Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Theoretical calculation studies on the rearrangement mechanisms of arenesulfenanilides to *o*- and *p*-aminodiphenyl sulfides

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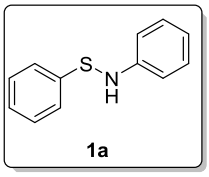
Supporting Information

Contents

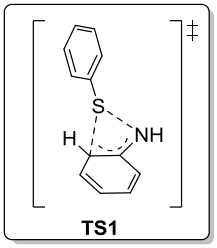
1. Coordinates of All Stationary Points in Thermal Rearrangement of Arenesulfenanilides



1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.022518	-0.406174	-0.627805
2	6	0	2.958259	0.401827	-1.010740
3	6	0	1.792386	0.448185	-0.234396
4	6	0	1.712962	-0.324077	0.928688
5	6	0	2.788755	-1.123060	1.304615
6	6	0	3.947984	-1.174111	0.533568
7	1	0	4.917234	-0.429597	-1.239406
8	1	0	3.027037	1.001861	-1.912492
9	1	0	0.814254	-0.293965	1.530632
10	1	0	2.713444	-1.715265	2.209470
11	1	0	4.779721	-1.800310	0.831822
12	7	0	0.717860	1.238500	-0.671753
13	1	0	0.856326	1.763750	-1.521177
14	6	0	-1.801321	0.467060	0.028532
15	6	0	-3.033923	0.627419	0.667550
16	6	0	-1.559526	-0.655707	-0.760370
17	6	0	-4.023160	-0.338148	0.510409
18	1	0	-3.221234	1.501774	1.282074
19	6	0	-2.557918	-1.616359	-0.910061
20	1	0	-0.601123	-0.773886	-1.248249
21	6	0	-3.790182	-1.464265	-0.278653
22	1	0	-4.978776	-0.208372	1.005279
23	1	0	-2.366071	-2.489819	-1.522839
24	1	0	-4.561831	-2.215114	-0.398542
25	16	0	-0.571563	1.745869	0.298604



TS1

With *endo*-H

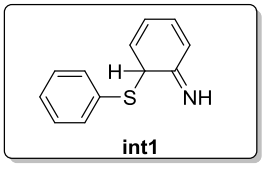
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.802353	-1.321326	-0.675794
2	6	0	2.456195	-1.003709	-0.788051
3	6	0	1.919628	0.111271	-0.106658
4	6	0	2.787022	0.894843	0.686331
5	6	0	4.132688	0.574045	0.792433
6	6	0	4.644490	-0.534412	0.113237
7	1	0	4.201200	-2.180023	-1.203547
8	1	0	1.794171	-1.603796	-1.399955
9	1	0	2.380278	1.751835	1.208939
10	1	0	4.787913	1.184474	1.403229
11	1	0	5.696021	-0.783162	0.197913
12	16	0	0.224735	0.503545	-0.246777
13	6	0	-2.266471	0.608706	1.005369
14	6	0	-2.518857	0.863074	-0.395099
15	6	0	-2.802192	-0.519056	1.625317
16	6	0	-3.266756	-0.127609	-1.125465
17	6	0	-3.546272	-1.428450	0.890491
18	1	0	-2.631540	-0.683295	2.682434
19	6	0	-3.772670	-1.229759	-0.493197
20	1	0	-3.412801	0.047083	-2.183885
21	1	0	-3.959966	-2.304043	1.377155
22	1	0	-4.346725	-1.961991	-1.048591
23	7	0	-2.033209	1.894947	-1.059489
24	1	0	-1.750012	1.362461	1.583308
25	1	0	-1.536772	2.523398	-0.425629

With exo-H
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.710794	1.309797	-0.733535
2	6	0	-2.376871	0.937815	-0.821302
3	6	0	-1.884847	-0.163246	-0.085050
4	6	0	-2.785316	-0.876198	0.737956
5	6	0	-4.118459	-0.500701	0.820806

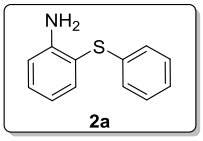
6	6	0	-4.585126	0.592507	0.086629
7	1	0	-4.075290	2.157208	-1.302857
8	1	0	-1.689560	1.485334	-1.454466
9	1	0	-2.412172	-1.723096	1.300556
10	1	0	-4.799057	-1.056696	1.455381
11	1	0	-5.627029	0.883950	0.152842
12	16	0	-0.206494	-0.633203	-0.191594
13	6	0	2.308163	-0.683828	0.978884
14	6	0	2.523276	-0.829365	-0.440213
15	6	0	2.770004	0.445762	1.654403
16	6	0	3.140259	0.274622	-1.130942
17	6	0	3.410769	1.458012	0.959808
18	1	0	2.625794	0.526457	2.725019
19	6	0	3.590963	1.367632	-0.442118
20	1	0	3.258120	0.206042	-2.206996
21	1	0	3.773849	2.332066	1.487539
22	1	0	4.078233	2.179979	-0.968794
23	7	0	2.061515	-1.924758	-1.015523
24	1	0	2.174098	-1.861621	-2.030505
25	1	0	1.874186	-1.521925	1.504508



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.382976	1.179678	0.447593
2	6	0	2.099249	0.860201	0.886001
3	6	0	1.487996	-0.320691	0.457173
4	6	0	2.169865	-1.179522	-0.410720
5	6	0	3.445664	-0.848483	-0.858490
6	6	0	4.055040	0.330203	-0.428691
7	1	0	3.854240	2.095228	0.786115
8	1	0	1.562894	1.521975	1.554436
9	1	0	1.700049	-2.104184	-0.724025
10	1	0	3.968657	-1.516117	-1.533467
11	1	0	5.051154	0.582588	-0.773005
12	16	0	-0.150154	-0.746978	1.042086

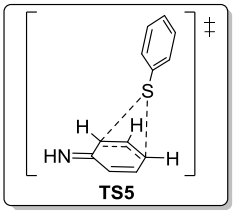
13	6	0	-1.147559	-0.411332	-0.533114
14	6	0	-2.573682	-0.787201	-0.183966
15	6	0	-0.949156	1.015987	-0.913980
16	6	0	-3.446390	0.301399	0.256529
17	6	0	-1.872592	1.949754	-0.633875
18	1	0	-0.004375	1.281241	-1.372129
19	6	0	-3.120281	1.588305	0.016586
20	1	0	-4.397529	0.037000	0.706794
21	1	0	-1.693774	2.990826	-0.875733
22	1	0	-3.806527	2.380662	0.295311
23	7	0	-2.910796	-2.017787	-0.296481
24	1	0	-3.877153	-2.155340	0.009226
25	1	0	-0.766379	-1.107502	-1.277802



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.423394	1.732675	-0.508634
2	6	0	1.320005	0.883331	-0.472120
3	6	0	1.494173	-0.461382	-0.145098
4	6	0	2.773175	-0.949535	0.140079
5	6	0	3.869856	-0.094664	0.091577
6	6	0	3.700645	1.251179	-0.230793
7	1	0	2.279442	2.777618	-0.759004
8	1	0	0.331126	1.264283	-0.691205
9	1	0	2.908345	-1.993486	0.400564
10	1	0	4.858045	-0.481948	0.312138
11	1	0	4.554897	1.916752	-0.262727
12	16	0	0.142249	-1.642692	-0.100007
13	6	0	-1.303239	-0.598157	-0.161273
14	6	0	-1.722943	0.110674	0.987114
15	6	0	-2.049414	-0.532434	-1.339863
16	6	0	-2.898084	0.876284	0.898813
17	6	0	-3.213320	0.224289	-1.409645
18	1	0	-1.699297	-1.084990	-2.203214
19	6	0	-3.629270	0.928951	-0.278746

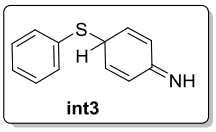
20	1	0	-3.229185	1.432530	1.769535
21	1	0	-3.783755	0.266904	-2.328857
22	1	0	-4.533039	1.526613	-0.314323
23	7	0	-0.971388	0.104891	2.145357
24	1	0	-1.450689	0.344746	2.998712
25	1	0	-0.302022	-0.647450	2.232506



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.502418	1.388431	0.548543
2	6	0	-2.167331	1.013030	0.515663
3	6	0	-1.779033	-0.230258	-0.033661
4	6	0	-2.786324	-1.078332	-0.547641
5	6	0	-4.120329	-0.699932	-0.506933
6	6	0	-4.483463	0.533719	0.039511
7	1	0	-3.785177	2.346143	0.970450
8	1	0	-1.398407	1.667250	0.907925
9	1	0	-2.493015	-2.029756	-0.973777
10	1	0	-4.882336	-1.361284	-0.903246
11	1	0	-5.526108	0.828515	0.066582
12	16	0	-0.101765	-0.700069	-0.072494
13	6	0	2.659192	-0.497291	-1.109206
14	6	0	2.816198	0.873477	-0.639938
15	6	0	2.599585	-1.549279	-0.222372
16	6	0	2.760157	1.082899	0.801162
17	6	0	2.479036	-1.294837	1.147048
18	1	0	2.525665	-2.565059	-0.588681
19	6	0	2.592370	0.034417	1.649320
20	1	0	2.855179	2.097012	1.173990
21	1	0	2.365383	-2.117485	1.841477
22	1	0	2.527310	0.198024	2.718410
23	7	0	3.029913	1.803273	-1.522812
24	1	0	3.135778	2.710711	-1.062671

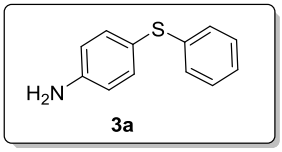
25	1	0	2.688736	-0.652146	-2.179847



int3

Standard orientation:

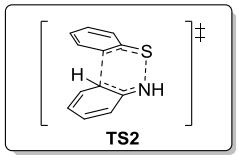
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.512722	-1.009787	-0.558591
2	6	0	-1.765090	-0.341642	0.416155
3	6	0	-2.227251	0.871382	0.933645
4	6	0	-3.426919	1.412602	0.475269
5	6	0	-4.163174	0.752358	-0.505928
6	6	0	-3.703525	-0.458429	-1.023122
7	1	0	-2.163211	-1.961473	-0.940911
8	1	0	-1.643526	1.383157	1.688675
9	1	0	-3.782125	2.352332	0.881966
10	1	0	-5.093647	1.176794	-0.864254
11	1	0	-4.278327	-0.979603	-1.779911
12	6	0	3.531084	0.597115	-0.149313
13	6	0	3.344439	-0.862816	-0.120042
14	6	0	2.141916	-1.430899	-0.264874
15	6	0	0.895093	-0.631367	-0.439633
16	6	0	1.117727	0.838917	-0.528478
17	6	0	2.324682	1.398329	-0.383294
18	1	0	4.231190	-1.475464	0.012815
19	1	0	2.031762	-2.509861	-0.240773
20	1	0	0.334435	-0.993781	-1.306393
21	1	0	0.240786	1.452681	-0.700958
22	1	0	2.464691	2.471652	-0.431790
23	7	0	4.657857	1.198292	0.005395
24	1	0	5.408666	0.521209	0.158484
25	16	0	-0.230829	-1.040017	1.023407



3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.502057	1.909526	-0.000091
2	6	0	-1.498282	0.942487	-0.000007
3	6	0	-1.839298	-0.411290	0.000040
4	6	0	-3.188511	-0.784935	0.000003
5	6	0	-4.181677	0.188130	-0.000083
6	6	0	-3.845001	1.541796	-0.000130
7	1	0	-2.226118	2.958123	-0.000126
8	1	0	-0.458532	1.241023	0.000024
9	1	0	-3.457522	-1.835463	0.000042
10	1	0	-5.222964	-0.113694	-0.000112
11	1	0	-4.620427	2.298400	-0.000195
12	16	0	-0.636082	-1.739085	0.000142
13	6	0	0.919614	-0.865352	0.000069
14	6	0	1.544232	-0.526881	-1.203360
15	6	0	1.544149	-0.526532	1.203444
16	6	0	2.761722	0.139615	-1.206721
17	6	0	2.761640	0.139963	1.206695
18	1	0	1.067410	-0.785515	2.140857
19	6	0	3.390483	0.483671	-0.000041
20	1	0	3.231640	0.400101	-2.149231
21	1	0	3.231493	0.400722	2.149162
22	1	0	1.067558	-0.786135	-2.140731
23	7	0	4.583819	1.197316	-0.000103
24	1	0	5.137941	1.142820	0.840834
25	1	0	5.137999	1.142576	-0.840986



With *endo*-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.572812	0.379660	0.397997

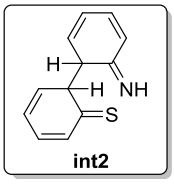
2	6	0	1.386371	0.660528	-0.357142
3	6	0	0.529053	-0.480910	-0.698645
4	6	0	1.160395	-1.798291	-0.701199
5	6	0	2.345340	-1.998736	-0.075482
6	6	0	3.033596	-0.898223	0.533897
7	1	0	3.130645	1.219499	0.793902
8	1	0	-0.170669	-0.288932	-1.505849
9	1	0	0.630129	-2.621122	-1.164906
10	1	0	2.789790	-2.986563	-0.041814
11	1	0	3.957571	-1.084712	1.069666
12	6	0	-1.369991	0.746436	0.695810
13	6	0	-2.586869	0.849892	-0.082713
14	6	0	-3.239547	-0.262023	-0.499649
15	6	0	-2.741248	-1.576378	-0.175281
16	6	0	-1.548366	-1.729240	0.442676
17	6	0	-0.701585	-0.569043	0.724444
18	1	0	-2.969230	1.846300	-0.264911
19	1	0	-4.169178	-0.174824	-1.050279
20	1	0	-3.343941	-2.442925	-0.421936
21	1	0	-1.171434	-2.714901	0.686139
22	1	0	0.003856	-0.697149	1.541231
23	7	0	-0.872014	1.828965	1.222804
24	16	0	0.901011	2.223693	-0.700275
25	1	0	-0.039385	1.621454	1.775259

With *exo*-H

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.594226	0.376777	0.407028
2	6	0	1.405760	0.663260	-0.340782
3	6	0	0.544889	-0.470764	-0.689645
4	6	0	1.167322	-1.791603	-0.692923
5	6	0	2.354033	-1.998907	-0.073514
6	6	0	3.049848	-0.902721	0.536195
7	1	0	3.148109	1.213193	0.813976
8	1	0	-0.151694	-0.274624	-1.498296
9	1	0	0.631128	-2.611308	-1.155414
10	1	0	2.793444	-2.989153	-0.043172
11	1	0	3.971668	-1.096196	1.073231

12	6	0	-1.402804	0.754610	0.664842
13	6	0	-2.610938	0.806551	-0.136091
14	6	0	-3.239650	-0.333260	-0.515651
15	6	0	-2.709194	-1.623790	-0.153916
16	6	0	-1.513262	-1.723702	0.470642
17	6	0	-0.702579	-0.537587	0.735149
18	1	0	-3.024903	1.781378	-0.370422
19	1	0	-4.168215	-0.284458	-1.073266
20	1	0	-3.285462	-2.512854	-0.381983
21	1	0	-1.107542	-2.691928	0.737038
22	1	0	-0.004477	-0.609837	1.562369
23	7	0	-0.852861	1.778503	1.254170
24	1	0	-1.392343	2.628272	1.071554
25	16	0	0.933400	2.230301	-0.673926

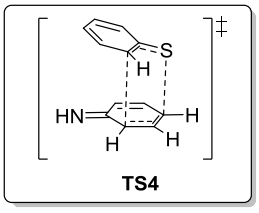


int2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.388645	-1.956341	-0.056365
2	6	0	1.176476	-1.800983	-0.615885
3	6	0	0.459488	-0.489009	-0.560477
4	6	0	1.364418	0.690957	-0.308804
5	6	0	2.571391	0.433958	0.435223
6	6	0	3.060642	-0.827567	0.549978
7	1	0	2.880272	-2.922145	-0.057383
8	1	0	0.659234	-2.639032	-1.066914
9	1	0	3.117123	1.286090	0.819898
10	1	0	4.001470	-0.994670	1.063053
11	16	0	0.971084	2.204541	-0.836013
12	6	0	-0.640106	-0.596236	0.644198
13	6	0	-1.392376	0.706792	0.766551
14	6	0	-1.543989	-1.751444	0.331652
15	6	0	-2.549674	0.870060	-0.116794
16	6	0	-2.722148	-1.559003	-0.282633

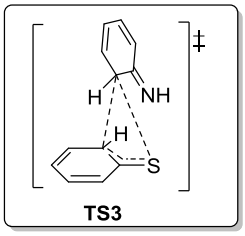
17	1	0	-1.194394	-2.750056	0.564018
18	6	0	-3.187678	-0.215832	-0.597715
19	1	0	-2.916579	1.873898	-0.300460
20	1	0	-3.349163	-2.402312	-0.548817
21	1	0	-4.084375	-0.103099	-1.197185
22	1	0	-0.067183	-0.757909	1.557363
23	7	0	-0.976384	1.569978	1.615369
24	1	0	-1.531432	2.428281	1.563609
25	1	0	-0.128171	-0.313669	-1.462129



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.582102	0.647823	1.177916
2	6	0	-0.103711	1.312571	-0.047725
3	6	0	-0.926684	1.173595	-1.215333
4	6	0	-2.206698	0.707074	-1.117025
5	6	0	-2.758704	0.309893	0.142026
6	6	0	-1.991622	0.329053	1.262068
7	1	0	-0.123716	1.023602	2.086143
8	1	0	-0.528934	1.529837	-2.157073
9	1	0	-2.831120	0.661590	-2.002373
10	1	0	-3.798113	0.010104	0.194568
11	1	0	-2.398703	0.020721	2.217635
12	6	0	-0.164281	-1.695579	-0.100708
13	6	0	0.686191	-1.479898	-1.268126
14	6	0	1.942628	-0.998895	-1.128662
15	6	0	2.466992	-0.651712	0.170951
16	6	0	1.690253	-0.754139	1.283209
17	6	0	0.283532	-1.044659	1.162747
18	1	0	0.301929	-1.777904	-2.237581
19	1	0	2.580579	-0.874815	-1.995668
20	1	0	3.507335	-0.363573	0.255799

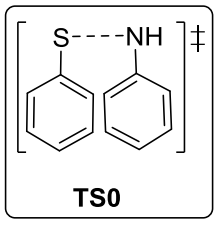
21	1	0	2.091475	-0.498365	2.256286
22	1	0	-0.200328	-1.459396	2.040229
23	7	0	-1.260681	-2.368287	-0.080526
24	1	0	-1.481050	-2.720659	-1.015377
25	16	0	1.355666	2.118506	-0.062933



TS3

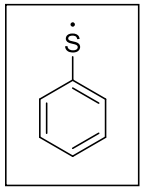
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.671014	-1.786940	0.960161
2	6	0	-2.070850	-0.810909	1.756377
3	6	0	-1.721003	0.415486	1.211517
4	6	0	-1.973182	0.706779	-0.158155
5	6	0	-2.592898	-0.303650	-0.944327
6	6	0	-2.930416	-1.524276	-0.392246
7	1	0	-2.936031	-2.747598	1.385482
8	1	0	-1.870437	-1.012347	2.802349
9	1	0	-2.781659	-0.094760	-1.989630
10	1	0	-3.392768	-2.285576	-1.009667
11	16	0	-1.474962	2.193994	-0.861520
12	6	0	1.214842	0.041143	-0.307447
13	6	0	1.615740	1.121583	0.457538
14	6	0	2.148671	-1.019884	-0.636574
15	6	0	2.932704	1.210132	0.903148
16	6	0	3.513405	-0.881307	-0.165275
17	6	0	3.879382	0.205429	0.577740
18	1	0	3.243774	2.058118	1.501399
19	1	0	4.227834	-1.658739	-0.413563
20	1	0	4.899153	0.304348	0.931717
21	1	0	0.211947	-0.059671	-0.684661
22	1	0	-1.260147	1.179376	1.824155
23	1	0	0.902472	1.906517	0.675453
24	7	0	1.691793	-2.032187	-1.330523
25	1	0	2.440420	-2.709769	-1.499795



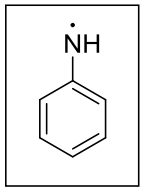
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.113380	1.419316	-0.079323
2	6	0	-2.730299	1.450186	-0.043477
3	6	0	-1.986883	0.251995	0.138182
4	6	0	-2.698071	-0.966779	0.300516
5	6	0	-4.082357	-0.977268	0.261505
6	6	0	-4.800286	0.208068	0.069669
7	1	0	-4.666683	2.341164	-0.219793
8	1	0	-2.198247	2.387834	-0.165016
9	1	0	-2.139715	-1.876550	0.482757
10	1	0	-4.613151	-1.913264	0.394268
11	1	0	-5.883466	0.191344	0.048006
12	7	0	-0.628324	0.230100	0.093628
13	1	0	-0.174315	1.139946	0.169508
14	6	0	2.083287	-0.471094	-0.227307
15	6	0	2.873391	0.153242	-1.214893
16	6	0	2.528628	-0.447540	1.109764
17	6	0	4.075554	0.759652	-0.873234
18	1	0	2.539467	0.144116	-2.245902
19	6	0	3.733872	0.165288	1.438362
20	1	0	1.931203	-0.924147	1.877705
21	6	0	4.515269	0.771055	0.453659
22	1	0	4.674224	1.228392	-1.646863
23	1	0	4.064713	0.168683	2.471480
24	1	0	5.453894	1.245697	0.714669
25	16	0	0.563625	-1.227540	-0.658547



