Supporting Information

Intra- versus Intermolecular Carbon-to-Carbon Proton Transfers in the Reactions of Arynes with Nitrogen Nucleophiles: A DFT Study

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S1. Discussion on the Addition of Nitrogen Nucleophiles to Arynes

To briefly investigate the addition of nitrogen nucleophiles to arynes, we performed DFT calculations on the reactions of benzyne with NMe_3, imine **11a**, and pyridine, respectively. For the reactions with NMe_3 and pyridine, no transition states could be located, suggesting that both reactions are barrierless. For the reaction with **11a**, we have successfully located the nucleophilic addition transition state **TS21** (Figure S1). The Gibbs energy of activation for this process is 10.7 kcal/mol. These computational results confirm that the addition of nitrogen nucleophiles to arynes is generally rapid.

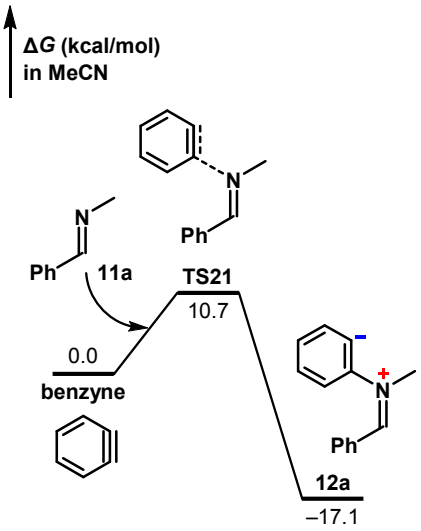
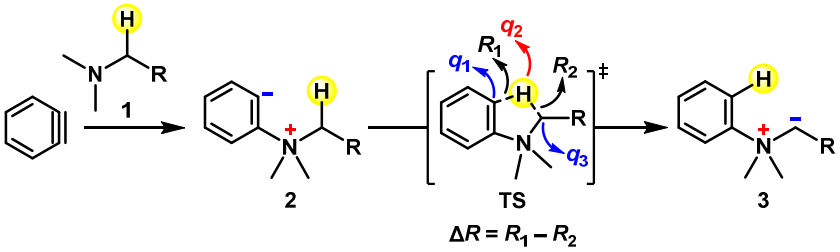


Figure S1. Gibbs energy profile for the nucleophilic addition of imine **11a** to benzyne. Computed at the SMD(MeCN)/M06-2X/maug-cc-pVTZ//SMD(MeCN)/M06-2X/6-31+G(d,p) level.

S2. Additional Data Related to Table 1

The C···H distances in the intramolecular 1,4-proton transfer transition states **TS1**–**TS9** and **TS9'** are listed in Table S1. As discussed in the main text, there exists a negative linear correlation between the Gibbs energy change (ΔG) and ΔR (Figure 2). The natural atomic charges obtained from natural population analysis[1] (NPA) are also listed in Table S1, although the correlations between $\Delta G/\Delta G^{\ddagger}$ and the atomic charges are insignificant.

Table S1. C···H Distances and Natural Atomic Charges in the Intramolecular 1,4-Proton Transfer Transition States



entry	TS	R_1 (Å)	R_2 (Å)	ΔR (Å)	q_1 (e)	q_2 (e)	q_3 (e)
1	**TS1**	1.359	1.466	−0.107	−0.367	+0.293	−0.692
2	**TS2**	1.555	1.292	0.263	−0.378	+0.318	−0.443
3	**TS3**	1.522	1.314	0.208	−0.376	+0.315	−0.459
4	**TS4**	1.520	1.298	0.222	−0.377	+0.327	−0.482
5	**TS5**	1.500	1.330	0.170	−0.375	+0.312	−0.460
6	**TS6**	1.418	1.403	0.015	−0.361	+0.307	−0.401
7	**TS7**	1.391	1.433	−0.042	−0.368	+0.306	−0.950
8	**TS8**	1.421	1.408	0.013	−0.371	+0.294	−0.416
9	**TS9**	1.549	1.287	0.262	−0.374	+0.332	−0.266
10	**TS9'**	1.459	1.367	0.092	−0.371	+0.302	−0.350

(1) *NBO* Version 3.1, Glendening, E. D.; Reed, A. E.; Carpenter, J. E.; Weinhold, F.

S3. Discussion on "Inert" Solvents

To verify whether benzene and *n*-hexane are indeed "inert" solvents or not, we investigated the intermolecular proton transfer from these solvents to the benzyne–NMe_3 adduct **2a** (Figure S2). To simplify the computations, only the zigzag conformation was considered for *n*-hexane, **TS23**, and **21**. DFT calculations suggested that the Gibbs energies of activation for the intermolecular proton transfer from benzene and *n*-hexane to **2a** are 27.5 and 36.8 kcal/mol, respectively. Meanwhile, both reactions are highly endergonic. These results indicate that benzene and *n*-hexane are indeed "inert" solvents.

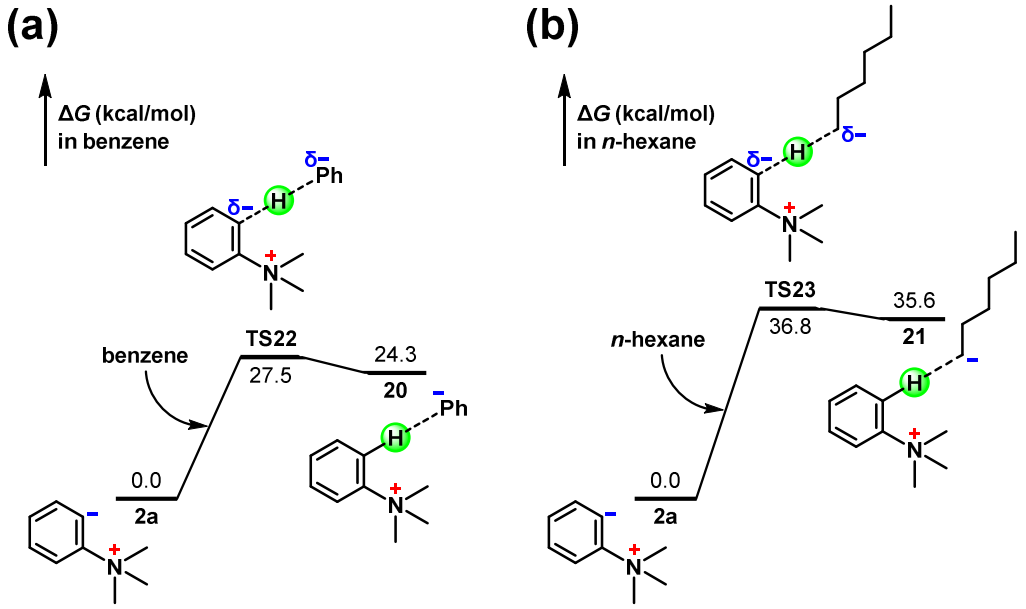
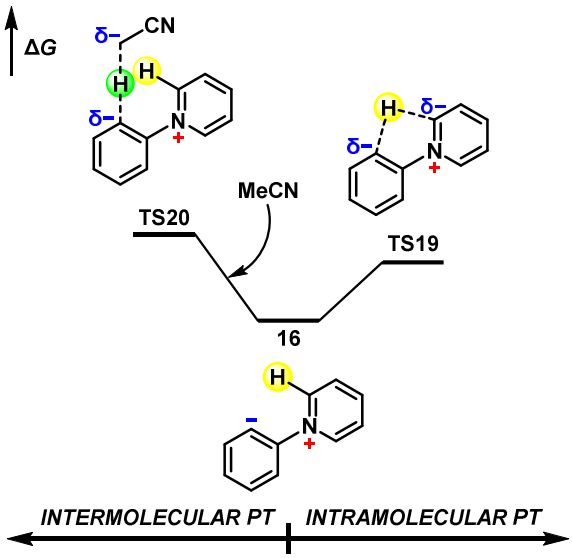


Figure S2. Gibbs energy profiles for the intermolecular proton transfer from (a) benzene and (b) *n*-hexane to **2a**. Computed at the SMD/M06-2X/maug-cc-pVTZ//SMD/M06-2X/6-31+G(d,p) level.

