-2.117695	1.123865	-1.904500
8	6	0	-2.618074	-0.363651	0.490253
9	7	0	-1.955814	0.917336	0.196308
10	1	0	-1.741511	1.511384	0.988774
11	6	0	0.868296	0.028755	-0.496800
12	6	0	1.493280	1.162416	0.087526
13	6	0	1.568820	-1.204781	-0.502557
14	6	0	2.765737	1.060837	0.626798
15	1	0	0.975588	2.115521	0.111067
16	6	0	2.843649	-1.301009	0.044016
17	1	0	1.086749	-2.078836	-0.930005
18	6	0	3.442516	-0.170082	0.608244
19	1	0	3.239654	1.932177	1.067380
20	1	0	3.367889	-2.251073	0.038273
21	1	0	4.437072	-0.242746	1.038172

N-phenyl-a-PC

Sum of electronic and zero-point Energies= -553.460423
Sum of electronic and thermal Energies= -553.450828
Sum of electronic and thermal Enthalpies= -553.449884
Sum of electronic and thermal Free Energies= -553.497188

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.532184	0.225876	-1.014505
2	8	0	3.288465	1.323978	-0.072381
3	6	0	0.617904	-0.822829	-0.632642
4	1	0	0.607906	-1.769725	1.364390
5	6	0	1.320805	-1.511329	0.577405
6	1	0	0.552058	-1.510610	-1.480158
7	1	0	1.855528	-2.418223	0.263991
8	6	0	2.454402	0.450446	-0.021072
9	7	0	2.228535	-0.455805	0.987037
10	1	0	2.946539	-0.581168	1.684601
11	6	0	-0.762131	-0.275497	-0.317619
12	6	0	-0.975666	1.073502	-0.014274
13	6	0	-1.851988	-1.157950	-0.313404
14	6	0	-2.259136	1.527783	0.304223
15	1	0	-0.145502	1.770880	-0.044566
16	6	0	-3.132568	-0.704971	0.007576
17	1	0	-1.701948	-2.205103	-0.568866
18	6	0	-3.338895	0.642230	0.320079
19	1	0	-2.413168	2.577789	0.535373
20	1	0	-3.967782	-1.399353	0.004287
21	1	0	-4.334923	0.999000	0.565144

N-phenyl-b

N-phenyl-b-RC

Sum of electronic and zero-point Energies= -553.437469
Sum of electronic and thermal Energies= -553.425826
Sum of electronic and thermal Enthalpies= -553.424882
Sum of electronic and thermal Free Energies= -553.479389

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.722518	0.997034	0.526225
2	8	0	4.034547	-0.205641	-1.455209
3	6	0	0.911982	-1.062580	1.396495
4	1	0	0.286243	-1.929822	1.595773
5	6	0	0.292840	0.089537	0.678584
6	1	0	1.689064	-0.877793	2.134016
7	1	0	0.684441	1.078141	0.908058
8	6	0	3.841867	0.377522	-0.460397
9	7	0	1.295666	-0.770148	0.007038
10	1	0	0.837092	-1.406538	-0.644365
11	6	0	-1.142005	0.091038	0.261168
12	6	0	-1.839437	1.307643	0.225916
13	6	0	-1.825074	-1.078511	-0.111933
14	6	0	-3.180773	1.357315	-0.161241
15	1	0	-1.324687	2.223531	0.504663
16	6	0	-3.163601	-1.031491	-0.503256
17	1	0	-1.317441	-2.040284	-0.095253
18	6	0	-3.848698	0.187348	-0.528716
19	1	0	-3.700382	2.311044	-0.179569
20	1	0	-3.672747	-1.948147	-0.787044
21	1	0	-4.890374	0.222827	-0.833393

N-phenyl-b-TS

Sum of electronic and zero-point Energies= -553.350516
Sum of electronic and thermal Energies= -553.340533
Sum of electronic and thermal Enthalpies= -553.339588
Sum of electronic and thermal Free Energies= -553.387220

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.242531	-0.690224	0.488353
2	8	0	-3.507555	0.761667	-1.268663
3	6	0	-1.171332	-0.269435	1.570838
4	1	0	-0.924588	0.683319	2.026221
5	6	0	-0.545660	-0.573915	0.273752
6	1	0	-1.816552	-0.948310	2.107484
7	1	0	-0.773715	-1.580402	-0.079551
8	6	0	-2.901632	0.142928	-0.399926
9	7	0	-1.449207	0.418924	-0.317784
10	1	0	-1.053510	1.193885	-0.845989
11	6	0	0.923114	-0.248990	0.101685
12	6	0	1.776073	-1.225854	-0.426738
13	6	0	1.452451	1.003109	0.451858
14	6	0	3.136702	-0.960008	-0.600596
15	1	0	1.374665	-2.195657	-0.707344
16	6	0	2.810712	1.269467	0.274002
17	1	0	0.810375	1.779358	0.860278
18	6	0	3.656561	0.287798	-0.251178
19	1	0	3.785805	-1.726448	-1.013022
20	1	0	3.207620	2.242984	0.545425
21	1	0	4.713102	0.496658	-0.388716