Standard orientation:

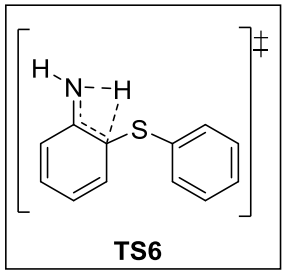
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.575111	-0.000002	-0.000044
2	6	0	-0.149575	1.217643	0.000008
3	6	0	-0.149575	-1.217644	0.000003
4	6	0	-1.534825	1.212324	0.000027
5	1	0	0.403128	2.148558	0.000019
6	6	0	-1.534827	-1.212322	0.000022
7	1	0	0.403124	-2.148560	0.000010
8	6	0	-2.231818	0.000000	0.000023
9	1	0	-2.079048	2.149411	0.000047
10	1	0	-2.079048	-2.149411	0.000039
11	1	0	-3.315537	0.000002	0.000046
12	16	0	2.301277	0.000000	-0.000024



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.077705	1.233039	0.000060
2	6	0	-0.302239	1.210769	-0.000030
3	6	0	-1.017917	-0.030852	-0.000073
4	6	0	-0.247094	-1.237380	-0.000006
5	6	0	1.131822	-1.196828	0.000078
6	6	0	1.804985	0.033778	0.000110
7	1	0	1.603890	2.180705	0.000089
8	1	0	-0.868702	2.136318	-0.000072

9	1	0	-0.789324	-2.174807	-0.000031
10	1	0	1.700257	-2.119609	0.000118
11	1	0	2.888097	0.059011	0.000182
12	7	0	-2.350279	-0.136548	-0.000137
13	1	0	-2.765850	0.799055	-0.000158



TS6

Standard orientation:

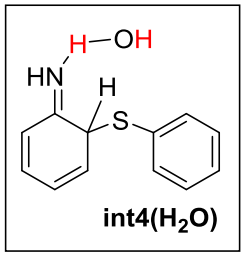
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.434594	-1.279480	-0.149591
2	6	0	-4.013108	0.011011	0.088317
3	6	0	-3.282046	1.171913	0.073072
4	6	0	-1.928930	1.022418	-0.340994
5	6	0	-1.221027	-0.275374	-0.206055
6	6	0	-2.078392	-1.436011	-0.246388
7	1	0	-4.086893	-2.144028	-0.165663
8	1	0	-5.081907	0.066322	0.267402
9	1	0	-3.737892	2.143404	0.221285
10	1	0	-0.435151	0.572940	-1.088348
11	1	0	-1.633394	-2.424663	-0.257020
12	7	0	-1.126659	1.762829	-1.072223
13	1	0	-1.223290	2.779652	-1.103966
14	16	0	-0.030219	-0.352551	1.182391
15	6	0	1.580771	-0.180724	0.420017
16	6	0	1.884274	-0.707764	-0.837849
17	6	0	2.581931	0.445286	1.167399
18	6	0	3.174062	-0.591430	-1.346915
19	1	0	1.113148	-1.202060	-1.415506
20	6	0	3.875539	0.540762	0.658942
21	1	0	2.344062	0.866665	2.137228
22	6	0	4.176202	0.028583	-0.600986
23	1	0	3.399106	-0.997864	-2.326480
24	1	0	4.644174	1.032390	1.244330

25	1	0	5.180062	0.113113	-0.999760

H_2O

Standard orientation:

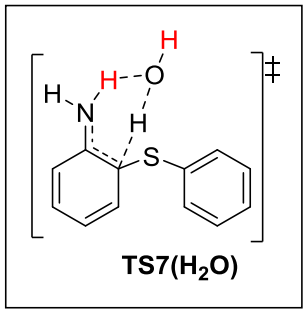
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	-0.000000	0.117108
2	1	0	0.000000	0.763443	-0.468431
3	1	0	-0.000000	-0.763443	-0.468431



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.619532	-1.399320	0.150376
2	6	0	-2.324668	-1.347081	0.663695
3	6	0	-1.570929	-0.178257	0.531307
4	6	0	-2.108306	0.938663	-0.118655
5	6	0	-3.395449	0.868823	-0.644420
6	6	0	-4.153965	-0.294364	-0.508397
7	1	0	-4.204799	-2.305273	0.258724
8	1	0	-1.893975	-2.205816	1.163871
9	1	0	-1.519027	1.844773	-0.209156
10	1	0	-3.811767	1.732047	-1.151025
11	1	0	-5.158669	-0.337757	-0.912843
12	16	0	0.067986	-0.096519	1.247889
13	6	0	1.086989	0.051730	-0.337251
14	6	0	2.456670	0.540508	0.084769
15	6	0	1.060647	-1.279873	-1.001047
16	6	0	3.507914	-0.459887	0.206871

17	6	0	2.122057	-2.103549	-0.971645
18	1	0	0.124830	-1.580097	-1.457033
19	6	0	3.349192	-1.696450	-0.315321
20	1	0	4.444025	-0.160952	0.666656
21	1	0	2.070021	-3.090297	-1.415608
22	1	0	4.163844	-2.410334	-0.256755
23	7	0	2.598482	1.797715	0.313227
24	1	0	3.542312	2.018919	0.632351
25	1	0	0.589178	0.827423	-0.916683
26	8	0	0.283169	3.235188	-0.485783
27	1	0	1.125809	2.889797	-0.116433
28	1	0	0.522002	4.010707	-1.000302



Standard orientation:

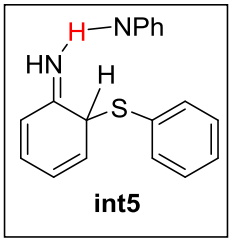
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.136740	-2.103369	-0.867484
2	6	0	-3.397369	-1.669802	-0.351160
3	6	0	-3.569423	-0.438212	0.214314
4	6	0	-2.478073	0.477970	0.266021
5	6	0	-1.123929	0.018292	-0.132344
6	6	0	-1.044473	-1.310881	-0.721190
7	1	0	-2.057707	-3.081224	-1.325613
8	1	0	-4.247609	-2.339858	-0.421107
9	1	0	-4.541821	-0.119487	0.572910
10	1	0	-0.797397	1.016995	-0.795975
11	1	0	-0.064076	-1.660070	-1.023433
12	7	0	-2.594525	1.762883	0.537935
13	1	0	-3.529030	2.126017	0.674578
14	16	0	0.073350	0.185663	1.284530
15	6	0	1.652747	0.000798	0.471426

16	6	0	2.680224	-0.573517	1.229777
17	6	0	1.916018	0.430909	-0.833727
18	6	0	3.960218	-0.692862	0.697046
19	1	0	2.471582	-0.931323	2.231249
20	6	0	3.194868	0.282572	-1.365169
21	1	0	1.138419	0.886333	-1.432488
22	6	0	4.222855	-0.271328	-0.604955
23	1	0	4.748174	-1.133770	1.296792
24	1	0	3.386592	0.614332	-2.379226
25	1	0	5.216182	-0.377938	-1.024154
26	8	0	-0.782659	2.457194	-1.008586
27	1	0	0.040553	2.781913	-0.628061
28	1	0	-1.776048	2.346327	-0.010132

$PhNH_2$

Standard orientation:

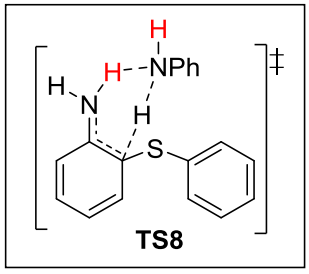
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.153210	1.219655	0.000001
2	6	0	0.239472	1.191601	-0.000005
3	6	0	0.925377	-0.027338	-0.000017
4	6	0	0.194445	-1.215393	-0.000009
5	6	0	-1.199128	-1.189015	0.000018
6	6	0	-1.876641	0.028063	0.000013
7	1	0	-1.672717	2.171155	0.000002
8	1	0	0.802616	2.119165	-0.000006
9	1	0	0.737144	-2.152692	-0.000029
10	1	0	-1.754535	-2.119923	0.000023
11	1	0	-2.960169	0.049402	0.000021
12	7	0	2.364561	-0.113866	-0.000036
13	1	0	2.756924	0.342538	-0.817297
14	1	0	2.756924	0.341982	0.817537



int5

Standard orientation:

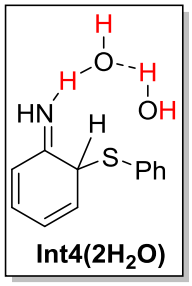
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.477610	4.215948	0.413474
2	6	0	1.296525	3.203761	-0.085021
3	6	0	0.726884	2.015310	-0.547624
4	6	0	-0.659990	1.840123	-0.507552
5	6	0	-1.468390	2.844061	0.015910
6	6	0	-0.902742	4.034851	0.472604
7	1	0	0.921084	5.139422	0.767865
8	1	0	2.372342	3.326160	-0.110883
9	1	0	-1.093200	0.923813	-0.886042
10	1	0	-2.540722	2.693284	0.060184
11	1	0	-1.535588	4.818069	0.873626
12	16	0	1.773191	0.721349	-1.211196
13	6	0	1.445972	-0.604993	0.094082
14	6	0	1.998233	-1.903306	-0.456239
15	6	0	2.068351	-0.137925	1.364027
16	6	0	3.324814	-2.300296	0.001169
17	6	0	3.222660	-0.655959	1.814930
18	1	0	1.577727	0.680802	1.876172
19	6	0	3.883114	-1.723323	1.087600
20	1	0	3.813808	-3.121832	-0.511795
21	1	0	3.688145	-0.270927	2.714189
22	1	0	4.847187	-2.070829	1.443228
23	7	0	1.269570	-2.568313	-1.279996
24	1	0	1.756578	-3.403622	-1.609446
25	1	0	0.363108	-0.668865	0.165124
26	1	0	-0.612087	-1.895668	-1.784916
27	1	0	-1.851987	-1.151798	-2.722919
28	6	0	-2.325441	-1.371272	-0.731363
29	6	0	-1.948124	-2.000174	0.469655
30	6	0	-3.560752	-0.699326	-0.770726
31	6	0	-2.771613	-1.937718	1.588185
32	1	0	-1.014457	-2.549295	0.506427
33	6	0	-4.378295	-0.653002	0.352200
34	1	0	-3.868482	-0.208182	-1.688542
35	6	0	-3.991715	-1.263889	1.545288
36	1	0	-2.458232	-2.430887	2.501990
37	1	0	-5.327039	-0.130486	0.294370
38	1	0	-4.630104	-1.221199	2.419017
39	7	0	-1.469819	-1.348368	-1.813160



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.231769	2.383492	1.353364
2	6	0	-2.429477	3.041191	0.108596
3	6	0	-1.658754	2.752636	-0.995687
4	6	0	-0.634856	1.790585	-0.896829
5	6	0	-0.254352	1.244779	0.424014
6	6	0	-1.190850	1.519143	1.510229
7	1	0	-2.906762	2.586014	2.175362
8	1	0	-3.234892	3.761009	0.016439
9	1	0	-1.863881	3.218922	-1.953089
10	1	0	-0.052208	0.135711	0.217469
11	1	0	-0.990681	1.051136	2.465805
12	7	0	0.027341	1.272643	-1.935869
13	1	0	-0.290770	1.515221	-2.863960
14	16	0	1.471449	1.809700	0.972307
15	6	0	2.496935	0.438668	0.462465
16	6	0	3.152890	0.475359	-0.770192
17	6	0	2.644601	-0.673084	1.297832
18	6	0	3.940954	-0.600707	-1.170171
19	1	0	3.027385	1.337924	-1.411640
20	6	0	3.429252	-1.748394	0.892059
21	1	0	2.136439	-0.691268	2.254043
22	6	0	4.074907	-1.714615	-0.344098
23	1	0	4.442797	-0.572815	-2.130273
24	1	0	3.536081	-2.611917	1.538294
25	1	0	4.682482	-2.554312	-0.660582
26	1	0	0.321739	0.270422	-1.765724
27	7	0	0.107379	-1.254078	-0.882308
28	6	0	-1.120355	-1.714213	-0.517912
29	6	0	-1.323127	-2.749609	0.437793
30	6	0	-2.288048	-1.108206	-1.058285
31	6	0	-2.594809	-3.159186	0.799217
32	1	0	-0.451634	-3.226121	0.876796

33	6	0	-3.558275	-1.520414	-0.674225
34	1	0	-2.175642	-0.333032	-1.804920
35	6	0	-3.729931	-2.546974	0.252876
36	1	0	-2.711054	-3.960929	1.521183
37	1	0	-4.426583	-1.038408	-1.111272
38	1	0	-4.722403	-2.867834	0.544970
39	1	0	0.843727	-1.767586	-0.404847

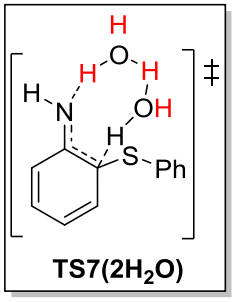


Int4(2H_2O)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.768756	-1.248976	-0.625130
2	6	0	2.450355	-1.161425	-1.067730
3	6	0	1.613722	-0.157889	-0.571988
4	6	0	2.091744	0.750895	0.378456
5	6	0	3.402995	0.637052	0.832916
6	6	0	4.245660	-0.354450	0.330227
7	1	0	4.416215	-2.024754	-1.017452
8	1	0	2.064269	-1.869983	-1.790194
9	1	0	1.447196	1.529801	0.769299
10	1	0	3.769479	1.336684	1.575418
11	1	0	5.267918	-0.429395	0.682439
12	16	0	-0.049542	-0.035159	-1.223802
13	6	0	-1.087929	-0.151733	0.353721
14	6	0	-2.521182	-0.146031	-0.142454
15	6	0	-0.673146	-1.373359	1.097116
16	6	0	-3.244037	-1.410075	-0.123349
17	6	0	-1.442871	-2.471565	1.151230
18	1	0	0.302431	-1.349141	1.566120
19	6	0	-2.737581	-2.496140	0.498514
20	1	0	-4.224210	-1.436665	-0.587833
21	1	0	-1.104965	-3.357618	1.675012

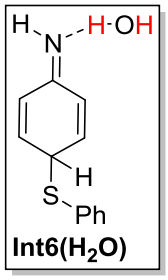
22	1	0	-3.311700	-3.416118	0.522716
23	7	0	-3.009362	0.965418	-0.569872
24	1	0	-3.962709	0.850217	-0.914831
25	1	0	-0.883860	0.757392	0.920882
26	8	0	-0.185601	2.789986	1.590373
27	1	0	-0.646142	3.119476	0.785097
28	1	0	-0.382086	3.418790	2.289529
29	8	0	-1.462668	3.286306	-0.764295
30	1	0	-2.076333	2.511104	-0.730774
31	1	0	-0.830065	3.056670	-1.453301



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.638507	-2.524109	0.956825
2	6	0	2.975368	-2.315307	0.480155
3	6	0	3.366299	-1.148360	-0.102101
4	6	0	2.445150	-0.061065	-0.243773
5	6	0	1.038964	-0.243182	0.207487
6	6	0	0.717744	-1.548388	0.800109
7	1	0	1.379513	-3.470186	1.415168
8	1	0	3.697293	-3.118244	0.584423
9	1	0	4.383833	-1.016252	-0.453165
10	1	0	0.806695	0.631122	0.935080
11	1	0	-0.307743	-1.690746	1.119234
12	7	0	2.818311	1.096514	-0.732712
13	1	0	3.791454	1.198716	-0.991036
14	16	0	-0.085326	0.084392	-1.268703
15	6	0	-1.710666	-0.068618	-0.536061
16	6	0	-2.605961	-0.970560	-1.120110
17	6	0	-2.107243	0.722465	0.548098
18	6	0	-3.907617	-1.068913	-0.633411

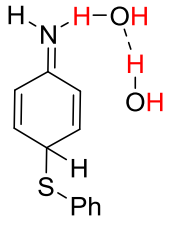
19	1	0	-2.279295	-1.590009	-1.946591
20	6	0	-3.402869	0.591745	1.042201
21	1	0	-1.401341	1.410607	1.005657
22	6	0	-4.306411	-0.292413	0.452471
23	1	0	-4.602090	-1.762300	-1.093730
24	1	0	-3.709583	1.197042	1.887735
25	1	0	-5.315625	-0.377258	0.838786
26	8	0	0.481236	2.100532	1.562430
27	1	0	0.865760	2.340167	2.410630
28	1	0	2.189608	2.018993	-0.688231
29	8	0	1.463161	3.213242	-0.354006
30	1	0	0.756449	3.452772	-0.960295
31	1	0	0.979331	2.799740	0.585821



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.116278	-0.714340	-0.591516
2	6	0	-2.248001	-0.249149	0.400851
3	6	0	-2.444183	1.017491	0.957391
4	6	0	-3.500253	1.814196	0.519255
5	6	0	-4.356419	1.354642	-0.479003
6	6	0	-4.162210	0.090395	-1.034518
7	1	0	-2.973924	-1.705789	-1.004748
8	1	0	-1.767786	1.371031	1.725587
9	1	0	-3.649234	2.795292	0.954877
10	1	0	-5.174570	1.977311	-0.821305
11	1	0	-4.831696	-0.273657	-1.805175
12	6	0	3.122742	-0.382889	-0.102508
13	6	0	2.652709	-1.774841	-0.134429
14	6	0	1.362389	-2.083294	-0.307684
15	6	0	0.306438	-1.042407	-0.456380

16	6	0	0.820667	0.354159	-0.481976
17	6	0	2.112813	0.659174	-0.308781
18	1	0	3.397636	-2.556775	-0.021969
19	1	0	1.038003	-3.118200	-0.327754
20	1	0	-0.302351	-1.249869	-1.341523
21	1	0	0.087516	1.138076	-0.634278
22	1	0	2.464808	1.684352	-0.313839
23	7	0	4.351670	-0.040156	0.085373
24	1	0	4.955905	-0.853167	0.209053
25	16	0	-0.898685	-1.275148	0.981464
26	8	0	4.675813	2.780402	-0.161459
27	1	0	4.736576	1.809761	-0.038366
28	1	0	5.227401	3.163051	0.525863

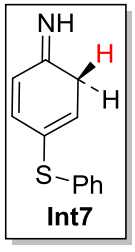


Int6(2H_2O)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.557522	-0.531385	-0.532945
2	6	0	-2.584343	-0.204856	0.416343
3	6	0	-2.557396	1.077035	0.972115
4	6	0	-3.495864	2.027143	0.574527
5	6	0	-4.457856	1.703958	-0.380043
6	6	0	-4.487098	0.424455	-0.933576
7	1	0	-3.586450	-1.532721	-0.945745
8	1	0	-1.800420	1.322738	1.706360
9	1	0	-3.470642	3.020202	1.007653
10	1	0	-5.184782	2.445396	-0.690187
11	1	0	-5.239300	0.167640	-1.670415
12	6	0	2.701755	-1.037690	-0.143395
13	6	0	2.055139	-2.354947	-0.223390
14	6	0	0.735694	-2.487916	-0.401009
15	6	0	-0.174000	-1.313586	-0.509241

16	6	0	0.521516	0.001307	-0.504319
17	6	0	1.842783	0.133220	-0.325675
18	1	0	2.692028	-3.230307	-0.138158
19	1	0	0.279756	-3.470879	-0.451774
20	1	0	-0.814693	-1.414025	-1.390438
21	1	0	-0.097558	0.881021	-0.637722
22	1	0	2.303255	1.115139	-0.318804
23	7	0	3.965650	-0.880480	0.071014
24	1	0	4.443263	-1.776615	0.171906
25	16	0	-1.383625	-1.427474	0.940379
26	8	0	5.295874	1.563469	0.293255
27	1	0	5.661805	1.606176	1.181145
28	1	0	4.866350	0.673740	0.218438
29	8	0	3.164104	3.194594	-0.349512
30	1	0	3.994601	2.730019	-0.116369
31	1	0	3.394562	3.780499	-1.075354

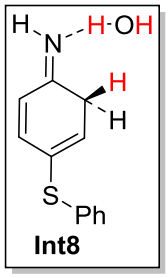


Int7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.544829	-0.686664	-0.774472
2	6	0	-1.782838	0.486323	-0.053159
3	6	0	-3.019736	0.682386	0.567916
4	6	0	-4.013048	-0.286854	0.458861
5	6	0	-3.774250	-1.463418	-0.249254
6	6	0	-2.536885	-1.659702	-0.859891
7	1	0	-0.591815	-0.835607	-1.266179
8	1	0	-3.197758	1.585770	1.139535
9	1	0	-4.970430	-0.126818	0.941179
10	1	0	-4.545034	-2.221149	-0.323277
11	1	0	-2.343202	-2.570224	-1.415294
12	6	0	3.358142	-0.723476	0.133730
13	6	0	2.279485	-0.909882	1.109191

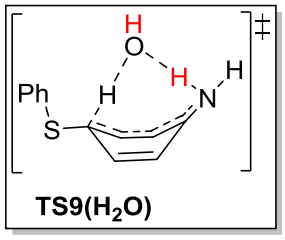
14	6	0	1.152601	-0.176000	1.062340
15	6	0	0.954880	0.863926	0.051230
16	6	0	1.938857	1.176322	-0.807413
17	6	0	3.287260	0.526285	-0.724555
18	1	0	2.394023	-1.700319	1.844530
19	1	0	0.349001	-0.356239	1.766307
20	1	0	1.787630	1.944292	-1.557377
21	1	0	3.994279	1.254807	-0.298436
22	7	0	4.344055	-1.522867	-0.034871
23	1	0	4.300126	-2.295731	0.633261
24	16	0	-0.566370	1.794319	0.063208
25	1	0	3.678876	0.296698	-1.718636