S4. Solvent Effect

To assess the solvent effect, we performed DFT calculations on the intra- and intermolecular proton transfers of the benzyne–pyridine adduct **16** both in the gas phase and in MeCN solution (Table S2). In both cases, we found that the dipole moment (μ) of the intermolecular proton transfer transition state **TS20** is larger than that of the intramolecular one (**TS19**). As a result, the Gibbs energy of solvation (ΔG_{solv}) for **TS20** is more negative than that for **TS19**. Consequently, the Gibbs energy difference between **TS20** and **TS19** is reduced from 2.6 kcal/mol in the gas phase to 0.8 kcal/mol in MeCN solution. These results indicate that the solvent effect is crucial.

Table S2. Solvent Effect on the Intra- and Intermolecular Proton Transfers of 16[a]



	μ_{gas} (D)[b]	μ_{MeCN} (D)[c]	ΔG_{gas}[b]	ΔG_{MeCN}[c]	ΔG_{solv}[d]
16	8.1	12.3	0.0	0.0	−24.1 (−27.3)
MeCN	4.0	5.2	0.0	0.0	−6.6 (−6.6)
TS19	5.6	7.8	4.6	15.1	−15.3 (−14.5)
TS20	6.7	9.6	7.2	15.9	−22.2 (−23.7)

[a]Energies are reported in kcal/mol. A standard state of 298 K and 1 atm was used.

[b]Computed at the M06-2X/6-31+G(d,p) level.

[c]Computed at the SMD(MeCN)/M06-2X/6-31+G(d,p) level.

[d]The Gibbs energies of solvation (ΔG_{solv}) were computed on the basis of the optimized geometries in the gas phase. The values given in parentheses were computed on the basis of the optimized geometries in MeCN solution.

S5. Tunneling Effect

To assess the influence of proton tunneling, we carried out direct dynamics calculations on the intramolecular 1,4-proton transfer of the benzyne–NMe_3 adduct **2a** with GAUSSRATE[2] as the interface between Gaussian 09[3] and POLYRATE[4] at the M06-2X/6-31+G(d,p) level. The rate constants were obtained using canonical variational transition state theory (CVT).[5] The local quadratic approximation (Page–McIver method) was employed to calculate the minimum energy path.[6] Quantum effects of multidimensional tunneling were calculated with small curvature tunneling (SCT) approximation.[7] We found that the quantum tunneling increases the rate constant in a factor of 16 at 298.15 K, corresponding to a decrease of 1.6 kcal/mol in terms of Gibbs energy of activation (according to the conventional transition state theory, in which $\kappa = 1$). Considering that the proton tunneling takes place in all proton transfer processes, the quantum effects could be cancelled out when comparing the Gibbs energy differences. Therefore, our conclusions in the main text should not be affected significantly if we ignore the proton tunneling.

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S6. Computed Energies of All of the Stationary Points

Table S3. Thermal Corrections to Gibbs Energy (TCGs) and Single-Point Energies (SPEs)

	TCG[a] (a.u.)	SPE[a] (a.u.)	SPE[b] (a.u.)
benzyne (in MeCN)	0.048297	−230.828664	−230.900117
$CHCl_3$ (in $CHCl_3$)	−0.008823	−1419.176639	−1419.317952
MeCN(in MeCN)	0.021662	−132.711320	−132.756820
benzene(in benzene)	0.073851	−232.160418	−232.231046
n-hexane (in *n*-hexane)	0.157684	−236.968664	−237.040209
N,*N*-dimethylaniline (in $CHCl_3$)	0.142230	−366.077996	−366.191271
C_2H_4 (in $CHCl_3$)	0.029175	−78.548642	−78.574398
methyl acrylate (in $CHCl_3$)	0.066099	−306.355989	−306.464792
2a (in THF)	0.170754	−405.281147	−405.404716
2a (in $CHCl_3$)	0.170570	−405.279474	−405.403061
2a (in benzene)	0.170291	−405.271214	−405.394911
2a (in *n*-hexane)	0.170275	−405.268314	−405.392055
2b (in THF)	0.204118	−557.870391	−558.046199
2c (in THF)	0.209737	−633.077992	−633.284461
2d (in THF)	0.167465	−497.490137	−497.644975
2e (in THF)	0.195040	−573.938838	−574.122798
2f (in THF)	0.247743	−636.254918	−636.445925
2g (in THF)	0.265306	−813.861165	−814.052632
2h (in THF)	0.147811	−404.054295	−404.176591
2i (in THF)	0.143758	−496.259367	−496.412854
2j (in $CHCl_3$)	0.197883	−444.577912	−444.712998
2k (in $CHCl_3$)	0.236905	−672.380046	−672.598253
3a (in THF)	0.170476	−405.275114	−405.399980
3b (in THF)	0.204471	−557.911995	−558.089421
3c (in THF)	0.208326	−633.111523	−633.319577
3d (in THF)	0.167347	−497.524963	−497.681132
3e (in THF)	0.193757	−573.963770	−574.149487
3f (in THF)	0.245880	−636.260284	−636.452994
3g (in THF)	0.264201	−813.862529	−814.055537
3h (in THF)	0.147245	−404.062837	−404.186477
3i (in THF)	0.143705	−496.301719	−496.456596
3i' (in THF)	0.143383	−496.279933	−496.434667
4 (in $CHCl_3$)	0.210383	−1863.767629	−1864.041370
5 (in $CHCl_3$)	0.210917	−1863.791711	−1864.064797
6 (in $CHCl_3$)	0.249737	−2091.569201	−2091.926317
7 (in $CHCl_3$)	0.250246	−2091.592309	−2091.948460
9 (in $CHCl_3$)	0.381370	−1547.634059	−1548.076117
10 (in $CHCl_3$)	0.313374	−1280.534715	−1280.882305
11a (in MeCN)	0.118446	−364.872032	−364.983778
12a (in MeCN)	0.194789	−595.756806	−595.936187
12b (in MeCN)	0.192021	−687.966056	−688.176607

13a (in MeCN)	0.194075	−595.782975	−595.963325
13b (in MeCN)	0.191490	−688.021074	−688.232811
14a (in MeCN)	0.235967	−728.474985	−728.698978
14b (in MeCN)	0.233581	−820.684235	−820.939358
15a (in MeCN)	0.234960	−728.494457	−728.720719
16 (in MeCN)	0.136401	−479.083278	−479.228320
17 (in MeCN)	0.136127	−479.104178	−479.248418
18 (in MeCN)	0.176392	−611.800461	−611.990099
19 (in MeCN)	0.176396	−611.817595	−612.009583
20 (in benzene)	0.265333	−637.409667	−637.603196
21 (in *n*-hexane)	0.347717	−642.195526	−642.390444
TS1 (in THF)	0.164708	−405.245051	−405.367494
TS2 (in THF)	0.199447	−557.856584	−558.031659
TS3 (in THF)	0.204442	−633.063177	−633.268868
TS4 (in THF)	0.162511	−497.478776	−497.632669
TS5 (in THF)	0.189674	−573.918296	−574.101480
TS6 (in THF)	0.241878	−636.226135	−636.416330
TS7 (in THF)	0.258617	−813.829589	−814.020604
TS8 (in THF)	0.142931	−404.026033	−404.147929
TS9 (in THF)	0.139789	−496.251011	−496.404073
TS9' (in THF)	0.138914	−496.238037	−496.391150
TS10 (in $CHCl_3$)	0.192003	−444.536162	−444.670485
TS11 (in $CHCl_3$)	0.206498	−1863.763906	−1864.035461
TS12 (in $CHCl_3$)	0.232901	−672.363987	−672.581219
TS13 (in $CHCl_3$)	0.246261	−2091.565364	−2091.919981
TS14 (in $CHCl_3$)	0.377306	−1547.615265	−1548.056489
TS15 (in $CHCl_3$)	0.178480	−1824.465091	−1824.725062
TS16 (in $CHCl_3$)	0.324666	−2699.712169	−2700.195555
TS17a (in MeCN)	0.190265	−595.720013	−595.898564
TS17b (in MeCN)	0.187209	−687.948771	−688.158892
TS18a (in MeCN)	0.232003	−728.458842	−728.681978
TS18b (in MeCN)	0.229217	−820.667190	−820.921413
TS19 (in MeCN)	0.131786	−479.054534	−479.198458
TS20 (in MeCN)	0.172864	−611.783997	−611.972577
TS21 (in MeCN)	0.188347	−595.703411	−595.885379
TS22 (in benzene)	0.260757	−637.401558	−637.593482
TS23 (in *n*-hexane)	0.344710	−642.191994	−642.385520

