Supporting Information

An Experimental and Computational Assessment of Acid-Catalyzed Azide-Nitrile Cycloadditions

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Table S1. Overall Energy Barriers Calculated at the M06-2X/6-311+G(d,p) Level for the Cycloaddition of NaN_3 with Acetonitrile and Benzonitrile, Catalyzed by Different Bronsted and Lewis acids.

Additive	Overall energy barrier for PhCN (kcal mol^{-1})	Overall energy barrier for MeCN (kcal mol^{-1})
9	+25.4	+24.6
NH_4^+	+26.8	+29.3
HN_3	+27.5	+30.0
$AlCl_3$	+28.3	+28.5
AcOH	+28.2	+29.3
$ZnBr_2$	+30.1	+35.0
H_3O^+	+40.2	+39.0
None	+33.1	+37.0

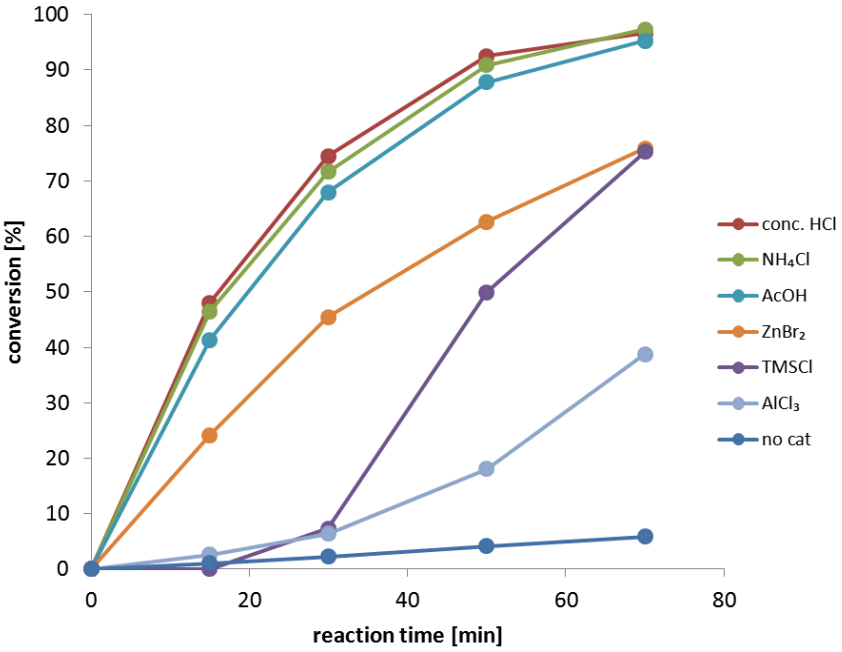


Figure S1. Comparison of the reaction progress for the cycloaddition of NaN_3 with benzonitrile, using different catalytic systems when a 50% catalyst loading is added to the reaction mixture. Inhibition of the reactions assisted by TMSCl and $AlCl_3$ can be clearly observed. Conditions: 1 mmol of benzonitrile, 2 equiv. of NaN3 and 50% of catalyst in 1 mL of NMP as solvent heated to a reaction temperature of 160 °C.

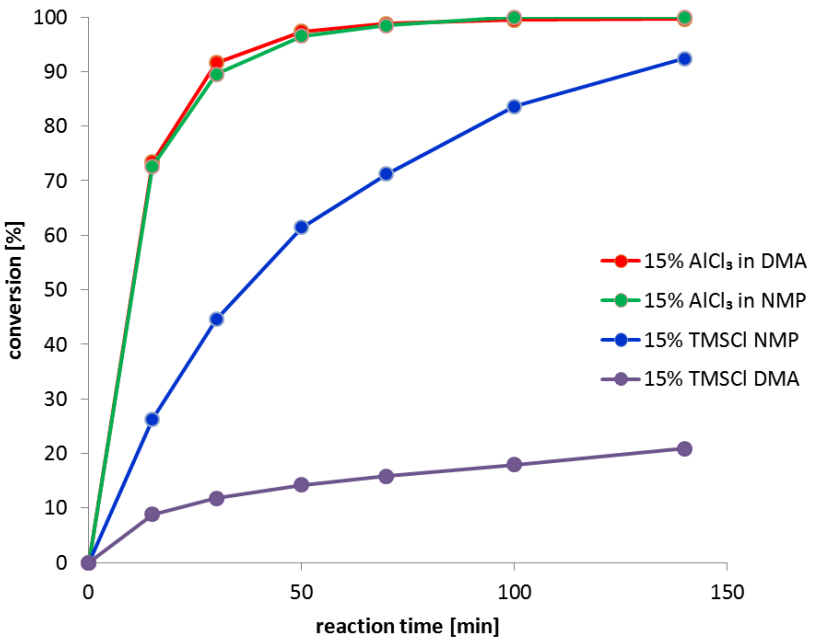


Figure S2. Comparison of the reaction progress for the cycloaddition of NaN_3 with benzonitrile, using different catalytic systems. No difference between DMA and NMP is appreciable for $AlCl_3$, while in the case of TMSCl the reaction is more efficient in NMP. Conditions: 1 mmol of benzonitrile, 2 equiv. of NaN3 and 15% of catalyst in 1mL of NMP as solvent heated to a reaction temperature of 160 °C.

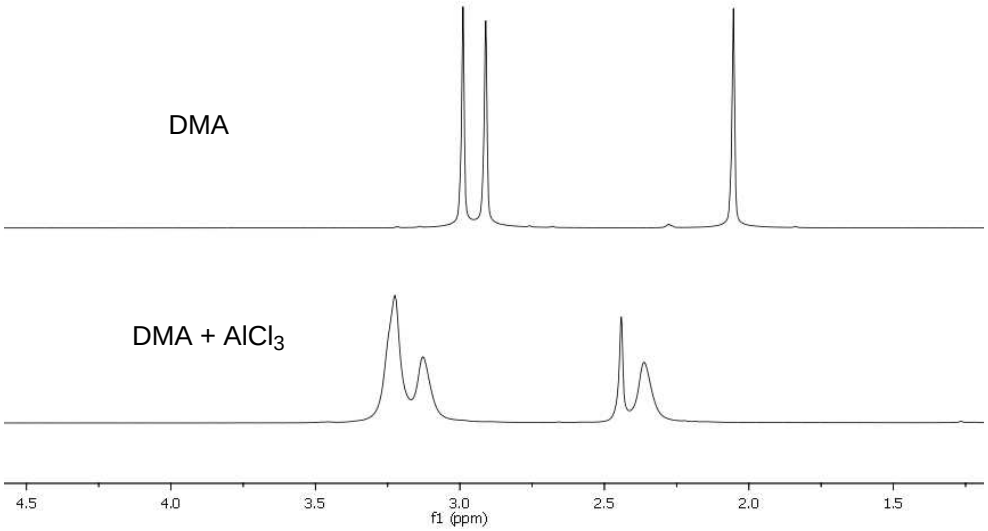


Figure S3. ^{1}HNMR spectra of pure *N*,*N*-dimethylacetamide (DMA) in $CDCl_3$(top) and the same mixture after addition of an excess of $AlCl_3$ (bottom).

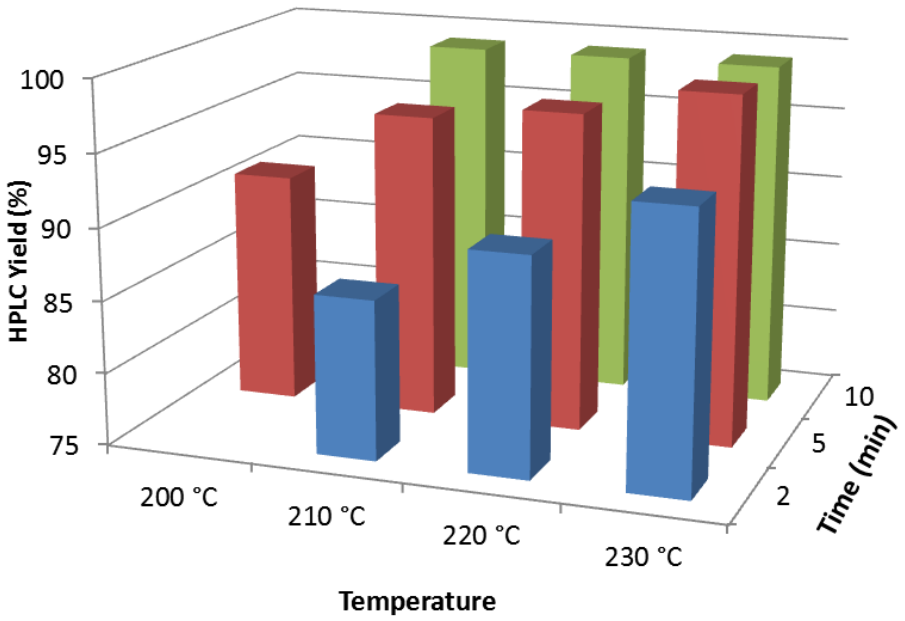
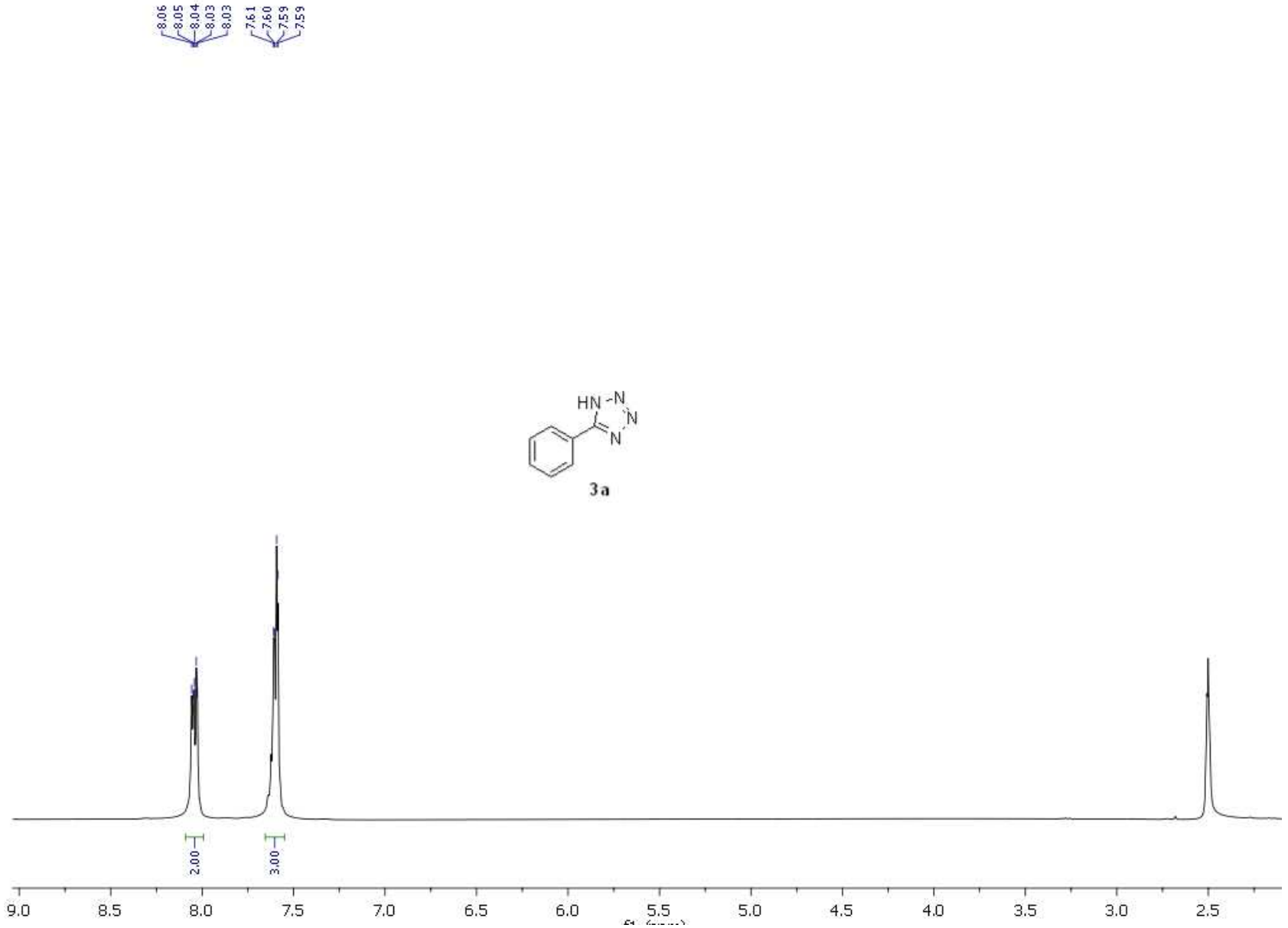