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.949912	0.808985	-0.737796
2	6	0	2.317781	-0.423860	-0.192205
3	6	0	3.620745	-0.616889	0.275770
4	6	0	4.549756	0.416335	0.189380
5	6	0	4.182313	1.651163	-0.342488
6	6	0	2.880002	1.843063	-0.800372
7	1	0	0.945101	0.956447	-1.113156
8	1	0	3.900507	-1.568700	0.711986
9	1	0	5.558931	0.258625	0.551983
10	1	0	4.904151	2.457089	-0.398635
11	1	0	2.586409	2.798773	-1.219228
12	6	0	-2.831211	0.410384	0.734810
13	6	0	-1.652714	0.552225	1.587056
14	6	0	-0.500742	-0.086717	1.307348
15	6	0	-0.368955	-0.970155	0.150287

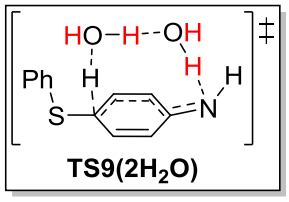
16	6	0	-1.428449	-1.218765	-0.636861
17	6	0	-2.782522	-0.655224	-0.341806
18	1	0	-1.719762	1.223460	2.437508
19	1	0	0.370277	0.056640	1.935700
20	1	0	-5.152926	0.866676	-0.528536
21	1	0	-1.330987	-1.871413	-1.496759
22	1	0	-3.438002	-1.477491	-0.017240
23	7	0	-3.897753	1.117683	0.849426
24	1	0	-3.834137	1.774179	1.627966
25	16	0	1.183048	-1.806629	-0.117764
26	8	0	-5.573974	0.548600	-1.355766
27	1	0	-6.194527	1.234074	-1.616502
28	1	0	-3.263223	-0.278142	-1.249440



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.912017	0.440241	-1.085615
2	6	0	-1.848929	-0.626352	-0.182150
3	6	0	-2.763036	-0.690903	0.871132
4	6	0	-3.721934	0.309967	1.028689
5	6	0	-3.766621	1.384224	0.143620
6	6	0	-2.858589	1.446599	-0.914755
7	1	0	-1.222320	0.475136	-1.920364
8	1	0	-2.713384	-1.519080	1.567495
9	1	0	-4.426647	0.252798	1.850337
10	1	0	-4.508546	2.163853	0.270205
11	1	0	-2.900253	2.269709	-1.619284
12	6	0	3.215411	0.447733	0.297633
13	6	0	3.057356	-0.261816	-0.953276
14	6	0	1.875388	-0.917876	-1.156035
15	6	0	0.895891	-0.988936	-0.104035
16	6	0	1.408295	-0.847845	1.236387

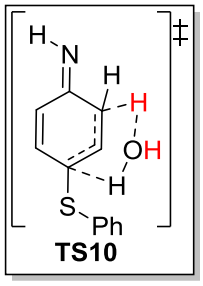
17	6	0	2.564557	-0.158476	1.443487
18	1	0	3.740066	-0.063388	-1.772089
19	1	0	1.609925	-1.290773	-2.138809
20	1	0	0.712366	0.598935	-0.192825
21	1	0	0.803274	-1.194871	2.066306
22	1	0	2.906247	0.117953	2.432990
23	7	0	3.624771	1.702310	0.405866
24	1	0	4.052450	2.010270	-0.470670
25	16	0	-0.619168	-1.925669	-0.372236
26	8	0	0.922395	1.725024	-0.161939
27	1	0	0.316832	2.128384	0.475850
28	1	0	1.909494	1.926047	0.110597



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.205022	0.040427	1.206036
2	6	0	2.142889	-0.675753	0.004619
3	6	0	2.979260	-0.315031	-1.052566
4	6	0	3.855036	0.762046	-0.918291
5	6	0	3.892107	1.494251	0.265621
6	6	0	3.064533	1.129943	1.329144
7	1	0	1.582925	-0.258937	2.040718
8	1	0	2.928119	-0.867925	-1.982439
9	1	0	4.497370	1.036830	-1.747024
10	1	0	4.566727	2.336322	0.365128
11	1	0	3.105729	1.679417	2.263138
12	6	0	-3.232439	-0.174448	0.200461
13	6	0	-2.517162	-0.660941	1.362812
14	6	0	-1.247398	-1.135535	1.240964
15	6	0	-0.585989	-1.180849	-0.042005
16	6	0	-1.454848	-1.115969	-1.192858
17	6	0	-2.712743	-0.608137	-1.080723
18	1	0	-2.975851	-0.547404	2.339656

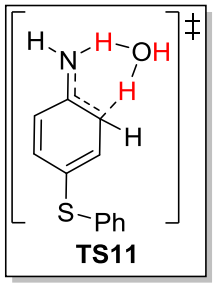
19	1	0	-0.684198	-1.422570	2.121908
20	1	0	-0.312105	0.263783	-0.210711
21	1	0	-1.044034	-1.368784	-2.163875
22	1	0	-3.334204	-0.445326	-1.952878
23	7	0	-4.220861	0.697173	0.227830
24	1	0	-4.494045	0.893651	1.191302
25	16	0	0.994016	-2.047823	-0.190853
26	8	0	-2.478704	2.614831	-0.486963
27	1	0	-2.683852	3.087785	-1.299539
28	1	0	-3.261244	1.993359	-0.295484
29	8	0	-0.242198	1.434605	-0.388148
30	1	0	-1.158942	1.924008	-0.419444
31	1	0	0.346991	1.825219	0.269984



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.384047	0.468906	1.126155
2	6	0	-1.817583	0.747972	-0.120235
3	6	0	-2.095020	-0.099231	-1.202819
4	6	0	-2.885940	-1.235996	-1.023307
5	6	0	-3.430230	-1.520840	0.232516
6	6	0	-3.187203	-0.659311	1.299891
7	1	0	-2.175176	1.126966	1.960682
8	1	0	-1.681356	0.132863	-2.176889
9	1	0	-3.096626	-1.883939	-1.866914
10	1	0	-4.046523	-2.400911	0.370618
11	1	0	-3.614431	-0.868825	2.273590
12	6	0	3.227013	-0.581889	0.106145
13	6	0	2.675258	0.185011	1.221054
14	6	0	1.562226	0.973485	1.093580
15	6	0	0.863930	1.094203	-0.149767

16	6	0	1.454974	0.483474	-1.285765
17	6	0	2.522105	-0.382992	-1.163647
18	1	0	3.179635	0.121169	2.179722
19	1	0	1.173388	1.505030	1.955888
20	1	0	0.303328	-0.558665	0.417568
21	1	0	1.006562	0.648631	-2.260173
22	1	0	2.961722	-0.841972	-2.041972
23	7	0	4.234306	-1.405742	0.154543
24	1	0	4.616781	-1.436222	1.100392
25	16	0	-0.614508	2.086749	-0.302348
26	8	0	0.256900	-1.580916	0.219401
27	1	0	-0.571307	-1.684230	-0.298048
28	1	0	1.047890	-1.597108	-0.416713

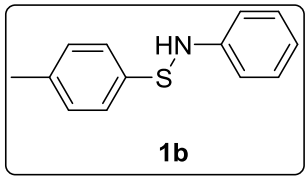


TS11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.785364	0.964530	-0.315878
2	6	0	2.224545	-0.357682	-0.214939
3	6	0	3.572286	-0.623584	0.047393
4	6	0	4.471631	0.427377	0.199375
5	6	0	4.035013	1.748233	0.108400
6	6	0	2.690373	2.009507	-0.146084
7	1	0	0.745551	1.175949	-0.529253
8	1	0	3.911448	-1.649070	0.138837
9	1	0	5.514563	0.211725	0.401170
10	1	0	4.735444	2.564779	0.235969
11	1	0	2.340792	3.032825	-0.222670
12	6	0	-2.964370	0.015873	0.747115
13	6	0	-1.929849	-0.193364	1.712689
14	6	0	-0.725099	-0.696077	1.319988
15	6	0	-0.451950	-1.066164	-0.042422

16	6	0	-1.448235	-0.986356	-0.966312
17	6	0	-2.758756	-0.460045	-0.632145
18	1	0	-2.098397	0.093759	2.744884
19	1	0	0.068897	-0.815849	2.048056
20	1	0	-4.455303	1.155711	-0.041567
21	1	0	-1.275006	-1.330976	-1.979310
22	1	0	-3.576225	-1.096872	-0.988233
23	7	0	-4.063113	0.710361	0.961524
24	1	0	-4.184325	1.132637	1.872894
25	16	0	1.137829	-1.760872	-0.459236
26	8	0	-4.384977	1.400553	-1.386689
27	1	0	-4.213741	2.322398	-1.606970
28	1	0	-3.203075	0.506496	-1.266258

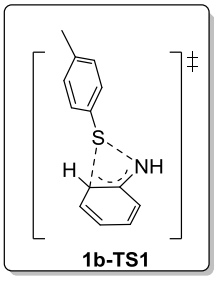


1b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.280653	-0.827827	-0.639930
2	6	0	3.328244	0.095107	-1.055996
3	6	0	2.200931	0.352375	-0.263686
4	6	0	2.047025	-0.327546	0.948717
5	6	0	3.011984	-1.243632	1.356857
6	6	0	4.132118	-1.504012	0.570408
7	1	0	5.146806	-1.013945	-1.264681
8	1	0	3.455161	0.622344	-1.996130
9	1	0	1.177037	-0.135191	1.562721
10	1	0	2.879734	-1.762070	2.299694
11	1	0	4.877092	-2.220328	0.894108
12	7	0	1.236781	1.257829	-0.731051
13	1	0	1.414061	1.694424	-1.622272
14	6	0	-1.346523	0.842822	0.037052
15	6	0	-2.545363	1.191020	0.664800
16	6	0	-1.259558	-0.350453	-0.673236
17	6	0	-3.644258	0.345089	0.575689
18	1	0	-2.623694	2.121716	1.217209
19	6	0	-2.371530	-1.187102	-0.752544

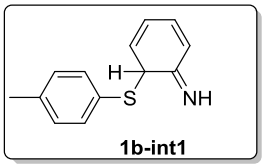
20	1	0	-0.332405	-0.622632	-1.160162
21	6	0	-3.578630	-0.860891	-0.131856
22	1	0	-4.571320	0.629633	1.062800
23	1	0	-2.292338	-2.114769	-1.309826
24	16	0	0.034027	1.976613	0.215200
25	6	0	-4.769421	-1.783415	-0.198638
26	1	0	-4.895883	-2.332279	0.740597
27	1	0	-5.693694	-1.228018	-0.377959
28	1	0	-4.656484	-2.518702	-0.997766



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.396546	1.096951	-0.757181
2	6	0	-2.040351	0.828816	-0.849576
3	6	0	-1.461918	-0.238105	-0.126598
4	6	0	-2.311335	-1.019111	0.688414
5	6	0	-3.666348	-0.743886	0.771564
6	6	0	-4.235494	0.315743	0.050085
7	1	0	-3.819093	1.923964	-1.318251
8	1	0	-1.399722	1.435903	-1.477369
9	1	0	-1.881329	-1.838944	1.250782
10	1	0	-4.300117	-1.355245	1.405578
11	16	0	0.243825	-0.570292	-0.239903
12	6	0	2.727287	-0.533559	1.031723
13	6	0	3.002944	-0.825842	-0.356627
14	6	0	3.211412	0.635653	1.617042
15	6	0	3.717794	0.169058	-1.113705
16	6	0	3.925415	1.549257	0.858278
17	1	0	3.023766	0.828361	2.666529
18	6	0	4.172767	1.311943	-0.515694
19	1	0	3.881679	-0.035382	-2.164191
20	1	0	4.298761	2.457040	1.317812

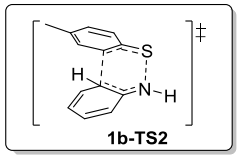
21	1	0	4.722489	2.047047	-1.091687
22	7	0	2.565937	-1.899153	-0.989218
23	1	0	2.236392	-1.287335	1.631559
24	6	0	-5.713506	0.587929	0.117996
25	1	0	-6.247291	0.009544	-0.644629
26	1	0	-6.126748	0.306580	1.088990
27	1	0	-5.933508	1.642807	-0.058793
28	1	0	2.089233	-2.524683	-0.337668



Standard orientation:

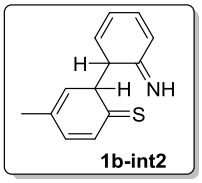
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.988286	1.000589	0.663864
2	6	0	1.675176	0.715924	1.031968
3	6	0	1.048118	-0.437377	0.557781
4	6	0	1.753943	-1.299489	-0.287503
5	6	0	3.058901	-0.999336	-0.660388
6	6	0	3.699909	0.152416	-0.188156
7	1	0	3.463555	1.900375	1.040154
8	1	0	1.128384	1.388915	1.680679
9	1	0	1.276434	-2.203485	-0.646636
10	1	0	3.592699	-1.674460	-1.321309
11	16	0	-0.629489	-0.822708	1.045842
12	6	0	-1.541115	-0.377786	-0.555381
13	6	0	-2.994652	-0.711571	-0.288244
14	6	0	-1.271398	1.055487	-0.860910
15	6	0	-3.845009	0.390480	0.162671
16	6	0	-2.170674	2.012522	-0.580037
17	1	0	-0.296580	1.302756	-1.262695
18	6	0	-3.459957	1.672787	-0.003420
19	1	0	-4.825189	0.144485	0.557766
20	1	0	-1.941165	3.055329	-0.765045
21	1	0	-4.128027	2.478745	0.280519
22	7	0	-3.373170	-1.921629	-0.471334
23	1	0	-4.356973	-2.033213	-0.214558
24	1	0	-1.151130	-1.055180	-1.312770

25	6	0	5.127242	0.449544	-0.570352
26	1	0	5.822103	-0.162028	0.014713
27	1	0	5.309928	0.230452	-1.625226
28	1	0	5.377364	1.496893	-0.391080



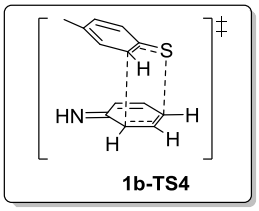
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.913688	1.502467	0.399351
2	6	0	0.714135	1.298007	-0.359913
3	6	0	0.383444	-0.088543	-0.700219
4	6	0	1.483827	-1.048850	-0.699485
5	6	0	2.659145	-0.784722	-0.074568
6	6	0	2.835922	0.508250	0.537234
7	1	0	2.095964	2.491336	0.802376
8	1	0	-0.333508	-0.192174	-1.508418
9	1	0	1.316754	-2.013424	-1.165086
10	1	0	3.754863	0.701941	1.081704
11	6	0	-1.853884	0.294592	0.693437
12	6	0	-3.011222	-0.095022	-0.085188
13	6	0	-3.168870	-1.375639	-0.499619
14	6	0	-2.190015	-2.383556	-0.173277
15	6	0	-1.035173	-2.048599	0.445411
16	6	0	-0.719288	-0.647525	0.725191
17	1	0	-3.757804	0.667225	-0.269279
18	1	0	-4.056622	-1.665515	-1.050041
19	1	0	-2.398168	-3.418447	-0.419645
20	1	0	-0.296843	-2.802633	0.688671
21	1	0	-0.020613	-0.482989	1.541261
22	7	0	-1.827768	1.486849	1.219318
23	16	0	-0.347178	2.543602	-0.701565
24	6	0	3.784628	-1.781693	-0.010940
25	1	0	4.690587	-1.380361	-0.475644
26	1	0	4.035438	-2.022211	1.027295
27	1	0	3.523449	-2.710079	-0.521356
28	1	0	-0.982301	1.626760	1.773484



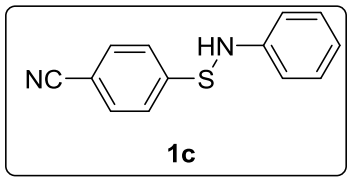
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.655536	-0.805865	-0.045609
2	6	0	1.466127	-1.091928	-0.607038
3	6	0	0.312267	-0.140530	-0.557154
4	6	0	0.710278	1.290649	-0.309828
5	6	0	1.922861	1.495172	0.440913
6	6	0	2.838241	0.502096	0.563487
7	1	0	1.292754	-2.061207	-1.060434
8	1	0	2.114255	2.486807	0.831029
9	1	0	3.768651	0.695998	1.088704
10	16	0	-0.211258	2.552027	-0.841149
11	6	0	-0.674718	-0.641142	0.645996
12	6	0	-1.857859	0.288455	0.762612
13	6	0	-1.082838	-2.050533	0.337088
14	6	0	-2.990691	0.006348	-0.122561
15	6	0	-2.246385	-2.312994	-0.279177
16	1	0	-0.385805	-2.845797	0.571621
17	6	0	-3.177701	-1.240697	-0.599593
18	1	0	-3.704456	0.800846	-0.310759
19	1	0	-2.513145	-3.329860	-0.543829
20	1	0	-4.050718	-1.471758	-1.200142
21	1	0	-0.084924	-0.575341	1.560394
22	7	0	-1.796255	1.247160	1.608952
23	1	0	-2.630905	1.836686	1.552070
24	1	0	-0.294532	-0.199515	-1.461198
25	6	0	3.808369	-1.772348	-0.026097
26	1	0	4.682678	-1.349943	-0.531540
27	1	0	4.109784	-1.999492	1.001782
28	1	0	3.549351	-2.710079	-0.520206



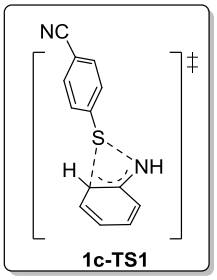
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.280386	0.675018	1.153910
2	6	0	0.242766	1.319691	-0.062592
3	6	0	-0.564532	1.190943	-1.242369
4	6	0	-1.852419	0.749763	-1.163483
5	6	0	-2.460358	0.370959	0.084408
6	6	0	-1.698574	0.393969	1.210960
7	1	0	0.167479	1.044168	2.070087
8	1	0	-0.143868	1.528600	-2.181108
9	1	0	-2.457195	0.707479	-2.064081
10	1	0	-2.126886	0.103229	2.163725
11	6	0	0.104326	-1.675417	-0.110864
12	6	0	0.994809	-1.499531	-1.253756
13	6	0	2.261923	-1.057007	-1.083760
14	6	0	2.762523	-0.715937	0.226277
15	6	0	1.953356	-0.787558	1.317274
16	6	0	0.541712	-1.037028	1.161921
17	1	0	0.627973	-1.792049	-2.231697
18	1	0	2.925915	-0.960140	-1.934607
19	1	0	3.807923	-0.456235	0.336664
20	1	0	2.335793	-0.537629	2.299470
21	1	0	0.025149	-1.434841	2.028498
22	7	0	-1.023681	-2.295893	-0.124086
23	1	0	-1.227399	-2.640205	-1.065763
24	16	0	1.720916	2.089135	-0.055638
25	6	0	-3.911685	-0.018600	0.101862
26	1	0	-4.539203	0.774312	-0.316872
27	1	0	-4.071976	-0.917832	-0.500194
28	1	0	-4.253357	-0.229355	1.115964



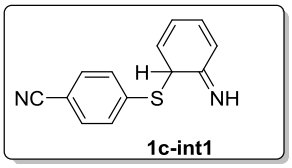
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.493033	-0.958497	-0.612728
2	6	0	3.573398	-0.008883	-1.043164
3	6	0	2.428526	0.257009	-0.281977
4	6	0	2.221705	-0.435620	0.914065
5	6	0	3.154394	-1.377919	1.338136
6	6	0	4.291966	-1.649174	0.581424
7	1	0	5.374552	-1.153152	-1.212534
8	1	0	3.740421	0.529931	-1.970278
9	1	0	1.339482	-0.233420	1.507363
10	1	0	2.983295	-1.906862	2.268564
11	1	0	5.011730	-2.385499	0.916742
12	7	0	1.486515	1.181823	-0.772851
13	1	0	1.731585	1.656852	-1.628537
14	6	0	-1.093894	0.989901	0.043911
15	6	0	-2.246114	1.428073	0.707074
16	6	0	-1.110423	-0.203495	-0.679032
17	6	0	-3.409517	0.678092	0.643865
18	1	0	-2.234268	2.354901	1.269901
19	6	0	-2.275412	-0.955124	-0.741347
20	1	0	-0.214581	-0.535593	-1.185869
21	6	0	-3.433856	-0.522362	-0.082014
22	1	0	-4.303965	1.014752	1.152440
23	1	0	-2.293291	-1.883014	-1.299100
24	16	0	0.367941	2.004507	0.196640
25	6	0	-4.631059	-1.297412	-0.147343
26	7	0	-5.600584	-1.924473	-0.200029