[a]Computed at the SMD/M06-2X/6-31+G(d,p) level. A standard state of 298 K and 1 atm was used.

[b]Computed at the SMD/M06-2X/maug-cc-pVTZ//SMD/M06-2X/6-31+G(d,p) level.

S7. Cartesian Coordinates of All of the Stationary Points

benzyne (in MeCN)

C	0.623355	-1.232024	0.000008
C	-0.623344	-1.232020	0.000051
C	-1.467471	-0.132172	0.000054
C	-0.703989	1.052276	0.000000
C	0.703980	1.052278	-0.000049
C	1.467471	-0.132164	-0.000048
H	-2.550983	-0.133084	0.000090
H	-1.227876	2.004550	-0.000005
H	1.227874	2.004547	-0.000090
H	2.550983	-0.133053	-0.000086

$CHCl_3$ (in $CHCl_3$)

Cl	-0.179875	1.676285	-0.084743
Cl	-1.362544	-0.993713	-0.084884
Cl	1.542425	-0.682339	-0.084884
C	-0.000095	-0.000380	0.462867
H	0.000456	-0.001698	1.549482

MeCN (in MeCN)

N	1.434912	0.000018	-0.000045
C	0.278026	-0.000035	0.000106
C	-1.180397	0.000032	-0.000023
H	-1.543266	-0.348874	-0.968668
H	-1.543449	1.013279	0.182159
H	-1.543446	-0.664513	0.786322

benzene (in benzene)

C	-0.492980	1.304782	-0.000154
C	-1.376584	0.225319	0.000062
C	-0.883541	-1.079279	0.000011
C	0.493104	-1.304709	0.000206
C	1.376542	-0.225471	0.000325
C	0.883464	1.079339	-0.000037
H	-0.876927	2.320574	-0.000210
H	-2.448239	0.400890	0.000553
H	-1.571358	-1.919641	-0.000668
H	0.876994	-2.320480	-0.001319
H	2.448168	-0.400893	-0.000439
H	1.571331	1.919658	-0.000402

n-hexane (in *n*-hexane)

C	-3.203917	0.209368	0.000182
C	-1.881037	-0.552620	-0.000262
C	-0.665979	0.373822	0.000021
C	0.665996	-0.373893	0.000121
C	1.880981	0.552608	-0.000214
C	3.203947	-0.209298	0.000127
H	-4.060892	-0.470946	-0.000490
H	-3.286156	0.851636	-0.883463
H	-3.286413	0.850298	0.884748
H	-1.833847	-1.208464	-0.879300
H	-1.833683	-1.209238	0.878195
H	-0.713192	1.031864	-0.879340
H	-0.713423	1.031669	0.879515
H	0.713256	-1.032086	-0.879126
H	0.713379	-1.031606	0.879716
H	1.833717	1.208487	-0.879222
H	1.833674	1.209199	0.878261
H	4.060926	0.471030	-0.000166
H	3.286353	-0.851272	-0.883701
H	3.286346	-0.850495	0.884520

N,*N*-dimethylaniline (in $CHCl_3$)

N	1.570854	-0.002534	-0.205009
C	2.277420	-1.235730	0.097729
C	2.283458	1.233916	0.065758
C	0.186821	0.000265	-0.096737
C	-0.545598	-1.206747	-0.054463
C	-1.935710	-1.196468	0.013551
C	-2.648627	0.001338	0.054006
C	-1.933838	1.198284	0.031279
C	-0.543502	1.207657	-0.037092
H	2.071925	-1.598323	1.116852
H	3.349103	-1.058954	0.002040
H	2.008508	-2.024382	-0.610610
H	1.981870	2.017422	-0.634599
H	3.350849	1.061533	-0.076262
H	2.119047	1.600654	1.091118
H	-0.032009	-2.160157	-0.078059
H	-2.464898	-2.145144	0.040166
H	-3.732238	0.001817	0.110217
H	-2.461419	2.147296	0.073559
H	-0.029263	2.160882	-0.043547

C_2H_4 (in $CHCl_3$)

C	0.665494	-0.000048	-0.000010
C	-0.665496	-0.000034	-0.000031
H	1.234618	-0.925923	-0.000017
H	1.234339	0.926136	0.000107
H	-1.234687	-0.925975	0.000142
H	-1.234259	0.926252	0.000017

methyl acrylate (in $CHCl_3$)

O	1.013824	-0.716354	0.000062
O	0.060438	1.317847	-0.000260
C	2.300009	-0.085269	0.000222
C	-0.041316	0.108343	-0.000198
C	-2.484223	-0.004690	0.000361
C	-1.318592	-0.649370	-0.000344
H	3.025772	-0.896922	0.000237
H	2.417785	0.533030	0.892846
H	2.417951	0.533158	-0.892290
H	-2.516989	1.081738	0.000868
H	-3.425698	-0.544461	0.000446
H	-1.248183	-1.732573	-0.000773

2a (in THF)

N	1.399608	-0.008352	0.000001
C	1.896969	-0.722309	-1.217778
C	1.897043	-0.722057	1.217895
C	1.987049	1.361421	-0.000166
C	-0.138241	-0.029387	0.000018
C	-0.723204	-1.294014	0.000031
C	-2.134304	-1.229335	0.000017
C	-2.869623	-0.038400	-0.000027
C	-2.200853	1.184220	0.000000
C	-0.804910	1.198859	0.000027
H	1.496122	-1.733435	-1.204280
H	2.988258	-0.728641	-1.191256
H	1.537579	-0.187050	-2.097690
H	1.537827	-0.186540	2.097720
H	2.988336	-0.728482	1.191269
H	1.496118	-1.733154	1.204666
H	1.668417	1.892507	-0.896936
H	3.072616	1.257870	-0.000206
H	1.668512	1.892699	0.896518
H	-2.706507	-2.159345	0.000049
H	-3.957625	-0.060735	-0.000081
H	-2.748556	2.122042	0.000009
H	-0.297911	2.156736	0.000112

2a (in $CHCl_3$)

N	1.400644	-0.006702	0.000004

C	1.893688	-0.723767	1.217387
C	1.990139	1.360950	0.000113
C	1.893917	-0.723617	-1.217367
C	-0.140154	-0.026739	-0.000169
C	-0.719517	-1.292153	-0.000054
C	-2.130680	-1.230111	-0.000014
C	-2.867481	-0.040504	-0.000015
C	-2.201812	1.184172	0.000018
C	-0.806177	1.201788	-0.000049
H	1.537884	-0.186706	2.097730
H	2.985179	-0.739270	1.191570
H	1.482022	-1.730754	1.203296
H	1.672504	1.893745	-0.896132
H	3.075967	1.257647	0.000029
H	1.672675	1.893532	0.896544
H	1.482226	-1.730590	-1.203462
H	2.985394	-0.739111	-1.191319
H	1.538288	-0.186438	-2.097710
H	-2.700609	-2.161408	0.000098
H	-3.955439	-0.064740	0.000057
H	-2.751994	2.120517	0.000131
H	-0.300136	2.160376	0.000042