Figure S4. Effect of temperature and heating time in the cycloaddition of NaN_3 with benzonitrile using $AlCl_3$ in NMP as catalyst system. For a better comparison of the results, 10 mol % catalyst was used instead of 15 mol %. Conditions: 1 mmol benzonitrile, 2 equiv NaN_3, 1mL NMP, 10 mol % $AlCl_3$.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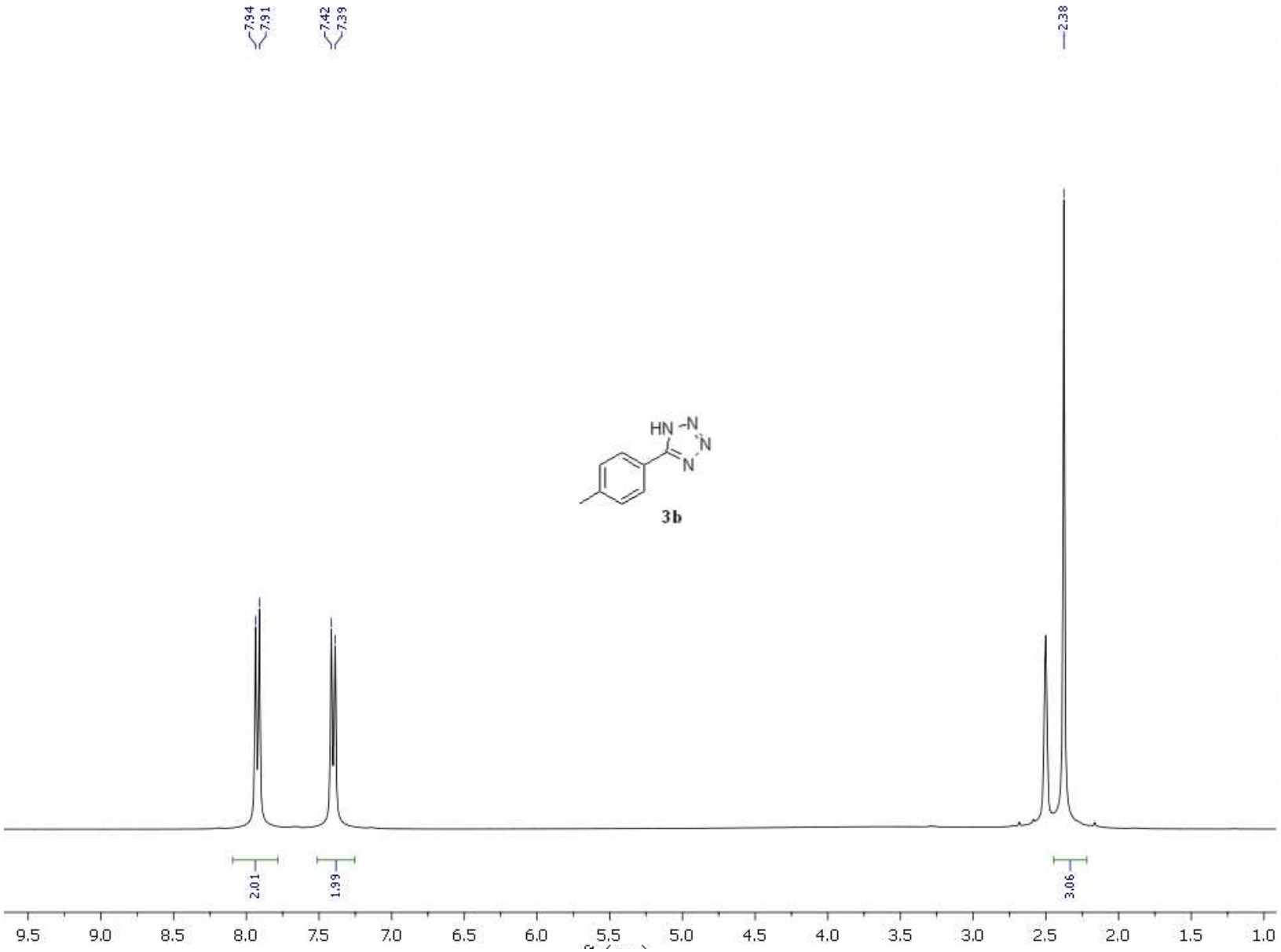
8.04
8.03
8.03
7.61
7.60
7.59
7.59
HN
N
N
N
3a
2.00
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5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7.39
2.38
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N
N
N
3b
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1.99
3.06
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9.0
8.5
8.0
7.5
7.0
6.5
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5.5
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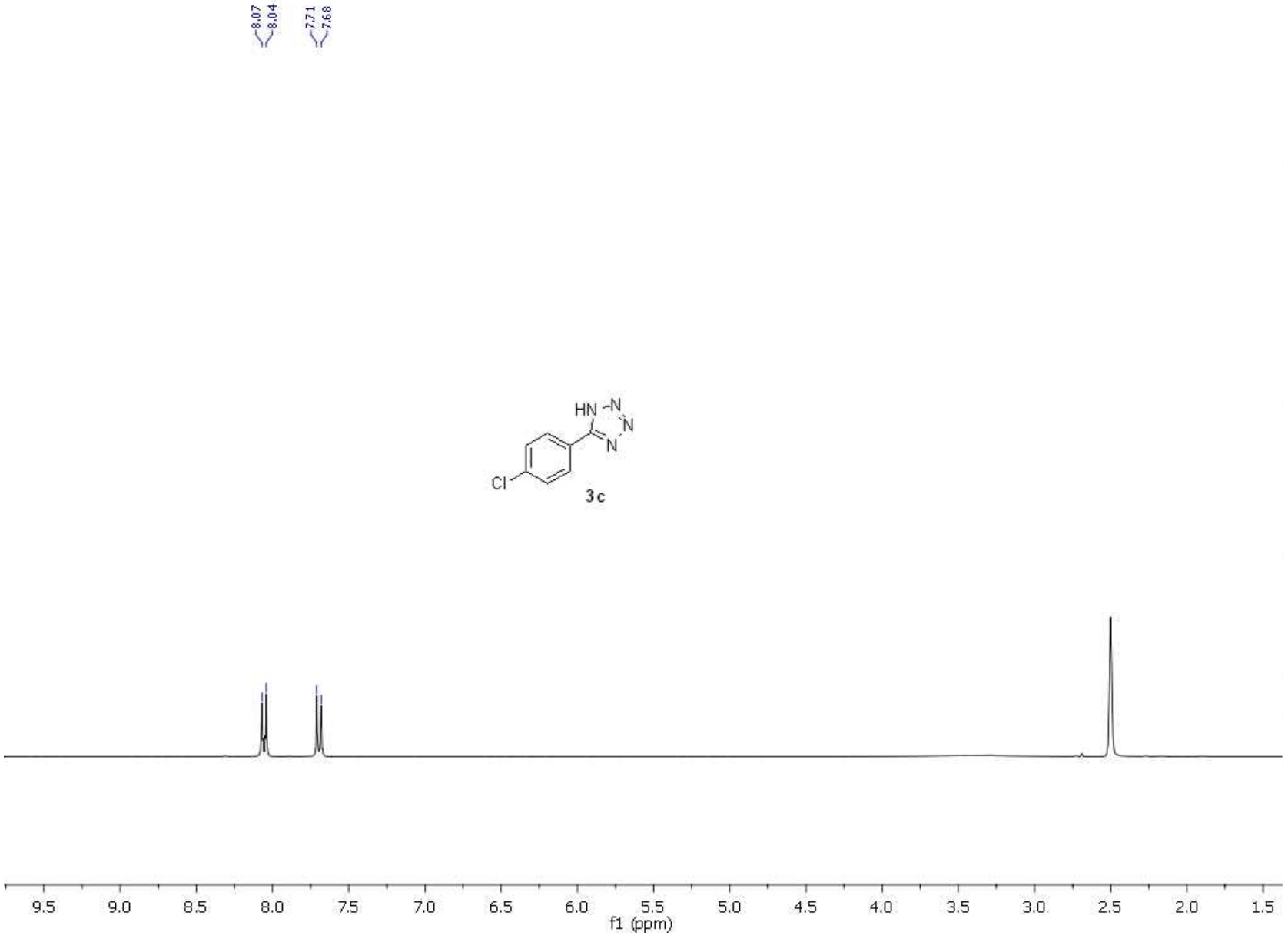
4.0
3.5
3.0
2.5
2.0
1.5
1.0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2.5
2.0
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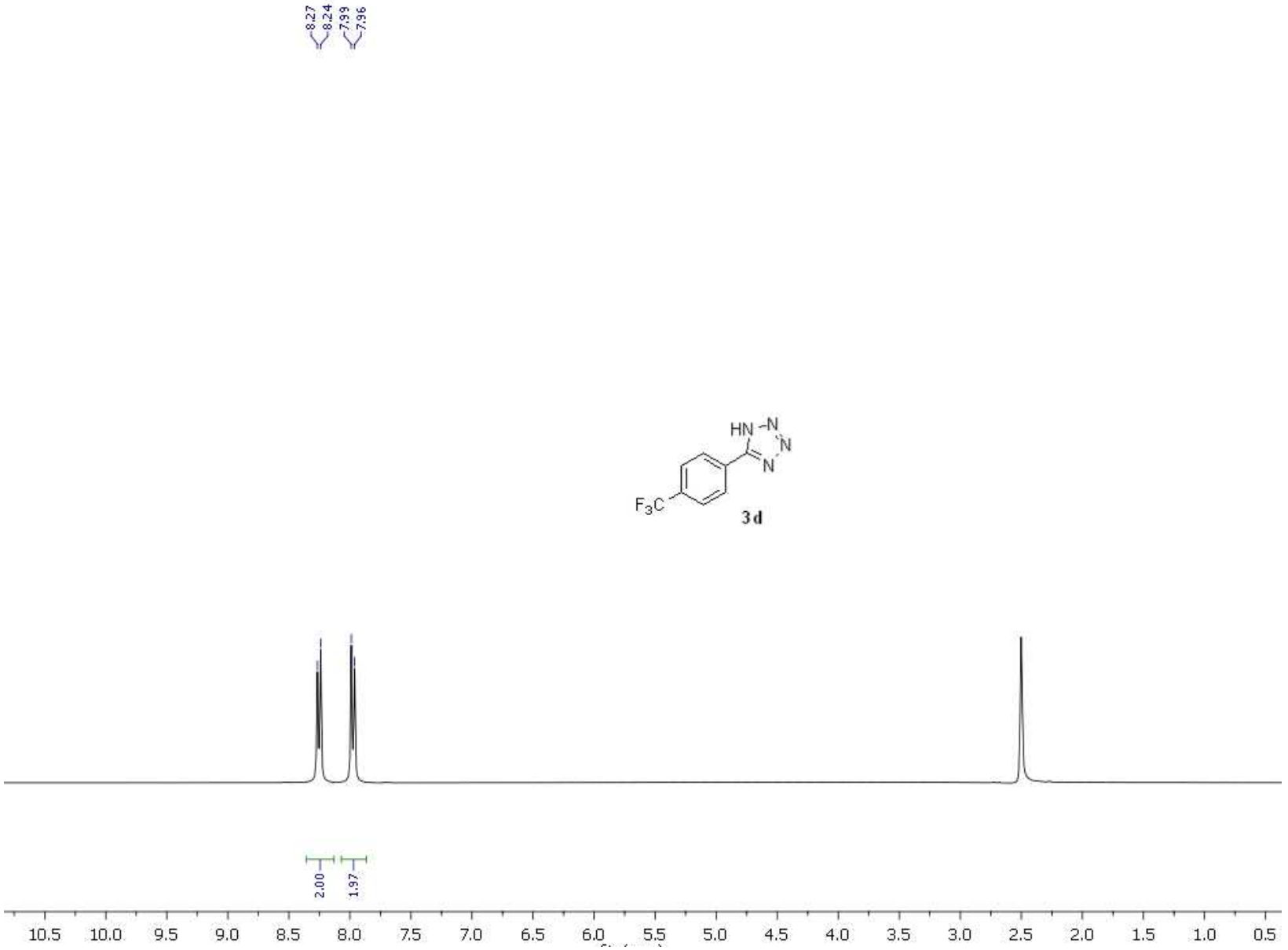
f1 (ppm)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N
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N
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9.0
8.5
8.0
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7.0