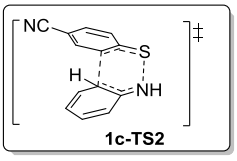
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.171152	1.016722	-0.790561
2	6	0	-1.812348	0.767595	-0.866858
3	6	0	-1.225899	-0.293642	-0.141894
4	6	0	-2.062882	-1.101077	0.659971
5	6	0	-3.422942	-0.860413	0.737225
6	6	0	-3.987186	0.203154	0.012926
7	1	0	-3.614703	1.832557	-1.347363
8	1	0	-1.176481	1.386034	-1.487434
9	1	0	-1.620741	-1.917439	1.216832
10	1	0	-4.059731	-1.483316	1.352750
11	16	0	0.490939	-0.591946	-0.239986
12	6	0	2.980553	-0.492253	1.053626
13	6	0	3.262678	-0.798571	-0.331920
14	6	0	3.442268	0.692464	1.619724
15	6	0	3.959877	0.196356	-1.107184
16	6	0	4.140871	1.606109	0.843776
17	1	0	3.251813	0.900243	2.665518
18	6	0	4.393899	1.355779	-0.526575
19	1	0	4.126671	-0.022829	-2.154107
20	1	0	4.498086	2.526956	1.289968
21	1	0	4.930301	2.092964	-1.111797
22	7	0	2.850263	-1.888805	-0.946476
23	1	0	2.497053	-1.244257	1.661711
24	6	0	-5.388993	0.456850	0.094162
25	7	0	-6.524531	0.663032	0.161368
26	1	0	2.380125	-2.513806	-0.289047



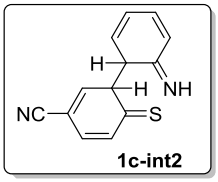
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.874014	0.711196	0.998528
2	6	0	1.544126	0.462299	1.313612
3	6	0	0.809279	-0.476899	0.583755
4	6	0	1.421312	-1.167262	-0.469440
5	6	0	2.741561	-0.906997	-0.804297
6	6	0	3.477540	0.034239	-0.068831
7	1	0	3.444588	1.437194	1.563744
8	1	0	1.065583	1.001716	2.120918
9	1	0	0.864033	-1.916205	-1.018215
10	1	0	3.215097	-1.437219	-1.620870
11	16	0	-0.881454	-0.818477	1.044948
12	6	0	-1.763211	-0.359768	-0.565864
13	6	0	-3.227239	-0.665442	-0.308889
14	6	0	-1.461424	1.068216	-0.871178
15	6	0	-4.061477	0.454630	0.126241
16	6	0	-2.346183	2.041135	-0.601908
17	1	0	-0.479548	1.296981	-1.267281
18	6	0	-3.648647	1.728162	-0.038192
19	1	0	-5.050870	0.229146	0.509980
20	1	0	-2.096247	3.078600	-0.789652
21	1	0	-4.303406	2.548270	0.235249
22	7	0	-3.620400	-1.870236	-0.488757
23	1	0	-4.608738	-1.968869	-0.244956
24	1	0	-1.388998	-1.046993	-1.321837
25	6	0	4.839977	0.300371	-0.407628
26	7	0	5.940973	0.517341	-0.682915



Standard orientation:

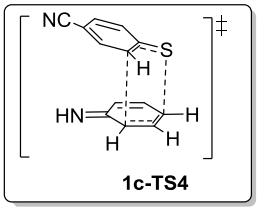
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.459365	1.885725	0.391024
2	6	0	0.303149	1.472876	-0.354104
3	6	0	0.198406	0.044590	-0.684463
4	6	0	1.442248	-0.713638	-0.704946
5	6	0	2.555098	-0.234577	-0.082774
6	6	0	2.542186	1.072949	0.528158
7	1	0	1.473457	2.894380	0.784971
8	1	0	-0.492081	-0.177184	-1.492289
9	1	0	1.453319	-1.690776	-1.169927
10	1	0	3.426271	1.409936	1.054765
11	6	0	-2.044728	0.030858	0.696376
12	6	0	-3.113197	-0.544400	-0.094595
13	6	0	-3.048053	-1.831737	-0.511456
14	6	0	-1.917304	-2.663274	-0.174502
15	6	0	-0.838611	-2.143127	0.451913
16	6	0	-0.764048	-0.706681	0.730982
17	1	0	-3.975808	0.081671	-0.284216
18	1	0	-3.868814	-2.266016	-1.070431
19	1	0	-1.950809	-3.718897	-0.417744
20	1	0	0.010239	-2.765566	0.707327
21	1	0	-0.111386	-0.429496	1.554981
22	7	0	-2.220804	1.205114	1.228549
23	16	0	-0.951202	2.518496	-0.694090
24	6	0	3.751929	-1.015318	-0.035661
25	7	0	4.722411	-1.639913	0.016140
26	1	0	-1.415033	1.484125	1.789466



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.548599	-0.285611	-0.041715

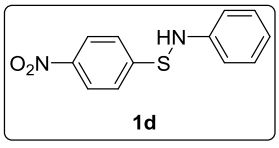
2	6	0	1.427295	-0.768372	-0.621866
3	6	0	0.146310	-0.011571	-0.559826
4	6	0	0.320258	1.462951	-0.305537
5	6	0	1.481483	1.855218	0.457849
6	6	0	2.546392	1.029378	0.584695
7	1	0	1.427514	-1.745104	-1.087968
8	1	0	1.507400	2.861601	0.855443
9	1	0	3.437655	1.350002	1.110057
10	16	0	-0.781081	2.563362	-0.839469
11	6	0	-0.739327	-0.675791	0.651011
12	6	0	-2.060253	0.048766	0.750177
13	6	0	-0.900084	-2.135695	0.351135
14	6	0	-3.130241	-0.434281	-0.124797
15	6	0	-2.001721	-2.594873	-0.263293
16	1	0	-0.081231	-2.801274	0.596786
17	6	0	-3.101583	-1.699031	-0.591102
18	1	0	-3.970584	0.223672	-0.316880
19	1	0	-2.092962	-3.644589	-0.517355
20	1	0	-3.923129	-2.081009	-1.186875
21	1	0	-0.171614	-0.502146	1.565048
22	7	0	-2.150303	1.026628	1.571466
23	1	0	-3.070576	1.470485	1.512626
24	1	0	-0.450670	-0.166708	-1.458928
25	6	0	3.756730	-1.050794	-0.037139
26	7	0	4.739209	-1.658128	-0.019751



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.084733	-0.683197	-1.153381
2	6	0	0.456270	-1.327722	0.056578
3	6	0	-0.338895	-1.224845	1.249195
4	6	0	-1.636575	-0.815716	1.198060
5	6	0	-2.243624	-0.444133	-0.053957
6	6	0	-1.506916	-0.434734	-1.202739

7	1	0	0.359241	-1.039510	-2.076393
8	1	0	0.101341	-1.560477	2.179272
9	1	0	-2.243570	-0.792009	2.094563
10	1	0	-1.965654	-0.158013	-2.143229
11	6	0	0.235277	1.682558	0.104514
12	6	0	1.120303	1.529440	1.256581
13	6	0	2.395350	1.108955	1.096429
14	6	0	2.911081	0.772774	-0.210364
15	6	0	2.110189	0.820490	-1.309011
16	6	0	0.693598	1.045697	-1.164708
17	1	0	0.741372	1.821143	2.229908
18	1	0	3.056850	1.029180	1.950808
19	1	0	3.963778	0.540503	-0.312805
20	1	0	2.506551	0.577308	-2.287135
21	1	0	0.176308	1.434183	-2.035310
22	7	0	-0.900917	2.282477	0.097349
23	1	0	-1.131283	2.640648	1.027310
24	16	0	1.949970	-2.059334	0.030723
25	6	0	-3.634190	-0.115580	-0.077872
26	7	0	-4.760121	0.142161	-0.076564

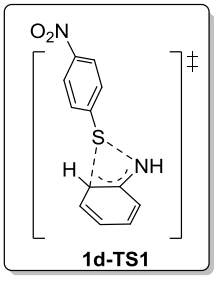


1d

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.830832	-1.097594	-0.536413
2	6	0	3.950418	-0.139760	-1.026613
3	6	0	2.813681	0.212761	-0.289268
4	6	0	2.574934	-0.401018	0.943128
5	6	0	3.468854	-1.352144	1.426889
6	6	0	4.598108	-1.709876	0.694155
7	1	0	5.706602	-1.360316	-1.118362
8	1	0	4.141914	0.337854	-1.982083
9	1	0	1.698952	-0.131506	1.518685
10	1	0	3.273643	-1.819547	2.385063
11	1	0	5.287476	-2.452659	1.075840
12	7	0	1.908823	1.142731	-0.839430

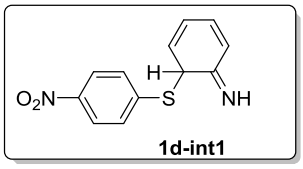
13	1	0	2.179483	1.561139	-1.716852
14	6	0	-0.672895	1.125451	-0.011878
15	6	0	-1.799544	1.657823	0.629198
16	6	0	-0.749433	-0.105323	-0.667881
17	6	0	-2.999285	0.964838	0.611487
18	1	0	-1.738688	2.612788	1.138886
19	6	0	-1.949481	-0.802499	-0.686668
20	1	0	0.127075	-0.507724	-1.156709
21	6	0	-3.060167	-0.260446	-0.048093
22	1	0	-3.883181	1.355385	1.095539
23	1	0	-2.035283	-1.757718	-1.185379
24	16	0	0.833611	2.074263	0.079934
25	7	0	-4.330383	-0.999516	-0.068012
26	8	0	-4.356062	-2.075073	-0.656145
27	8	0	-5.291562	-0.497638	0.504927



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.748043	1.082039	-0.611600
2	6	0	-1.384776	0.865446	-0.720583
3	6	0	-0.791978	-0.310263	-0.207523
4	6	0	-1.623715	-1.268670	0.414116
5	6	0	-2.988788	-1.064730	0.521752
6	6	0	-3.532628	0.111708	0.008865
7	1	0	-3.214426	1.977445	-0.997604
8	1	0	-0.752150	1.598699	-1.203828
9	1	0	-1.175329	-2.171749	0.807679
10	1	0	-3.637106	-1.789591	0.993475
11	16	0	0.930437	-0.563844	-0.341317
12	6	0	3.418543	-0.649865	0.967090
13	6	0	3.706497	-0.721356	-0.449245
14	6	0	3.864967	0.431023	1.720525
15	6	0	4.393576	0.394410	-1.049655

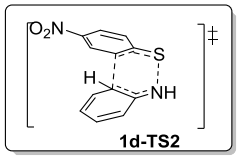
16	6	0	4.554175	1.467207	1.105998
17	1	0	3.670355	0.463530	2.785442
18	6	0	4.812869	1.448084	-0.285693
19	1	0	4.564366	0.350937	-2.117738
20	1	0	4.899517	2.306707	1.698155
21	1	0	5.341417	2.277356	-0.740048
22	7	0	3.308051	-1.700420	-1.235115
23	1	0	2.940467	-1.495849	1.441276
24	7	0	-4.983839	0.336256	0.126545
25	8	0	-5.438171	1.378469	-0.331868
26	8	0	-5.651924	-0.531868	0.677025
27	1	0	2.842980	-2.429827	-0.691285



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.640596	-0.308154	1.265927
2	6	0	1.294590	-0.595156	1.435636
3	6	0	0.427593	-0.624502	0.333043
4	6	0	0.932979	-0.355310	-0.946930
5	6	0	2.273353	-0.045446	-1.121015
6	6	0	3.113544	-0.027033	-0.011980
7	1	0	3.320656	-0.280127	2.105599
8	1	0	0.905720	-0.787543	2.427794
9	1	0	0.287440	-0.398754	-1.813623
10	1	0	2.678512	0.167309	-2.100341
11	16	0	-1.256050	-1.092870	0.638127
12	6	0	-2.203998	-0.116318	-0.662576
13	6	0	-3.651338	-0.545321	-0.476850
14	6	0	-1.945888	1.338641	-0.447415
15	6	0	-4.490152	0.320472	0.350774
16	6	0	-2.840199	2.119419	0.178120
17	1	0	-0.988467	1.731504	-0.765865
18	6	0	-4.111225	1.582995	0.635450
19	1	0	-5.457569	-0.060240	0.660594

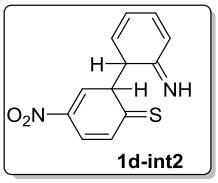
20	1	0	-2.619998	3.163847	0.364037
21	1	0	-4.770651	2.230787	1.202336
22	7	0	-4.022601	-1.624934	-1.054305
23	1	0	-4.996422	-1.841038	-0.828975
24	1	0	-1.867608	-0.476287	-1.632827
25	7	0	4.535100	0.300443	-0.195676
26	8	0	5.254150	0.295330	0.797205
27	8	0	4.918171	0.559941	-1.331205



Standard orientation:

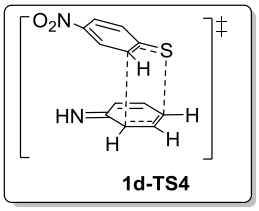
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.014668	2.070853	0.330715
2	6	0	-0.115128	1.552794	-0.390122
3	6	0	-0.117193	0.112128	-0.685842
4	6	0	1.176079	-0.556184	-0.691025
5	6	0	2.231507	0.034852	-0.086329
6	6	0	2.157483	1.345369	0.482084
7	1	0	0.957268	3.088477	0.696054
8	1	0	-0.793141	-0.181691	-1.482703
9	1	0	1.278853	-1.542199	-1.121322
10	1	0	3.025990	1.746065	0.985102
11	6	0	-2.342544	-0.044512	0.709304
12	6	0	-3.367131	-0.717613	-0.061987
13	6	0	-3.205176	-2.005627	-0.449437
14	6	0	-2.012570	-2.740337	-0.100831
15	6	0	-0.973788	-2.125788	0.507360
16	6	0	-1.009793	-0.682496	0.754930
17	1	0	-4.275560	-0.163531	-0.261285
18	1	0	-3.992470	-2.514271	-0.993573
19	1	0	-1.965576	-3.800349	-0.321512
20	1	0	-0.077488	-2.675247	0.768362
21	1	0	-0.376244	-0.335652	1.567376
22	7	0	-2.603706	1.125570	1.214564
23	16	0	-1.447923	2.491409	-0.743642
24	7	0	3.517389	-0.690296	-0.025010
25	8	0	4.466427	-0.104330	0.480314

26	8	0	3.557316	-1.829369	-0.473086
27	1	0	-1.819085	1.477892	1.764153



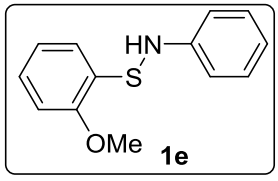
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.230608	-0.010402	-0.041378
2	6	0	1.168126	-0.607265	-0.603335
3	6	0	-0.162571	0.056368	-0.559365
4	6	0	-0.097517	1.547163	-0.344381
5	6	0	1.039296	2.048843	0.392286
6	6	0	2.166153	1.310596	0.536429
7	1	0	1.262746	-1.595322	-1.031287
8	1	0	0.993156	3.066573	0.757291
9	1	0	3.042607	1.699173	1.035538
10	16	0	-1.287211	2.543367	-0.892734
11	6	0	-0.989129	-0.646815	0.672917
12	6	0	-2.361153	-0.022945	0.761958
13	6	0	-1.036590	-2.121300	0.407858
14	6	0	-3.395371	-0.609600	-0.091997
15	6	0	-2.102878	-2.678985	-0.186879
16	1	0	-0.166046	-2.715083	0.660089
17	6	0	-3.271104	-1.879641	-0.527243
18	1	0	-4.285334	-0.023784	-0.293685
19	1	0	-2.112772	-3.738155	-0.416479
20	1	0	-4.063995	-2.339032	-1.106903
21	1	0	-0.432982	-0.406844	1.579039
22	7	0	-2.520248	0.966920	1.557888
23	1	0	-3.472164	1.337539	1.495930
24	1	0	-0.748279	-0.169039	-1.450827
25	7	0	3.526850	-0.721351	-0.023433
26	8	0	4.480662	-0.126869	0.462738
27	8	0	3.569965	-1.853754	-0.486158



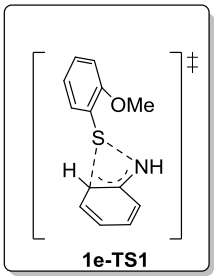
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.208976	0.702568	1.146949
2	6	0	0.761459	1.334514	-0.065921
3	6	0	-0.029010	1.231319	-1.262287
4	6	0	-1.326463	0.816320	-1.220575
5	6	0	-1.912193	0.458734	0.030853
6	6	0	-1.214201	0.464248	1.192153
7	1	0	0.654233	1.054950	2.070504
8	1	0	0.416440	1.563738	-2.190804
9	1	0	-1.938481	0.772273	-2.110286
10	1	0	-1.701603	0.199174	2.119905
11	6	0	0.500649	-1.671896	-0.109996
12	6	0	1.402933	-1.540183	-1.250812
13	6	0	2.681404	-1.136315	-1.077232
14	6	0	3.186630	-0.802726	0.234525
15	6	0	2.373721	-0.837036	1.324452
16	6	0	0.955933	-1.043697	1.165206
17	1	0	1.030894	-1.829325	-2.227489
18	1	0	3.353865	-1.068752	-1.924020
19	1	0	4.241166	-0.584313	0.348050
20	1	0	2.762489	-0.597575	2.306484
21	1	0	0.423370	-1.423384	2.030386
22	7	0	-0.650771	-2.242860	-0.119207
23	1	0	-0.875305	-2.597811	-1.051822
24	16	0	2.263546	2.048113	-0.035007
25	7	0	-3.340014	0.084409	0.057099
26	8	0	-3.875630	-0.061463	1.146417
27	8	0	-3.897786	-0.064129	-1.023907



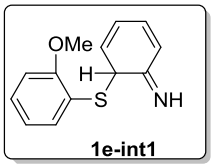
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.472771	0.378800	-0.261692
2	6	0	-3.415727	-0.144603	-0.996647
3	6	0	-2.224879	-0.516825	-0.356649
4	6	0	-2.112581	-0.349297	1.027169
5	6	0	-3.180629	0.171599	1.751724
6	6	0	-4.365723	0.540482	1.119250
7	1	0	-5.386262	0.659757	-0.773447
8	1	0	-3.510011	-0.272901	-2.070289
9	1	0	-1.192392	-0.625174	1.524891
10	1	0	-3.077974	0.294968	2.823903
11	1	0	-5.190544	0.948743	1.690119
12	7	0	-1.181299	-1.044569	-1.131122
13	1	0	-1.281610	-0.979289	-2.132610
14	6	0	1.194549	0.061644	-0.385132
15	6	0	2.514889	0.006969	0.093546
16	6	0	0.623176	1.290653	-0.687523
17	6	0	3.247286	1.179520	0.257622
18	6	0	1.356246	2.467420	-0.521037
19	1	0	-0.397097	1.330883	-1.044648
20	6	0	2.661913	2.410157	-0.051256
21	1	0	4.265033	1.145510	0.621762
22	1	0	0.899003	3.420825	-0.755987
23	1	0	3.236508	3.319064	0.080890
24	16	0	0.338509	-1.510197	-0.556935
25	8	0	2.976477	-1.249381	0.361529
26	6	0	4.301655	-1.397416	0.850951
27	1	0	4.429851	-0.879500	1.807074
28	1	0	4.448350	-2.466140	0.993955
29	1	0	5.033848	-1.021194	0.129010



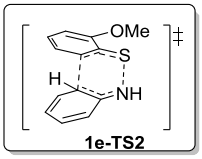
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.183462	-2.345155	0.028090
2	6	0	1.878196	-1.952451	-0.216780
3	6	0	1.492063	-0.593925	-0.207123
4	6	0	2.499830	0.382020	0.066000
5	6	0	3.815349	-0.020042	0.311070
6	6	0	4.149603	-1.372365	0.291066
7	1	0	3.452162	-3.394271	0.013720
8	1	0	1.108979	-2.685294	-0.426559
9	1	0	4.585342	0.710053	0.517390
10	1	0	5.175943	-1.663730	0.483100
11	16	0	-0.155469	-0.151611	-0.518838
12	6	0	-2.470387	1.000989	0.518560
13	6	0	-2.830600	0.525696	-0.798113
14	6	0	-3.088379	0.474708	1.652384
15	6	0	-3.780531	-0.553486	-0.875654
16	6	0	-4.024237	-0.539861	1.527955
17	1	0	-2.830885	0.860248	2.631662
18	6	0	-4.364981	-1.056419	0.254558
19	1	0	-4.012223	-0.935770	-1.861797
20	1	0	-4.500718	-0.945809	2.412752
21	1	0	-5.089747	-1.858888	0.182601
22	7	0	-2.278209	0.956807	-1.917818
23	1	0	-1.795314	1.841594	0.598352
24	8	0	2.106503	1.673370	0.071250
25	6	0	3.074901	2.685372	0.314927
26	1	0	3.863309	2.671370	-0.444344
27	1	0	2.534040	3.627927	0.258866
28	1	0	3.520688	2.578676	1.309180
29	1	0	-1.634363	1.724577	-1.720428



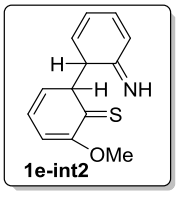
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.224975	0.417003	0.277919
2	6	0	-1.947866	0.462446	-0.291659
3	6	0	-1.190620	-0.724312	-0.391153
4	6	0	-1.735897	-1.921117	0.073168
5	6	0	-3.004582	-1.964117	0.646732
6	6	0	-3.742716	-0.789841	0.744755
7	1	0	-3.819859	1.315809	0.361794
8	1	0	-1.146932	-2.825138	-0.026096
9	1	0	-3.410397	-2.902889	1.002810
10	1	0	-4.733973	-0.803859	1.183120
11	16	0	0.440643	-0.726256	-1.121406
12	6	0	1.491404	-0.721715	0.455798
13	6	0	2.925631	-0.784522	-0.028916
14	6	0	1.147439	0.493720	1.246154
15	6	0	3.634583	0.490138	-0.140030
16	6	0	1.934293	1.581250	1.239742
17	1	0	0.206078	0.485495	1.781734
18	6	0	3.174126	1.594160	0.484104
19	1	0	4.580827	0.498033	-0.671066
20	1	0	1.645361	2.473592	1.782431
21	1	0	3.744218	2.516017	0.441007
22	7	0	3.411626	-1.937030	-0.307643
23	1	0	4.364980	-1.846865	-0.667171
24	1	0	1.245677	-1.647220	0.973436
25	8	0	-1.375140	1.598656	-0.758916
26	6	0	-2.096508	2.817512	-0.660191
27	1	0	-1.445495	3.578438	-1.086169
28	1	0	-3.030543	2.777135	-1.230311
29	1	0	-2.316357	3.067879	0.383269