N-phenyl-b-PC

Sum of electronic and zero-point Energies= -553.461475
Sum of electronic and thermal Energies= -553.451987
Sum of electronic and thermal Enthalpies= -553.451043
Sum of electronic and thermal Free Energies= -553.497517

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.657940	-0.579263	0.845680
2	8	0	-3.762833	0.857568	-0.531340
3	6	0	-1.282546	-0.963742	1.033579
4	1	0	-0.859939	-0.374589	1.854352
5	6	0	-0.588184	-0.626105	-0.310032
6	1	0	-1.248321	-2.025247	1.282533
7	1	0	-0.652679	-1.493024	-0.984678
8	6	0	-2.740850	0.306031	-0.198905
9	7	0	-1.481819	0.439881	-0.752466
10	1	0	-1.427373	0.824403	-1.685444
11	6	0	0.866589	-0.223499	-0.176940
12	6	0	1.872597	-1.129236	-0.536354
13	6	0	1.231538	1.032120	0.330410
14	6	0	3.221075	-0.794921	-0.382604
15	1	0	1.600935	-2.100688	-0.942994
16	6	0	2.577796	1.369239	0.479903
17	1	0	0.458139	1.747138	0.595303
18	6	0	3.576532	0.456132	0.125994
19	1	0	3.989734	-1.507573	-0.666912
20	1	0	2.847741	2.346582	0.869367
21	1	0	4.623394	0.721273	0.240703

THE STRUCTURES IN THE GAS PHASE: AT MP2/6-31 ++G(d, p) LEVEL

O-Native

O-RC

Sum of electronic and zero-point Energies= -341.400144
Sum of electronic and thermal Energies= -341.392893
Sum of electronic and thermal Enthalpies= -341.391948
Sum of electronic and thermal Free Energies= -341.433829

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.929760	-0.720633	-0.160831
2	8	0	-1.260064	1.240233	0.118282
3	8	0	-2.141047	-0.942427	-0.070305
4	6	0	1.801031	0.319613	-0.665319
5	1	0	2.567227	-0.029466	-1.345660
6	1	0	2.655483	-0.706603	1.096060
7	6	0	1.852981	-0.070631	0.745251
8	1	0	1.293997	1.236239	-0.940273
9	1	0	1.385502	0.565403	1.487070
10	6	0	-1.675913	0.137192	0.021007

O-TS

Sum of electronic and zero-point Energies= -341.289847
Sum of electronic and thermal Energies= -341.284403

Sum of electronic and thermal Enthalpies= -341.283459
Sum of electronic and thermal Free Energies= -341.319042

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.244895	-0.884140	-0.343296
2	8	0	-0.484788	1.244984	0.199194
3	8	0	-2.060659	-0.448404	-0.030678
4	6	0	1.539142	0.584078	-0.331208
5	1	0	1.782722	0.432694	-1.373273
6	1	0	2.143336	-1.400838	0.297713
7	6	0	1.415378	-0.613401	0.469964
8	1	0	1.560778	1.590753	0.047205
9	1	0	1.192083	-0.462526	1.522490
10	6	0	-1.000270	0.119389	0.011927

O-PC

Sum of electronic and zero-point Energies= -341.410135
Sum of electronic and thermal Energies= -341.405357
Sum of electronic and thermal Enthalpies= -341.404412
Sum of electronic and thermal Free Energies= -341.438444

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.063593	-1.115041	0.131691
2	8	0	0.063640	1.115049	-0.131717
3	8	0	2.053006	-0.000027	0.000014
4	6	0	-1.300940	0.744527	0.152122
5	1	0	-1.510802	0.953851	1.201284
6	1	0	-1.952531	-1.330901	0.488802
7	6	0	-1.300985	-0.744505	-0.152113
8	1	0	-1.952475	1.330986	-0.488740
9	1	0	-1.510884	-0.953880	-1.201255
10	6	0	0.849389	-0.000006	-0.000009

O-methyl-a

O-methyl-a-RC

Sum of electronic and zero-point Energies= -380.563311
Sum of electronic and thermal Energies= -380.554720
Sum of electronic and thermal Enthalpies= -380.553776
Sum of electronic and thermal Free Energies= -380.599164

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.481314	-0.330549	0.632061
2	8	0	1.826764	0.957931	-0.720281
3	8	0	2.497849	-1.043017	0.339163
4	6	0	-1.414288	0.151939	-0.368857
5	1	0	-0.923294	0.447653	-1.292049
6	6	0	-1.123699	0.957802	0.820179
7	6	0	2.138338	-0.047727	-0.180834
8	6	0	-2.685124	-0.632587	-0.511165
9	1	0	-3.087210	-0.874889	0.471475
10	1	0	-2.499962	-1.561839	-1.049852
11	1	0	-3.426061	-0.054403	-1.065380
12	1	0	-0.457523	1.808725	0.742360
13	1	0	-1.843695	0.983274	1.629964