6.5
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2.5
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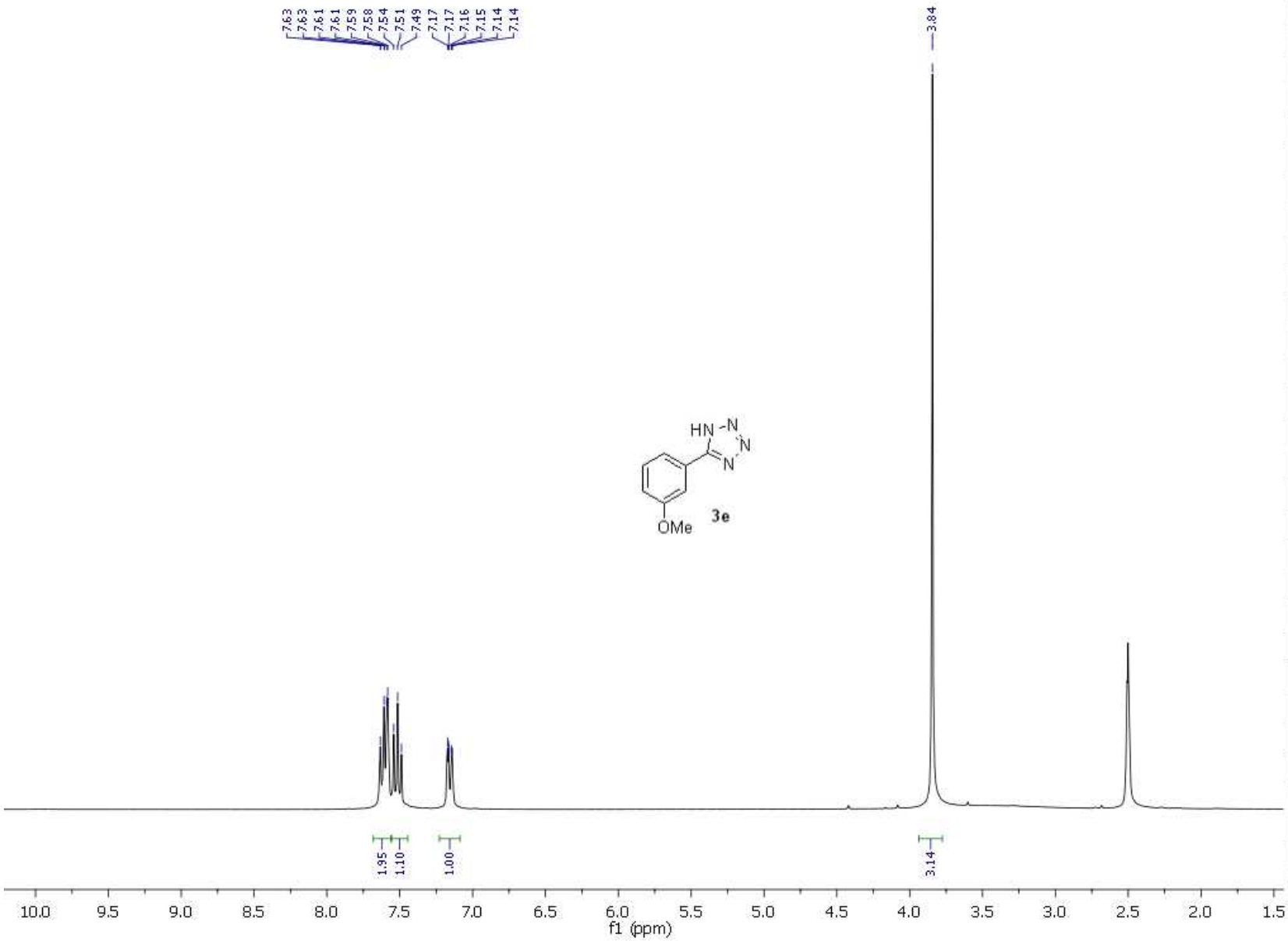
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7.14
7.14
3.84
HN
N
N
N
OMe
3e
1.95
1.10
1.00
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9.0
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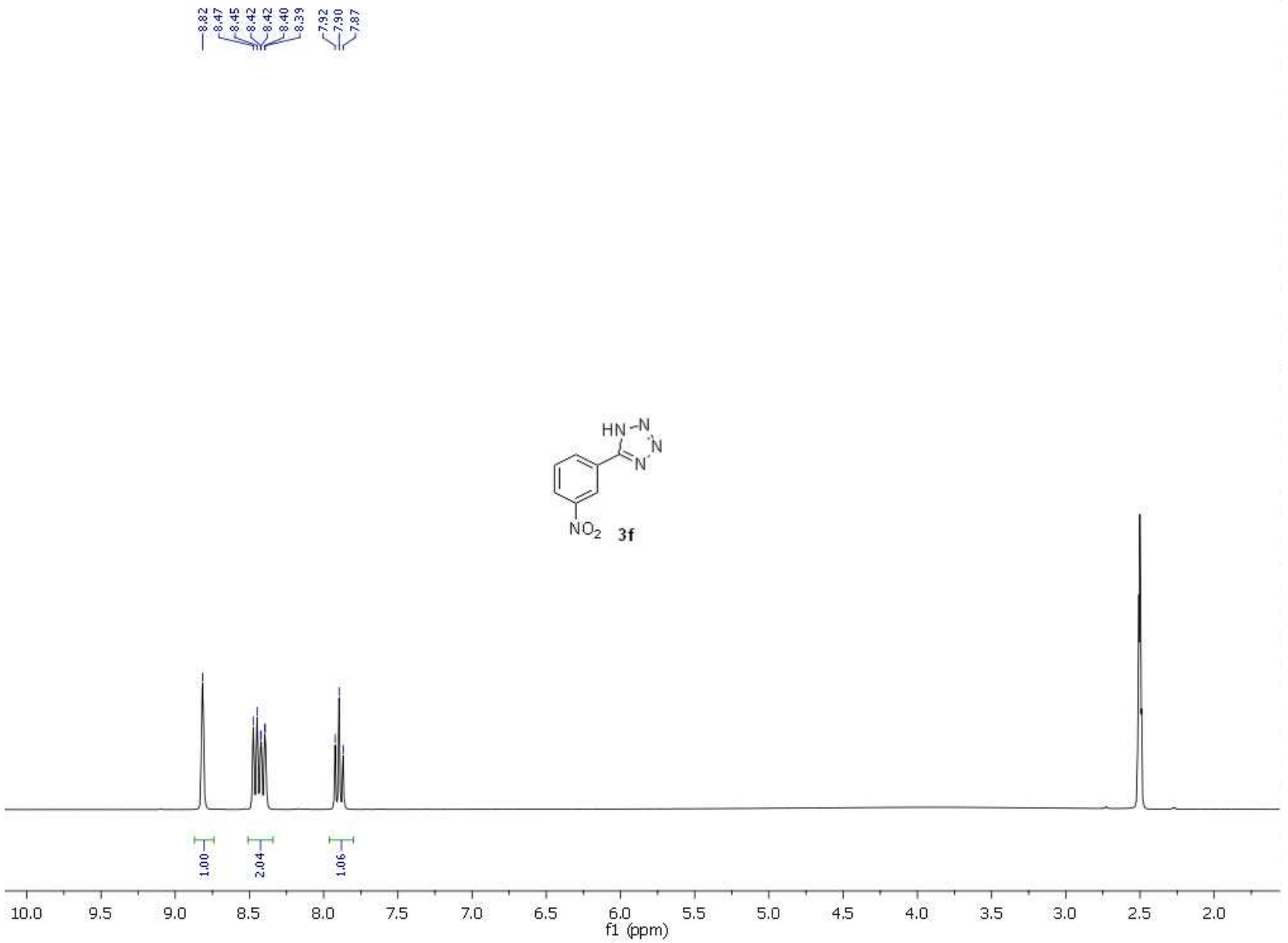
f1 (ppm)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N
N
NO2
3f
1.00
2.04
1.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
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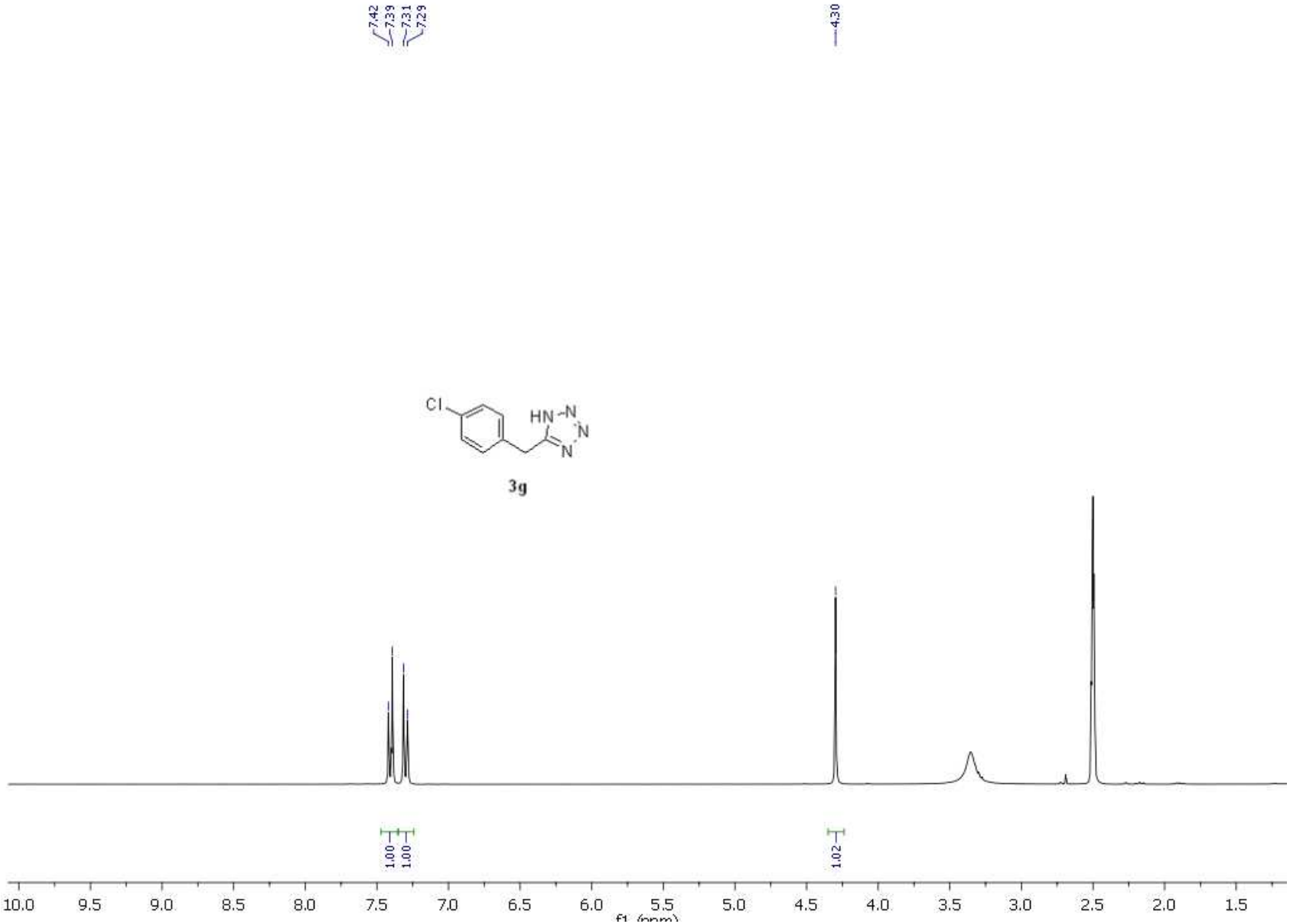
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)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4.30
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N
N
N
3g
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1.00
1.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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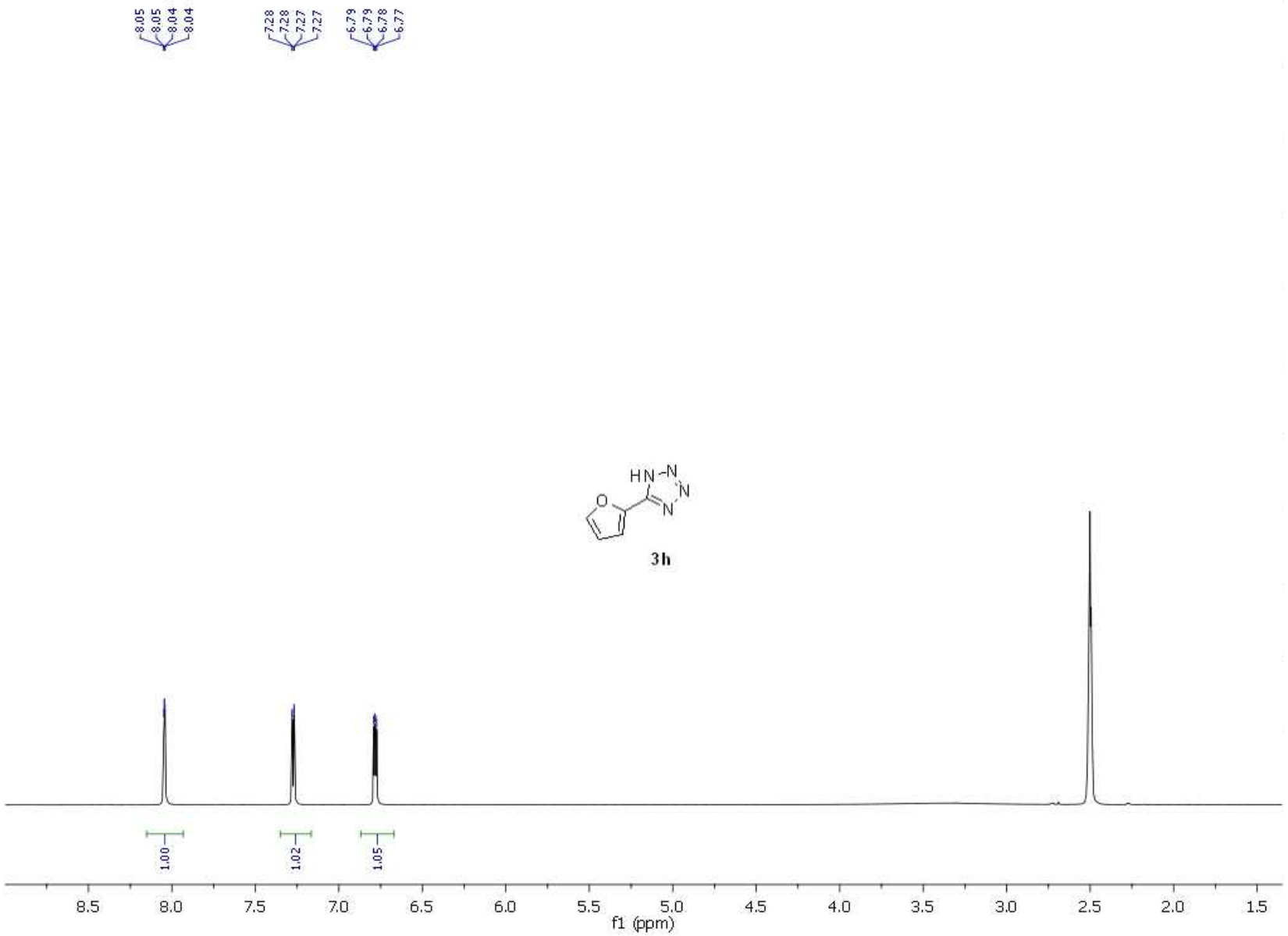
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)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8.04
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7.27
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6.79
6.78
6.77
HN
N
N
O
3h
1.00
1.02
1.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
f1 (ppm)