Standard orientation:

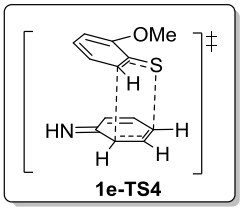
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.066125	0.188768	-0.037088
2	6	0	-0.857966	-0.272337	-0.698112
3	6	0	0.227700	0.706235	-0.826580
4	6	0	-0.133704	2.121263	-0.807395
5	6	0	-1.335058	2.500145	-0.314775
6	6	0	-2.289372	1.531179	0.135734
7	1	0	0.979651	0.418174	-1.554034
8	1	0	0.595466	2.850166	-1.136631
9	1	0	-1.599912	3.549673	-0.255932
10	1	0	-3.212024	1.883130	0.576301
11	6	0	1.639680	-0.954274	0.701993
12	6	0	2.921430	-1.253626	0.097084
13	6	0	3.825296	-0.271594	-0.135995
14	6	0	3.535975	1.097426	0.215157
15	6	0	2.312491	1.448713	0.670190
16	6	0	1.230539	0.463973	0.741159
17	1	0	3.135363	-2.295192	-0.107042
18	1	0	4.795560	-0.511604	-0.555691
19	1	0	4.318810	1.841377	0.121530
20	1	0	2.091239	2.475863	0.932118
21	1	0	0.453225	0.686006	1.467851
22	7	0	0.877551	-1.946102	1.067351
23	16	0	-0.607018	-1.863828	-1.116344
24	8	0	-2.932664	-0.783613	0.322484
25	6	0	-4.182066	-0.404087	0.881481
26	1	0	-4.757231	0.210032	0.180588
27	1	0	-4.713325	-1.333930	1.073588
28	1	0	-4.048559	0.142504	1.821436
29	1	0	0.019570	-1.614025	1.508984



Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

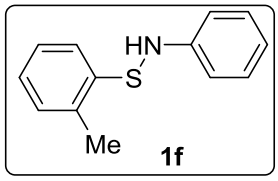
Number	Number	Type	X	Y	Z
1	6	0	-3.477951	1.119211	-0.246312
2	6	0	-2.256345	1.393454	-0.735815
3	6	0	-1.124101	0.429670	-0.575159
4	6	0	-1.561899	-0.987001	-0.307824
5	6	0	-2.825060	-1.159213	0.363489
6	6	0	-3.739632	-0.155565	0.386019
7	1	0	-4.280804	1.843339	-0.321269
8	1	0	-2.042789	2.348051	-1.200807
9	1	0	-3.053070	-2.137745	0.766545
10	1	0	-4.709195	-0.321825	0.842904
11	16	0	-0.618800	-2.270693	-0.741991
12	6	0	-0.215911	0.979500	0.673051
13	6	0	0.898375	0.005178	0.960559
14	6	0	0.281823	2.340855	0.295739
15	6	0	2.133857	0.173593	0.164586
16	6	0	1.500731	2.488061	-0.246803
17	1	0	-0.385237	3.185617	0.410316
18	6	0	2.413686	1.368186	-0.408885
19	1	0	1.840838	3.465578	-0.570366
20	1	0	3.339888	1.530744	-0.943590
21	1	0	-0.880518	0.999788	1.536423
22	7	0	0.717942	-0.910913	1.829922
23	1	0	1.528956	-1.532867	1.863922
24	1	0	-0.453265	0.447859	-1.434546
25	8	0	2.927251	-0.919936	0.179462
26	6	0	4.160403	-0.859145	-0.526134
27	1	0	4.812203	-0.085094	-0.107938
28	1	0	4.623512	-1.836010	-0.405151
29	1	0	3.988811	-0.661167	-1.588800



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

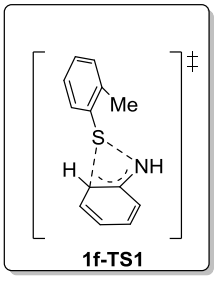
1	6	0	0.475747	0.696225	-1.481987
2	6	0	-0.328663	-0.454657	-1.031646
3	6	0	-1.487266	-0.147319	-0.210790
4	6	0	-1.957665	1.140166	-0.142087
5	6	0	-1.301998	2.207712	-0.830353
6	6	0	-0.153018	1.999684	-1.518722
7	1	0	1.112241	0.452189	-2.325702
8	1	0	-2.855496	1.365766	0.416814
9	1	0	-1.750474	3.193361	-0.797973
10	1	0	0.354093	2.814327	-2.020021
11	6	0	1.134686	1.150125	1.082707
12	6	0	0.764194	-0.013207	1.882810
13	6	0	1.332431	-1.219254	1.653541
14	6	0	2.294150	-1.398067	0.591520
15	6	0	2.595619	-0.372410	-0.249968
16	6	0	1.843864	0.858519	-0.194987
17	1	0	0.073123	0.134870	2.705856
18	1	0	1.078314	-2.070663	2.273372
19	1	0	2.809853	-2.346384	0.505671
20	1	0	3.316238	-0.511829	-1.046523
21	1	0	2.331378	1.735284	-0.607820
22	7	0	0.879206	2.377719	1.369232
23	1	0	0.343980	2.437010	2.239221
24	16	0	0.151003	-2.002064	-1.391871
25	8	0	-2.076434	-1.211836	0.375158
26	6	0	-3.238743	-0.990610	1.158412
27	1	0	-4.052986	-0.576862	0.554049
28	1	0	-3.529060	-1.967788	1.539076
29	1	0	-3.030256	-0.317054	1.997326



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.320929	0.335526	-0.415388

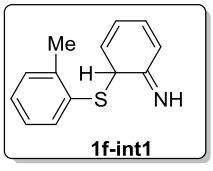
2	6	0	-3.226624	-0.262672	-1.029317
3	6	0	-2.009029	-0.377721	-0.344972
4	6	0	-1.908360	0.113297	0.960588
5	6	0	-3.013926	0.702884	1.566388
6	6	0	-4.224968	0.821601	0.887904
7	1	0	-5.255529	0.415510	-0.958768
8	1	0	-3.311765	-0.644960	-2.041521
9	1	0	-0.969406	0.031203	1.492068
10	1	0	-2.921395	1.078024	2.579241
11	1	0	-5.079889	1.284034	1.365548
12	7	0	-0.908339	-0.943065	-1.007423
13	1	0	-1.066685	-1.276339	-1.945737
14	6	0	1.586367	-0.174506	-0.223419
15	6	0	2.857328	-0.376580	0.342561
16	6	0	1.215476	1.068073	-0.732296
17	6	0	3.737460	0.706487	0.372616
18	6	0	2.113478	2.131085	-0.687675
19	1	0	0.229416	1.197233	-1.158072
20	6	0	3.378378	1.953068	-0.134989
21	1	0	4.722861	0.563909	0.803763
22	1	0	1.818998	3.096275	-1.083188
23	1	0	4.081139	2.776853	-0.097106
24	16	0	0.460354	-1.577043	-0.236404
25	6	0	3.258603	-1.718721	0.896785
26	1	0	2.595403	-2.030886	1.710630
27	1	0	3.212885	-2.498219	0.128794
28	1	0	4.277145	-1.689421	1.286066



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.526432	-1.881435	-0.201587

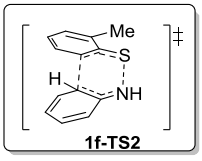
2	6	0	2.203419	-1.527029	-0.408410
3	6	0	1.754978	-0.202832	-0.196174
4	6	0	2.689235	0.783409	0.234353
5	6	0	4.014399	0.400941	0.433115
6	6	0	4.436702	-0.911563	0.221123
7	1	0	3.851109	-2.901680	-0.369056
8	1	0	1.479167	-2.260991	-0.739555
9	1	0	4.733363	1.144359	0.760199
10	1	0	5.475471	-1.174757	0.385149
11	16	0	0.075259	0.173203	-0.467480
12	6	0	-2.373954	0.901082	0.672420
13	6	0	-2.654380	0.598064	-0.712731
14	6	0	-2.938591	0.135344	1.690944
15	6	0	-3.461679	-0.562312	-0.987237
16	6	0	-3.739927	-0.952241	1.380342
17	1	0	-2.745996	0.391262	2.725896
18	6	0	-3.995265	-1.301855	0.032397
19	1	0	-3.629348	-0.810749	-2.027574
20	1	0	-4.175853	-1.545010	2.176081
21	1	0	-4.613680	-2.164629	-0.185272
22	7	0	-2.146625	1.263142	-1.733767
23	1	0	-1.810260	1.794726	0.902029
24	6	0	2.271837	2.207755	0.473075
25	1	0	1.857002	2.652681	-0.434757
26	1	0	1.488011	2.264195	1.232787
27	1	0	3.121360	2.809403	0.801034
28	1	0	-1.607351	2.063984	-1.400684



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.299537	0.934865	-0.010700
2	6	0	2.023867	0.803407	0.548820
3	6	0	1.370715	-0.435051	0.407949
4	6	0	1.990739	-1.493073	-0.263023

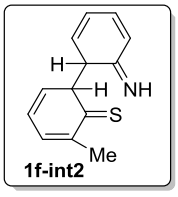
5	6	0	3.254142	-1.334663	-0.822907
6	6	0	3.910259	-0.113124	-0.693848
7	1	0	3.818745	1.881986	0.089120
8	1	0	1.473981	-2.442598	-0.337150
9	1	0	3.724318	-2.160132	-1.344275
10	1	0	4.897587	0.023622	-1.119753
11	16	0	-0.263671	-0.699096	1.100552
12	6	0	-1.296464	-0.692083	-0.488724
13	6	0	-2.730333	-0.796030	-0.011167
14	6	0	-0.979146	0.545865	-1.256646
15	6	0	-3.463560	0.462513	0.133625
16	6	0	-1.787835	1.617124	-1.223391
17	1	0	-0.041700	0.567614	-1.798413
18	6	0	-3.025970	1.590057	-0.463311
19	1	0	-4.408407	0.438962	0.666583
20	1	0	-1.521458	2.523960	-1.753706
21	1	0	-3.612880	2.499798	-0.397498
22	7	0	-3.194217	-1.964205	0.235755
23	1	0	-4.149079	-1.903352	0.597386
24	1	0	-1.027953	-1.601210	-1.023487
25	6	0	1.392314	1.964023	1.272193
26	1	0	0.411262	2.199450	0.855343
27	1	0	1.236912	1.734831	2.329683
28	1	0	2.027328	2.849064	1.203835



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.374777	0.108826	0.196112
2	6	0	-1.198128	-0.324768	-0.525647
3	6	0	-0.143337	0.666672	-0.765815
4	6	0	-0.527512	2.072375	-0.739727
5	6	0	-1.694559	2.442731	-0.162225
6	6	0	-2.586626	1.452802	0.361065
7	1	0	0.564239	0.380207	-1.537084
8	1	0	0.162886	2.807261	-1.134694

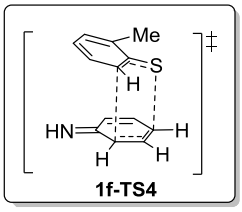
9	1	0	-1.971862	3.488596	-0.097469
10	1	0	-3.488652	1.784631	0.864670
11	6	0	1.440485	-0.916904	0.680109
12	6	0	2.674536	-1.192248	-0.026379
13	6	0	3.527788	-0.189787	-0.347282
14	6	0	3.230109	1.175759	0.009510
15	6	0	2.038894	1.501025	0.560810
16	6	0	0.997435	0.488678	0.735457
17	1	0	2.899481	-2.230744	-0.234141
18	1	0	4.466081	-0.409674	-0.843574
19	1	0	3.981182	1.939104	-0.158386
20	1	0	1.812147	2.525766	0.827707
21	1	0	0.266778	0.701535	1.511263
22	7	0	0.738232	-1.921231	1.123395
23	16	0	-0.928583	-1.924139	-0.937566
24	6	0	-3.383335	-0.895601	0.677404
25	1	0	-3.847451	-1.416706	-0.163811
26	1	0	-2.911116	-1.668846	1.288855
27	1	0	-4.165062	-0.406735	1.261366
28	1	0	-0.084795	-1.596914	1.632222



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.744479	2.416518	-0.135875
2	6	0	-0.552135	2.097903	-0.665382
3	6	0	-0.074223	0.682652	-0.644298
4	6	0	-1.176063	-0.337929	-0.514283
5	6	0	-2.353412	0.054740	0.243758
6	6	0	-2.601030	1.385373	0.404766
7	1	0	-2.080497	3.446442	-0.099581
8	1	0	0.114873	2.857751	-1.053430
9	1	0	-3.505709	1.691340	0.920659
10	16	0	-0.992818	-1.845607	-1.160723
11	6	0	0.931954	0.543392	0.637759

12	6	0	1.420641	-0.879964	0.759042
13	6	0	2.050099	1.523226	0.444793
14	6	0	2.613640	-1.225101	-0.016817
15	6	0	3.227636	1.137012	-0.071317
16	1	0	1.860822	2.563386	0.680696
17	6	0	3.476959	-0.260612	-0.393529
18	1	0	2.814064	-2.273707	-0.207852
19	1	0	4.014197	1.860715	-0.252228
20	1	0	4.393127	-0.519244	-0.913070
21	1	0	0.325757	0.780778	1.512168
22	7	0	0.766893	-1.682319	1.513576
23	1	0	1.160635	-2.625770	1.468596
24	1	0	0.537724	0.446449	-1.514677
25	6	0	-3.302816	-0.990790	0.751404
26	1	0	-3.763124	-1.537371	-0.075045
27	1	0	-2.766065	-1.727517	1.354396
28	1	0	-4.089597	-0.535822	1.355783

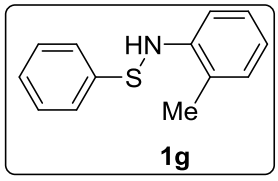


1f-TS4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.483318	-0.133048	-1.483531
2	6	0	0.214604	1.021329	-0.606641
3	6	0	1.117873	1.236764	0.503586
4	6	0	2.306113	0.552601	0.522752
5	6	0	2.680137	-0.379502	-0.493329
6	6	0	1.820169	-0.680278	-1.498714
7	1	0	-0.018234	-0.069714	-2.442964
8	1	0	3.008365	0.747259	1.326891
9	1	0	3.663564	-0.832212	-0.456653
10	1	0	2.085713	-1.397068	-2.266295
11	6	0	-0.088012	-1.709569	0.631040
12	6	0	-0.773438	-0.925521	1.653905
13	6	0	-1.971442	-0.351606	1.397723

14	6	0	-2.586983	-0.462773	0.096583
15	6	0	-1.948925	-1.103324	-0.919903
16	6	0	-0.583277	-1.536680	-0.762362
17	1	0	-0.325225	-0.875946	2.640419
18	1	0	-2.494755	0.193691	2.174347
19	1	0	-3.588497	-0.075837	-0.043960
20	1	0	-2.416660	-1.186622	-1.893286
21	1	0	-0.248227	-2.325811	-1.426386
22	7	0	0.905980	-2.502403	0.828186
23	1	0	1.180714	-2.492832	1.813667
24	16	0	-1.132665	1.965025	-0.885819
25	6	0	0.798233	2.267806	1.546119
26	1	0	0.790086	3.271600	1.113310
27	1	0	-0.199057	2.102736	1.960207
28	1	0	1.532764	2.239990	2.353139

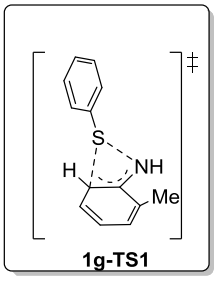


1g

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.574434	0.774318	0.416236
2	6	0	2.675820	-0.270780	0.626289
3	6	0	1.549611	-0.364620	-0.217726
4	6	0	1.353676	0.576423	-1.231350
5	6	0	2.271125	1.604506	-1.420556
6	6	0	3.387512	1.712075	-0.597023
7	1	0	4.442085	0.848359	1.063612
8	1	0	0.480610	0.497585	-1.865563
9	1	0	2.103809	2.325381	-2.212408
10	1	0	4.102562	2.513345	-0.737866
11	7	0	0.644997	-1.422378	-0.011512
12	1	0	0.733016	-1.938864	0.848693
13	6	0	-1.927099	-0.453316	-0.155117
14	6	0	-3.220139	-0.414962	-0.685323
15	6	0	-1.564189	0.420580	0.868278
16	6	0	-4.146716	0.492970	-0.183297
17	1	0	-3.502052	-1.092031	-1.484922
18	6	0	-2.499679	1.328419	1.361395

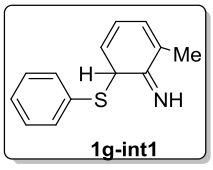
19	1	0	-0.559813	0.401763	1.269506
20	6	0	-3.791167	1.369106	0.842058
21	1	0	-5.148916	0.515749	-0.595663
22	1	0	-2.211200	2.009457	2.153929
23	1	0	-4.513635	2.077358	1.229313
24	16	0	-0.795912	-1.659557	-0.857763
25	6	0	2.902759	-1.277769	1.723720
26	1	0	2.093489	-1.268728	2.464831
27	1	0	2.974104	-2.297537	1.329136
28	1	0	3.829857	-1.063966	2.256688



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.961283	0.931367	1.223804
2	6	0	-2.613360	0.912034	0.893950
3	6	0	-2.133932	0.068291	-0.132172
4	6	0	-3.060778	-0.750107	-0.814700
5	6	0	-4.407941	-0.724126	-0.483059
6	6	0	-4.862842	0.115149	0.536896
7	1	0	-4.315124	1.583326	2.014280
8	1	0	-1.906136	1.543481	1.417447
9	1	0	-2.698363	-1.398065	-1.603280
10	1	0	-5.108483	-1.356535	-1.016395
11	1	0	-5.915493	0.133441	0.794503
12	16	0	-0.436053	0.040953	-0.540461
13	6	0	1.976500	-1.433377	-0.496076
14	6	0	2.294429	-0.069200	-0.855137
15	6	0	2.448255	-1.987608	0.686490
16	6	0	3.007834	0.745895	0.115261
17	6	0	3.184032	-1.200856	1.562420
18	1	0	2.235587	-3.022427	0.925139
19	6	0	3.444188	0.156072	1.278398

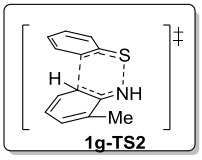
20	1	0	3.555462	-1.627918	2.487037
21	1	0	3.992988	0.749503	2.001253
22	7	0	1.894120	0.500244	-1.972238
23	1	0	1.450163	-2.039920	-1.220945
24	6	0	3.223837	2.194836	-0.180068
25	1	0	3.749862	2.327782	-1.128298
26	1	0	2.257826	2.695769	-0.295823
27	1	0	3.787574	2.678750	0.618804
28	1	0	1.398505	-0.174354	-2.556724



Standard orientation:

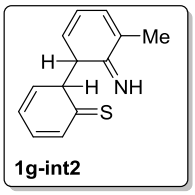
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.679334	1.180838	0.570439
2	6	0	2.376063	0.847753	0.934652
3	6	0	1.800486	-0.336401	0.467139
4	6	0	2.537911	-1.184600	-0.364996
5	6	0	3.833954	-0.840288	-0.738827
6	6	0	4.407478	0.341513	-0.270193
7	1	0	4.122382	2.099082	0.938558
8	1	0	1.796524	1.501814	1.573907
9	1	0	2.093962	-2.110927	-0.709468
10	1	0	4.399992	-1.499791	-1.386563
11	1	0	5.419150	0.604294	-0.556567
12	16	0	0.135359	-0.779215	0.954474
13	6	0	-0.782728	-0.421320	-0.666986
14	6	0	-2.228893	-0.758880	-0.365533
15	6	0	-0.527749	0.993020	-1.050346
16	6	0	-3.101077	0.348631	0.072040
17	6	0	-1.436168	1.946453	-0.792515
18	1	0	0.435065	1.231606	-1.484335
19	6	0	-2.702900	1.619787	-0.164853
20	1	0	-1.229964	2.983276	-1.031988
21	1	0	-3.361863	2.438954	0.106049
22	7	0	-2.577521	-1.984554	-0.494146
23	1	0	-3.549487	-2.124990	-0.215607
24	1	0	-0.395017	-1.137526	-1.388746

25	6	0	-4.436905	0.023771	0.676372
26	1	0	-5.093758	-0.480330	-0.041319
27	1	0	-4.330030	-0.640238	1.540321
28	1	0	-4.942893	0.932428	1.004841