O-methyl-a-TS

Sum of electronic and zero-point Energies= -380.460608
Sum of electronic and thermal Energies= -380.453621
Sum of electronic and thermal Enthalpies= -380.452677
Sum of electronic and thermal Free Energies= -380.491964

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.165030	0.865636	-0.444562

2	8	0	-0.830139	-0.984256	0.827899
3	8	0	-2.349296	0.019059	-0.613831
4	6	0	1.306627	-0.208008	0.451093
5	1	0	1.228533	-0.928990	1.250179
6	6	0	0.789901	1.142065	0.601118
7	6	0	-1.332437	-0.199866	-0.002473
8	6	0	2.059799	-0.619150	-0.744434
9	1	0	2.110157	0.158322	-1.499263
10	1	0	1.625317	-1.525871	-1.167606
11	1	0	3.061533	-0.895946	-0.393387
12	1	0	0.335662	1.362775	1.563978
13	1	0	1.451174	1.935950	0.258228

O-methyl-a-PC

Sum of electronic and zero-point Energies= -380.573850
Sum of electronic and thermal Energies= -380.567742
Sum of electronic and thermal Enthalpies= -380.566798
Sum of electronic and thermal Free Energies= -380.603982

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.672512	1.068724	-0.417453
2	8	0	-0.150471	-0.826836	0.664030
3	8	0	-2.237572	-0.584057	-0.233545
4	6	0	1.099893	-0.109893	0.504419

5	1	0	1.619657	-0.176020	1.458835
6	6	0	0.603338	1.303069	0.210287
7	6	0	-1.132250	-0.158218	-0.016068
8	6	0	1.906619	-0.730748	-0.616650
9	1	0	1.374610	-0.635266	-1.563590
10	1	0	2.077572	-1.786349	-0.414532
11	1	0	2.871003	-0.228260	-0.703491
12	1	0	0.446267	1.888347	1.117100
13	1	0	1.229728	1.849639	-0.490508

O- methyl-b

O-methyl-b-RC

Sum of electronic and zero-point Energies= -380.563300
Sum of electronic and thermal Energies= -380.554721
Sum of electronic and thermal Enthalpies= -380.553777
Sum of electronic and thermal Free Energies= -380.599039

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.484970	-0.348308	0.633140
2	8	0	1.812530	0.964489	-0.712059
3	8	0	2.509537	-1.038975	0.325649
4	6	0	-1.113646	0.946001	0.827727
5	1	0	-1.835105	0.974449	1.636082

6	6	0	-1.411094	0.150239	-0.366452
7	1	0	-0.438292	1.790201	0.756277
8	1	0	-0.915721	0.445627	-1.287403
9	6	0	2.137095	-0.042810	-0.183403
10	6	0	-2.690743	-0.618540	-0.514585
11	1	0	-3.424468	-0.028347	-1.065701
12	1	0	-2.516322	-1.546548	-1.058958
13	1	0	-3.096540	-0.862370	0.466134

O-methyl-b-TS

Sum of electronic and zero-point Energies= -380.455373
Sum of electronic and thermal Energies= -380.448535
Sum of electronic and thermal Enthalpies= -380.447591
Sum of electronic and thermal Free Energies= -380.486455

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.076498	-0.580021	0.425353
2	8	0	1.356074	1.103829	-0.247188
3	8	0	2.206614	-1.043806	0.006120
4	6	0	-0.754327	1.243766	0.313835
5	1	0	-0.998940	1.267437	1.367625
6	6	0	-1.119072	0.032590	-0.389691
7	1	0	-0.433732	2.163199	-0.144787
8	1	0	-0.855744	0.038077	-1.446461
9	6	0	1.425255	-0.127267	-0.022614
10	6	0	-2.439898	-0.631911	-0.096229

11	1	0	-3.248244	-0.125373	-0.623797
12	1	0	-2.385492	-1.666243	-0.432208
13	1	0	-2.639111	-0.620186	0.973541

O-methyl-b-PC

Sum of electronic and zero-point Energies= -380.574161
Sum of electronic and thermal Energies= -380.567995
Sum of electronic and thermal Enthalpies= -380.567051
Sum of electronic and thermal Free Energies= -380.604344

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.060753	-0.952728	0.077028
2	8	0	-0.918109	1.121630	0.014568
3	8	0	-2.320653	-0.676002	-0.114116
4	6	0	0.511466	1.270545	-0.094025
5	1	0	0.771674	1.433654	-1.142038
6	6	0	1.033743	-0.064054	0.415869
7	1	0	0.812059	2.124087	0.507506
8	1	0	1.117815	-0.053015	1.505927
9	6	0	-1.211592	-0.217129	-0.017140
10	6	0	2.304381	-0.558004	-0.227217
11	1	0	3.124811	0.122791	0.003356
12	1	0	2.560656	-1.546455	0.148366
13	1	0	2.181114	-0.612401	-1.307884

O-phenyl-a

O-phenyl-a-RC

Sum of electronic and zero-point Energies= -571.675261
Sum of electronic and thermal Energies= -571.663353
Sum of electronic and thermal Enthalpies= -571.662408
Sum of electronic and thermal Free Energies= -571.717115