Complete Ref. 17

Gaussian 09, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Cartesian coordinates, energies, and imaginary frequency (transition states) for all the calculated structures.

H_2O

```
Sum of electronic and zero-point Energies=            -76.408132
 Sum of electronic and thermal Energies=               -76.405296
 Sum of electronic and thermal Enthalpies=             -76.404352
 Sum of electronic and thermal Free Energies=          -76.425778
```

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.117893
2	1	0	0.000000	0.760951	-0.471573
3	1	0	0.000000	-0.760951	-0.471573

HN_3

```
 Sum of electronic and zero-point Energies=           -164.743620
 Sum of electronic and thermal Energies=              -164.740415
 Sum of electronic and thermal Enthalpies=            -164.739471
 Sum of electronic and thermal Free Energies=         -164.766588
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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.229330	0.014952	-0.000036
2	7	0	0.109277	0.012713	-0.000003
3	7	0	-1.114369	-0.138801	0.000036
4	1	0	-1.569673	0.777945	0.000020

N_3^-

Sum of electronic and zero-point Energies= -164.297745
Sum of electronic and thermal Energies= -164.294771
Sum of electronic and thermal Enthalpies= -164.293827
Sum of electronic and thermal Free Energies= -164.314180

Standard orientation:

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1	7	0	-1.171087	0.000120	0.000032
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3	7	0	1.171086	0.000120	-0.000032

NH_3

Sum of electronic and zero-point Energies= -56.518338
Sum of electronic and thermal Energies= -56.515472
Sum of electronic and thermal Enthalpies= -56.514528
Sum of electronic and thermal Free Energies= -56.536372

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.000000	0.115024
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3	1	0	-0.814581	-0.470298	-0.268390
4	1	0	0.814581	-0.470298	-0.268390

MeCN

Sum of electronic and zero-point Energies= -132.697500
Sum of electronic and thermal Energies= -132.693934
Sum of electronic and thermal Enthalpies= -132.692990
Sum of electronic and thermal Free Energies= -132.721475

Standard orientation:

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3	6	0	1.175443	-0.000079	0.000098
4	1	0	1.539006	-0.590628	0.841322
5	1	0	1.538447	-0.433891	-0.931848
6	1	0	1.538918	1.023741	0.090441

PhCN

Sum of electronic and zero-point Energies= -324.350398
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Sum of electronic and thermal Enthalpies= -324.343401
Sum of electronic and thermal Free Energies= -324.380618

Standard orientation:

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1	6	0	-1.475818	1.209067	-0.000154
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6	6	0	-2.167650	0.000008	-0.000197
7	1	0	-2.017979	2.147007	-0.000194
8	1	0	0.464295	2.149479	-0.000020
9	1	0	0.464189	-2.149547	-0.000026
10	1	0	-2.018004	-2.146981	-0.000196
11	1	0	-3.251610	0.000044	-0.000251
12	6	0	2.035964	-0.000060	0.000235
13	7	0	3.186783	0.000040	0.000393

AcOH

Sum of electronic and zero-point Energies= -229.013437
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Sum of electronic and thermal Enthalpies= -229.007984
Sum of electronic and thermal Free Energies= -229.040481

Standard orientation:

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3	8	0	-0.789090	-1.024767	-0.000254
4	1	0	-1.733063	-0.799657	-0.000637
5	6	0	1.388605	-0.123216	-0.000096
6	1	0	1.662604	-0.705100	0.882123
7	1	0	1.661639	-0.705747	-0.882190
8	1	0	1.920225	0.824955	-0.000734

TS1 (R = Me)

Imaginary Freq.: -592.6803
Sum of electronic and zero-point Energies= -297.391884
Sum of electronic and thermal Energies= -297.385793
Sum of electronic and thermal Enthalpies= -297.384849
Sum of electronic and thermal Free Energies= -297.421331

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	2.140143	0.197536	-0.013049
4	1	0	2.254877	0.854669	-0.876097
5	1	0	2.296557	0.785915	0.891859
6	1	0	2.875695	-0.603605	-0.061831
7	7	0	-1.462359	0.547078	-0.017068
8	7	0	-1.864962	-0.527168	-0.018558
9	7	0	0.121039	-1.378085	0.003780
10	1	0	-0.218147	1.996628	-0.346520

TS1 (R = Ph)

Imaginary Freq.: -558.2118
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Sum of electronic and thermal Energies= -489.039188
Sum of electronic and thermal Enthalpies= -489.038243
Sum of electronic and thermal Free Energies= -489.082935

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	7	0	-3.588487	-0.330970	-0.027924
5	7	0	-1.716684	-1.382707	-0.387471
6	1	0	-1.618918	1.749491	0.929452
7	6	0	0.485211	-0.195589	-0.071785
8	6	0	0.991851	1.093151	-0.244424
9	6	0	1.355669	-1.265341	0.162205
10	6	0	2.364689	1.307924	-0.182740
11	1	0	0.326066	1.923341	-0.446529
12	6	0	2.724141	-1.040665	0.231280
13	1	0	0.952040	-2.262767	0.291568
14	6	0	3.230711	0.245645	0.057924
15	1	0	2.756519	2.308404	-0.323822

16	1	0	3.395647	-1.870285	0.419116
17	1	0	4.299472	0.419090	0.108724

TS1′ (R = Me)

Imaginary Freq.: -617.0397
Sum of electronic and zero-point Energies= -297.376624
Sum of electronic and thermal Energies= -297.370708
Sum of electronic and thermal Enthalpies= -297.369764
Sum of electronic and thermal Free Energies= -297.405891

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	6	0	-2.171624	-0.171318	-0.002853
4	1	0	-2.883184	0.652549	-0.006043
5	1	0	-2.317328	-0.793257	-0.887160
6	1	0	-2.326494	-0.794220	0.878978
7	7	0	1.337617	-0.705440	-0.016868
8	7	0	1.748803	0.466793	0.129219
9	7	0	-0.100732	1.323168	-0.010742
10	1	0	2.379381	0.767185	-0.622876

TS1′ (R = Ph)

Imaginary Freq.: -580.7466
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Sum of electronic and thermal Energies= -489.023584
Sum of electronic and thermal Enthalpies= -489.022640
Sum of electronic and thermal Free Energies= -489.066967

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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3	7	0	2.960984	-0.771596	0.005713
4	7	0	3.474722	0.358545	-0.118957
5	7	0	1.701320	1.364896	0.027503
6	1	0	4.102679	0.599156	0.657108
7	6	0	-0.508094	0.172899	-0.000134
8	6	0	-1.020808	-1.124881	0.010686
9	6	0	-1.379329	1.270158	-0.009738
10	6	0	-2.398327	-1.320837	0.012390
11	1	0	-0.354617	-1.976416	0.019133
12	6	0	-2.751558	1.064920	-0.009265
13	1	0	-0.972586	2.274577	-0.017824

14	6	0	-3.263366	-0.231528	0.001867
15	1	0	-2.793404	-2.329798	0.021243
16	1	0	-3.421932	1.916362	-0.016704
17	1	0	-4.335527	-0.391085	0.002557

3 (R = Me)

Sum of electronic and zero-point Energies= -297.481653
Sum of electronic and thermal Energies= -297.476542
Sum of electronic and thermal Enthalpies= -297.475598
Sum of electronic and thermal Free Energies= -297.510766

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	7	0	0.183002	-1.131052	-0.000182
5	6	0	-0.592745	-0.064192	-0.000245
6	6	0	-2.075110	-0.022579	0.000123
7	1	0	-2.458666	-1.041379	-0.009194
8	1	0	-2.440001	0.491545	0.890663
9	1	0	-2.440136	0.507866	-0.880702
10	1	0	-0.020410	1.992589	-0.000152

3 (R = Ph)

Sum of electronic and zero-point Energies= -489.139116
Sum of electronic and thermal Energies= -489.131337
Sum of electronic and thermal Enthalpies= -489.130393
Sum of electronic and thermal Free Energies= -489.172666

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.802037	-1.120141	-0.139815
2	7	0	3.074284	-0.690753	-0.084440
3	7	0	3.126104	0.580326	0.073999
4	7	0	1.864329	1.003205	0.124749
5	6	0	1.040802	-0.048209	-0.007467
6	6	0	-0.424738	-0.010557	-0.002647
7	6	0	-1.129201	-1.215024	0.069127
8	6	0	-1.115711	1.201245	-0.074204
9	6	0	-2.517964	-1.203721	0.071536
10	1	0	-0.586580	-2.151182	0.127793
11	6	0	-2.505543	1.204217	-0.070301
12	1	0	-0.582293	2.143099	-0.142590
13	6	0	-3.207876	0.004409	0.002286
14	1	0	-3.062207	-2.139037	0.129628

15	1	0	-3.039000	2.145628	-0.128781
16	1	0	-4.291800	0.010763	0.004095
17	1	0	1.655991	1.988110	0.258438

3 (R = Ph)(Gas Phase)

Sum of electronic and zero-point Energies= -489.115877
Sum of electronic and thermal Energies= -489.108000
Sum of electronic and thermal Enthalpies= -489.107056
Sum of electronic and thermal Free Energies= -489.149743

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.795620	-1.107441	-0.202100
2	7	0	3.073600	-0.684834	-0.117023
3	7	0	3.132890	0.571390	0.111527
4	7	0	1.864556	0.999143	0.179510
5	6	0	1.039609	-0.047972	-0.015738
6	6	0	-0.424601	-0.008796	-0.010910
7	6	0	-1.126290	-1.211021	0.093811
8	6	0	-1.120713	1.196077	-0.113773
9	6	0	-2.514059	-1.201079	0.105537
10	1	0	-0.569971	-2.137645	0.165791
11	6	0	-2.509836	1.200339	-0.098573
12	1	0	-0.588923	2.134880	-0.225901
13	6	0	-3.207801	0.002436	0.012664
14	1	0	-3.056228	-2.135071	0.189087
15	1	0	-3.045777	2.137905	-0.181351
16	1	0	-4.290977	0.006601	0.023199
17	1	0	1.667350	1.965618	0.387670

3′ (R = Me)

Sum of electronic and zero-point Energies= -297.478103
Sum of electronic and thermal Energies= -297.472909
Sum of electronic and thermal Enthalpies= -297.471965
Sum of electronic and thermal Free Energies= -297.508298

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.134019	1.119212	-0.000196
2	7	0	1.382558	0.746815	0.000164
3	7	0	1.369995	-0.556251	0.000062
4	7	0	0.166434	-1.089688	-0.000040
5	6	0	-0.606370	-0.014651	-0.000330
6	6	0	-2.092340	-0.037254	0.000150
7	1	0	-2.447001	-1.067054	-0.010055

8	1	0	-2.477878	0.463506	0.889705
9	1	0	-2.478598	0.481651	-0.878574
10	1	0	2.224688	-1.107283	0.000078

3′ (R = Ph)

Sum of electronic and zero-point Energies= -489.130442
Sum of electronic and thermal Energies= -489.123450
Sum of electronic and thermal Enthalpies= -489.122506
Sum of electronic and thermal Free Energies= -489.162944

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.792708	-0.000176	1.087639
2	7	0	-3.003737	-0.000272	0.576527
3	7	0	-3.041057	0.000060	-0.727034
4	7	0	-1.800286	0.000414	-1.124652
5	6	0	-1.041750	0.000253	-0.003861
6	6	0	0.438617	0.000228	0.001114
7	6	0	1.136089	-1.208335	0.001928
8	6	0	1.136475	1.208556	0.002285
9	6	0	2.527370	-1.206011	0.006133
10	1	0	0.591616	-2.146071	0.000253
11	6	0	2.527758	1.205716	0.006389
12	1	0	0.592322	2.146464	0.000883
13	6	0	3.223279	-0.000261	0.008903
14	1	0	3.066776	-2.146072	0.008145
15	1	0	3.067487	2.145593	0.008550
16	1	0	4.307352	-0.000438	0.012950
17	1	0	-3.848068	-0.000532	1.144518

3′ (R = Ph) (Gas Phase)

Sum of electronic and zero-point Energies= -489.120021
Sum of electronic and thermal Energies= -489.112251
Sum of electronic and thermal Enthalpies= -489.111307
Sum of electronic and thermal Free Energies= -489.153694

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.791452	-1.122555	0.000057
2	7	0	-3.027973	-0.739453	-0.000055
3	7	0	-2.997173	0.573229	0.000132
4	7	0	-1.788124	1.096002	-0.000085
5	6	0	-1.033626	0.006159	-0.000102
6	6	0	0.433580	0.008744	-0.000064
7	6	0	1.126453	-1.201992	-0.000035

8	6	0	1.134868	1.215219	-0.000008
9	6	0	2.515760	-1.202413	0.000033
10	1	0	0.569335	-2.130949	-0.000153