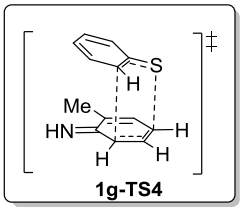
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.663981	-0.890133	0.365129
2	6	0	-1.417819	-0.878128	-0.344357
3	6	0	-0.863448	0.434101	-0.694832
4	6	0	-1.802789	1.550888	-0.749087
5	6	0	-3.022185	1.459798	-0.165229
6	6	0	-3.435042	0.233235	0.451581
7	1	0	-3.007597	-1.835435	0.767119
8	1	0	-0.110252	0.408783	-1.475988
9	1	0	-1.477204	2.472431	-1.215891
10	1	0	-3.699294	2.305945	-0.169862
11	1	0	-4.395142	0.191420	0.953626
12	6	0	1.234771	-0.247081	0.778242
13	6	0	2.458936	-0.098940	-0.006400
14	6	0	2.805740	1.142127	-0.441443
15	6	0	2.010057	2.305650	-0.146699
16	6	0	0.805278	2.190139	0.455877
17	6	0	0.266665	0.866025	0.755549
18	1	0	3.728422	1.272929	-0.996835
19	1	0	2.396575	3.283166	-0.412517
20	1	0	0.198297	3.061453	0.667459
21	1	0	-0.470310	0.830344	1.553544
22	7	0	0.996155	-1.391999	1.347796
23	16	0	-0.547310	-2.279371	-0.627441
24	6	0	3.292711	-1.316654	-0.257332
25	1	0	3.613575	-1.767026	0.685121
26	1	0	2.699769	-2.076142	-0.774773
27	1	0	4.171037	-1.072365	-0.856993
28	1	0	0.122632	-1.367754	1.874478



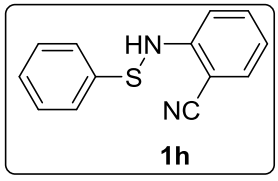
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.058471	1.404587	-0.142673
2	6	0	-1.827223	1.557519	-0.660090
3	6	0	-0.801157	0.474694	-0.555425
4	6	0	-1.378941	-0.892983	-0.296581
5	6	0	-2.638540	-0.944788	0.399611
6	6	0	-3.439994	0.149762	0.467040
7	1	0	-3.779705	2.212638	-0.178587
8	1	0	-1.524184	2.495087	-1.109946
9	1	0	-2.961116	-1.902558	0.787606
10	1	0	-4.410702	0.076094	0.945249
11	16	0	-0.588908	-2.265350	-0.768747
12	6	0	0.202711	0.890231	0.667579
13	6	0	1.241251	-0.188857	0.858463
14	6	0	0.807451	2.216596	0.324808
15	6	0	2.423031	-0.135043	-0.027944
16	6	0	2.006348	2.274841	-0.275080
17	1	0	0.230919	3.113178	0.516634
18	6	0	2.766816	1.065225	-0.547148
19	1	0	2.429826	3.228377	-0.570325
20	1	0	3.661154	1.148109	-1.156792
21	1	0	-0.417635	0.934573	1.562540
22	7	0	1.013566	-1.076325	1.751566
23	1	0	1.740970	-1.793377	1.761309
24	1	0	-0.161521	0.439501	-1.437975
25	6	0	3.230400	-1.380369	-0.243510
26	1	0	3.705980	-1.720259	0.683154
27	1	0	2.590804	-2.192241	-0.602875
28	1	0	4.020690	-1.207732	-0.975297



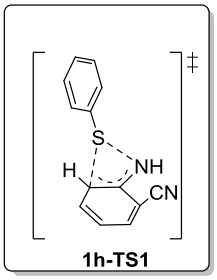
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.603184	1.285002	0.907606
2	6	0	-0.105767	1.381192	-0.476130
3	6	0	-0.905016	0.755216	-1.489535
4	6	0	-2.185604	0.359423	-1.225818
5	6	0	-2.760474	0.522338	0.074954
6	6	0	-2.013786	1.015768	1.095541
7	1	0	-0.165339	2.014891	1.579844
8	1	0	-0.490040	0.686558	-2.487270
9	1	0	-2.794265	-0.056712	-2.021048
10	1	0	-3.800205	0.262638	0.231824
11	1	0	-2.437632	1.131908	2.085836
12	6	0	-0.166565	-1.375197	0.756454
13	6	0	0.673380	-1.686575	-0.412998
14	6	0	1.925014	-1.165722	-0.470554
15	6	0	2.449982	-0.301778	0.556213
16	6	0	1.677051	0.083795	1.606830
17	6	0	0.274986	-0.240933	1.616731
18	1	0	2.566675	-1.408241	-1.310623
19	1	0	3.490198	-0.004791	0.504397
20	1	0	2.075234	0.735755	2.374463
21	1	0	-0.213321	-0.246934	2.585170
22	7	0	-1.259450	-1.969778	1.081091
23	1	0	-1.502299	-2.693157	0.402653
24	16	0	1.348895	2.127023	-0.804861
25	6	0	0.151164	-2.634816	-1.450756
26	1	0	0.016623	-3.643234	-1.043919
27	1	0	-0.820663	-2.303409	-1.830581
28	1	0	0.841778	-2.705480	-2.291842



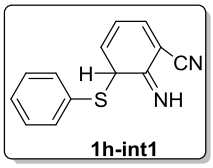
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.532226	-0.812258	0.559957
2	6	0	-2.641902	0.241329	0.309956
3	6	0	-1.442411	0.012713	-0.407264
4	6	0	-1.168039	-1.287459	-0.847768
5	6	0	-2.062873	-2.317133	-0.593438
6	6	0	-3.249249	-2.091452	0.109015
7	1	0	-4.441288	-0.604646	1.110297
8	1	0	-0.250350	-1.476133	-1.387795
9	1	0	-1.827463	-3.314523	-0.946107
10	1	0	-3.938019	-2.903320	0.303151
11	7	0	-0.574989	1.072957	-0.632187
12	1	0	-0.820403	1.972393	-0.242330
13	6	0	2.044100	0.346221	-0.344866
14	6	0	3.322546	0.059558	-0.830629
15	6	0	1.734471	0.125597	0.995280
16	6	0	4.291536	-0.440499	0.033404
17	1	0	3.560488	0.224911	-1.876145
18	6	0	2.711497	-0.381746	1.849784
19	1	0	0.743185	0.346202	1.368253
20	6	0	3.990234	-0.664780	1.376347
21	1	0	5.283073	-0.658444	-0.346078
22	1	0	2.467143	-0.554160	2.891597
23	1	0	4.745469	-1.057828	2.046047
24	16	0	0.858341	0.997281	-1.527133
25	6	0	-2.923289	1.555638	0.779765
26	7	0	-3.096676	2.640571	1.143041



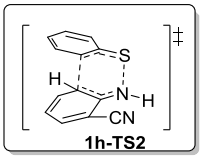
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.026372	0.920321	1.337998
2	6	0	-2.682753	0.834289	1.005945
3	6	0	-2.267832	0.093286	-0.124560
4	6	0	-3.251721	-0.552502	-0.908071
5	6	0	-4.593315	-0.461095	-0.570676
6	6	0	-4.983935	0.274111	0.552055
7	1	0	-4.334135	1.491829	2.205778
8	1	0	-1.929755	1.334105	1.602379
9	1	0	-2.936000	-1.117371	-1.776395
10	1	0	-5.340111	-0.958608	-1.178362
11	1	0	-6.033588	0.344661	0.812654
12	16	0	-0.580712	-0.012643	-0.534972
13	6	0	1.703941	-1.572929	-0.643326
14	6	0	2.143161	-0.216466	-0.870112
15	6	0	2.106589	-2.280290	0.488170
16	6	0	2.947289	0.391932	0.175097
17	6	0	2.906594	-1.672167	1.442454
18	1	0	1.788760	-3.307596	0.618651
19	6	0	3.320553	-0.334266	1.285921
20	1	0	3.219307	-2.222734	2.321149
21	1	0	3.934105	0.133735	2.045281
22	7	0	1.777231	0.519770	-1.896068
23	1	0	1.148178	-2.064976	-1.429308
24	6	0	3.357718	1.749658	0.041727
25	7	0	3.717782	2.845978	-0.015657
26	1	0	1.230036	-0.034284	-2.555926



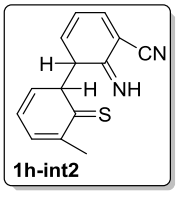
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.926667	1.121770	0.603317
2	6	0	2.605810	0.843261	0.949367
3	6	0	1.993402	-0.321779	0.480782
4	6	0	2.709048	-1.207106	-0.331292
5	6	0	4.023063	-0.916118	-0.686669
6	6	0	4.634007	0.247061	-0.218732
7	1	0	4.399993	2.024267	0.972227
8	1	0	2.044086	1.523326	1.577431
9	1	0	2.236566	-2.120393	-0.672667
10	1	0	4.573839	-1.603498	-1.318099
11	1	0	5.659641	0.467437	-0.490379
12	16	0	0.306513	-0.698521	0.950825
13	6	0	-0.564642	-0.352114	-0.694821
14	6	0	-2.010433	-0.737201	-0.472107
15	6	0	-0.331802	1.077848	-1.031247
16	6	0	-2.909704	0.363409	-0.056773
17	6	0	-1.265423	2.018618	-0.799101
18	1	0	0.645938	1.344689	-1.413014
19	6	0	-2.550084	1.660477	-0.249686
20	1	0	-1.061410	3.063110	-0.999331
21	1	0	-3.252219	2.447262	0.000260
22	7	0	-2.342679	-1.955441	-0.645590
23	1	0	-3.326394	-2.116334	-0.416120
24	1	0	-0.124440	-1.037510	-1.416097
25	6	0	-4.199381	0.022600	0.440802
26	7	0	-5.237746	-0.293183	0.839811



Standard orientation:

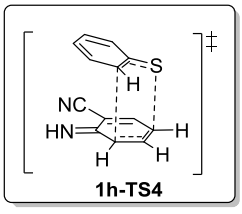
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.681743	-1.168995	0.364596
2	6	0	-1.444352	-1.002675	-0.341333
3	6	0	-1.066518	0.368599	-0.709918
4	6	0	-2.146893	1.349763	-0.789821
5	6	0	-3.345367	1.104260	-0.208319
6	6	0	-3.594390	-0.156189	0.429805
7	1	0	-2.899377	-2.145055	0.780628
8	1	0	-0.314662	0.427951	-1.490632
9	1	0	-1.948417	2.296279	-1.277836
10	1	0	-4.131717	1.849473	-0.233578
11	1	0	-4.543484	-0.316188	0.928688
12	6	0	1.074411	-0.029703	0.814007
13	6	0	2.284913	0.296884	0.063855
14	6	0	2.497547	1.567444	-0.387764
15	6	0	1.541762	2.608609	-0.140600
16	6	0	0.348721	2.327862	0.432834
17	6	0	-0.025243	0.948408	0.741844
18	1	0	3.417633	1.801050	-0.908963
19	1	0	1.796039	3.625408	-0.414243
20	1	0	-0.375109	3.112043	0.616684
21	1	0	-0.764949	0.837339	1.530064
22	7	0	0.984220	-1.195026	1.378045
23	16	0	-0.385484	-2.269577	-0.597803
24	6	0	3.270622	-0.714497	-0.137414
25	7	0	4.092963	-1.502502	-0.328385
26	1	0	0.110671	-1.290986	1.895796



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.374116	1.036425	-0.168131
2	6	0	-2.175611	1.353336	-0.686230

3	6	0	-1.010595	0.420515	-0.566298
4	6	0	-1.397448	-1.013980	-0.295719
5	6	0	-2.641171	-1.229156	0.399746
6	6	0	-3.582685	-0.252799	0.456619
7	1	0	-4.201377	1.734591	-0.218887
8	1	0	-2.007897	2.315434	-1.155138
9	1	0	-2.831219	-2.218034	0.797067
10	1	0	-4.535599	-0.451834	0.934480
11	16	0	-0.416351	-2.258404	-0.749804
12	6	0	-0.080815	0.965250	0.659375
13	6	0	1.088173	0.037855	0.877945
14	6	0	0.345251	2.357840	0.313723
15	6	0	2.262020	0.281180	0.007006
16	6	0	1.531227	2.595060	-0.273769
17	1	0	-0.354887	3.164788	0.492217
18	6	0	2.465817	1.517408	-0.516891
19	1	0	1.811049	3.597479	-0.574564
20	1	0	3.362455	1.715014	-1.092374
21	1	0	-0.710240	0.938184	1.548814
22	7	0	0.992864	-0.871968	1.765125
23	1	0	1.817022	-1.478486	1.779988
24	1	0	-0.371646	0.462417	-1.449065
25	6	0	3.216627	-0.762398	-0.152399
26	7	0	3.979123	-1.625790	-0.250203

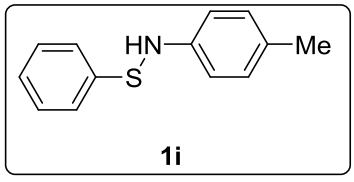


1h-TS4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.290574	1.127278	0.598768
2	6	0	1.185124	0.584989	-0.770427
3	6	0	0.067316	1.029337	-1.552282
4	6	0	-0.684946	2.096717	-1.153063
5	6	0	-0.398822	2.794521	0.063654
6	6	0	0.589481	2.360588	0.887459
7	1	0	2.278619	1.026036	1.034502

8	1	0	-0.116243	0.538581	-2.499463
9	1	0	-1.501035	2.440198	-1.777993
10	1	0	-0.968384	3.681651	0.311382
11	1	0	0.806400	2.877808	1.814333
12	6	0	-0.974075	-0.229384	1.144338
13	6	0	-1.183654	-1.225857	0.074168
14	6	0	-0.277477	-2.223874	-0.130326
15	6	0	0.919267	-2.310991	0.657837
16	6	0	1.211740	-1.357417	1.584884
17	6	0	0.412168	-0.163020	1.679900
18	1	0	-0.463405	-2.970491	-0.892026
19	1	0	1.561184	-3.173423	0.533580
20	1	0	2.115834	-1.431152	2.176704
21	1	0	0.461577	0.373201	2.620979
22	7	0	-1.847882	0.583943	1.607371
23	1	0	-2.744976	0.485159	1.125600
24	16	0	2.278531	-0.545368	-1.321798
25	6	0	-2.385277	-1.146735	-0.682582
26	7	0	-3.368488	-1.032312	-1.280627

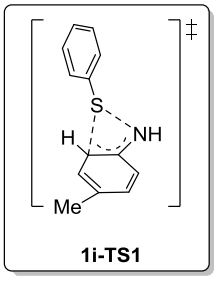


1i

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.651402	-0.277590	0.795725
2	6	0	2.489288	-0.998187	1.042117
3	6	0	1.341420	-0.774244	0.272347
4	6	0	1.388939	0.177866	-0.747955
5	6	0	2.564722	0.883871	-0.985949
6	6	0	3.715678	0.679254	-0.222149
7	1	0	4.529113	-0.471817	1.403690
8	1	0	2.470891	-1.742509	1.831986
9	1	0	0.510991	0.358799	-1.354439
10	1	0	2.580772	1.615476	-1.787130
11	7	0	0.163365	-1.479958	0.576475
12	1	0	0.224880	-2.155078	1.323033
13	6	0	-2.232909	-0.381552	-0.108927

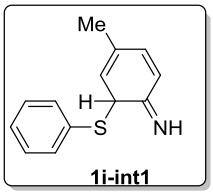
14	6	0	-3.443582	-0.334488	-0.805776
15	6	0	-1.926573	0.597488	0.834059
16	6	0	-4.345857	0.693857	-0.552595
17	1	0	-3.681502	-1.097292	-1.539757
18	6	0	-2.838161	1.622592	1.079150
19	1	0	-0.985668	0.553664	1.366351
20	6	0	-4.047855	1.677082	0.390540
21	1	0	-5.284861	0.724878	-1.093237
22	1	0	-2.596181	2.383758	1.812209
23	1	0	-4.751931	2.477059	0.585353
24	16	0	-1.113192	-1.724702	-0.509474
25	6	0	4.973361	1.475240	-0.465658
26	1	0	5.046246	2.324074	0.223092
27	1	0	5.866870	0.862197	-0.322608
28	1	0	4.998673	1.874598	-1.481865



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.042115	1.200841	1.080856
2	6	0	2.737904	0.726249	1.094636
3	6	0	2.262123	-0.106086	0.057678
4	6	0	3.147888	-0.445271	-0.988573
5	6	0	4.451627	0.030156	-0.996036
6	6	0	4.903268	0.854848	0.037111
7	1	0	4.393443	1.839139	1.883553
8	1	0	2.062976	0.984725	1.901217
9	1	0	2.788951	-1.085367	-1.785145
10	1	0	5.120823	-0.239436	-1.805181
11	1	0	5.921969	1.224948	0.029255
12	16	0	0.618613	-0.697636	0.076716
13	6	0	-1.945876	-0.643638	-1.089166
14	6	0	-2.067876	-1.413776	0.126132
15	6	0	-2.648797	0.546305	-1.246467

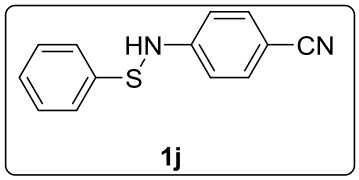
16	6	0	-2.875157	-0.851386	1.178432
17	6	0	-3.446981	1.049301	-0.224283
18	1	0	-2.566703	1.094788	-2.178006
19	6	0	-3.542876	0.324664	0.997400
20	1	0	-2.931344	-1.405945	2.106694
21	1	0	-4.156591	0.727964	1.795912
22	7	0	-1.428423	-2.542486	0.361779
23	1	0	-1.379615	-1.059561	-1.911006
24	6	0	-4.195569	2.340093	-0.379282
25	1	0	-5.265742	2.196059	-0.199253
26	1	0	-3.846795	3.077209	0.352209
27	1	0	-4.067947	2.763482	-1.376193
28	1	0	-0.903027	-2.832215	-0.464608



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.316439	1.153680	0.656618
2	6	0	2.084683	0.617001	1.026001
3	6	0	1.619871	-0.551876	0.417603
4	6	0	2.397095	-1.180304	-0.560254
5	6	0	3.621011	-0.633225	-0.936338
6	6	0	4.083299	0.533236	-0.327654
7	1	0	3.673827	2.058841	1.134116
8	1	0	1.474431	1.099974	1.778730
9	1	0	2.040118	-2.095721	-1.016697
10	1	0	4.218109	-1.122961	-1.696964
11	1	0	5.039220	0.953986	-0.617079
12	16	0	0.044493	-1.251575	0.901905
13	6	0	-1.016077	-0.717045	-0.581240
14	6	0	-2.412712	-1.182174	-0.231765
15	6	0	-0.873067	0.752985	-0.770752
16	6	0	-3.279830	-0.191107	0.405988
17	6	0	-1.786078	1.628703	-0.314808
18	1	0	0.039130	1.102998	-1.239216

19	6	0	-2.987499	1.122427	0.344117
20	1	0	-4.199833	-0.540666	0.863122
21	1	0	-3.671953	1.846085	0.776448
22	7	0	-2.733308	-2.391204	-0.507191
23	1	0	-3.680794	-2.595255	-0.180038
24	1	0	-0.646943	-1.291730	-1.428521
25	6	0	-1.619847	3.118063	-0.437691
26	1	0	-2.451092	3.562912	-0.994534
27	1	0	-1.606322	3.590492	0.550558
28	1	0	-0.690364	3.372498	-0.949016

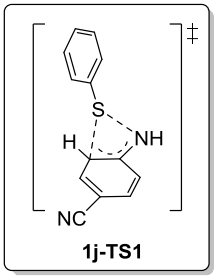


1j

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.289035	-0.456015	0.965088
2	6	0	2.109076	-1.152218	1.155381
3	6	0	1.038866	-1.000264	0.257843
4	6	0	1.178891	-0.132729	-0.833842
5	6	0	2.363487	0.559697	-1.023849
6	6	0	3.432718	0.410315	-0.129493
7	1	0	4.109488	-0.580079	1.660509
8	1	0	2.009650	-1.823228	2.001635
9	1	0	0.356871	-0.006381	-1.525125
10	1	0	2.465354	1.228933	-1.868819
11	7	0	-0.140292	-1.701575	0.495025
12	1	0	-0.189792	-2.257106	1.335241
13	6	0	-2.412004	-0.304756	-0.116404
14	6	0	-3.598663	-0.091546	-0.822916
15	6	0	-1.996345	0.605606	0.852641
16	6	0	-4.369175	1.034315	-0.550952
17	1	0	-3.920318	-0.799708	-1.579290
18	6	0	-2.775766	1.731076	1.114686
19	1	0	-1.074416	0.441058	1.394132
20	6	0	-3.961308	1.950539	0.418062
21	1	0	-5.290306	1.195060	-1.098906
22	1	0	-2.448506	2.439413	1.866997

23	1	0	-4.561974	2.827640	0.625834
24	16	0	-1.474784	-1.777717	-0.540812
25	6	0	4.648197	1.129517	-0.326144
26	7	0	5.634353	1.712523	-0.483573

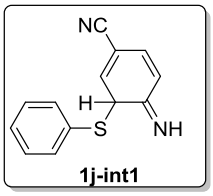


1j-TS1

Standard orientation:

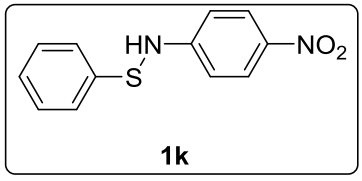
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.048638	1.350312	1.119694
2	6	0	2.788975	0.771113	1.108634
3	6	0	2.395756	-0.074621	0.045429
4	6	0	3.316322	-0.318820	-1.000026
5	6	0	4.575088	0.261404	-0.980643
6	6	0	4.944100	1.097159	0.077282
7	1	0	4.339662	1.998230	1.938127
8	1	0	2.085505	0.955597	1.910878
9	1	0	3.017730	-0.967792	-1.813890
10	1	0	5.273724	0.067554	-1.786097
11	1	0	5.928660	1.550047	0.089182
12	16	0	0.812896	-0.793485	0.032325
13	6	0	-1.723065	-0.870301	-1.098802
14	6	0	-1.804199	-1.693422	0.086580
15	6	0	-2.460375	0.303514	-1.200241
16	6	0	-2.619704	-1.211998	1.172111
17	6	0	-3.258558	0.718127	-0.135009
18	1	0	-2.416101	0.901210	-2.101581
19	6	0	-3.330651	-0.053608	1.061113
20	1	0	-2.646242	-1.811014	2.073240
21	1	0	-3.950978	0.299210	1.875059
22	7	0	-1.104844	-2.795820	0.271286
23	1	0	-1.162518	-1.234555	-1.948357
24	6	0	-4.008722	1.924315	-0.236935
25	7	0	-4.619864	2.903317	-0.313326

26	1	0	-0.584442	-3.034246	-0.574608



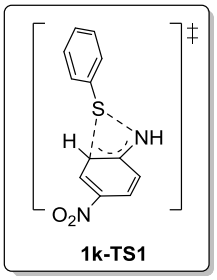
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.335186	1.344341	0.539902
2	6	0	2.139181	0.756660	0.946530
3	6	0	1.764923	-0.487744	0.432805
4	6	0	2.593497	-1.143219	-0.482993
5	6	0	3.782334	-0.546320	-0.893584
6	6	0	4.154517	0.696650	-0.382502
7	1	0	3.622351	2.309733	0.939706
8	1	0	1.490877	1.257723	1.654388
9	1	0	2.305821	-2.116271	-0.862732
10	1	0	4.421776	-1.055517	-1.605150
11	1	0	5.082342	1.157343	-0.700550
12	16	0	0.237393	-1.256942	0.966824
13	6	0	-0.844841	-0.902234	-0.548493
14	6	0	-2.166861	-1.585443	-0.271688
15	6	0	-0.916577	0.573763	-0.688629
16	6	0	-3.205397	-0.765164	0.355102
17	6	0	-1.983565	1.268328	-0.235843
18	1	0	-0.058437	1.087503	-1.101869
19	6	0	-3.130679	0.578427	0.350990
20	1	0	-4.077025	-1.270079	0.757316
21	1	0	-3.929169	1.181116	0.766231
22	7	0	-2.279908	-2.817278	-0.595984
23	1	0	-3.193658	-3.184475	-0.320255
24	1	0	-0.352270	-1.386017	-1.389264
25	6	0	-2.003047	2.695576	-0.298663
26	7	0	-2.037653	3.849892	-0.338961



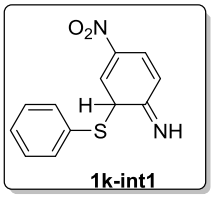
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.874911	0.744091	0.972216
2	6	0	-1.664626	1.399390	1.101368
3	6	0	-0.614578	1.144152	0.199963
4	6	0	-0.804896	0.214314	-0.833813
5	6	0	-2.018426	-0.439322	-0.965119
6	6	0	-3.045384	-0.173302	-0.063249
7	1	0	-3.690166	0.932022	1.656513
8	1	0	-1.523618	2.118453	1.900658
9	1	0	0.001523	0.010284	-1.524512
10	1	0	-2.180026	-1.158891	-1.755349
11	7	0	0.592037	1.808652	0.376648
12	1	0	0.675680	2.415517	1.178034
13	6	0	2.792945	0.263709	-0.130296
14	6	0	3.969629	-0.051868	-0.814754
15	6	0	2.335516	-0.555392	0.899355
16	6	0	4.688112	-1.189039	-0.460172
17	1	0	4.323984	0.585603	-1.617901
18	6	0	3.063447	-1.692973	1.244290
19	1	0	1.421684	-0.312635	1.424749
20	6	0	4.238400	-2.014484	0.569918
21	1	0	5.601541	-1.429603	-0.991456
22	1	0	2.703921	-2.330310	2.043824
23	1	0	4.798720	-2.900570	0.842127
24	16	0	1.925288	1.743660	-0.664355
25	7	0	-4.323835	-0.870106	-0.201093
26	8	0	-5.205532	-0.617328	0.615725
27	8	0	-4.445296	-1.669409	-1.124991



Standard orientation:

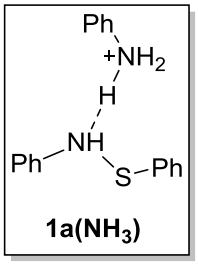
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.250189	-1.455740	1.189202
2	6	0	-3.035660	-0.789133	1.147681
3	6	0	-2.711532	0.045952	0.052377
4	6	0	-3.653914	0.188518	-0.993301
5	6	0	-4.867335	-0.478819	-0.942900
6	6	0	-5.167850	-1.302071	0.146374
7	1	0	-4.489225	-2.094774	2.030991
8	1	0	-2.315151	-0.895389	1.948935
9	1	0	-3.407262	0.828603	-1.831173
10	1	0	-5.583609	-0.363544	-1.747810
11	1	0	-6.117309	-1.823449	0.182221
12	16	0	-1.186293	0.873778	0.001100
13	6	0	1.332823	1.092952	-1.124157
14	6	0	1.354418	1.964261	0.029482
15	6	0	2.141732	-0.038120	-1.175972
16	6	0	2.196052	1.582456	1.134886
17	6	0	2.944886	-0.334059	-0.089526
18	1	0	2.153731	-0.685240	-2.041394
19	6	0	2.981372	0.467681	1.073882
20	1	0	2.180358	2.217635	2.010938
21	1	0	3.624393	0.174634	1.891246
22	7	0	0.576127	3.020010	0.170083
23	1	0	0.757585	1.387605	-1.990648
24	7	0	3.793346	-1.534115	-0.145496
25	8	0	4.510058	-1.766449	0.822448
26	8	0	3.734296	-2.231224	-1.152968
27	1	0	0.047221	3.190324	-0.687037



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.347815	-1.669269	0.460826
2	6	0	-2.230635	-0.956065	0.889675
3	6	0	-2.039702	0.359958	0.460884
4	6	0	-2.971395	0.961285	-0.390779
5	6	0	-4.081702	0.240651	-0.821672
6	6	0	-4.270945	-1.073856	-0.396374
7	1	0	-3.492011	-2.690747	0.792265
8	1	0	-1.503385	-1.414576	1.547836
9	1	0	-2.824227	1.987689	-0.704829
10	1	0	-4.802230	0.707822	-1.482716
11	1	0	-5.137464	-1.631797	-0.731155
12	16	0	-0.617100	1.292971	1.023227
13	6	0	0.474990	1.150992	-0.516255
14	6	0	1.638312	2.099104	-0.307493
15	6	0	0.836565	-0.284770	-0.611220
16	6	0	2.852144	1.526777	0.278649
17	6	0	2.039867	-0.705199	-0.189461
18	1	0	0.097992	-0.994321	-0.957555
19	6	0	3.057125	0.195775	0.311121
20	1	0	3.619729	2.211342	0.622531
21	1	0	3.974333	-0.231846	0.690774
22	7	0	1.475258	3.319313	-0.653246
23	1	0	2.303403	3.875830	-0.429769
24	1	0	-0.135024	1.494915	-1.348392
25	7	0	2.337658	-2.148628	-0.205618
26	8	0	3.464858	-2.489725	0.136384
27	8	0	1.452794	-2.918893	-0.557130

2. Coordinates of All Stationary Points in Acid-catalyzed Rearrangement of Arenesulfenanilides

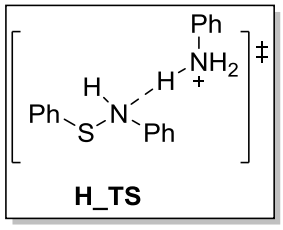


1a(NH_3)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.214953	2.674498	1.529741
2	6	0	-1.405680	1.547445	1.400008
3	6	0	-0.776471	1.287641	0.185598
4	6	0	-0.971046	2.134047	-0.907156
5	6	0	-1.788158	3.251620	-0.773155
6	6	0	-2.407713	3.526976	0.446259
7	1	0	-2.702874	2.876191	2.475325
8	1	0	-1.273558	0.869711	2.236370
9	1	0	-0.520943	1.897149	-1.864931
10	1	0	-1.944918	3.906258	-1.621823
11	1	0	-3.043541	4.397665	0.546705
12	7	0	0.098364	0.150993	0.052511
13	1	0	0.236341	-0.285473	0.961651
14	6	0	-2.058425	-1.510085	-0.449768
15	6	0	-3.169910	-0.805196	-0.922807
16	6	0	-2.204298	-2.493825	0.534537
17	6	0	-4.428821	-1.081481	-0.398260
18	1	0	-3.044959	-0.052867	-1.690316
19	6	0	-3.467320	-2.763653	1.051330
20	1	0	-1.338457	-3.046697	0.878493
21	6	0	-4.576481	-2.056655	0.586726
22	1	0	-5.293634	-0.540104	-0.761828
23	1	0	-3.587912	-3.529205	1.808082
24	1	0	-5.559197	-2.272446	0.988460
25	16	0	-0.438902	-1.133890	-1.088901
26	7	0	2.413104	1.041750	-0.935947
27	1	0	2.384868	0.954571	-1.953977
28	1	0	1.436306	0.665846	-0.518839
29	6	0	3.526858	0.271683	-0.357353
30	6	0	4.548253	0.933385	0.308724

31	6	0	3.494861	-1.112757	-0.475075
32	6	0	5.577604	0.180638	0.871036
33	1	0	4.552944	2.015104	0.389562
34	6	0	4.532276	-1.852149	0.086977
35	1	0	2.680568	-1.608613	-0.991738
36	6	0	5.569999	-1.207451	0.758575
37	1	0	6.383184	0.682243	1.392010
38	1	0	4.526654	-2.931336	0.000179
39	1	0	6.373583	-1.788037	1.193940
40	1	0	2.494241	2.034992	-0.716477

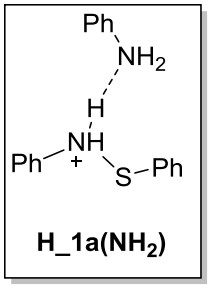


H_TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.534237	2.610631	-0.720155
2	6	0	0.595708	1.292746	-0.282223
3	6	0	-0.247605	0.878496	0.747787
4	6	0	-1.158696	1.759710	1.322748
5	6	0	-1.207052	3.081177	0.883367
6	6	0	-0.362114	3.507598	-0.137138
7	1	0	1.187499	2.938094	-1.519579
8	1	0	1.275885	0.590515	-0.746218
9	1	0	-1.833904	1.417387	2.099650
10	1	0	-1.913006	3.769082	1.331699
11	1	0	-0.404541	4.532958	-0.482920
12	7	0	-0.185768	-0.489231	1.217231
13	1	0	-0.783763	-0.583263	2.037447
14	6	0	-2.398053	-1.166893	-0.292215
15	6	0	-3.462851	-1.630695	0.489181
16	6	0	-2.615070	-0.235533	-1.313655
17	6	0	-4.746617	-1.152076	0.249258
18	1	0	-3.284603	-2.367424	1.263167
19	6	0	-3.902655	0.238496	-1.543368
20	1	0	-1.783725	0.108797	-1.914480

21	6	0	-4.964336	-0.217477	-0.763366
22	1	0	-5.576528	-1.513082	0.844300
23	1	0	-4.077848	0.958465	-2.333298
24	1	0	-5.966346	0.149845	-0.949768
25	16	0	-0.748430	-1.747924	0.027250
26	1	0	1.097570	-0.863518	1.584414
27	7	0	2.253616	-1.182914	1.833823
28	1	0	2.567598	-0.690406	2.669437
29	1	0	2.278246	-2.181635	2.042558
30	6	0	3.104570	-0.860586	0.687509
31	6	0	3.021867	-1.656332	-0.448693
32	6	0	3.898914	0.277541	0.725079
33	6	0	3.761102	-1.300395	-1.574199
34	1	0	2.388092	-2.535753	-0.464799
35	6	0	4.632593	0.625005	-0.406466
36	1	0	3.944403	0.892983	1.616949
37	6	0	4.562838	-0.160572	-1.555116
38	1	0	3.708553	-1.915592	-2.463617
39	1	0	5.258870	1.507989	-0.386308
40	1	0	5.136830	0.111312	-2.432027



H_1a(NH_2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.317615	0.641036	-1.039860
2	6	0	1.971172	0.600185	-0.699447
3	6	0	1.478561	1.559872	0.177810
4	6	0	2.285109	2.564582	0.699553
5	6	0	3.633704	2.593046	0.351968
6	6	0	4.147762	1.632431	-0.515330
7	1	0	3.718003	-0.105852	-1.713278
8	1	0	1.324238	-0.168785	-1.100229
9	1	0	1.875458	3.315115	1.367606

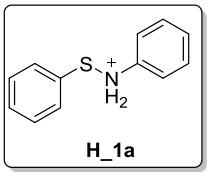
10	1	0	4.274998	3.366405	0.755078
11	1	0	5.195675	1.658120	-0.787266
12	7	0	0.067828	1.523055	0.560907
13	1	0	-0.241063	0.539902	0.897039
14	6	0	-2.476454	1.017686	-0.434977
15	6	0	-2.689584	-0.117429	-1.226753
16	6	0	-3.357555	1.335728	0.606316
17	6	0	-3.778453	-0.942943	-0.961930
18	1	0	-2.010262	-0.339010	-2.040033
19	6	0	-4.429565	0.491819	0.877742
20	1	0	-3.209369	2.239056	1.185598
21	6	0	-4.638897	-0.645165	0.095232
22	1	0	-3.957556	-1.814785	-1.579359
23	1	0	-5.113058	0.730485	1.683263
24	1	0	-5.483791	-1.291366	0.300333
25	16	0	-1.089002	2.065808	-0.794929
26	1	0	-0.080244	2.160715	1.343444
27	7	0	-0.635509	-1.001191	1.476923
28	1	0	-1.588160	-1.213691	1.193194
29	1	0	-0.589795	-1.057606	2.490585
30	6	0	0.317241	-1.877339	0.855149
31	6	0	0.018595	-2.482005	-0.364881
32	6	0	1.582678	-2.030154	1.420445
33	6	0	0.994532	-3.226568	-1.024957
34	1	0	-0.971708	-2.378760	-0.792393
35	6	0	2.549321	-2.779958	0.758643
36	1	0	1.815881	-1.556605	2.368248
37	6	0	2.263421	-3.373663	-0.469864
38	1	0	0.756337	-3.699869	-1.969884
39	1	0	3.529201	-2.898657	1.204686
40	1	0	3.017793	-3.957748	-0.981748

$PhN^{+}H_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.224745	1.210280	0.001616
2	6	0	0.168193	1.220636	-0.005856
3	6	0	0.825317	-0.000055	-0.010190
4	6	0	0.168319	-1.220394	-0.005811
5	6	0	-1.225050	-1.210183	0.001589

6	6	0	-1.915970	-0.000115	0.006141
7	1	0	-1.764657	2.148350	0.000710
8	1	0	0.711531	2.159348	-0.009313
9	1	0	0.711122	-2.159427	-0.009296
10	1	0	-1.764465	-2.148538	0.000717
11	1	0	-2.998635	0.000192	0.009220
12	7	0	2.320836	-0.000071	0.008259
13	1	0	2.695291	0.820574	-0.478013
14	1	0	2.692667	0.009339	0.965004
15	1	0	2.694908	-0.830350	-0.461772

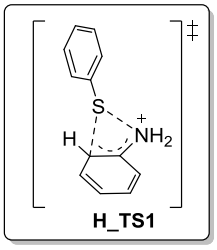


H_1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.060293	-1.210437	-0.080518
2	6	0	-2.684012	-1.218594	-0.284228
3	6	0	-2.024561	-0.000046	-0.393858
4	6	0	-2.683972	1.218522	-0.284200
5	6	0	-4.060253	1.210402	-0.080489
6	6	0	-4.744867	-0.000007	0.020660
7	1	0	-4.595086	-2.148170	-0.001384
8	1	0	-2.141674	-2.154940	-0.355132
9	1	0	-2.141602	2.154850	-0.355077
10	1	0	-4.595015	2.148151	-0.001332
11	1	0	-5.815850	0.000008	0.179993
12	7	0	-0.574987	-0.000068	-0.580448
13	1	0	-0.271221	-0.826193	-1.099235
14	6	0	2.031762	0.000059	0.410803
15	6	0	2.686789	-1.220391	0.176813
16	6	0	2.686772	1.220436	0.176388
17	6	0	3.988382	-1.213184	-0.308301
18	1	0	2.182839	-2.154582	0.393213
19	6	0	3.988366	1.213079	-0.308718
20	1	0	2.182806	2.154696	0.392461
21	6	0	4.634597	-0.000090	-0.552176
22	1	0	4.503542	-2.149012	-0.485282

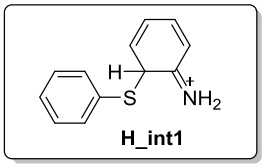
23	1	0	4.503513	2.148853	-0.486025
24	1	0	5.652011	-0.000148	-0.924232
25	16	0	0.392475	0.000160	1.059473
26	1	0	-0.271215	0.825909	-1.099467



Standard orientation:

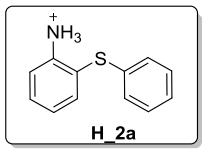
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.882915	1.363972	-0.472484
2	6	0	-2.545002	1.092433	-0.662827
3	6	0	-1.961976	-0.082113	-0.093641
4	6	0	-2.788310	-0.965952	0.667249
5	6	0	-4.124639	-0.681525	0.847721
6	6	0	-4.671474	0.479853	0.279683
7	1	0	-4.327889	2.253542	-0.900031
8	1	0	-1.913304	1.756620	-1.238718
9	1	0	-2.341140	-1.853985	1.095307
10	1	0	-4.753895	-1.347552	1.424442
11	1	0	-5.723200	0.697888	0.425060
12	16	0	-0.311239	-0.416783	-0.320424
13	6	0	2.455560	-0.901373	0.813401
14	6	0	2.494691	-0.642907	-0.583557
15	6	0	3.055628	-0.010101	1.694068
16	6	0	3.087321	0.551890	-1.059290
17	6	0	3.665196	1.143641	1.213594
18	1	0	3.047366	-0.221615	2.755603
19	6	0	3.672195	1.421213	-0.166772
20	1	0	3.090873	0.760964	-2.122627
21	1	0	4.136395	1.834375	1.901427
22	1	0	4.144089	2.325530	-0.529896
23	7	0	1.893233	-1.504917	-1.447026
24	1	0	1.977032	-1.362258	-2.443767
25	1	0	2.004310	-1.816887	1.174471

26	1	0	1.648911	-2.437857	-1.148176



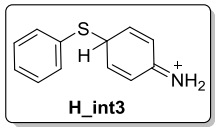
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.454232	1.180069	0.465053
2	6	0	2.162363	0.869971	0.879739
3	6	0	1.546308	-0.291376	0.400799
4	6	0	2.220394	-1.142520	-0.482664
5	6	0	3.506169	-0.817474	-0.899954
6	6	0	4.122017	0.341788	-0.426482
7	1	0	3.938826	2.073537	0.838991
8	1	0	1.635030	1.513462	1.572761
9	1	0	1.748744	-2.055685	-0.825560
10	1	0	4.033113	-1.473800	-1.581513
11	1	0	5.126779	0.587364	-0.748059
12	16	0	-0.079019	-0.720078	0.990837
13	6	0	-1.150229	-0.258974	-0.536637
14	6	0	-2.515786	-0.745968	-0.189029
15	6	0	-1.015979	1.200146	-0.722823
16	6	0	-3.546416	0.178952	0.074871
17	6	0	-2.040055	2.045898	-0.475892
18	1	0	-0.041267	1.560870	-1.025747
19	6	0	-3.306954	1.522307	-0.068973
20	1	0	-4.524484	-0.179929	0.371827
21	1	0	-1.916585	3.115826	-0.578266
22	1	0	-4.113323	2.217408	0.136809
23	7	0	-2.709500	-2.053045	-0.102075
24	1	0	-3.601602	-2.433689	0.183448
25	1	0	-0.724584	-0.824840	-1.365981
26	1	0	-1.946240	-2.704882	-0.225633



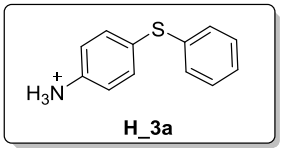
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.424260	-1.195372	-1.349143
2	6	0	-1.337265	-0.353209	-1.119591
3	6	0	-1.416289	0.612461	-0.109786
4	6	0	-2.582783	0.745239	0.650790
5	6	0	-3.671209	-0.086915	0.393864
6	6	0	-3.591741	-1.062354	-0.598197
7	1	0	-2.363724	-1.940726	-2.132985
8	1	0	-0.446477	-0.435957	-1.730139
9	1	0	-2.642961	1.499171	1.427329
10	1	0	-4.578340	0.027102	0.974730
11	1	0	-4.437315	-1.710587	-0.791229
12	16	0	-0.054558	1.745737	0.230612
13	6	0	1.343463	0.655811	0.019927
14	6	0	1.466915	-0.529959	0.750451
15	6	0	2.385201	0.992234	-0.845800
16	6	0	2.549422	-1.382830	0.625161
17	6	0	3.495829	0.159284	-0.969074
18	1	0	2.313561	1.903465	-1.425873
19	6	0	3.577746	-1.028216	-0.246677
20	1	0	2.607319	-2.302800	1.197155
21	1	0	4.295444	0.435398	-1.644986
22	1	0	4.435933	-1.678505	-0.354733
23	7	0	0.376366	-0.869787	1.690774
24	1	0	0.619517	-1.669197	2.279605
25	1	0	0.164403	-0.058327	2.286983
26	1	0	-0.499174	-1.069370	1.177389