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.231403	-0.638790	0.453188
2	8	0	-3.549645	1.116814	-0.123605
3	8	0	-3.907755	-1.030159	-1.040000
4	6	0	-0.340864	0.504924	0.409705
5	1	0	-0.335992	-0.470377	2.387371
6	6	0	-0.948901	0.076600	1.679772
7	1	0	-0.777851	1.372104	-0.079000
8	1	0	-1.787343	0.631567	2.085272
9	6	0	-3.707707	0.034471	-0.574532
10	6	0	1.083526	0.228195	0.091925
11	6	0	1.932688	1.290051	-0.248385
12	6	0	1.596119	-1.074406	0.160317
13	6	0	3.282757	1.053032	-0.519073
14	1	0	1.534330	2.296911	-0.315872

15	6	0	2.947100	-1.308336	-0.108977
16	1	0	0.927771	-1.893627	0.396100
17	6	0	3.795108	-0.246039	-0.439730
18	1	0	3.932473	1.878419	-0.783736
19	1	0	3.337179	-2.317878	-0.060955
20	1	0	4.840904	-0.430986	-0.651963

O-phenyl-a-TS

Sum of electronic and zero-point Energies= -571.583465
Sum of electronic and thermal Energies= -571.573070
Sum of electronic and thermal Enthalpies= -571.572126
Sum of electronic and thermal Free Energies= -571.620652

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.718411	-0.976589	0.163938
2	8	0	-2.504252	1.249789	-0.038514
3	8	0	-2.941020	-0.305872	-1.703147
4	6	0	-0.441485	0.448411	1.103625
5	1	0	-0.951304	-1.448254	2.018151
6	6	0	-1.394716	-0.595004	1.505142
7	1	0	-0.714833	1.486955	1.240854
8	1	0	-2.242478	-0.196623	2.060297
9	6	0	-2.537651	0.179671	-0.668600
10	6	0	0.803647	0.194877	0.467998
11	6	0	1.617012	1.315708	0.173770
12	6	0	1.272309	-1.115066	0.192210
13	6	0	2.891447	1.130780	-0.354231
14	1	0	1.231957	2.311667	0.359012
15	6	0	2.540079	-1.282205	-0.345326
16	1	0	0.617649	-1.961045	0.351567
17	6	0	3.351013	-0.165392	-0.611679
18	1	0	3.517497	1.984411	-0.578799
19	1	0	2.903891	-2.276253	-0.570875

20	1	0	4.337150	-0.310173	-1.035864

O-phenyl-a-PC

Sum of electronic and zero-point Energies= -571.684108
Sum of electronic and thermal Energies= -571.674515
Sum of electronic and thermal Enthalpies= -571.673571
Sum of electronic and thermal Free Energies= -571.720404

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.420625	0.416780	-0.788927
2	8	0	-2.651869	-0.610481	0.786884
3	8	0	-3.626704	0.962692	-0.551964
4	6	0	-1.281526	-0.981370	1.036031
5	1	0	-0.886609	-0.366520	1.847062
6	6	0	-0.596709	-0.667279	-0.292113
7	1	0	-1.251982	-2.034159	1.305328
8	1	0	-0.696988	-1.505674	-0.987936
9	6	0	-2.664367	0.321271	-0.217709
10	6	0	0.834058	-0.242846	-0.179174
11	6	0	1.164939	1.024341	0.321556
12	6	0	1.851720	-1.138986	-0.528900
13	6	0	2.505230	1.388226	0.466482
14	1	0	0.378226	1.729249	0.563635
15	6	0	3.192926	-0.777886	-0.369458
16	1	0	1.596462	-2.112518	-0.934178
17	6	0	3.520836	0.485975	0.129321
18	1	0	2.756981	2.372847	0.841307
19	1	0	3.975454	-1.475009	-0.643087
20	1	0	4.559391	0.771171	0.243711

O-phenyl-b

O-phenyl-b-RC

Sum of electronic and zero-point Energies= -571.675298
Sum of electronic and thermal Energies= -571.663381
Sum of electronic and thermal Enthalpies= -571.662437
Sum of electronic and thermal Free Energies= -571.717112

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.229053	-0.653053	0.450965
2	8	0	3.542718	1.119593	-0.110187
3	8	0	3.914743	-1.014175	-1.051485
4	6	0	0.949082	0.059119	1.680033
5	1	0	0.333953	-0.488121	2.385523
6	6	0	0.342844	0.493969	0.411372
7	1	0	1.789335	0.609652	2.087627
8	1	0	0.783139	1.361205	-0.074029
9	6	0	3.707924	0.043596	-0.573590
10	6	0	-1.082817	0.224333	0.093339
11	6	0	-1.599560	-1.077132	0.151983
12	6	0	-1.927926	1.291732	-0.240733
13	6	0	-2.951880	-1.304089	-0.117433
14	1	0	-0.934161	-1.900135	0.382983
15	6	0	-3.279248	1.061533	-0.511594
16	1	0	-1.525955	2.297661	-0.300679
17	6	0	-3.795837	-0.236586	-0.442193
18	1	0	-3.345434	-2.312650	-0.077024
19	1	0	-3.925919	1.890894	-0.771362
20	1	0	-4.842564	-0.416275	-0.654497