11	6	0	2.523341	1.207730	-0.000007
12	1	0	0.586012	2.149382	-0.000049
13	6	0	3.215925	0.000037	0.000075
14	1	0	3.052883	-2.143192	0.000049
15	1	0	3.066565	2.145033	-0.000050
16	1	0	4.299367	-0.003263	0.000154
17	1	0	-3.838918	1.131524	0.000339

TS2 (R = Me)

Imaginary Freq.: -482.7628
Sum of electronic and zero-point Energies= -296.947494
Sum of electronic and thermal Energies= -296.941887
Sum of electronic and thermal Enthalpies= -296.940943
Sum of electronic and thermal Free Energies= -296.976739

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.681082	0.281484	0.000036
2	7	0	0.233727	-1.081736	-0.000005
3	6	0	-2.104601	-0.198920	-0.000008
4	1	0	-2.287563	-0.818353	-0.880600
5	1	0	-2.287872	-0.817698	0.880979
6	1	0	-2.795899	0.642691	-0.000405
7	7	0	1.375008	-0.608099	-0.000007
8	7	0	1.955396	0.401055	0.000008
9	7	0	-0.123354	1.359920	-0.000017

TS2 (R = Ph)

Imaginary Freq.: -422.6281
Sum of electronic and zero-point Energies= -488.607676
Sum of electronic and thermal Energies= -488.599336
Sum of electronic and thermal Enthalpies= -488.598392
Sum of electronic and thermal Free Energies= -488.642094

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.037602	0.382797	0.064688
2	7	0	-1.799987	-1.033714	-0.185751
3	7	0	-2.981760	-0.682619	-0.130328
4	7	0	-3.681648	0.229560	0.024144
5	7	0	-1.693985	1.393790	0.235207
6	6	0	0.433214	0.140484	0.022256

7	6	0	0.988316	-1.138408	0.112970
8	6	0	1.286665	1.243806	-0.090518
9	6	0	2.370740	-1.307583	0.096022
10	1	0	0.338185	-1.998670	0.202577
11	6	0	2.665201	1.072238	-0.114817
12	1	0	0.856275	2.236216	-0.161495
13	6	0	3.212807	-0.206057	-0.020029
14	1	0	2.788772	-2.305071	0.174037
15	1	0	3.314004	1.936233	-0.205755
16	1	0	4.288377	-0.341489	-0.035691

5 (R = Me)

Sum of electronic and zero-point Energies= -297.033112
Sum of electronic and thermal Energies= -297.028993
Sum of electronic and thermal Enthalpies= -297.028048
Sum of electronic and thermal Free Energies= -297.060635

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.193801	1.100207	-0.004003
2	7	0	-1.453380	0.650743	0.004042
3	7	0	-1.452316	-0.652270	0.004262
4	7	0	-0.192735	-1.099920	-0.004136
5	6	0	0.563749	0.000822	-0.008034
6	6	0	2.056298	0.000214	0.003765
7	1	0	2.450583	-0.726973	-0.708313
8	1	0	2.434249	0.988376	-0.260657
9	1	0	2.440504	-0.258941	0.993422

5 (R = Ph)

Sum of electronic and zero-point Energies= -488.695927
Sum of electronic and thermal Energies= -488.688309
Sum of electronic and thermal Enthalpies= -488.687365
Sum of electronic and thermal Free Energies= -488.729463

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.844588	-1.098720	0.082891
2	7	0	-3.098613	-0.651979	0.048761
3	7	0	-3.098664	0.651995	-0.048865
4	7	0	-1.844622	1.098686	-0.082855
5	6	0	-1.087601	-0.000010	0.000074
6	6	0	0.384444	-0.000002	0.000047
7	6	0	1.092687	1.205065	0.038603
8	6	0	1.092697	-1.205062	-0.038556

9	6	0	2.483339	1.203358	0.038153
10	1	0	0.548428	2.141870	0.072325
11	6	0	2.483349	-1.203345	-0.038187
12	1	0	0.548442	-2.141870	-0.072259
13	6	0	3.184021	0.000011	-0.000040
14	1	0	3.021398	2.144206	0.070281
15	1	0	3.021416	-2.144187	-0.070352
16	1	0	4.268107	0.000016	-0.000078

$INT_{1\rightarrow3}$ (R = Me)

Sum of electronic and zero-point Energies= -297.447060
Sum of electronic and thermal Energies= -297.440993
Sum of electronic and thermal Enthalpies= -297.440048
Sum of electronic and thermal Free Energies= -297.476909

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.762207	0.143719	-0.000016
2	7	0	0.294108	-0.814279	-0.000528
3	6	0	-2.097157	-0.531578	0.000208
4	1	0	-2.189733	-1.164826	0.885400
5	1	0	-2.896739	0.207319	-0.006057
6	1	0	-2.185335	-1.175596	-0.877543
7	7	0	1.423872	-0.298712	-0.000158
8	7	0	2.467645	0.091541	0.000447
9	7	0	-0.500967	1.383741	-0.000123
10	1	0	-1.364615	1.924227	-0.000416

$INT_{1\rightarrow3}$ (R = Ph)

Sum of electronic and zero-point Energies= -489.104583
Sum of electronic and thermal Energies= -489.095668
Sum of electronic and thermal Enthalpies= -489.094724
Sum of electronic and thermal Free Energies= -489.139912

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.965193	0.447313	0.088251
2	7	0	1.747398	-0.692569	-0.242854
3	7	0	2.968472	-0.488068	-0.150105
4	7	0	4.075752	-0.381028	-0.092163
5	7	0	1.530677	1.541739	0.393167
6	1	0	0.848635	2.259637	0.630697
7	6	0	-0.493397	0.156540	0.022751
8	6	0	-0.962821	-1.149290	0.184802
9	6	0	-1.403401	1.197319	-0.181447

10	6	0	-2.329331	-1.406442	0.163771
11	1	0	-0.260204	-1.958813	0.341208
12	6	0	-2.767055	0.933708	-0.215479
13	1	0	-1.052539	2.212051	-0.334240
14	6	0	-3.232584	-0.367096	-0.037842
15	1	0	-2.687577	-2.419766	0.303135
16	1	0	-3.466684	1.743698	-0.385432
17	1	0	-4.297342	-0.569632	-0.060526

TS3 (R = Me)

Imaginary Freq.: -406.5686
Sum of electronic and zero-point Energies= -297.399724
Sum of electronic and thermal Energies= -297.393682
Sum of electronic and thermal Enthalpies= -297.392738
Sum of electronic and thermal Free Energies= -297.429245

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.963789	0.423750	0.000077
2	7	0	0.486135	-1.282861	0.000490
3	6	0	-2.190446	-0.355326	-0.000211
4	1	0	-2.217015	-0.981346	-0.891793
5	1	0	-2.216355	-0.983638	0.889748
6	1	0	-3.029973	0.342986	0.000973
7	7	0	1.378247	-0.531602	-0.000286
8	7	0	2.093215	0.395854	-0.000253
9	7	0	-0.302089	1.394191	0.000192
10	1	0	0.800198	1.382380	0.000880

TS4 (R = Me)

Imaginary Freq.: -337.3674
Sum of electronic and zero-point Energies= -373.817324
Sum of electronic and thermal Energies= -373.807979
Sum of electronic and thermal Enthalpies= -373.807035
Sum of electronic and thermal Free Energies= -373.851767

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.124171	-0.678192	-0.006040
2	7	0	0.952542	1.441089	0.029059
3	6	0	2.583678	-0.719614	0.006624
4	1	0	2.958440	-0.193118	-0.870592
5	1	0	2.942656	-0.217211	0.904304
6	1	0	2.897055	-1.764235	-0.004613
7	7	0	-0.225775	1.512623	0.004311

8	7	0	-1.380955	1.477845	-0.022770
9	7	0	0.077626	-1.189089	-0.024717
10	1	0	-2.688161	-0.191435	0.059642
11	1	0	-0.990730	-1.214962	-0.023931
12	8	0	-2.530643	-1.139604	-0.066921
13	1	0	-3.085275	-1.612639	0.565875

TS4 (R = Ph)

Imaginary Freq.: -281.3093
Sum of electronic and zero-point Energies= -565.469269
Sum of electronic and thermal Energies= -565.457142
Sum of electronic and thermal Enthalpies= -565.456198
Sum of electronic and thermal Free Energies= -565.508958

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.424315	-0.335452	0.091440
2	7	0	-1.079081	1.730657	-0.308493
3	7	0	-2.232308	1.495293	-0.260221
4	7	0	-3.338979	1.161267	-0.192363
5	7	0	-1.367737	-1.007234	0.195744
6	1	0	-4.226819	-0.708859	0.105013
7	1	0	-2.407676	-1.318108	0.214040
8	8	0	-3.861092	-1.606333	0.158421
9	1	0	-4.299093	-2.057805	0.891762
10	6	0	1.011728	-0.172024	0.047502
11	6	0	1.743321	-1.319440	-0.287928
12	6	0	1.651958	1.027097	0.361641
13	6	0	3.128611	-1.252271	-0.318103
14	1	0	1.223979	-2.240994	-0.523140
15	6	0	3.039137	1.072499	0.341644
16	1	0	1.065811	1.898603	0.616640
17	6	0	3.774816	-0.059479	-0.002064
18	1	0	3.702293	-2.131678	-0.585259
19	1	0	3.547832	1.996242	0.589604
20	1	0	4.857597	-0.012200	-0.023487

TS5 (R = Me)

Imaginary Freq.: -593.6290
Sum of electronic and zero-point Energies= -353.943184
Sum of electronic and thermal Energies= -353.934047
Sum of electronic and thermal Enthalpies= -353.933103
Sum of electronic and thermal Free Energies= -353.977787

Standard orientation:

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.077338	-0.477312	0.019071
2	7	0	-0.959296	1.161391	-0.069239
3	6	0	-2.557652	-0.715026	-0.014072
4	1	0	-3.039714	-0.210403	0.825825
5	1	0	-2.980078	-0.305165	-0.934010
6	1	0	-2.757630	-1.784519	0.035566
7	7	0	0.203481	1.481999	-0.005697
8	7	0	1.315059	1.696037	0.062733
9	7	0	-0.100615	-1.194068	0.088061
10	1	0	2.819128	-0.629155	-0.863881
11	1	0	1.323238	-1.101997	0.026136
12	7	0	2.498033	-1.144298	-0.045055
13	1	0	2.916556	-0.717360	0.780769
14	1	0	2.831798	-2.104797	-0.116019

TS5 (R = Ph)

Imaginary Freq.: -154.0027
Sum of electronic and zero-point Energies= -545.600780
Sum of electronic and thermal Energies= -545.588705
Sum of electronic and thermal Enthalpies= -545.587761
Sum of electronic and thermal Free Energies= -545.640893

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.500590	0.103661	-0.000016
2	7	0	0.983636	-1.483266	0.000045
3	7	0	2.188298	-1.505041	0.000037
4	7	0	3.320043	-1.415484	0.000025
5	7	0	1.303344	1.009990	-0.000056
6	1	0	4.378069	1.240306	-0.827599
7	1	0	2.855354	1.326708	-0.000034
8	6	0	-0.992656	0.073791	-0.000005
9	6	0	-1.656674	1.305733	0.000039
10	6	0	-1.743772	-1.103172	-0.000045
11	6	0	-3.044199	1.359655	0.000044
12	1	0	-1.070551	2.217405	0.000071
13	6	0	-3.135669	-1.046031	-0.000042
14	1	0	-1.243455	-2.062162	-0.000084
15	6	0	-3.789514	0.181431	0.000003
16	1	0	-3.546024	2.320737	0.000083
17	1	0	-3.708416	-1.966619	-0.000075
18	1	0	-4.872951	0.221996	0.000006
19	7	0	3.916524	1.618976	-0.000020
20	1	0	4.377888	1.240955	0.827956
21	1	0	4.018528	2.634042	-0.000418

TS6 (R = Me)

Imaginary Freq.: -440.5758
Sum of electronic and zero-point Energies= -461.717432
Sum of electronic and thermal Energies= -461.707665
Sum of electronic and thermal Enthalpies= -461.706721
Sum of electronic and thermal Free Energies= -461.754415

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.579232	0.430932	-0.220477
2	7	0	2.264446	0.808980	0.119021
3	7	0	2.839379	-0.239255	0.227165
4	7	0	3.284159	-1.285783	0.308871
5	7	0	0.251885	-0.719282	-0.318422
6	1	0	-1.229940	-0.925590	-0.545866
7	6	0	-0.014288	1.798626	-0.285930
8	7	0	-2.344121	-1.056985	-0.685292
9	7	0	-2.956491	-0.399427	0.127707
10	7	0	-3.580402	0.196002	0.861667
11	1	0	0.498182	2.393210	-1.043642
12	1	0	-1.074344	1.724710	-0.533068
13	1	0	0.104445	2.300575	0.675997

TS6 (R = Ph)

Imaginary Freq.: -277.3090
Sum of electronic and zero-point Energies= -653.376091
Sum of electronic and thermal Energies= -653.363247
Sum of electronic and thermal Enthalpies= -653.362302
Sum of electronic and thermal Free Energies= -653.417597

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.185687	-0.114331	-0.285980
2	7	0	2.326791	1.115589	0.173290
3	7	0	3.412213	0.599797	0.153830
4	7	0	4.386831	0.012512	0.101441
5	7	0	1.551932	-1.233276	-0.528589
6	1	0	0.205338	-2.263769	-0.424909
7	6	0	-0.121511	0.588180	-0.259473
8	6	0	-1.059713	0.267961	-1.244829
9	6	0	-0.465888	1.469538	0.765609
10	6	0	-2.336531	0.816551	-1.195963
11	1	0	-0.783606	-0.411920	-2.043494
12	6	0	-1.750582	2.001132	0.820903
13	1	0	0.265419	1.721327	1.524228
14	6	0	-2.687194	1.675880	-0.157065
15	1	0	-3.058470	0.569190	-1.966066
16	1	0	-2.020716	2.669358	1.630715
17	1	0	-3.686642	2.093647	-0.112021

18	7	0	-0.679877	-2.844030	-0.228017
19	7	0	-1.391647	-2.252279	0.567812
20	7	0	-2.107234	-1.770786	1.293422

TS7 (R = Me)

Imaginary Freq.:-615.4071
Sum of electronic and zero-point Energies= -526.402062
Sum of electronic and thermal Energies= -526.390207