2a (in benzene)

N	1.403671	-0.002655	-0.000002
C	1.884945	-0.727779	1.215960
C	1.997231	1.359870	0.000113
C	1.885297	-0.727704	-1.215870
C	-0.144195	-0.019399	-0.000202
C	-0.709939	-1.286517	-0.000068
C	-2.121066	-1.232423	-0.000025
C	-2.861500	-0.046171	0.000000
C	-2.203607	1.183400	0.000026
C	-0.808850	1.209615	-0.000101
H	1.541198	-0.183885	2.096939
H	2.976140	-0.769694	1.190052
H	1.442872	-1.722482	1.200432
H	1.680437	1.895003	-0.895177
H	3.083614	1.257926	0.000102
H	1.680446	1.894829	0.895513
H	1.442845	-1.722243	-1.200703
H	2.976452	-0.769988	-1.189417
H	1.542184	-0.183499	-2.096908
H	-2.685242	-2.166789	0.000046
H	-3.949285	-0.074937	0.000090
H	-2.760079	2.115866	0.000104
H	-0.307165	2.171126	-0.000054

2a (in *n*-hexane)

N	1.404837	-0.001447	-0.000003
C	1.882572	-0.728814	1.215632
C	1.999879	1.359547	-0.000356
C	1.882478	-0.729416	-1.215312
C	-0.145388	-0.016743	0.000043
C	-0.706970	-1.284216	0.000022
C	-2.118082	-1.233435	0.000000
C	-2.859809	-0.048235	-0.000002
C	-2.204440	1.182969	-0.000005
C	-0.809957	1.212415	0.000011
H	1.543681	-0.181762	2.096514
H	2.973495	-0.780196	1.188756
H	1.429736	-1.718959	1.199842
H	1.682724	1.894659	-0.895529
H	3.086403	1.257974	-0.000337
H	1.682729	1.895114	0.894548
H	1.429647	-1.719557	-1.198992
H	2.973402	-0.780790	-1.188501
H	1.543517	-0.182805	-2.096441
H	-2.680087	-2.168884	-0.000005
H	-3.947526	-0.078341	-0.000011
H	-2.763085	2.114058	-0.000019
H	-0.310185	2.175181	0.000000

2b (in THF)

O	1.453214	-0.980377	1.486683
N	0.575783	1.130489	-0.231160
C	2.774242	-2.041297	-0.201157
C	1.926407	-0.941013	0.370376
C	1.723716	0.231360	-0.575562
C	0.898795	1.911272	1.003669
C	0.427833	2.108965	-1.358660
C	-0.731769	0.317975	-0.148149
C	-0.929858	-0.606237	-1.168488
C	-2.165664	-1.280286	-1.043854
C	-3.090999	-1.043417	-0.021436
C	-2.809839	-0.090040	0.956551
C	-1.604956	0.611583	0.900367
H	2.167396	-2.589153	-0.931897
H	3.094857	-2.719461	0.589999
H	3.640185	-1.633553	-0.731925
H	1.548442	-0.156439	-1.578195
H	2.635679	0.838956	-0.580487
H	0.151511	2.692794	1.131849
H	1.877051	2.372124	0.858834
H	0.915942	1.241614	1.859554
H	0.205457	1.547961	-2.265215
H	1.359238	2.669999	-1.460488
H	-0.398628	2.778149	-1.117227
H	-2.432937	-2.037431	-1.783797
H	-4.025908	-1.598901	0.016699
H	-3.510909	0.107948	1.762034
H	-1.391025	1.341794	1.672970

2c (in THF)

O	2.786043	-0.701378	-0.521778
O	1.510176	-0.428591	1.306410
N	-0.130235	1.437057	-0.164146
C	3.479339	-1.772307	0.138866
C	1.818716	-0.116658	0.180265
C	1.227789	1.015940	-0.632999
C	-0.014589	2.170617	1.134719
C	-0.661037	2.402958	-1.182914
C	-1.079303	0.221370	-0.124485
C	-1.015486	-0.622255	-1.227347
C	-1.932777	-1.693108	-1.131092
C	-2.809556	-1.882452	-0.057568
C	-2.805100	-0.980009	1.005800
C	-1.922096	0.099890	0.981502
H	4.220727	-2.124613	-0.575795
H	2.779279	-2.571502	0.389055
H	3.964876	-1.404975	1.045270
H	1.891683	1.883929	-0.569352
H	1.139247	0.692495	-1.667233
H	-0.980086	2.612582	1.375663
H	0.719962	2.965834	1.001077
H	0.304265	1.480692	1.912376
H	-0.740816	1.880717	-2.135088
H	0.026183	3.248775	-1.254272
H	-1.644784	2.734693	-0.849815
H	-1.973804	-2.429609	-1.935961
H	-3.491701	-2.730179	-0.044487
H	-3.472587	-1.110251	1.852569
H	-1.915955	0.787850	1.819482

2d (in THF)

N	-0.795835	0.307100	0.234122
N	-4.103160	-0.555318	-0.455160
C	-1.205438	1.716712	-0.035622

C	-1.169312	-0.036756	1.646195
C	-1.497096	-0.608389	-0.725558
C	-2.953267	-0.571003	-0.565515
C	0.721445	0.046497	0.055726
C	1.113442	-1.276750	0.207785
C	2.508729	-1.439656	0.061278
C	3.394464	-0.390306	-0.206936
C	2.907693	0.908835	-0.348715
C	1.538935	1.145648	-0.216069
H	-0.710193	2.369621	0.681703
H	-2.285756	1.793036	0.094842
H	-0.932014	1.980348	-1.057250
H	-0.924467	-1.083802	1.813995
H	-2.234709	0.152231	1.788757
H	-0.578748	0.600011	2.304972
H	-1.115953	-1.615579	-0.535860
H	-1.232704	-0.304617	-1.741478
H	2.940070	-2.437210	0.160636
H	4.460783	-0.581267	-0.307993
H	3.577486	1.736765	-0.560861
H	1.171602	2.158994	-0.329601

2e (in THF)

O	3.064946	-1.256649	0.537238
N	1.055471	-2.121048	-0.068167
N	0.699804	1.024766	-0.131033
C	1.991009	-1.155496	-0.048493
C	1.659227	0.106365	-0.845216
C	1.276109	1.378210	1.200339
C	0.606423	2.282109	-0.944071
C	-0.708934	0.405001	-0.060894
C	-1.195887	-0.119523	-1.255032
C	-2.495001	-0.655861	-1.114993
C	-3.217683	-0.660898	0.083578
C	-2.653418	-0.106341	1.231079
C	-1.371554	0.442738	1.167706
H	1.221999	-2.983336	0.434359
H	0.182573	-1.992364	-0.567575
H	2.585895	0.663136	-0.985572
H	1.195893	-0.137729	-1.801319
H	0.682806	2.175821	1.644513
H	2.297294	1.727220	1.043094
H	1.278583	0.499467	1.845104
H	0.242244	2.016504	-1.935228
H	1.598042	2.735334	-0.996595
H	-0.098539	2.951216	-0.449723
H	-2.980232	-1.101490	-1.985354
H	-4.214588	-1.094657	0.125591
H	-3.195296	-0.097703	2.172093
H	-0.944903	0.867913	2.069078

2f (in THF)