O-phenyl-b-TS

Sum of electronic and zero-point Energies= -571.565225
Sum of electronic and thermal Energies= -571.554858
Sum of electronic and thermal Enthalpies= -571.553913
Sum of electronic and thermal Free Energies= -571.602699

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.377078	0.603162	-0.035999
2	8	0	-3.187061	-0.791009	0.397114
3	8	0	-3.525555	1.072180	-0.951915
4	6	0	-1.148602	-0.906904	1.189412
5	1	0	-0.884644	-0.256855	2.013459
6	6	0	-0.535576	-0.579243	-0.082885
7	1	0	-1.678233	-1.817553	1.415007
8	1	0	-0.809157	-1.251810	-0.896550
9	6	0	-2.980094	0.249628	-0.265188
10	6	0	0.920157	-0.222988	-0.085709
11	6	0	1.356350	1.008149	0.420731
12	6	0	1.847439	-1.153490	-0.574730
13	6	0	2.722062	1.304702	0.429987
14	1	0	0.628975	1.732526	0.764535
15	6	0	3.211605	-0.854119	-0.553865
16	1	0	1.503628	-2.097809	-0.983151
17	6	0	3.650551	0.373782	-0.047357
18	1	0	3.059684	2.261824	0.807982
19	1	0	3.926460	-1.571343	-0.937780
20	1	0	4.707497	0.609245	-0.039467

O-phenyl-b-PC

Sum of electronic and zero-point Energies= -571.683284
Sum of electronic and thermal Energies= -571.673737
Sum of electronic and thermal Enthalpies= -571.672793
Sum of electronic and thermal Free Energies= -571.719792

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.268158	0.230511	0.963935
2	8	0	1.472759	-0.483403	-1.010792
3	8	0	3.060727	1.156358	-0.965984
4	6	0	0.618593	-1.103692	-0.011098
5	1	0	0.847400	-0.682557	2.139784
6	6	0	1.448261	-0.915240	1.264442
7	1	0	0.532825	-2.154562	-0.286792
8	1	0	2.099056	-1.768029	1.462384
9	6	0	2.340903	0.376159	-0.396702
10	6	0	-0.734800	-0.453744	0.005551
11	6	0	-1.861213	-1.184545	-0.391246
12	6	0	-0.881213	0.891200	0.382364
13	6	0	-3.126298	-0.588871	-0.395270
14	1	0	-1.748995	-2.219961	-0.694237
15	6	0	-2.143470	1.487023	0.371806
16	1	0	-0.017652	1.472295	0.686323
17	6	0	-3.267289	0.749521	-0.019239
18	1	0	-3.992115	-1.162176	-0.702890
19	1	0	-2.249520	2.525304	0.661136
20	1	0	-4.244992	1.215103	-0.026634

N-Native

N-RC

Sum of electronic and zero-point Energies= -321.553559
Sum of electronic and thermal Energies= -321.546335
Sum of electronic and thermal Enthalpies= -321.545391
Sum of electronic and thermal Free Energies= -321.586772

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.281851	1.250602	0.000264
2	8	0	-2.173850	-0.935491	-0.000306
3	6	0	1.838092	0.168523	-0.738592
4	1	0	2.683745	-0.276893	-1.246450
5	1	0	2.677552	-0.283974	1.251293
6	6	0	1.834419	0.164312	0.741782
7	1	0	1.347678	0.974262	-1.266511
8	1	0	1.341312	0.967042	1.271761
9	6	0	-1.690210	0.140753	-0.000171
10	7	0	0.917770	-0.723892	-0.003259
11	1	0	1.277134	-1.675605	-0.005059

N-TS

Sum of electronic and zero-point Energies= -321.448635
Sum of electronic and thermal Energies= -321.443307
Sum of electronic and thermal Enthalpies= -321.442362
Sum of electronic and thermal Free Energies= -321.477538

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.472182	1.253228	0.230272
2	8	0	-2.078271	-0.388348	-0.069980
3	6	0	1.537755	0.557688	-0.440402
4	1	0	1.771631	0.305041	-1.465392
5	1	0	2.153686	-1.369435	0.311329
6	6	0	1.450302	-0.559835	0.487898
7	1	0	1.569592	1.595844	-0.161756
8	1	0	1.347754	-0.311603	1.539252
9	6	0	-0.949329	0.089764	0.019514
10	7	0	0.183871	-0.846132	-0.181179
11	1	0	0.041500	-1.741668	-0.639571

N-PC

Sum of electronic and zero-point Energies= -321.569885
Sum of electronic and thermal Energies= -321.564983
Sum of electronic and thermal Enthalpies= -321.564039
Sum of electronic and thermal Free Energies= -321.598179