Sum of electronic and thermal Enthalpies= -526.389263
Sum of electronic and thermal Free Energies= -526.442528

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.040121	-0.708470	-0.038198
2	7	0	0.904128	-0.650967	-0.396820
3	7	0	0.656323	1.365528	-0.535877
4	7	0	1.750087	1.629035	-0.005639
5	7	0	2.706655	1.016217	0.274624
6	8	0	-1.839183	-1.121866	-0.367881
7	6	0	-2.518351	-0.074458	0.081791
8	8	0	-1.989141	0.980679	0.368969
9	6	0	-3.986106	-0.340555	0.198205
10	6	0	3.168151	-1.605189	0.292885
11	1	0	-0.872820	-0.923895	-0.407652
12	1	0	-0.177215	1.609959	0.022065
13	1	0	-4.149553	-1.129135	0.936226
14	1	0	-4.371839	-0.696332	-0.758758
15	1	0	-4.507385	0.563833	0.501736
16	1	0	3.475626	-1.420148	1.323142
17	1	0	2.873800	-2.645929	0.170680
18	1	0	4.012738	-1.375512	-0.358250

TS7 (R = Ph)

Imaginary Freq.: -582.9740
Sum of electronic and zero-point Energies= -718.057676
Sum of electronic and thermal Energies= -718.043254
Sum of electronic and thermal Enthalpies= -718.042310
Sum of electronic and thermal Free Energies= -718.101248

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.617993	0.406154	-0.260522
2	7	0	-0.482651	0.011939	-0.506620
3	7	0	-1.492434	1.779576	-0.665253
4	7	0	-0.536907	2.458291	-0.257889

5	7	0	0.600299	2.287397	-0.059287
6	8	0	-2.884562	-1.383018	-0.331014
7	6	0	-3.838637	-0.668254	0.251606
8	8	0	-3.685501	0.490841	0.583095
9	6	0	-5.103347	-1.442794	0.448512
10	1	0	-2.051428	-0.861100	-0.413566
11	1	0	-2.296130	1.719414	-0.017600
12	1	0	-5.463396	-1.800121	-0.518333
13	1	0	-5.857241	-0.817227	0.919497
14	1	0	-4.898274	-2.316757	1.070239
15	6	0	1.988284	-0.067917	-0.065904
16	6	0	2.299339	-1.359048	-0.509227
17	6	0	2.961836	0.717230	0.552849
18	6	0	3.584484	-1.854252	-0.339629
19	1	0	1.533937	-1.958679	-0.988033
20	6	0	4.244019	0.207388	0.728064
21	1	0	2.719934	1.712935	0.900251
22	6	0	4.557490	-1.072184	0.280176
23	1	0	3.826880	-2.851431	-0.687749
24	1	0	4.999194	0.814417	1.213299
25	1	0	5.560105	-1.462392	0.413143

TS8 (R = Me)

Imaginary Freq.: -452.2804
Sum of electronic and zero-point Energies= -526.428733
Sum of electronic and thermal Energies= -526.416535
Sum of electronic and thermal Enthalpies= -526.415591
Sum of electronic and thermal Free Energies= -526.470110

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.197048	-0.831900	0.008759
2	7	0	-1.072940	-1.103897	-0.146194
3	7	0	-0.276616	1.762312	-0.309752
4	7	0	-1.388743	1.550851	-0.076784
5	7	0	-2.494642	1.209509	0.136303
6	8	0	1.551646	-0.999137	-0.274695
7	6	0	2.475082	-0.255220	0.023911
8	8	0	2.303406	1.021383	0.298016
9	6	0	3.898773	-0.696440	0.090214
10	6	0	-3.593665	-1.235691	0.168317
11	1	0	-0.035869	-0.928435	-0.231715
12	1	0	1.360108	1.281090	0.162900
13	1	0	4.363120	-0.321070	1.002660
14	1	0	4.432079	-0.262576	-0.759960
15	1	0	3.959573	-1.780729	0.045232
16	1	0	-4.183144	-0.792692	-0.633893
17	1	0	-3.643184	-2.324289	0.131071
18	1	0	-3.961366	-0.865181	1.124911

TS8 (R = Ph)

Imaginary Freq.: -249.9418
Sum of electronic and zero-point Energies= -718.081039
Sum of electronic and thermal Energies= -718.066237
Sum of electronic and thermal Enthalpies= -718.065293
Sum of electronic and thermal Free Energies= -718.125626

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.682875	0.046171	-0.087041
2	7	0	0.366957	-0.452359	-0.180060
3	7	0	1.836322	2.040165	-0.243270
4	7	0	0.696564	2.157159	-0.092269
5	7	0	-0.471525	2.145427	0.039604
6	8	0	2.843769	-1.177545	-0.195242
7	6	0	3.940986	-0.689874	0.048614
8	8	0	4.124885	0.596612	0.242160
9	6	0	5.186979	-1.501215	0.157807
10	1	0	1.415590	-0.651175	-0.208778
11	1	0	3.280515	1.097202	0.130242
12	1	0	4.972565	-2.547781	-0.041698
13	1	0	5.599026	-1.386381	1.162824
14	1	0	5.926753	-1.123370	-0.550450
15	6	0	-2.119386	-0.148639	-0.017156
16	6	0	-2.535309	-1.486683	-0.085744
17	6	0	-3.048403	0.884238	0.108627
18	6	0	-3.888410	-1.782510	-0.028264
19	1	0	-1.798839	-2.275479	-0.184840
20	6	0	-4.400719	0.570805	0.166146
21	1	0	-2.714805	1.910136	0.159814
22	6	0	-4.820605	-0.754498	0.097702
23	1	0	-4.214872	-2.814157	-0.081714
24	1	0	-5.128671	1.367101	0.264875
25	1	0	-5.878272	-0.988151	0.142211

TS9 (R = Ph)

Imaginary Freq.: -142.9814
Sum of electronic and zero-point Energies= -717.647388
Sum of electronic and thermal Energies= -717.632800
Sum of electronic and thermal Enthalpies= -717.631856
Sum of electronic and thermal Free Energies= -717.692368

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.527618	0.176060	-0.227926
2	7	0	0.401643	-0.543172	-0.507827

3	7	0	1.974371	2.208699	-0.163506
4	7	0	0.857762	2.060203	-0.026086
5	7	0	-0.314880	1.803851	0.094994
6	8	0	2.998203	-0.753418	-0.859761
7	6	0	3.740155	-0.734070	0.228764
8	8	0	3.291117	-0.684423	1.356232
9	6	0	5.214815	-0.778901	-0.074119
10	1	0	2.000783	-0.625349	-0.647396
11	1	0	5.500229	0.134427	-0.601617
12	1	0	5.436490	-1.621734	-0.731335
13	1	0	5.788166	-0.862370	0.846624
14	6	0	-1.994148	-0.068725	-0.078488
15	6	0	-2.424839	-1.400099	-0.107731
16	6	0	-2.940959	0.946646	0.070526
17	6	0	-3.773059	-1.710591	0.011935
18	1	0	-1.687291	-2.185949	-0.222817
19	6	0	-4.293954	0.633081	0.182839
20	1	0	-2.622343	1.980215	0.093922
21	6	0	-4.714389	-0.692508	0.156393
22	1	0	-4.090762	-2.747200	-0.006781
23	1	0	-5.020344	1.430558	0.293132
24	1	0	-5.767781	-0.932307	0.248317

TS10 (R = Ph)

Imaginary Freq.: -469.9221
Sum of electronic and zero-point Energies= -718.096179
Sum of electronic and thermal Energies= -718.082119
Sum of electronic and thermal Enthalpies= -718.081175
Sum of electronic and thermal Free Energies= -718.139495

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.667365	0.903866	0.029961
2	7	0	-0.540211	0.560478	0.230719
3	7	0	-1.309137	2.464739	0.089690
4	7	0	-0.235318	2.828017	-0.111097
5	7	0	0.925155	2.275082	-0.194554
6	8	0	-2.625911	-1.554973	0.363958
7	6	0	-3.613504	-0.932071	0.047056
8	8	0	-3.567938	0.365485	-0.276507
9	6	0	-4.997008	-1.491251	-0.039367
10	1	0	-0.795275	-0.405977	0.430475
11	1	0	-2.650318	0.680117	-0.207835
12	1	0	-4.998175	-2.528973	0.284161
13	1	0	-5.348524	-1.421425	-1.071090
14	1	0	-5.670372	-0.899530	0.583303
15	6	0	1.866932	0.032636	0.000057
16	6	0	3.137527	0.587403	0.171817
17	6	0	1.728734	-1.343653	-0.198024
18	6	0	4.259640	-0.232893	0.153039
19	1	0	3.244341	1.653343	0.328982

20	6	0	2.854880	-2.156607	-0.224458
21	1	0	0.748632	-1.782566	-0.348831
22	6	0	4.120936	-1.603359	-0.047248
23	1	0	5.242905	0.200741	0.293829
24	1	0	2.743143	-3.222182	-0.387028
25	1	0	4.998001	-2.240279	-0.065883

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Sum of electronic and zero-point Energies= -7417.907015
Sum of electronic and thermal Energies= -7417.890331
Sum of electronic and thermal Enthalpies= -7417.889387
Sum of electronic and thermal Free Energies= -7417.956266

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.762441	3.925103	0.167945
2	7	0	0.957963	2.900346	0.648496
3	7	0	1.159916	1.855576	1.178417
4	30	0	0.873059	0.088121	0.197320
5	35	0	-0.356267	-1.536004	1.548077
6	35	0	2.879784	-0.656310	-0.942826
7	6	0	-1.729867	0.260380	-1.137891
8	6	0	-2.404930	-0.746923	-2.033305
9	7	0	-2.600760	0.727785	-0.259232
10	6	0	-3.681976	-1.104493	-1.263102
11	1	0	-2.612686	-0.254922	-2.988922
12	6	0	-3.924365	0.111347	-0.355486
13	1	0	-4.532148	-1.303810	-1.912832
14	1	0	-4.271790	-0.165086	0.641360
15	8	0	-0.534135	0.625232	-1.224591
16	6	0	-2.297197	1.753737	0.718770
17	1	0	-1.905180	1.304151	1.635179
18	1	0	-1.563205	2.445268	0.304834
19	1	0	-3.212491	2.300815	0.945950
20	1	0	-4.627316	0.830813	-0.785698
21	1	0	-3.501707	-1.986618	-0.647226
22	1	0	-1.742126	-1.591066	-2.222605

7 (R = Me)

Sum of electronic and zero-point Energies= -7550.582308
Sum of electronic and thermal Energies= -7550.562051
Sum of electronic and thermal Enthalpies= -7550.561107
Sum of electronic and thermal Free Energies= -7550.635302

Standard orientation:

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

1	6	0	-1.227706	0.567056	-1.714047
2	7	0	-2.353837	1.415525	-2.339647
3	7	0	-2.235697	2.591915	-2.039384
4	7	0	-2.095515	3.667571	-1.738798
5	7	0	-0.334313	1.086523	-1.043536
6	30	0	1.022674	0.032032	-0.013272
7	35	0	2.224214	1.350637	1.671719
8	35	0	2.439685	-1.476192	-1.339103
9	6	0	-1.491229	-1.298078	1.140105
10	6	0	-2.302643	-2.566018	1.019756
11	7	0	-2.306791	-0.274972	1.386577
12	6	0	-3.747114	-2.073048	0.886982
13	1	0	-1.950881	-3.164713	0.179410
14	6	0	-3.713830	-0.663391	1.494675
15	1	0	-4.028234	-2.013874	-0.165282
16	1	0	-4.006015	-0.653442	2.549802
17	8	0	-0.249977	-1.246391	1.058824
18	6	0	-1.892361	1.065996	1.746448
19	1	0	-0.806329	1.111336	1.817283
20	1	0	-2.234869	1.783593	0.997156
21	1	0	-2.327606	1.322317	2.716318
22	1	0	-2.140429	-3.140371	1.937323
23	1	0	-4.464038	-2.714814	1.395995
24	1	0	-4.336078	0.052641	0.954661
25	6	0	-1.537119	-0.858233	-2.090076
26	1	0	-0.758940	-1.525227	-1.718944
27	1	0	-2.507403	-1.152498	-1.679830
28	1	0	-1.600963	-0.951993	-3.177435

7 (R = Ph)

Sum of electronic and zero-point Energies= -7742.244381
Sum of electronic and thermal Energies= -7742.221014
Sum of electronic and thermal Enthalpies= -7742.220069
Sum of electronic and thermal Free Energies= -7742.302691

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.544733	-2.093841	-0.122103
2	7	0	0.923225	-3.525743	0.227607
3	7	0	-0.025700	-4.127407	0.707673
4	7	0	-0.914780	-4.657821	1.145229
5	7	0	-0.596128	-1.657614	0.052179
6	30	0	-1.380143	0.169865	-0.129613
7	35	0	-2.914628	0.655220	1.735096
8	35	0	-2.259540	0.609898	-2.382111
9	6	0	1.239513	1.798809	0.569717
10	6	0	2.165477	2.891721	0.091627
11	7	0	1.815115	1.138932	1.573201
12	6	0	3.506022	2.577975	0.764373
13	1	0	2.200730	2.903299	-0.997836

14	6	0	3.135709	1.653339	1.934171
15	1	0	4.158609	2.049696	0.069845
16	1	0	3.060481	2.187395	2.886845
17	8	0	0.103259	1.604002	0.106933
18	6	0	1.174523	0.148227	2.413091
19	1	0	0.120920	0.062165	2.152432
20	1	0	1.661789	-0.823250	2.297974
21	1	0	1.254648	0.463896	3.456754
22	6	0	1.770790	-1.421864	-0.656112
23	6	0	3.040319	-1.706626	-0.147253
24	6	0	1.633002	-0.459015	-1.657808
25	6	0	4.154036	-1.017273	-0.617572
26	1	0	3.154705	-2.459299	0.624459
27	6	0	2.749836	0.212349	-2.143913
28	1	0	0.648529	-0.240698	-2.059820
29	6	0	4.011855	-0.060975	-1.620838
30	1	0	5.133938	-1.230623	-0.204774
31	1	0	2.634576	0.949222	-2.931278
32	1	0	4.882078	0.467175	-1.994971
33	1	0	1.739963	3.842530	0.427017
34	1	0	4.024005	3.471316	1.108987
35	1	0	3.832102	0.820699	2.057281

TS11 (R = Me)

Imaginary Freq.: -205.5774
Sum of electronic and zero-point Energies= -7550.579551
Sum of electronic and thermal Energies= -7550.559560
Sum of electronic and thermal Enthalpies= -7550.558616
Sum of electronic and thermal Free Energies= -7550.632253

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.210874	0.631775	1.699782
2	7	0	2.402424	1.953111	2.220209
3	7	0	1.944536	2.956674	1.758394
4	7	0	1.414315	3.844567	1.270057
5	7	0	0.271103	0.992032	1.067958