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.607860	-1.095350	-0.350712
2	6	0	-1.802041	-0.248622	0.419037
3	6	0	-2.234907	1.041870	0.742478
4	6	0	-3.473257	1.485237	0.286001
5	6	0	-4.270126	0.648996	-0.493954
6	6	0	-3.838147	-0.639212	-0.811417
7	1	0	-2.279474	-2.104251	-0.569977
8	1	0	-1.613036	1.680986	1.357214
9	1	0	-3.816237	2.480161	0.542300
10	1	0	-5.232702	0.997266	-0.848180
11	1	0	-4.466141	-1.292600	-1.404564
12	6	0	3.462081	0.456439	-0.153483
13	6	0	3.270069	-0.970748	-0.103525
14	6	0	2.041895	-1.492438	-0.291729
15	6	0	0.855511	-0.644472	-0.504623
16	6	0	1.125726	0.795552	-0.629740
17	6	0	2.356634	1.321710	-0.438727
18	1	0	4.127361	-1.608590	0.077669
19	1	0	1.890552	-2.564861	-0.254449
20	1	0	0.222425	-1.028800	-1.305920
21	1	0	0.281458	1.440189	-0.843581
22	1	0	2.522749	2.391432	-0.485794
23	7	0	4.666217	0.962523	0.064606
24	1	0	5.458967	0.370190	0.270455
25	16	0	-0.244102	-0.838232	1.059935
26	1	0	4.832729	1.959162	0.035991

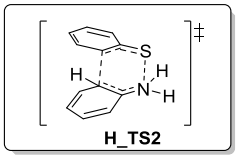


H_3a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.429405	0.827172	-1.208479
2	6	0	-2.393922	-0.104318	-1.213602

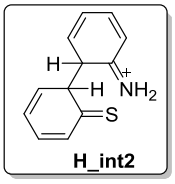
3	6	0	-1.875575	-0.560992	0.000008
4	6	0	-2.393825	-0.104226	1.213607
5	6	0	-3.429325	0.827275	1.208487
6	6	0	-3.944381	1.293794	0.000013
7	1	0	-3.838754	1.180208	-2.147239
8	1	0	-1.994710	-0.480630	-2.147262
9	1	0	-1.994551	-0.480429	2.147283
10	1	0	-3.838597	1.180351	2.147266
11	1	0	-4.754536	2.012962	-0.000006
12	16	0	-0.563393	-1.781315	0.000011
13	6	0	0.893038	-0.779129	0.000000
14	6	0	2.127734	-1.455503	0.000032
15	6	0	0.879538	0.622416	-0.000039
16	6	0	3.320678	-0.752150	0.000036
17	6	0	2.072466	1.335527	-0.000035
18	1	0	-0.060544	1.156215	-0.000054
19	6	0	3.269159	0.637019	0.000010
20	1	0	4.264631	-1.286702	0.000062
21	1	0	2.048937	2.420682	-0.000069
22	1	0	2.149490	-2.538457	0.000069
23	7	0	4.550197	1.401870	-0.000046
24	1	0	4.364812	2.409102	0.000712
25	1	0	5.120166	1.196115	0.827794
26	1	0	5.119491	1.197222	-0.828630



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.580991	0.340169	0.462374
2	6	0	1.426342	0.637478	-0.337619
3	6	0	0.552329	-0.496439	-0.709647
4	6	0	1.153082	-1.825261	-0.686416
5	6	0	2.321095	-2.034914	-0.034790
6	6	0	3.007521	-0.946578	0.607416
7	1	0	3.150941	1.168153	0.864813
8	1	0	-0.130636	-0.287123	-1.525643

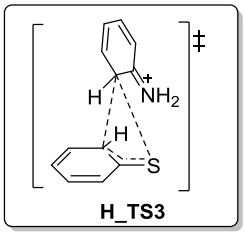
9	1	0	0.630873	-2.637549	-1.175407
10	1	0	2.762231	-3.023766	-0.005999
11	1	0	3.911533	-1.155187	1.167413
12	6	0	-1.430687	0.725364	0.662277
13	6	0	-2.630427	0.829527	-0.086326
14	6	0	-3.256165	-0.308640	-0.512880
15	6	0	-2.733194	-1.608016	-0.218769
16	6	0	-1.538219	-1.728865	0.408549
17	6	0	-0.739232	-0.554771	0.733096
18	1	0	-3.065206	1.805614	-0.264807
19	1	0	-4.188020	-0.227904	-1.059944
20	1	0	-3.303518	-2.484947	-0.496301
21	1	0	-1.119712	-2.701377	0.630918
22	1	0	-0.035748	-0.665993	1.553510
23	7	0	-0.884277	1.803096	1.220892
24	1	0	-1.333550	2.706949	1.156044
25	16	0	1.044512	2.185514	-0.809068
26	1	0	-0.082054	1.738920	1.830662



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.354855	-2.004900	-0.005259
2	6	0	1.170276	-1.840780	-0.619164
3	6	0	0.480986	-0.514997	-0.605224
4	6	0	1.396873	0.656490	-0.329801
5	6	0	2.563025	0.389265	0.468539
6	6	0	3.016290	-0.884197	0.625654
7	1	0	2.841396	-2.972481	0.005067
8	1	0	0.673542	-2.669097	-1.108174
9	1	0	3.130553	1.233114	0.841083
10	1	0	3.933645	-1.063190	1.174734
11	16	0	1.039822	2.158362	-0.915434
12	6	0	-0.670036	-0.588291	0.615507
13	6	0	-1.402030	0.705053	0.689453

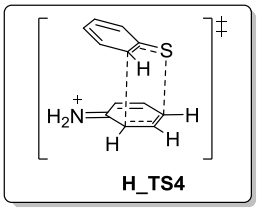
14	6	0	-1.545289	-1.744732	0.279443
15	6	0	-2.620790	0.864127	-0.019665
16	6	0	-2.758961	-1.571364	-0.277244
17	1	0	-1.135196	-2.733985	0.432072
18	6	0	-3.267979	-0.242413	-0.487275
19	1	0	-3.055076	1.851301	-0.121413
20	1	0	-3.363366	-2.419963	-0.570218
21	1	0	-4.215707	-0.121489	-0.999424
22	1	0	-0.085378	-0.766188	1.519897
23	7	0	-0.890664	1.699895	1.386721
24	1	0	-1.320442	2.616328	1.386087
25	1	0	-0.095936	-0.336583	-1.511054
26	1	0	-0.013858	1.609612	1.881454



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.170442	-1.681091	0.956192
2	6	0	-2.124111	-1.022872	1.621350
3	6	0	-1.601646	0.137130	1.094240
4	6	0	-2.125501	0.677701	-0.133200
5	6	0	-3.198212	-0.022239	-0.788609
6	6	0	-3.703853	-1.179227	-0.246766
7	1	0	-3.582020	-2.589684	1.380428
8	1	0	-1.738680	-1.424144	2.550177
9	1	0	-3.593222	0.392360	-1.707307
10	1	0	-4.515620	-1.703891	-0.734771
11	16	0	-1.507630	2.098686	-0.787767
12	6	0	1.516154	0.135054	-0.397698
13	6	0	1.880609	1.163981	0.454831
14	6	0	2.445080	-0.904695	-0.692275
15	6	0	3.140140	1.172135	1.051759
16	6	0	3.721990	-0.891368	-0.075081
17	6	0	4.054124	0.134086	0.780113

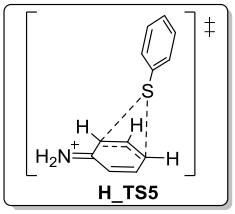
18	1	0	3.419953	1.974452	1.722233
19	1	0	4.430415	-1.681145	-0.295693
20	1	0	5.031672	0.146306	1.245921
21	1	0	0.539180	0.113835	-0.860356
22	1	0	-0.809288	0.673373	1.597827
23	1	0	1.180927	1.968008	0.644539
24	7	0	2.107621	-1.894789	-1.549018
25	1	0	2.768182	-2.615292	-1.798061
26	1	0	1.231231	-1.881196	-2.046679



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.597346	0.510709	1.172369
2	6	0	-0.238719	1.274119	-0.059424
3	6	0	-1.116967	1.125581	-1.192072
4	6	0	-2.365222	0.604038	-1.040671
5	6	0	-2.829938	0.141397	0.242132
6	6	0	-1.999426	0.113503	1.312049
7	1	0	-0.166705	0.941365	2.071505
8	1	0	-0.792401	1.540075	-2.138239
9	1	0	-3.046518	0.579916	-1.883100
10	1	0	-3.869204	-0.147249	0.349755
11	1	0	-2.350062	-0.207381	2.286719
12	6	0	0.093016	-1.616561	-0.208071
13	6	0	0.970597	-1.362592	-1.287670
14	6	0	2.177203	-0.762188	-1.043216
15	6	0	2.604150	-0.426215	0.284121
16	6	0	1.765075	-0.615503	1.331824
17	6	0	0.385318	-1.018921	1.110742
18	1	0	0.699210	-1.683014	-2.286001
19	1	0	2.852360	-0.577524	-1.870159
20	1	0	3.608051	-0.053028	0.437467
21	1	0	2.065737	-0.363908	2.340887

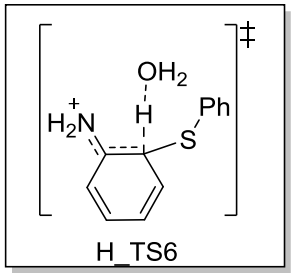
22	1	0	-0.060310	-1.554576	1.944667
23	7	0	-1.005193	-2.343236	-0.357623
24	1	0	-1.271088	-2.707423	-1.262193
25	16	0	1.119610	2.209396	-0.102069
26	1	0	-1.632934	-2.519143	0.412493



H_TS5

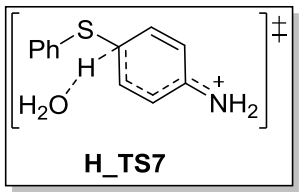
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.605269	1.193254	0.782709
2	6	0	-2.260056	0.894762	0.761848
3	6	0	-1.778437	-0.206548	-0.011949
4	6	0	-2.714889	-0.985122	-0.761063
5	6	0	-4.057919	-0.675202	-0.729693
6	6	0	-4.503000	0.410558	0.039334
7	1	0	-3.973986	2.024590	1.370266
8	1	0	-1.546693	1.478667	1.329318
9	1	0	-2.343476	-1.818331	-1.343839
10	1	0	-4.769708	-1.265076	-1.293260
11	1	0	-5.560033	0.649370	0.060708
12	16	0	-0.125791	-0.599868	-0.027917
13	6	0	2.649404	-0.500357	-1.098984
14	6	0	2.692976	0.833283	-0.585977
15	6	0	2.648802	-1.575492	-0.231086
16	6	0	2.687370	1.035350	0.825055
17	6	0	2.578661	-1.363845	1.147491
18	1	0	2.640623	-2.582675	-0.626774
19	6	0	2.623725	-0.045034	1.664318
20	1	0	2.734014	2.044200	1.217378
21	1	0	2.545594	-2.206014	1.826370
22	1	0	2.605780	0.106276	2.736283
23	7	0	2.791915	1.879270	-1.424328
24	1	0	2.853592	2.823997	-1.077213
25	1	0	2.674963	-0.654907	-2.171123
26	1	0	2.840365	1.749256	-2.423152



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.840439	-1.820147	0.083491
2	6	0	3.626140	-0.828455	0.709373
3	6	0	3.270241	0.503149	0.687387
4	6	0	2.094763	0.923683	0.021490
5	6	0	1.209790	-0.092118	-0.497140
6	6	0	1.681002	-1.447678	-0.546540
7	1	0	3.161435	-2.853176	0.084372
8	1	0	4.547375	-1.115026	1.203428
9	1	0	3.920144	1.248925	1.130685
10	1	0	0.531096	-0.284363	0.787139
11	1	0	1.056919	-2.179414	-1.044388
12	7	0	1.760128	2.229621	-0.045944
13	1	0	2.415561	2.931416	0.261170
14	16	0	-0.090372	0.426076	-1.666642
15	6	0	-1.589805	0.169650	-0.700119
16	6	0	-2.273340	-1.042383	-0.806969
17	6	0	-2.069735	1.172288	0.154997
18	6	0	-3.416148	-1.266307	-0.038634
19	1	0	-1.914142	-1.803335	-1.488140
20	6	0	-3.205825	0.935686	0.931395
21	1	0	-1.568002	2.131554	0.200013
22	6	0	-3.875945	-0.286569	0.837489
23	1	0	-3.944627	-2.207618	-0.126782
24	1	0	-3.580292	1.713169	1.586765
25	1	0	-4.762523	-0.463706	1.433635
26	8	0	-0.111166	-0.437384	1.799056
27	1	0	-0.974499	0.012881	1.670505
28	1	0	0.323271	-0.090563	2.592828
29	1	0	1.053213	2.508979	-0.713109



H_TS7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.601488	0.979991	0.558144
2	6	0	-1.887250	0.444539	-0.526015
3	6	0	-2.284147	-0.772931	-1.082696
4	6	0	-3.360488	-1.471649	-0.535764
5	6	0	-4.051741	-0.956180	0.558119
6	6	0	-3.679199	0.275125	1.099610
7	1	0	-2.329492	1.954657	0.947833
8	1	0	-1.764745	-1.162948	-1.948689
9	1	0	-3.663823	-2.415183	-0.972997
10	1	0	-4.890191	-1.499611	0.975756
11	1	0	-4.235926	0.697260	1.927919
12	6	0	3.561555	-0.420863	0.147122
13	6	0	3.147736	0.868356	0.569937
14	6	0	1.885560	1.324033	0.276041
15	6	0	0.929171	0.500310	-0.392701
16	6	0	1.392554	-0.761863	-0.878261
17	6	0	2.646332	-1.228086	-0.579544
18	1	0	3.843448	1.503927	1.105332
19	1	0	1.587919	2.321268	0.580016
20	1	0	0.326124	-0.019724	0.869590
21	1	0	0.721304	-1.376396	-1.465167
22	1	0	2.959736	-2.205238	-0.928178
23	7	0	4.798534	-0.874766	0.431376
24	1	0	5.477087	-0.289143	0.891034
25	16	0	-0.475756	1.342787	-1.192331
26	8	0	-0.270028	-0.440771	1.798653
27	1	0	0.051697	-0.093857	2.644985
28	1	0	-1.209481	-0.167088	1.665897
29	1	0	5.117360	-1.767676	0.091149

3. Computed Energies

Table S1. Sum of electronic and zero-point energies (*E*, in Hartree), sum of electronic and thermal enthalpies (*H*, in Hartree), and sum of electronic and thermal free energies (*G*, in Hartree) for the thermal rearrangement of benzenesulfenanilide (**1a**). Relative energies (ΔE, ΔH, ΔG *and* ΔG_{sol} in aniline) at 298 K are reported in kcal/mol.

Structure	E	H	G	Gsol+ZPC	ΔE	ΔH	ΔG	ΔG_{sol}
1a(singlet)	-916.846161	-916.833174	-916.886925	-916.906023	0.0	0.0	0.0	0.0
1a(triplet)	-916.791825	-916.777854	-916.835326	-916.785169	34.1	34.7	32.4	75.8
TS1 with *exo*-H	-916.772518	-916.759809	-916.81237	-916.8366	46.2	46.0	46.8	43.6
TS1 with *endo*-H	-916.774108	-916.761441	-916.813907	-916.837364	45.2	45.0	45.8	43.1
Int1	-916.815107	-916.802054	-916.855899	-916.889703	19.5	19.5	19.5	10.2
TS2 with *exo*-H	-916.774937	-916.762738	-916.812494	-916.857127	44.7	44.2	46.7	30.7
TS2 with *endo*-H	-916.775487	-916.763376	-916.812803	-916.857726	44.3	43.8	46.5	30.3
Int2	-916.778008	-916.765314	-916.816536	-916.861729	42.8	42.6	44.2	27.8
TS3	-916.757441	-916.744352	-916.798301	-916.8232484	55.7	55.7	55.6	51.9
TS4	-916.782173	-916.770061	-916.818924	-916.863559	40.2	39.6	42.7	26.6
Int3	-916.818685	-916.805673	-916.859344	-916.891743	17.2	17.3	17.3	9.0
TS5	-916.769829	-916.756978	-916.809863	-916.834011	47.9	47.8	48.4	45.2
TS6	-916.741677	-916.728836	-916.781951	-916.808411	65.6	65.5	65.9	61.3
H_2O	-76.437825	-76.434045	-76.455468	-76.468796				
Int4(H_2O)	-993.268497	-993.252444	-993.31219	-993.347782	9.7	9.3	19.0	17.0
TS7(H_2O)	-993.231257	-993.216755	-993.272749	-993.298645	33.1	31.7	43.7	47.8
Int4($2H_2O$)	-1069.722085	-1069.703384	-1069.769298	-1069.804618	-0.2	-1.3	17.9	24.5
TS7($2H_2O$)	-1069.69499	-1069.678244	-1069.738792	-1069.769646	16.8	14.4	37.1	46.4
Int6(H_2O)	-993.268667	-993.252346	-993.31453	-993.352974	9.6	9.3	17.5	13.7
TS9(H_2O)	-993.206362	-993.192033	-993.247937	-993.276239	48.7	47.2	59.3	61.9
Int6($2H_2O$)	-1069.720074	-1069.701037	-1069.76979	-1069.812114	1.1	0.1	17.6	19.8
TS9($2H_2O$)	-1069.6864	-1069.669609	-1069.730464	-1069.759698	22.2	19.9	42.3	52.7
TS10	-993.197282	-993.18252	-993.238436	-993.272228	54.4	53.1	65.2	64.4
Int7	-916.819701	-916.806574	-916.86018	-916.887991	16.6	16.7	16.8	11.3
Int8	-993.270138	-993.253751	-993.315796	-993.348867	8.7	8.5	16.7	16.3
TS11	-993.238251	-993.223691	-993.280478	-993.30842	28.7	27.3	38.9	41.7
$PhNH_2$	-287.585389	-287.579165	-287.614259	-287.625607				
Int5	-1204.426578	-1204.405796	-1204.480348	-1204.516205	3.1	4.1	13.1	9.7
TS8	-1204.387678	-1204.368483	-1204.437242	-1204.469444	27.5	27.5	40.1	39.0
2a	-916.868477	-916.855511	-916.908103	-916.925937	-14.0	-14.0	-13.3	-12.5
3a	-916.86494	-916.851823	-916.905152	-916.925423	-11.8	-11.7	-11.4	-12.2
PhS·	-629.828915	-629.822395	-629.859401	-629.870345	40.7	40.7	28.6	25.3
PhNH·	-286.95233	-286.945964	-286.981892	-286.995426				
TS0(triplet)	-916.765224	-916.752366	-916.80762	-916.848626	50.8	50.7	49.8	36.0

Table S2. Sum of electronic and zero-point energies (*E*, in Hartree), sum of electronic and thermal enthalpies (*H*, in Hartree), and sum of electronic and thermal free energies (*G*, in Hartree) for the acid-catalyzed rearrangement of benzenesulfenanilide (**1a**). Relative energies (ΔE, ΔH, ΔG *and* ΔG_{sol} in aniline) at 298 K are reported in kcal/mol.

Structure	E	H	G	Gsol+ZPC	ΔE	ΔH	ΔG	ΔGsol
H_1a	-917.190287	-917.177076	-917.23188	-917.323671	0.0	0.0	0.0	0.0
H_TS1	-917.165071	-917.151953	-917.205218	-917.280688	15.8	15.8	16.7	27.0
H_Int1	-917.196293	-917.18293	-917.236816	-917.336621	-3.8	-3.7	-3.1	-8.1
H_TS2	-917.154994	-917.142406	-917.192905	-917.306081	22.1	21.8	24.5	11.0
H_Int2	-917.156178	-917.143269	-917.19463	-917.309717	21.4	21.2	23.4	8.8
H_TS3	-917.14527	-917.131473	-917.188007	-917.265224	28.2	28.6	27.5	36.7
H_Int3	-917.200392	-917.187075	-917.240983	-917.339103	-6.3	-6.3	-5.7	-9.7
H_TS4	-917.161851	-917.149439	-917.198709	-917.313679	17.8	17.3	20.8	6.3
H_TS5	-917.164427	-917.151092	-917.20474	-917.279723	16.2	16.3	17.0	27.6
H_2O	-76.437825	-76.434045	-76.455468	-76.468796				
H_TS6	-993.63471	-993.619318	-993.676988	-993.780452	-4.1	-5.1	6.5	7.5
H_TS7	-993.634118	-993.618596	-993.677035	-993.778831	-3.8	-4.7	6.5	8.6
H_2a	-917.212814	-917.199656	-917.252413	-917.346274	-14.1	-14.2	-12.9	-14.2
H_3a	-917.20311	-917.189549	-917.244822	-917.349291	-8.0	-7.8	-8.1	-16.1