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.073776	-1.133555	0.100937
2	8	0	2.072433	-0.022094	0.036555
3	6	0	-1.301035	-0.757878	-0.136676
4	1	0	-1.536386	-0.947044	-1.184963
5	1	0	-2.077457	1.267035	-0.414465
6	6	0	-1.336867	0.735923	0.180679
7	1	0	-1.930480	-1.364517	0.507974
8	1	0	-1.523221	0.916092	1.243558
9	6	0	0.858833	-0.007154	-0.012746
10	7	0	0.021597	1.081102	-0.208060
11	1	0	0.421101	1.980571	0.016838

N-methyl-a

N-methyl-a-RC

Sum of electronic and zero-point Energies= -360.714079
Sum of electronic and thermal Energies= -360.705516
Sum of electronic and thermal Enthalpies= -360.704572
Sum of electronic and thermal Free Energies= -360.749502

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.846758	1.067942	-0.578472
2	8	0	-2.585429	-1.043990	0.175710
3	6	0	1.433694	0.199743	-0.349345
4	1	0	1.894028	0.694170	1.746252
5	6	0	1.138496	0.789341	0.975448
6	1	0	0.971227	0.671243	-1.209511
7	1	0	0.501872	1.660122	1.052064
8	6	0	-2.176973	0.001364	-0.188720
9	7	0	0.439322	-0.442809	0.534017
10	1	0	0.856844	-1.255094	0.986110
11	6	0	2.752196	-0.476576	-0.613160
12	1	0	2.636610	-1.289141	-1.331684
13	1	0	3.475904	0.233738	-1.015217
14	1	0	3.161275	-0.890225	0.310617

N-methyl-a-TS

Sum of electronic and zero-point Energies= -360.615925
Sum of electronic and thermal Energies= -360.609043
Sum of electronic and thermal Enthalpies= -360.608099
Sum of electronic and thermal Free Energies= -360.647195

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.860428	-0.925382	0.913958
2	8	0	2.322120	-0.064804	-0.660013
3	6	0	-1.301246	-0.224371	0.433098
4	1	0	-1.484551	1.904527	0.191681
5	6	0	-0.826935	1.144247	0.608637
6	1	0	-1.221116	-0.938714	1.236963
7	1	0	-0.468488	1.401609	1.600934
8	6	0	1.284225	-0.149670	-0.000142
9	7	0	0.233694	0.837434	-0.343737
10	1	0	0.305560	1.364634	-1.207395
11	6	0	-2.060166	-0.653669	-0.761127
12	1	0	-1.602793	-1.539586	-1.203046
13	1	0	-3.053786	-0.958039	-0.413539
14	1	0	-2.146335	0.125794	-1.513793

N-methyl-a-PC

Sum of electronic and zero-point Energies= -360.733119
Sum of electronic and thermal Energies= -360.726851
Sum of electronic and thermal Enthalpies= -360.725907
Sum of electronic and thermal Free Energies= -360.763238

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.144674	-0.887394	0.590111
2	8	0	2.273359	-0.594877	-0.195491
3	6	0	-1.097880	-0.138728	0.503614
4	1	0	-1.327353	1.866217	-0.343256
5	6	0	-0.627307	1.304900	0.275050
6	1	0	-1.594787	-0.259067	1.465162
7	1	0	-0.473953	1.831986	1.221446
8	6	0	1.145764	-0.173209	-0.027496
9	7	0	0.621413	1.046799	-0.421165
10	1	0	1.293760	1.779521	-0.594152
11	6	0	-1.942922	-0.692723	-0.625773
12	1	0	-2.110553	-1.757827	-0.475858
13	1	0	-2.908635	-0.185607	-0.653663
14	1	0	-1.438560	-0.546083	-1.580850

N- methyl-b

N-methyl-b-RC

Sum of electronic and zero-point Energies= -360.714079
Sum of electronic and thermal Energies= -360.705519
Sum of electronic and thermal Enthalpies= -360.704575
Sum of electronic and thermal Free Energies= -360.749473

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.842580	1.071191	-0.574926
2	8	0	2.586715	-1.041982	0.170387
3	6	0	-1.138794	0.779040	0.984545
4	1	0	-1.896129	0.676803	1.752676
5	6	0	-1.431498	0.202697	-0.346591
6	1	0	-0.501723	1.648554	1.071328
7	1	0	-0.966935	0.682103	-1.201255
8	6	0	2.175710	0.003877	-0.189632
9	7	0	-0.439425	-0.449408	0.532619
10	1	0	-0.859180	-1.265486	0.975822
11	6	0	-2.749952	-0.470026	-0.619628
12	1	0	-3.472531	0.244806	-1.015714
13	1	0	-2.633678	-1.275318	-1.346199
14	1	0	-3.161007	-0.892803	0.299146

N-methyl-b-TS

Sum of electronic and zero-point Energies= -360.611301
Sum of electronic and thermal Energies= -360.604568
Sum of electronic and thermal Enthalpies= -360.603624
Sum of electronic and thermal Free Energies= -360.642052