N	-0.639492	1.540026	0.042212
C	1.519567	0.349260	-0.557305
C	1.307018	-1.013789	-0.798382
C	2.268363	-1.952337	-0.426777
C	3.454044	-1.539925	0.182514
C	3.680121	-0.183072	0.412935
C	2.716885	0.754509	0.042354
C	0.494734	1.376541	-0.960906
C	-0.078613	1.934250	1.365247
C	-1.499775	2.670311	-0.435277
C	-1.482322	0.256271	0.078385
C	-2.100012	-0.091728	-1.121773
C	-2.829247	-1.296565	-1.019185
C	-2.915052	-2.068844	0.145519
C	-2.262255	-1.646208	1.301880
C	-1.529705	-0.457730	1.277196
H	0.385877	-1.335858	-1.276583
H	2.091957	-3.006562	-0.617816
H	4.202131	-2.272847	0.469784
H	4.605105	0.145837	0.876926
H	2.896619	1.812909	0.217612
H	0.954181	2.364318	-1.052963
H	0.002647	1.106208	-1.896200
H	-0.902607	2.114286	2.055912
H	0.495800	2.851289	1.225248
H	0.572407	1.149905	1.745451
H	-1.875969	2.418669	-1.423850
H	-0.894404	3.577813	-0.459856
H	-2.330307	2.781561	0.262753
H	-3.360382	-1.670561	-1.896872
H	-3.487548	-2.994297	0.153995
H	-2.314853	-2.226411	2.218429
H	-1.026711	-0.142118	2.183996

2g (in THF)

Si	-1.841965	-0.651808	-0.049219
N	0.155159	1.568144	-0.085383
C	-3.483172	-0.710380	-0.967195
C	-2.173259	-0.649036	1.802769
C	-0.814219	-2.151024	-0.506824
C	-1.088631	0.986201	-0.711201
C	0.618185	2.724726	-0.918106
C	-0.185514	2.116601	1.258248
C	1.247357	0.490695	-0.060334
C	1.698413	0.058170	-1.306793
C	2.656755	-0.973835	-1.199150
C	3.101218	-1.515429	0.012689
C	2.598281	-1.019999	1.214609
C	1.653414	0.007600	1.186854
H	-4.133225	0.125203	-0.684923
H	-4.013529	-1.641167	-0.736378
H	-3.332762	-0.672882	-2.052025
H	-1.253818	-0.727797	2.392857
H	-2.789464	-1.524545	2.041386
H	-2.723408	0.241561	2.125744
H	-0.583198	-2.160754	-1.577209
H	-1.382979	-3.059206	-0.272161
H	0.131168	-2.187092	0.044701
H	-0.837577	0.801536	-1.760392
H	-1.848684	1.776212	-0.682822
H	1.506236	3.151766	-0.449045
H	-0.187907	3.459350	-0.956003
H	0.861115	2.353307	-1.910044
H	-0.576069	1.330016	1.898541
H	-0.947845	2.884061	1.120069
H	0.708849	2.556648	1.700123
H	3.086050	-1.394529	-2.110855
H	3.837017	-2.317196	0.022976
H	2.932816	-1.417653	2.168330
H	1.275651	0.385728	2.130487

2h (in THF)

N	-1.369083	-0.011991	0.118700
C	-1.872248	0.083083	1.505323
C	-2.164338	-0.804769	-0.828505
C	-2.139368	0.675091	-0.934794
C	0.124118	-0.072345	0.023195
C	0.714491	-1.329355	0.049752
C	2.128190	-1.229959	0.004844
C	2.832833	-0.023004	-0.052663
C	2.144444	1.194316	-0.065704
C	0.753341	1.174324	-0.023083
H	-2.962642	0.109844	1.489921
H	-1.474886	0.995438	1.952228
H	-1.518098	-0.794264	2.047813
H	-3.026343	-1.293002	-0.389101

H	-1.561933	-1.390023	-1.511982
H	-2.980072	1.255458	-0.571521
H	-1.525683	1.125809	-1.705941
H	2.724366	-2.144389	0.016247
H	3.920519	-0.024544	-0.087837
H	2.678932	2.138574	-0.110263
H	0.180652	2.100730	-0.030655

2i (in THF)

N	-0.744321	-0.465274	0.112664
N	-3.986279	0.967034	0.175369
C	-1.193302	-0.824263	1.479738
C	-1.344425	-1.161894	-1.034792
C	-1.664620	0.271510	-0.772311
C	-2.951850	0.656285	-0.233601
C	0.703141	-0.051897	0.037599
C	0.981274	1.301362	0.119534
C	2.379682	1.534965	0.078149
C	3.340756	0.525944	-0.032206
C	2.951499	-0.816371	-0.106064
C	1.595017	-1.121998	-0.067786
H	-2.234951	-1.144864	1.456575
H	-1.070495	0.058960	2.107737
H	-0.556328	-1.636933	1.828545
H	-2.075626	-1.920258	-0.777404
H	-0.654085	-1.371749	-1.843199
H	-1.162707	1.042671	-1.349087
H	2.747735	2.560779	0.132495
H	4.398551	0.778693	-0.063489
H	3.689174	-1.608144	-0.194686
H	1.249919	-2.153327	-0.123287

2j (in $CHCl_3$)

N	-1.197746	-0.266449	-0.348412
C	-1.767454	-1.444800	0.361221
C	-1.484998	-0.432993	-1.808178
C	-1.902330	0.991133	0.118130
C	-1.746171	1.262753	1.601494
C	0.323629	-0.104072	-0.176668
C	0.879945	1.003634	-0.811396
C	2.276994	1.080853	-0.618918
C	3.023615	0.156017	0.120301
C	2.382533	-0.925833	0.721301
C	1.001344	-1.066885	0.575188
H	-1.346111	-2.355893	-0.063724
H	-2.848362	-1.436040	0.211725
H	-1.542009	-1.389424	1.424192
H	-1.099886	0.442299	-2.327652
H	-2.564202	-0.532193	-1.942305
H	-0.970981	-1.329236	-2.158074
H	-2.953115	0.867933	-0.159144
H	-1.456710	1.792103	-0.470952
H	-0.692149	1.286123	1.891145
H	-2.275489	0.536478	2.223128
H	-2.171369	2.248551	1.808368
H	2.827727	1.909262	-1.069074
H	4.099849	0.275578	0.228741
H	2.940162	-1.656720	1.299590
H	0.514231	-1.912517	1.048079

2k (in $CHCl_3$)

O	2.983442	-1.401221	-0.268926
O	3.135296	0.822176	-0.020579
N	-0.479256	1.236335	0.245872
C	4.287411	-1.534498	0.314866
C	2.522225	-0.154813	-0.395488
C	0.323238	1.083707	1.491389
C	-1.101839	2.598575	0.271731
C	0.433246	1.182467	-0.959602
C	1.182478	-0.131771	-1.093907
C	-1.606998	0.195532	0.096190
C	-2.334078	0.270042	-1.088168
C	-3.355072	-0.703901	-1.150403
C	-3.612961	-1.639070	-0.141789
C	-2.836353	-1.638070	1.015753
C	-1.808213	-0.703118	1.147398
H	4.496235	-2.602838	0.322944
H	4.288661	-1.137181	1.332004
H	5.027166	-1.004444	-0.288556
H	-0.323895	1.251001	2.351981
H	1.120367	1.827038	1.475657
H	0.750136	0.082163	1.542498
H	-1.656338	2.733176	-0.655193
H	-0.307377	3.341205	0.369587
H	-1.781050	2.646776	1.123680
H	1.128137	2.020560	-0.863641
H	-0.224814	1.330901	-1.813587
H	1.392612	-0.299647	-2.156830
H	0.578702	-0.985680	-0.772250
H	-3.993640	-0.744951	-2.034957
H	-4.415189	-2.365724	-0.254130
H	-3.018874	-2.352469	1.813085
H	-1.214469	-0.712368	2.054827

3a (in THF)