6	30	0	-1.069599	-0.074692	-0.037007
7	35	0	-2.165329	1.283914	-1.728781
8	35	0	-2.452060	-1.513400	1.353259
9	6	0	1.547997	-1.349504	-1.005410
10	6	0	2.347693	-2.599748	-0.727704
11	7	0	2.375322	-0.339216	-1.254161
12	6	0	3.772203	-2.233425	-1.157385
13	1	0	2.269212	-2.809755	0.343106
14	6	0	3.788475	-0.698587	-1.120092
15	1	0	4.535324	-2.662886	-0.510927
16	1	0	4.356554	-0.254396	-1.938821
17	8	0	0.301664	-1.295579	-0.988801
18	6	0	1.991553	1.019438	-1.581504
19	1	0	0.910717	1.079598	-1.702668

20	1	0	2.305637	1.703518	-0.789119
21	1	0	2.477095	1.308262	-2.516564
22	6	0	1.895818	-0.556237	2.265396
23	1	0	2.877332	-0.672823	1.800341
24	1	0	2.042444	-0.422824	3.337895
25	1	0	1.285806	-1.442287	2.083016
26	1	0	1.918734	-3.444912	-1.265864
27	1	0	3.951273	-2.574932	-2.177686
28	1	0	4.171567	-0.301592	-0.174517

TS11 (R = Ph)

Imaginary Freq.: -166.7308
Sum of electronic and zero-point Energies= -7742.240738
Sum of electronic and thermal Energies= -7742.218004
Sum of electronic and thermal Enthalpies= -7742.217060
Sum of electronic and thermal Free Energies= -7742.295729

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.055835	-0.495490	-1.344915
2	7	0	1.720020	-2.095087	-2.355065
3	7	0	0.706510	-2.692624	-2.520471
4	7	0	-0.322556	-3.193994	-2.625361
5	7	0	-0.109582	-0.500805	-1.179252
6	30	0	-1.553830	0.312906	0.036888
7	35	0	-3.519722	-1.050212	0.371857
8	35	0	-1.836155	2.646537	-0.565144
9	6	0	0.724274	-0.249788	1.974894
10	6	0	1.817054	0.480120	2.715917
11	7	0	1.144209	-1.468320	1.653100
12	6	0	3.071026	-0.349499	2.424386
13	1	0	1.875604	1.519231	2.393000
14	6	0	2.521457	-1.738672	2.071002
15	1	0	3.598903	0.067482	1.565587
16	1	0	2.506741	-2.419026	2.928211
17	8	0	-0.409996	0.221504	1.747193
18	6	0	0.319656	-2.546384	1.143502
19	1	0	-0.705213	-2.202846	1.009103
20	1	0	0.713210	-2.905206	0.189836
21	1	0	0.328791	-3.368273	1.864632
22	6	0	2.295235	0.243960	-1.084183
23	6	0	3.578793	-0.260060	-1.298034
24	6	0	2.126090	1.532408	-0.557105
25	6	0	4.684626	0.525600	-0.989743
26	1	0	3.705749	-1.253537	-1.702657
27	6	0	3.237097	2.309261	-0.255509
28	1	0	1.125551	1.922062	-0.396345
29	6	0	4.518411	1.807828	-0.472754
30	1	0	5.680873	0.131618	-1.154125
31	1	0	3.100678	3.305532	0.149643
32	1	0	5.385545	2.414214	-0.236201

33	1	0	1.544847	0.466502	3.776625
34	1	0	3.759664	-0.389950	3.266417
35	1	0	3.062105	-2.218282	1.251739

TS12 (R = Me)

Imaginary Freq.: -361.4371
Sum of electronic and zero-point Energies= -7550.570161
Sum of electronic and thermal Energies= -7550.550842
Sum of electronic and thermal Enthalpies= -7550.549898
Sum of electronic and thermal Free Energies= -7550.621894

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.152235	0.705232	1.806170
2	7	0	2.053536	1.737004	2.473690
3	7	0	1.535300	2.826806	2.136440
4	7	0	0.672856	3.286971	1.531544
5	7	0	0.192414	1.080144	1.127009
6	30	0	-0.995301	-0.044367	-0.044046
7	35	0	-2.324037	1.203193	-1.666940
8	35	0	-2.173237	-1.784448	1.220518
9	6	0	1.686729	-1.065937	-1.131738
10	6	0	2.534003	-2.304713	-0.958950
11	7	0	2.475628	-0.000104	-1.239724
12	6	0	3.959090	-1.829066	-1.262715
13	1	0	2.411077	-2.651662	0.070843
14	6	0	3.895077	-0.307664	-1.061063
15	1	0	4.708091	-2.291198	-0.622112
16	1	0	4.485572	0.247466	-1.791539
17	8	0	0.441061	-1.064351	-1.163499
18	6	0	2.037817	1.364713	-1.451551
19	1	0	0.961579	1.382486	-1.618478
20	1	0	2.280201	1.982304	-0.583202
21	1	0	2.547248	1.767465	-2.330253
22	6	0	1.691386	-0.665244	2.112816
23	1	0	2.690246	-0.774907	1.680786
24	1	0	1.785634	-0.797088	3.193062
25	1	0	1.027724	-1.431902	1.713272
26	1	0	2.175269	-3.092911	-1.620928
27	1	0	4.210509	-2.047810	-2.301545
28	1	0	4.205816	-0.002146	-0.056307

TS12 (R = Ph)

Imaginary Freq.: -356.6233
Sum of electronic and zero-point Energies= -7742.233773
Sum of electronic and thermal Energies= -7742.211547
Sum of electronic and thermal Enthalpies= -7742.210603
Sum of electronic and thermal Free Energies= -7742.288859

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.063388	-0.548439	-1.588877
2	7	0	1.521992	-1.649374	-2.553514
3	7	0	0.460237	-2.253473	-2.809644
4	7	0	-0.667750	-2.282956	-2.591931
5	7	0	-0.126442	-0.472185	-1.283859
6	30	0	-1.442184	0.272889	0.023847
7	35	0	-3.446733	-1.090054	0.313843
8	35	0	-1.832789	2.678461	-0.208809
9	6	0	0.798507	-0.485829	1.927889
10	6	0	1.912806	0.158698	2.716206
11	7	0	1.200151	-1.676716	1.490938
12	6	0	3.151045	-0.644565	2.310586
13	1	0	1.971528	1.225053	2.501074
14	6	0	2.577535	-1.997756	1.868689
15	1	0	3.643033	-0.160420	1.465404
16	1	0	2.564827	-2.735364	2.678071
17	8	0	-0.330968	0.015123	1.764192
18	6	0	0.355232	-2.688667	0.889443
19	1	0	-0.660459	-2.310006	0.782324
20	1	0	0.744660	-2.969509	-0.092112
21	1	0	0.345004	-3.573101	1.532968
22	6	0	2.234961	0.271892	-1.158806
23	6	0	3.550843	-0.119202	-1.425092
24	6	0	2.004258	1.468074	-0.472359
25	6	0	4.615504	0.676560	-1.011630
26	1	0	3.740957	-1.042807	-1.955829
27	6	0	3.070235	2.261735	-0.063394
28	1	0	0.985501	1.786461	-0.276010
29	6	0	4.379307	1.868555	-0.331996
30	1	0	5.632006	0.363637	-1.222515
31	1	0	2.876972	3.189755	0.463461
32	1	0	5.210821	2.488058	-0.014813
33	1	0	3.101457	-2.428042	1.012093
34	1	0	3.874732	-0.753694	3.116629
35	1	0	1.666451	0.034665	3.776227

$AlCl_3$-N_3^- Complex

Sum of electronic and zero-point Energies= -899.412956
Sum of electronic and thermal Energies= -899.398831
Sum of electronic and thermal Enthalpies= -899.397887
Sum of electronic and thermal Free Energies= -899.460196

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.774590	1.346469	0.755015

2	7	0	0.311038	2.209335	1.451269
3	7	0	-0.066779	3.041492	2.118711
4	13	0	-0.000834	0.000055	-0.242339
5	7	0	-1.376719	0.657316	-1.282735
6	7	0	-2.516412	0.279817	-1.354456
7	7	0	-3.598895	-0.031719	-1.462728
8	7	0	-0.772525	-1.343883	0.761358
9	7	0	-0.305693	-2.206285	1.456043
10	7	0	0.075225	-3.037913	2.122374
11	7	0	1.371705	-0.659246	-1.285885
12	7	0	2.511699	-0.282985	-1.359475
13	7	0	3.594316	0.027500	-1.469431

TS13 (R = Me)

Imaginary Freq.: -297.8074
Sum of electronic and zero-point Energies= -1920.284937
Sum of electronic and thermal Energies= -1920.271996
Sum of electronic and thermal Enthalpies= -1920.271052
Sum of electronic and thermal Free Energies= -1920.327633

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.880174	1.141935	0.024250
2	7	0	-3.250731	-0.450946	-0.004945
3	6	0	-2.876364	2.213180	0.021568
4	1	0	-3.460297	2.147704	-0.896586
5	1	0	-3.544214	2.084208	0.872325
6	1	0	-2.357326	3.170753	0.077884
7	7	0	-2.454887	-1.329594	0.000213
8	7	0	-1.586162	-2.087713	0.007402
9	7	0	-0.780496	0.747065	0.028930
10	13	0	0.940943	0.045597	0.001184
11	17	0	1.266025	-1.035468	-1.816105
12	17	0	1.315475	-1.091479	1.773303
13	17	0	2.252309	1.757666	0.009559

TS13 (R = Ph)

Imaginary Freq.: -138.6920
Sum of electronic and zero-point Energies= -2111.937705
Sum of electronic and thermal Energies= -2111.921934
Sum of electronic and thermal Enthalpies= -2111.920990
Sum of electronic and thermal Free Energies= -2111.985297

Standard orientation:

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

1	6	0	-0.993031	0.334258	-0.005115
2	7	0	-1.032206	2.642554	-0.029956
3	7	0	0.145066	2.693029	-0.023934
4	7	0	1.301158	2.612388	-0.017089
5	7	0	0.136051	0.054978	-0.003164
6	13	0	1.957149	-0.385243	0.004546
7	17	0	2.912313	0.241155	1.809358
8	17	0	2.922101	0.213399	-1.804609
9	17	0	1.896209	-2.547725	0.021023
10	6	0	-2.400494	0.016804	-0.003625
11	6	0	-3.423001	0.965628	0.033536
12	6	0	-2.690332	-1.356639	-0.035135
13	6	0	-4.742150	0.532353	0.037865
14	1	0	-3.179010	2.017287	0.058383
15	6	0	-4.013012	-1.771762	-0.031367
16	1	0	-1.880082	-2.076499	-0.062214
17	6	0	-5.037604	-0.828095	0.004885
18	1	0	-5.543057	1.261362	0.067436
19	1	0	-4.243141	-2.830164	-0.056078
20	1	0	-6.070986	-1.155836	0.007983

Al-INT$_{1\rightarrow3}$ (R = Me)

Sum of electronic and zero-point Energies= -1920.300593
Sum of electronic and thermal Energies= -1920.288774
Sum of electronic and thermal Enthalpies= -1920.287830
Sum of electronic and thermal Free Energies= -1920.341104

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.702953	-0.743943	0.007858
2	7	0	-3.140727	-0.475355	0.008614
3	7	0	-3.387386	0.734149	0.001350
4	7	0	-3.632813	1.824135	-0.005354
5	7	0	-0.865549	0.185261	0.010651
6	6	0	-1.498551	-2.233039	-0.006689
7	1	0	-2.026863	-2.692854	0.831604
8	1	0	-1.913452	-2.651373	-0.927456
9	1	0	-0.439406	-2.480136	0.053022
10	13	0	0.958267	0.148551	0.001466
11	17	0	1.738806	-0.799820	1.789728
12	17	0	1.731071	-0.906469	-1.730093
13	17	0	1.725217	2.169686	-0.064934

Al-INT$_{1\rightarrow3}$ (R = Ph)

Sum of electronic and zero-point Energies= -2111.959271
Sum of electronic and thermal Energies= -2111.943650
Sum of electronic and thermal Enthalpies= -2111.942706
Sum of electronic and thermal Free Energies= -2112.006625

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.739170	1.212578	-0.154897
2	7	0	1.216460	2.589938	-0.203466
3	7	0	0.285155	3.400646	-0.204801
4	7	0	-0.542313	4.150873	-0.214563
5	7	0	-0.478285	0.936315	-0.147748
6	13	0	-1.628942	-0.449180	0.058122
7	17	0	-2.106517	-1.315427	-1.869908
8	17	0	-0.907100	-2.018414	1.371304
9	17	0	-3.471387	0.287419	0.925655
10	6	0	1.905893	0.280019	-0.112698
11	6	0	3.090615	0.636407	0.536097
12	6	0	1.796039	-0.981326	-0.701568
13	6	0	4.141135	-0.271571	0.618568
14	1	0	3.183359	1.616487	0.989201
15	6	0	2.854527	-1.879345	-0.635669
16	1	0	0.889957	-1.255483	-1.230854
17	6	0	4.025818	-1.529236	0.032127
18	1	0	5.049863	0.004112	1.141203
19	1	0	2.764207	-2.852333	-1.104984
20	1	0	4.847610	-2.233836	0.092255

TS14 (R = Me)

Imaginary Freq.: -370.4724
Sum of electronic and zero-point Energies= -1920.284621
Sum of electronic and thermal Energies= -1920.272633
Sum of electronic and thermal Enthalpies= -1920.271689
Sum of electronic and thermal Free Energies= -1920.326611

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.902388	-0.651293	0.015783
2	7	0	3.259569	-0.107075	0.008964
3	7	0	3.077669	1.149126	-0.007533
4	7	0	2.240516	1.929712	-0.014475
5	7	0	0.926822	0.129677	0.009561
6	6	0	1.918446	-2.153081	-0.008612
7	1	0	1.049942	-2.550702	0.516108
8	1	0	1.879396	-2.486751	-1.048882
9	1	0	2.834470	-2.534866	0.441102
10	13	0	-0.896854	0.058711	0.002121
11	17	0	-1.693121	2.001177	-0.489246
12	17	0	-1.617387	-0.521182	1.955051
13	17	0	-1.604889	-1.366745	-1.463131

TS14 (R = Ph)

Imagianry Freq.: -380.6021
Sum of electronic and zero-point Energies= -2111.943383
Sum of electronic and thermal Energies= -2111.928627
Sum of electronic and thermal Enthalpies= -2111.927683
Sum of electronic and thermal Free Energies= -2111.989058

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.767871	1.253561	-0.145369
2	7	0	1.128761	2.666746	-0.220321
3	7	0	0.007297	3.257661	-0.251160
4	7	0	-1.115507	3.028721	-0.240873
5	7	0	-0.437919	0.923308	-0.131630
6	13	0	-1.632636	-0.440542	0.067850
7	17	0	-0.964618	-1.840497	1.572727
8	17	0	-1.892844	-1.479454	-1.809304