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.332413	1.115524	-0.299273
2	8	0	2.264447	-0.974556	0.053589
3	6	0	-0.757448	1.210660	0.448537
4	1	0	-1.005300	1.113282	1.498201
5	6	0	-1.137440	0.086799	-0.396109
6	1	0	-0.445932	2.179434	0.098452
7	1	0	-0.960481	0.249072	-1.456814
8	6	0	1.372744	-0.132559	-0.034919
9	7	0	-0.008359	-0.593187	0.241669
10	1	0	-0.174781	-1.432195	0.792405
11	6	0	-2.447406	-0.616089	-0.107054
12	1	0	-3.281008	-0.031553	-0.492160
13	1	0	-2.446503	-1.590889	-0.594497
14	1	0	-2.585051	-0.755456	0.965471

N-methyl-b-PC

Sum of electronic and zero-point Energies= -360.731562
Sum of electronic and thermal Energies= -360.725279
Sum of electronic and thermal Enthalpies= -360.724335
Sum of electronic and thermal Free Energies= -360.761692

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.917474	1.134885	0.012249
2	8	0	-2.386710	-0.615993	-0.073893
3	6	0	0.519769	1.250591	-0.069798
4	1	0	0.797612	1.427854	-1.111667
5	6	0	1.045123	-0.103028	0.408690
6	1	0	0.827232	2.088236	0.551020
7	1	0	1.115507	-0.107311	1.503761
8	6	0	-1.245153	-0.202666	-0.032625
9	7	0	-0.065742	-0.933081	-0.041847
10	1	0	-0.151747	-1.894544	0.257421
11	6	0	2.375922	-0.500639	-0.200112
12	1	0	3.153047	0.205713	0.095934
13	1	0	2.677761	-1.491318	0.139672
14	1	0	2.300288	-0.513753	-1.286979

N-phenyl-a

N-phenyl-a-RC

Sum of electronic and zero-point Energies= -551.826076
Sum of electronic and thermal Energies= -551.814250
Sum of electronic and thermal Enthalpies= -551.813306
Sum of electronic and thermal Free Energies= -551.867258

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-3.545310	0.982344	0.591592
2	8	0	-4.069165	-0.184349	-1.393368
3	6	0	-0.332270	0.102516	0.595689
4	1	0	-0.330131	-1.881754	1.559819
5	6	0	-0.960929	-1.035570	1.315537
6	1	0	-0.748937	1.085997	0.782890
7	1	0	-1.772424	-0.842527	2.004792
8	6	0	-3.772103	0.380287	-0.401030
9	7	0	-1.289648	-0.789072	-0.101790
10	1	0	-0.776836	-1.433144	-0.702715
11	6	0	1.110664	0.097878	0.239696
12	6	0	1.801536	-1.085402	-0.070410
13	6	0	1.801022	1.317052	0.167338
14	6	0	3.154845	-1.051129	-0.414552
15	1	0	1.297056	-2.045090	-0.024575
16	6	0	3.156575	1.353369	-0.171148
17	1	0	1.274979	2.238059	0.393301
18	6	0	3.835435	0.169691	-0.474472
19	1	0	3.672923	-1.973865	-0.646634
20	1	0	3.673661	2.304164	-0.217759
21	1	0	4.884382	0.195556	-0.742281

N-phenyl-a-TS

Sum of electronic and zero-point Energies= -551.735427
Sum of electronic and thermal Energies= -551.725367
Sum of electronic and thermal Enthalpies= -551.724423
Sum of electronic and thermal Free Energies= -551.772088

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.427319	-1.003898	-0.729648
2	8	0	-2.345431	-1.149342	1.571851
3	6	0	-0.570889	0.538191	-1.121532
4	1	0	-1.056305	2.521805	-0.389464
5	6	0	-1.504508	1.570830	-0.667924
6	1	0	-0.886137	-0.124527	-1.913951
7	1	0	-2.344155	1.714646	-1.340256
8	6	0	-2.273984	-0.604424	0.463035
9	7	0	-1.905700	0.844493	0.544646
10	1	0	-1.366870	1.049557	1.381466
11	6	0	0.709304	0.266530	-0.539063
12	6	0	1.390577	1.181316	0.298915
13	6	0	1.311111	-0.970126	-0.862397
14	6	0	2.648923	0.857114	0.789935
15	1	0	0.945037	2.137781	0.543663
16	6	0	2.565436	-1.291716	-0.347832
17	1	0	0.764643	-1.673283	-1.480045
18	6	0	3.233926	-0.380229	0.475741
19	1	0	3.178304	1.558508	1.422223
20	1	0	3.017984	-2.246775	-0.581074
21	1	0	4.210030	-0.628150	0.874029

N-phenyl-a-PC

Sum of electronic and zero-point Energies= -551.842675
Sum of electronic and thermal Energies= -551.833049
Sum of electronic and thermal Enthalpies= -551.832104
Sum of electronic and thermal Free Energies= -551.878966