N	-1.442048	-0.016958	0.047060
C	-1.980043	-0.571168	1.376878
C	-1.952889	-0.871413	-1.068909
C	-2.037932	1.335979	-0.142938
C	0.046251	0.022838	-0.002477
C	0.750916	1.224527	-0.017231
C	2.148823	1.208564	-0.020389
C	2.845549	0.006105	-0.019606
C	2.132390	-1.194770	-0.008686
C	0.742835	-1.190097	0.006063
H	-1.498952	0.070440	2.131698
H	-1.496225	-1.554055	1.469758
H	-1.561817	-0.497027	-2.017585
H	-3.040524	-0.821380	-1.044349
H	-1.639416	-1.901194	-0.910033
H	-1.760105	1.971550	0.697143
H	-3.117801	1.205056	-0.148722
H	-1.695262	1.766854	-1.086045
H	0.244089	2.180535	-0.023871
H	2.685128	2.152432	-0.027518
H	3.930877	-0.000470	-0.025611
H	2.659420	-2.143787	-0.003852
H	0.209522	-2.133627	0.043338

3b (in THF)

O	-1.440122	-1.122526	-1.347341
N	-0.565278	1.084766	0.207808
C	-3.197510	-1.722527	0.172163
C	-2.030651	-0.847625	-0.260008
C	-1.696980	0.194244	0.582177
C	-0.908867	1.827533	-1.052284
C	-0.386040	2.108182	1.291531
C	0.725799	0.331486	0.085070
C	1.056235	-0.546269	1.114941
C	2.268703	-1.227237	1.077034
C	3.151272	-1.036122	0.012806
C	2.810726	-0.154859	-1.008070
C	1.598478	0.539280	-0.976357
H	-3.646120	-1.402736	1.117249
H	-2.850707	-2.756106	0.274757
H	-3.965046	-1.708558	-0.608518
H	-2.167156	0.434448	1.523568
H	-0.134258	2.563099	-1.271527

H	-1.855891	2.330069	-0.863817
H	-1.015828	1.094614	-1.850288
H	-0.184458	1.593344	2.230166
H	-1.310158	2.682539	1.366731
H	0.450434	2.754388	1.023379
H	0.357919	-0.710620	1.928810
H	2.518448	-1.914645	1.879192
H	4.092902	-1.574977	-0.020513
H	3.483410	-0.001821	-1.846159
H	1.357437	1.207302	-1.792971

3c (in THF)

O	2.952120	-0.661728	-0.567095
O	1.511725	-0.594714	1.193446
N	-0.054410	1.384905	-0.134765
C	3.676455	-1.647005	0.154509
C	1.853798	-0.140897	0.086268
C	1.260770	0.900163	-0.626006
C	0.118404	2.089270	1.180447
C	-0.561821	2.409675	-1.108486
C	-1.079934	0.290224	-0.053032
C	-1.236261	-0.522389	-1.174689
C	-2.195178	-1.529261	-1.168242
C	-2.992474	-1.735767	-0.040728
C	-2.821484	-0.924298	1.075261
C	-1.867864	0.097825	1.074956
H	4.500367	-1.947251	-0.495039
H	3.051798	-2.515043	0.383303
H	4.074769	-1.243285	1.090448
H	1.445495	1.080663	-1.673778
H	-0.828943	2.536278	1.485065
H	0.864907	2.863924	1.017225
H	0.476879	1.364873	1.908997
H	-0.674835	1.944024	-2.086560
H	0.173367	3.213431	-1.158197
H	-1.522774	2.781021	-0.751207
H	-0.595835	-0.382304	-2.039271
H	-2.311605	-2.159426	-2.044390
H	-3.734001	-2.528431	-0.032866
H	-3.425271	-1.080462	1.963740
H	-1.750679	0.703945	1.963541

3d (in THF)

N	-0.965762	0.759499	0.174757
N	-2.603866	-2.163009	-0.790364
C	-1.419230	1.208017	-1.186360
C	-0.956112	1.953607	1.086134
C	-1.981984	-0.186007	0.730248
C	-2.283768	-1.274175	-0.092406
C	0.442340	0.229188	0.079780
C	0.748907	-1.038774	0.557860
C	2.063194	-1.504184	0.474748
C	3.062226	-0.710928	-0.079337
C	2.744290	0.562257	-0.552527
C	1.438160	1.037181	-0.473986
H	-0.776180	2.011469	-1.541032
H	-2.446207	1.556262	-1.085143
H	-1.370485	0.357110	-1.865523
H	-0.647872	1.619658	2.077224
H	-1.969888	2.350418	1.116676
H	-0.257942	2.697356	0.704154
H	-1.782443	-0.407946	1.773157
H	-0.017494	-1.669000	0.989548
H	2.294536	-2.497095	0.847015
H	4.081442	-1.078505	-0.143367
H	3.513237	1.194366	-0.985275
H	1.218543	2.033389	-0.843114

3e (in THF)

O	-1.429470	-1.227545	-1.264137
N	-3.196785	-1.630045	0.142611
N	-0.593226	1.058143	0.181554
C	-2.041136	-0.893483	-0.215237
C	-1.692454	0.164114	0.618685
C	-0.959358	1.749969	-1.102784
C	-0.421102	2.129224	1.220815
C	0.716031	0.331351	0.075406
C	1.088368	-0.482806	1.142978
C	2.318640	-1.131353	1.118762
C	3.177264	-0.974554	0.029390
C	2.794061	-0.159487	-1.030322
C	1.564506	0.504521	-1.011473
H	-3.146577	-2.577591	-0.214354
H	-3.424972	-1.616797	1.130481
H	-2.278689	0.538415	1.444302
H	-0.200910	2.490909	-1.358870
H	-1.913684	2.241868	-0.923231
H	-1.061058	0.988334	-1.874014
H	-0.205516	1.657239	2.178425
H	-1.353073	2.692649	1.279384
H	0.402584	2.776314	0.918114
H	0.405897	-0.623237	1.974205
H	2.601406	-1.767341	1.951868
H	4.132706	-1.489134	0.006862
H	3.446623	-0.034393	-1.888725
H	1.292179	1.121475	-1.857825

3f (in THF)

N	-0.646597	1.463778	0.093059
C	1.628240	0.405968	-0.243435
C	1.419172	-0.759878	0.552382
C	2.451874	-1.658297	0.822259
C	3.743368	-1.462826	0.336118
C	3.980185	-0.315940	-0.439987
C	2.968444	0.585151	-0.716439
C	0.646044	1.345153	-0.656348
C	-0.408958	1.853941	1.527001
C	-1.428640	2.583154	-0.536542
C	-1.499377	0.237401	-0.026792
C	-1.525430	-0.426296	-1.250873
C	-2.336673	-1.546542	-1.406092
C	-3.116526	-2.007957	-0.345103
C	-3.085223	-1.333070	0.871431
C	-2.280944	-0.203268	1.037115
H	0.437947	-0.977500	0.961911
H	2.231664	-2.531626	1.432748
H	4.539181	-2.167919	0.552760
H	4.977188	-0.123305	-0.830390
H	3.186355	1.460745	-1.325073
H	0.981794	2.338741	-0.935633
H	-1.348345	2.108880	2.018767
H	0.242899	2.725741	1.502062
H	0.088075	1.032919	2.042267
H	-1.570705	2.348944	-1.590630
H	-0.850324	3.501737	-0.427879
H	-2.387279	2.670660	-0.024051
H	-0.891160	-0.073744	-2.056600
H	-2.347727	-2.066121	-2.359087
H	-3.739208	-2.888818	-0.465759
H	-3.684470	-1.681001	1.706996
H	-2.273038	0.295044	1.998005

3g (in THF)

Si	-1.845617	-0.551909	0.081378
N	0.148291	1.574096	0.102058
C	-3.561591	-0.642906	0.874239
C	-0.906116	-2.128408	0.555116