9	17	0	-3.544226	0.351171	0.671398
10	6	0	1.970459	0.378063	-0.097315
11	6	0	3.162262	0.832264	0.472096
12	6	0	1.898774	-0.918019	-0.612448
13	6	0	4.265373	-0.012249	0.539531
14	1	0	3.219411	1.836880	0.872497
15	6	0	3.008124	-1.753008	-0.557212
16	1	0	0.983729	-1.267261	-1.077705
17	6	0	4.191351	-1.303474	0.024164
18	1	0	5.183853	0.340650	0.994314
19	1	0	2.947761	-2.754170	-0.967995
20	1	0	5.054504	-1.957668	0.072088

9

Sum of electronic and zero-point Energies= -578.829000
Sum of electronic and thermal Energies= -578.817609
Sum of electronic and thermal Enthalpies= -578.816664
Sum of electronic and thermal Free Energies= -578.867383

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.102044	-0.290718	0.072790
2	6	0	-0.606901	-1.621910	-0.470258
3	6	0	-2.078511	-1.323367	-0.803099
4	6	0	-2.416036	-0.055297	0.010174
5	7	0	-1.211375	0.227016	0.800785
6	7	0	0.264034	0.551943	-1.144559
7	1	0	-0.522749	-2.358330	0.331269
8	1	0	-0.020493	-1.955487	-1.326058

9	1	0	-2.203421	-1.131878	-1.868714
10	1	0	-2.718417	-2.163174	-0.535967
11	1	0	-3.265966	-0.185073	0.682417
12	1	0	-2.637417	0.787070	-0.658964
13	7	0	0.957695	1.533732	-0.896973
14	6	0	-1.111829	1.596250	1.275440
15	1	0	-0.171046	1.741407	1.810667
16	1	0	-1.178679	2.324866	0.453970
17	1	0	-1.933801	1.791644	1.966337
18	7	0	1.616033	2.432395	-0.747791
19	7	0	1.056884	-0.360957	0.980168
20	7	0	2.851479	-1.696289	0.257188
21	7	0	1.971524	-1.070809	0.556149

9 (Ionic)

Sum of electronic and zero-point Energies= -578.828636
Sum of electronic and thermal Energies= -578.816386
Sum of electronic and thermal Enthalpies= -578.815442
Sum of electronic and thermal Free Energies= -578.867940

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.147964	-1.042497	-0.232239
2	6	0	1.325318	-1.488845	-1.036920
3	6	0	2.438583	-0.572285	-0.514399
4	6	0	1.974288	-0.209531	0.894784
5	7	0	0.501259	-0.349954	0.805812
6	7	0	-1.091492	-1.443322	-0.623170
7	1	0	1.124705	-1.400052	-2.103773
8	1	0	1.504336	-2.544469	-0.805755
9	1	0	3.413689	-1.054105	-0.512645
10	1	0	2.486977	0.330722	-1.125134
11	1	0	2.205802	0.812480	1.188493
12	1	0	2.325670	-0.908582	1.658462
13	7	0	-2.108835	-0.896152	-0.123832
14	6	0	-0.358258	0.137839	1.881154
15	1	0	-0.997248	0.944988	1.518002
16	1	0	-0.961768	-0.680761	2.277257
17	1	0	0.285604	0.516310	2.671357
18	7	0	-3.104714	-0.508743	0.168253
19	7	0	-1.130597	1.631501	-1.033120
20	7	0	-0.186358	2.170482	-0.593301
21	7	0	0.755719	2.686957	-0.132149

10 (R = Me)

Sum of electronic and zero-point Energies= -711.525504
Sum of electronic and thermal Energies= -711.510935
Sum of electronic and thermal Enthalpies= -711.509991

Sum of electronic and thermal Free Energies= -711.567546

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.576721	-0.105185	0.159305
2	6	0	-0.714440	-1.651249	0.090327
3	6	0	-2.172947	-1.941196	0.472478
4	6	0	-2.862622	-0.619485	0.157431
5	7	0	-1.867678	0.343194	0.611924
6	7	0	-0.300705	0.354386	-1.284318
7	1	0	0.005000	-2.140806	0.748482
8	1	0	-0.525729	-1.972818	-0.933514
9	1	0	-2.582900	-2.781599	-0.087029
10	1	0	-2.261065	-2.153001	1.539391
11	1	0	-3.799307	-0.470296	0.697319
12	1	0	-3.061779	-0.519408	-0.921992
13	7	0	0.125914	1.498006	-1.392921
14	6	0	-2.189739	1.740792	0.404724
15	1	0	-1.380898	2.368678	0.786824
16	1	0	-2.361204	1.980234	-0.655561
17	1	0	-3.098536	1.982561	0.958731
18	7	0	0.543822	2.527084	-1.574683
19	7	0	0.426689	0.442197	1.041580
20	6	0	1.665152	0.159415	1.038968
21	6	0	2.574935	0.752770	2.073009
22	1	0	3.069756	-0.048651	2.626855
23	1	0	3.351504	1.347106	1.586213
24	1	0	2.002289	1.376383	2.755319
25	7	0	2.431029	-0.694008	0.202947
26	7	0	2.011590	-1.190797	-0.851198
27	7	0	1.815218	-1.706284	-1.821688

10 (R = Ph)

Sum of electronic and zero-point Energies= -903.184629
Sum of electronic and thermal Energies= -903.166878
Sum of electronic and thermal Enthalpies= -903.165934
Sum of electronic and thermal Free Energies= -903.231944

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.558469	-0.180163	-0.172514
2	6	0	-2.107764	0.610905	-1.391572
3	6	0	-3.164637	-0.306680	-2.023449
4	6	0	-3.531438	-1.233484	-0.871158
5	7	0	-2.233935	-1.449020	-0.243133
6	7	0	-1.991961	0.615902	1.072151
7	1	0	-1.309146	0.871886	-2.086887
8	1	0	-2.570813	1.528981	-1.030872

9	1	0	-4.016188	0.254336	-2.407129
10	1	0	-2.732927	-0.890148	-2.838238
11	1	0	-3.953186	-2.188090	-1.190496
12	1	0	-4.240756	-0.750902	-0.179465
13	7	0	-1.402046	0.321806	2.105728
14	6	0	-2.235573	-2.264490	0.955321
15	1	0	-1.217367	-2.363466	1.339236
16	1	0	-2.880515	-1.849914	1.744721
17	1	0	-2.603727	-3.261101	0.705443
18	7	0	-0.888070	0.125899	3.087385
19	7	0	-0.139860	-0.429828	-0.102521
20	6	0	0.788578	0.426555	-0.237938
21	7	0	0.733295	1.825633	-0.448210
22	7	0	-0.261692	2.510070	-0.182191
23	7	0	-1.051618	3.273807	0.015047
24	6	0	2.208759	-0.038671	-0.232079
25	6	0	3.265747	0.864671	-0.100961
26	6	0	2.481564	-1.405447	-0.346425
27	6	0	4.579056	0.405102	-0.079966
28	1	0	3.064980	1.924502	-0.007340
29	6	0	3.793446	-1.859121	-0.329477
30	1	0	1.659688	-2.103003	-0.452368
31	6	0	4.846169	-0.955079	-0.194748
32	1	0	5.392137	1.113645	0.027801
33	1	0	3.996472	-2.919702	-0.423718
34	1	0	5.869929	-1.311496	-0.180683

TS15 (R = Me)

Imaginary Freq.: -381.7727
Sum of electronic and zero-point Energies= -711.509215
Sum of electronic and thermal Energies= -711.495424
Sum of electronic and thermal Enthalpies= -711.494480
Sum of electronic and thermal Free Energies= -711.549698

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.613315	0.058239	-0.386558
2	6	0	-1.259739	-0.609485	-1.598448
3	6	0	-2.749522	-0.652786	-1.222544
4	6	0	-2.773528	-0.492557	0.312506
5	7	0	-1.363522	-0.461681	0.718952
6	7	0	-0.844471	1.558217	-0.567679
7	1	0	-0.842616	-1.613795	-1.686155
8	1	0	-1.045627	-0.057386	-2.512338
9	1	0	-3.292157	0.165881	-1.695321
10	1	0	-3.208472	-1.587468	-1.542912
11	1	0	-3.280652	-1.312578	0.825129
12	1	0	-3.272217	0.444145	0.596312
13	7	0	-0.097504	2.267034	0.094302
14	6	0	-1.127850	0.141423	2.017939
15	1	0	-0.057900	0.164947	2.238090

16	1	0	-1.529410	1.163968	2.082093
17	1	0	-1.619328	-0.462366	2.783730
18	7	0	0.568035	2.974724	0.661704
19	7	0	0.806674	-0.142471	-0.280570
20	6	0	1.428134	-1.166502	0.137864
21	6	0	0.896754	-2.442047	0.711844
22	1	0	0.022920	-2.774458	0.153893
23	1	0	1.675965	-3.202372	0.694854
24	1	0	0.589558	-2.262690	1.745233
25	7	0	2.847420	-1.124966	0.086308
26	7	0	3.118835	0.030072	-0.416172
27	7	0	2.543723	0.944280	-0.799449

TS15 (R = Ph)

Imaginary Freq.: -381.5244
Sum of electronic and zero-point Energies= -903.162934
Sum of electronic and thermal Energies= -903.146282
Sum of electronic and thermal Enthalpies= -903.145338
Sum of electronic and thermal Free Energies= -903.207583

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.056398	-0.644650	0.505584
2	6	0	0.261330	-1.109997	1.750969
3	6	0	-0.668509	-2.217366	1.237389
4	6	0	0.063663	-2.714503	-0.004182
5	7	0	0.594079	-1.476641	-0.564247
6	7	0	2.519126	-0.868616	0.841010
7	1	0	-0.264887	-0.276268	2.214591
8	1	0	0.975881	-1.505824	2.472987
9	1	0	-0.820556	-3.001201	1.979070
10	1	0	-1.641190	-1.808168	0.953836
11	1	0	-0.589983	-3.197274	-0.734511
12	1	0	0.869854	-3.417212	0.261561
13	7	0	3.314044	-0.297596	0.100375
14	6	0	1.431825	-1.602364	-1.738975
15	1	0	1.718200	-0.613338	-2.107660
16	1	0	2.343030	-2.188734	-1.547212
17	1	0	0.864495	-2.103674	-2.525704
18	7	0	4.109855	0.197600	-0.519698
19	7	0	0.925173	0.769871	0.181114
20	6	0	-0.152834	1.387031	-0.078826
21	7	0	-0.090426	2.790960	-0.257072
22	7	0	1.157510	3.074598	-0.078389
23	7	0	2.123538	2.510894	0.170341
24	6	0	-1.535188	0.845282	-0.181439
25	6	0	-2.436101	1.108115	0.848787
26	6	0	-1.921152	0.082344	-1.283627
27	6	0	-3.720134	0.573050	0.793101
28	1	0	-2.130214	1.713825	1.694919
29	6	0	-3.211888	-0.431470	-1.341471

30	1	0	-1.215320	-0.107957	-2.082728
31	6	0	-4.107107	-0.197742	-0.299367
32	1	0	-4.416900	0.763265	1.601207
33	1	0	-3.515842	-1.020966	-2.198928
34	1	0	-5.108680	-0.610351	-0.343140

TS16 (R = Ph)

Imaginary Freq.: -270.1240
Sum of electronic and zero-point Energies= -738.804852
Sum of electronic and thermal Energies= -738.789220
Sum of electronic and thermal Enthalpies= -738.788276
Sum of electronic and thermal Free Energies= -738.849295

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.809253	-0.208040	-0.327467
2	6	0	-2.541644	-0.311577	-1.641945
3	6	0	-3.881918	-0.939774	-1.209548
4	6	0	-3.936618	-0.729722	0.305441
5	7	0	-2.514120	-0.662889	0.680335
6	1	0	-1.972116	-0.934821	-2.331806
7	1	0	-2.649788	0.682528	-2.071673
8	1	0	-4.727465	-0.474845	-1.711305
9	1	0	-3.880537	-2.006233	-1.433292
10	1	0	-4.408838	-1.545621	0.850588
11	1	0	-4.408648	0.217309	0.587278
12	6	0	-2.110646	-0.584161	2.073208
13	1	0	-1.033501	-0.720885	2.162359
14	1	0	-2.394247	0.395790	2.469965
15	1	0	-2.623976	-1.368577	2.626723
16	7	0	-0.426426	-0.267255	-0.262098
17	6	0	0.717024	-0.138018	-0.174226
18	7	0	0.347837	2.441884	0.596794
19	7	0	-0.736936	2.205719	0.282883
20	7	0	-1.815807	1.864190	-0.067993
21	6	0	2.125932	-0.232484	-0.119491
22	6	0	2.931816	0.874601	-0.421628
23	6	0	2.669057	-1.486724	0.204579
24	6	0	4.306019	0.711040	-0.397992
25	1	0	2.476927	1.826072	-0.663912
26	6	0	4.046720	-1.619828	0.228522
27	1	0	2.017449	-2.322579	0.427553
28	6	0	4.858584	-0.527175	-0.072215
29	1	0	4.948423	1.550976	-0.631011
30	1	0	4.487958	-2.576522	0.478782
31	1	0	5.936083	-0.642958	-0.053125

TS16 with azide anion (R = Ph)

Imaginary Freq.: -268.4387
Sum of electronic and zero-point Energies= -903.114749
Sum of electronic and thermal Energies= -903.095222
Sum of electronic and thermal Enthalpies= -903.094278
Sum of electronic and thermal Free Energies= -903.164503

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.836907	-0.480202	-0.278851
2	6	0	-2.480394	0.269381	-1.420640
3	6	0	-3.884945	-0.366484	-1.466538
4	6	0	-4.029565	-1.087275	-0.123634
5	7	0	-2.635863	-1.386515	0.237680
6	7	0	0.440249	1.915376	-1.254735
7	1	0	-1.904251	0.114933	-2.333052
8	1	0	-2.488753	1.333322	-1.191966
9	1	0	-4.663256	0.379817	-1.609675
10	1	0	-3.937834	-1.090811	-2.279059
11	1	0	-4.591660	-2.018501	-0.176899
12	1	0	-4.457886	-0.448340	0.656166
13	7	0	0.246055	2.867672	-0.596661
14	6	0	-2.319542	-2.173495	1.415489
15	1	0	-1.265624	-2.450660	1.407317
16	1	0	-2.539277	-1.583249	2.311062
17	1	0	-2.931882	-3.073691	1.408601
18	7	0	0.052247	3.809963	0.065469
19	7	0	-0.470367	-0.674447	-0.216270
20	6	0	0.671129	-0.508588	-0.131114
21	7	0	0.373314	1.061587	2.002722
22	7	0	-0.717273	1.081776	1.627232
23	7	0	-1.803542	1.033161	1.158633
24	6	0	2.083265	-0.630017	-0.145030
25	6	0	2.907653	0.460332	0.161532
26	6	0	2.606024	-1.887800	-0.481657
27	6	0	4.279268	0.277943	0.123097
28	1	0	2.465597	1.414081	0.417573
29	6	0	3.982701	-2.044707	-0.510768
30	1	0	1.941054	-2.711048	-0.712508
31	6	0	4.812912	-0.966956	-0.211275
32	1	0	4.935616	1.107285	0.355666
33	1	0	4.406282	-3.007569	-0.768140
34	1	0	5.888530	-1.098365	-0.237246