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.554164	0.025137	-1.083917
2	8	0	3.191603	1.345849	-0.186334
3	6	0	0.619772	-0.951215	-0.567517
4	1	0	0.583688	-1.726746	1.482384
5	6	0	1.309264	-1.466360	0.713279
6	1	0	0.536206	-1.736020	-1.319870
7	1	0	1.949345	-2.328007	0.498684
8	6	0	2.378773	0.450428	-0.062855
9	7	0	2.075431	-0.285393	1.065893
10	1	0	2.774824	-0.297365	1.793667
11	6	0	-0.730372	-0.332150	-0.309125
12	6	0	-0.874800	1.030753	-0.020810
13	6	0	-1.860791	-1.161473	-0.313199
14	6	0	-2.139022	1.551537	0.272748
15	1	0	-0.013550	1.686180	-0.046387
16	6	0	-3.122435	-0.640696	-0.014790
17	1	0	-1.756208	-2.214027	-0.558525
18	6	0	-3.262532	0.719047	0.282183
19	1	0	-2.245192	2.607555	0.489363
20	1	0	-3.990461	-1.288654	-0.025436
21	1	0	-4.239951	1.127710	0.507380

N-phenyl-b

N-phenyl-b-RC

Sum of electronic and zero-point Energies= -551.826025
Sum of electronic and thermal Energies= -551.814219
Sum of electronic and thermal Enthalpies= -551.813275
Sum of electronic and thermal Free Energies= -551.867176

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.549283	0.996505	0.572329
2	8	0	4.055116	-0.216394	-1.389498
3	6	0	0.966914	-1.013240	1.327143
4	1	0	0.340696	-1.861184	1.577024
5	6	0	0.332325	0.116182	0.599009
6	1	0	1.777341	-0.810380	2.014798
7	1	0	0.743365	1.103312	0.779445
8	6	0	3.765350	0.370919	-0.408181
9	7	0	1.294383	-0.775279	-0.092111
10	1	0	0.784027	-1.426279	-0.687631
11	6	0	-1.110437	0.101794	0.241919
12	6	0	-1.805029	1.317968	0.156478
13	6	0	-1.796288	-1.086730	-0.058692
14	6	0	-3.160239	1.346173	-0.184047
15	1	0	-1.282699	2.242908	0.375045
16	6	0	-3.149219	-1.060607	-0.404823
17	1	0	-1.288352	-2.044092	-0.002422
18	6	0	-3.833946	0.157201	-0.478158
19	1	0	-3.680644	2.294625	-0.241091
20	1	0	-3.663484	-1.987354	-0.629454
21	1	0	-4.882707	0.176546	-0.747476

N-phenyl-b-TS

Sum of electronic and zero-point Energies= -551.720283
Sum of electronic and thermal Energies= -551.710222
Sum of electronic and thermal Enthalpies= -551.709278
Sum of electronic and thermal Free Energies= -551.756803

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.192114	0.578706	0.609121
2	8	0	3.490426	-0.600412	-1.361788
3	6	0	1.207281	0.176127	1.524780
4	1	0	0.910297	-0.782525	1.928611
5	6	0	0.544536	0.581231	0.287933
6	1	0	1.787279	0.826026	2.157008
7	1	0	0.788431	1.592526	-0.031623
8	6	0	2.876529	-0.125805	-0.407908
9	7	0	1.426968	-0.418159	-0.329468
10	1	0	1.005571	-1.169931	-0.872359
11	6	0	-0.910838	0.257891	0.112070
12	6	0	-1.772651	1.254882	-0.362901
13	6	0	-1.420997	-1.018357	0.399109
14	6	0	-3.132646	0.984837	-0.538771
15	1	0	-1.379557	2.238500	-0.592780
16	6	0	-2.778799	-1.287879	0.214227
17	1	0	-0.769693	-1.805329	0.764025
18	6	0	-3.636867	-0.287271	-0.254589
19	1	0	-3.791203	1.761742	-0.906592
20	1	0	-3.164301	-2.275663	0.434213
21	1	0	-4.689213	-0.498515	-0.396598

N-phenyl-b-PC

Sum of electronic and zero-point Energies= -551.843624
Sum of electronic and thermal Energies= -551.833944
Sum of electronic and thermal Enthalpies= -551.833000
Sum of electronic and thermal Free Energies= -551.879656

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-2.647346	-0.636291	0.822631
2	8	0	-3.776880	0.836381	-0.515247
3	6	0	-1.252534	-0.958953	1.013576
4	1	0	-0.853015	-0.342144	1.821422
5	6	0	-0.588422	-0.596468	-0.322616
6	1	0	-1.175612	-2.013615	1.266029
7	1	0	-0.681175	-1.437180	-1.022560
8	6	0	-2.739105	0.298995	-0.185065
9	7	0	-1.465847	0.502657	-0.699762
10	1	0	-1.428669	0.891773	-1.632282
11	6	0	0.860257	-0.211190	-0.194548
12	6	0	1.856906	-1.131263	-0.545582
13	6	0	1.227891	1.041928	0.317236
14	6	0	3.207499	-0.810090	-0.377965
15	1	0	1.576249	-2.095860	-0.955833
16	6	0	2.577591	1.364340	0.478898
17	1	0	0.457439	1.760341	0.571757
18	6	0	3.569656	0.438795	0.135256
19	1	0	3.970987	-1.527369	-0.653464
20	1	0	2.854855	2.336001	0.869426
21	1	0	4.615237	0.692180	0.259626