C	-2.124379	-0.741602	-1.800106
C	-1.111037	1.000956	0.741605
C	-0.131732	2.183719	-1.239785
C	0.676647	2.692795	0.954219
C	1.178144	0.504549	0.019219
C	1.639457	-0.052032	1.214024
C	2.579028	-1.075971	1.181303
C	3.055761	-1.559900	-0.038740
C	2.587043	-1.004342	-1.223699
C	1.650228	0.034010	-1.201907
H	-3.494147	-0.657733	1.967595
H	-4.084938	-1.552276	0.555755
H	-4.180499	0.215379	0.587270
H	0.043500	-2.221997	0.013825
H	-1.514099	-3.008153	0.307577
H	-0.687043	-2.157958	1.628522
H	-2.706582	0.092550	-2.210829
H	-2.672509	-1.668926	-2.013463
H	-1.175566	-0.794550	-2.349669
H	-1.830386	1.830807	0.738631
H	0.779596	2.610178	-1.667839
H	-0.869656	2.967877	-1.076263
H	-0.556166	1.427718	-1.896581
H	0.850030	2.322382	1.960427
H	-0.090068	3.467800	0.984329
H	1.597557	3.082002	0.513419
H	1.238369	0.286078	2.162112
H	2.928588	-1.506078	2.114670
H	3.782855	-2.365645	-0.061697
H	2.944855	-1.370459	-2.180872
H	1.308191	0.443853	-2.143551

3h (in THF)

N	1.402280	-0.050569	0.084402
C	1.888884	0.022631	1.477824
C	2.187547	0.667222	-0.934405
C	2.181817	-0.837113	-0.960671
C	-0.050060	-0.025338	0.000789
C	-0.746607	-1.227995	-0.026751
C	-2.139834	-1.202569	-0.046993
C	-2.820052	0.016428	-0.046088
C	-2.106746	1.214807	-0.019236
C	-0.712434	1.197902	0.009901
H	2.978076	0.072206	1.459750
H	1.567720	-0.879543	2.003330
H	1.477737	0.908235	1.968624
H	2.990324	1.260276	-0.495926
H	1.579174	1.209761	-1.654914
H	3.065973	-1.193598	-0.416368
H	-0.195052	-2.162732	-0.049654
H	-2.693906	-2.135717	-0.071916
H	-3.905329	0.032007	-0.070929
H	-2.633201	2.164101	-0.022780
H	-0.142571	2.123138	0.033747

3i (in THF)

N	-0.780567	0.441832	-0.124083
N	-3.952884	-1.061040	-0.072220
C	-1.199331	0.709779	-1.521861
C	-1.408912	1.258279	0.939005
C	-1.708487	-0.198822	0.871380
C	-2.943359	-0.615357	0.307469
C	0.637787	0.113278	-0.017896
C	1.022354	-1.220818	-0.048257
C	2.381079	-1.527624	-0.006201
C	3.329122	-0.506233	0.070195
C	2.922228	0.827692	0.099859
C	1.565525	1.146065	0.050143
H	-2.240950	1.029509	-1.526609
H	-1.086584	-0.212799	-2.094369
H	-0.561733	1.493404	-1.934417
H	-2.085724	2.012436	0.541000
H	-0.717970	1.607325	1.701319
H	0.266616	-1.999143	-0.090934
H	2.697232	-2.565640	-0.026300
H	4.386052	-0.750524	0.110171
H	3.658510	1.622630	0.162930
H	1.230678	2.179835	0.068325

3i' (in THF)

N	-0.769231	-0.519199	0.157454
N	-3.929740	1.033917	-0.022933
C	-1.208218	-0.537920	1.575115
C	-1.368814	-1.469896	-0.858353
C	-1.684376	0.013049	-0.873369
C	-2.917857	0.592125	-0.371398
C	0.641434	-0.157749	0.027321
C	1.583365	-1.170547	-0.097230
C	2.932937	-0.826846	-0.157507
C	3.319878	0.512603	-0.100169
C	2.357948	1.515648	0.022953
C	1.006099	1.182390	0.093344
H	-2.260987	-0.815143	1.619915
H	-1.049559	0.444336	2.025468
H	-0.607475	-1.290771	2.087754
H	-2.168751	-1.979948	-0.308938
H	-1.204731	0.646129	-1.616747
H	1.255396	-2.203325	-0.159830
H	3.680880	-1.607184	-0.256463
H	4.371723	0.775288	-0.155233
H	2.656854	2.558180	0.063721
H	0.245072	1.952269	0.194454

4 (in $CHCl_3$)

Cl	2.601004	-1.381900	-1.019072
Cl	2.476817	-0.261679	1.681965
Cl	3.310545	1.417272	-0.565360
N	-1.975611	-1.173251	-0.425927
C	2.259471	0.079240	-0.051574
C	-1.430951	-1.480959	-1.786518
C	-3.342212	-1.762033	-0.344531
C	-1.080780	-1.853859	0.591493
C	-1.497673	-1.620959	2.029350
C	-1.939719	0.346539	-0.226819
C	-0.673757	0.926845	-0.251338
C	-0.707926	2.324400	-0.068987
C	-1.883540	3.061157	0.112178
C	-3.111766	2.403907	0.121801
C	-3.150346	1.018375	-0.047685
H	1.174974	0.363558	-0.211157
H	-2.062158	-0.989661	-2.527895
H	-1.441477	-2.563419	-1.928015
H	-0.417477	-1.087487	-1.842530
H	-3.798046	-1.520992	0.613701
H	-3.245650	-2.843861	-0.447687
H	-3.949713	-1.369067	-1.159562
H	-0.084924	-1.451406	0.410573
H	-1.090571	-2.916565	0.333512
H	-2.459634	-2.080126	2.269451
H	-1.537052	-0.553881	2.262751
H	-0.741479	-2.077611	2.673909
H	0.232767	2.879042	-0.063568
H	-1.844802	4.139899	0.246903
H	-4.038151	2.953027	0.261625
H	-4.114350	0.522595	-0.032802

5 (in $CHCl_3$)

Cl	3.122647	-1.330976	-0.375689

Cl	2.424772	0.682243	1.671188
Cl	3.028859	1.527014	-1.088177
N	-1.449814	-1.328493	-0.453792
C	2.123152	0.228493	-0.119543
C	-0.560131	-1.323352	-1.671392
C	-2.484271	-2.387905	-0.657960
C	-0.580601	-1.693119	0.748998
C	-1.314335	-1.656860	2.073017
C	-2.041171	0.031543	-0.270918
C	-1.158931	1.098644	-0.099689
C	-1.672751	2.378051	0.087870
C	-3.051137	2.593641	0.102906
C	-3.916648	1.519049	-0.071766
C	-3.417797	0.227578	-0.258948
H	-1.158082	-1.013043	-2.528649
H	-0.182497	-2.337707	-1.810114
H	0.272017	-0.639184	-1.494398
H	-3.158592	-2.424537	0.195211
H	-1.958858	-3.336943	-0.760387
H	-3.036456	-2.168976	-1.572171
H	0.254012	-0.988780	0.731004
H	-0.192597	-2.690469	0.526468
H	-2.108161	-2.404629	2.141612
H	-1.730089	-0.667234	2.279526
H	-0.582044	-1.877539	2.854319
H	-0.079816	0.937939	-0.110231
H	-0.984792	3.206510	0.223484
H	-3.445883	3.593864	0.250175
H	-4.990878	1.672698	-0.062262
H	-4.117596	-0.587865	-0.386973

6 (in $CHCl_3$)

Cl	2.258398	-1.183342	1.892787
Cl	2.212229	-0.471837	-0.947055
Cl	2.096931	-3.280628	-0.135932
O	1.438278	2.820346	-1.525907
O	1.631568	2.797860	0.709862
N	-2.106054	0.804737	1.140788
C	1.628887	-1.618483	0.284266
C	2.755240	3.383133	-1.610371
C	0.991995	2.567807	-0.293949
C	-2.201137	0.107699	2.464909
C	-3.085926	1.929928	1.153071
C	-0.707915	1.365481	1.033020
C	-0.405677	1.996718	-0.314648
C	-2.360163	-0.231791	0.037576
C	-1.392075	-1.224181	-0.088687
C	-1.688076	-2.145959	-1.114365
C	-2.833268	-2.085072	-1.915818
C	-3.757388	-1.061361	-1.718307
C	-3.523534	-0.108499	-0.724840
H	0.507287	-1.531348	0.302267
H	2.956025	3.499563	-2.673989
H	3.484034	2.709445	-1.154482
H	2.786040	4.351842	-1.106887
H	-3.212152	-0.287505	2.568952
H	-1.985433	0.829671	3.255249
H	-1.477788	-0.706371	2.469632
H	-3.101074	2.425271	0.183831
H	-2.780771	2.633372	1.928619
H	-4.075084	1.538118	1.387055
H	-0.032233	0.530789	1.215269
H	-0.601834	2.089147	1.843446
H	-1.082106	2.825997	-0.551575
H	-0.479936	1.265752	-1.124182
H	-0.987689	-2.960825	-1.310079
H	-3.004632	-2.827915	-2.691733
H	-4.653480	-0.992393	-2.327745
H	-4.249830	0.684756	-0.588555

7 (in $CHCl_3$)

Cl	-2.942802	-2.159677	1.026155
Cl	-2.425352	-1.401600	-1.780598
Cl	-4.319559	0.163551	-0.151609
O	3.913421	-1.426591	-1.270440
O	3.126482	-2.188741	0.687379
N	0.807876	0.506927	1.269855
C	-2.666946	-0.676520	-0.070530
C	5.132408	-2.150221	-1.041900
C	2.976089	-1.546108	-0.329195
C	-0.314752	0.446010	2.276365
C	2.097280	0.450999	2.024891
C	0.676315	-0.726468	0.382409
C	1.713568	-0.812026	-0.720921
C	0.664962	1.758114	0.461823
C	-0.496656	1.905868	-0.296752
C	-0.667022	3.059246	-1.056130
C	0.308007	4.057093	-1.058757
C	1.458084	3.896205	-0.293352
C	1.646165	2.743868	0.473782
H	5.761063	-1.942647	-1.905868
H	4.926245	-3.219742	-0.966347
H	5.613279	-1.801036	-0.125914
H	-0.275792	1.350584	2.883226
H	-0.161466	-0.441665	2.891901
H	-1.260484	0.368742	1.736682
H	2.938906	0.528907	1.337550
H	2.131323	-0.506621	2.541960
H	2.118347	1.270216	2.743877
H	-0.335689	-0.688360	-0.023537
H	0.747746	-1.584252	1.055652
H	1.969324	0.167744	-1.137563
H	1.275399	-1.379551	-1.550382
H	-1.268762	1.134532	-0.290992
H	-1.571508	3.172006	-1.645382
H	0.169128	4.954713	-1.652795
H	2.223555	4.665445	-0.284064
H	2.551130	2.650139	1.059991

9 (in $CHCl_3$)

S	-0.042859	3.378315	0.120181
O	-0.870337	2.887914	-0.985622
O	0.510984	4.731363	-0.006698
O	-4.203764	-0.154392	-1.536851
O	-4.535550	-1.898923	-0.167472
N	1.274589	2.392489	0.418977
N	-1.087427	-1.968251	1.050980
C	-0.977181	3.279507	1.622840
C	-5.591249	0.186694	-1.410374
C	-3.799109	-1.230027	-0.862243
C	-2.104959	-1.128518	1.766770
C	-0.748343	-3.071691	2.009357
C	-1.744259	-2.558608	-0.180934
C	-2.336438	-1.514362	-1.114864
C	0.162677	-1.131498	0.661010
C	-0.015618	0.242091	0.776999
C	1.119182	0.949985	0.394824
C	2.324945	0.397494	-0.011436
C	2.438642	-0.992496	-0.087158
C	1.325356	-1.815571	0.222726
C	2.484858	2.726938	-0.384076
C	3.354379	1.465869	-0.255092
C	3.709885	-1.546006	-0.472264
C	4.803489	-1.965080	-0.788011
C	6.118714	-2.480699	-1.168779
C	1.556018	-3.307442	0.072940
H	-1.851416	3.919051	1.480045
H	-0.350135	3.646287	2.436049
H	-1.255449	2.233929	1.764774

H	-5.727309	1.082822	-2.013165
H	-5.836106	0.388416	-0.365600
H	-6.216302	-0.626434	-1.785783
H	-1.667927	-0.787459	2.704508
H	-2.972158	-1.765565	1.943791
H	-2.357659	-0.257624	1.170958
H	-0.264961	-3.895505	1.497252
H	-1.674532	-3.429307	2.460702
H	-0.090731	-2.662685	2.777238
H	-2.518672	-3.244730	0.173353
H	-0.980627	-3.127312	-0.703929
H	-2.270890	-1.886567	-2.143296
H	-1.771057	-0.576693	-1.092980
H	2.954968	3.629162	0.004280
H	2.210124	2.885972	-1.434858
H	4.032277	1.541229	0.604432
H	3.960453	1.296380	-1.148381
H	6.907172	-1.996432	-0.585817
H	6.316614	-2.296555	-2.228608
H	6.176348	-3.558372	-0.992327
H	2.337861	-3.478233	-0.668691
H	0.685792	-3.870723	-0.259546
H	1.903334	-3.752947	1.012724

10 (in $CHCl_3$)

S	3.310230	-0.486606	0.192268
O	4.295479	-1.564465	0.048287
O	3.152781	0.101659	1.525294
N	1.880869	-1.117244	-0.401605
N	-1.064223	2.906576	-0.020008
C	3.699873	0.803343	-0.958525
C	-1.449510	3.330243	1.363807
C	-2.069778	3.353185	-1.036448
C	0.194260	3.656966	-0.344884
C	-0.841622	1.370455	-0.064287
C	0.486635	0.992508	-0.212399
C	0.635501	-0.390524	-0.230965
C	-0.392537	-1.320641	-0.163065
C	-1.705741	-0.865776	-0.029379
C	-1.971770	0.524522	0.058014
C	1.630908	-2.534763	-0.015645
C	0.133452	-2.721700	-0.307177
C	-2.764707	-1.838738	0.007521
C	-3.629634	-2.688871	0.024714
C	-4.678505	-3.708653	0.046332
C	-3.433079	0.888980	0.242555
H	4.641833	1.239348	-0.617637
H	2.882453	1.525481	-0.928325
H	3.808709	0.355445	-1.946722
H	-2.347280	2.812985	1.687415
H	-1.617035	4.409261	1.365352
H	-0.623545	3.072906	2.027457
H	-1.748084	2.979245	-2.009183
H	-2.092639	4.444186	-1.041843
H	-3.058403	2.975820	-0.804070
H	0.971248	3.386244	0.362945
H	-0.051231	4.718173	-0.277842
H	0.516283	3.394611	-1.350371
H	1.824129	-2.675090	1.055789
H	2.277988	-3.198805	-0.586769
H	-0.328134	-3.436737	0.378194
H	-0.025928	-3.082870	-1.330960
H	-5.661042	-3.248189	0.182003
H	-4.516157	-4.415103	0.865271
H	-4.691424	-4.271388	-0.891437
H	-3.960871	0.886523	-0.719227
H	-3.614108	1.850967	0.714981
H	-3.915526	0.136590	0.870318

11a (in MeCN)

N	2.296776	-0.438810	0.000286
C	3.690118	-0.032311	-0.000379
C	1.417322	0.478126	0.000303
C	-0.034700	0.200839	0.000211
C	-0.539453	-1.107247	0.000148
C	-1.913324	-1.325317	-0.000109
C	-2.798177	-0.242025	-0.000162
C	-2.302415	1.061068	-0.000114
C	-0.924783	1.280322	-0.000017
H	4.185973	-0.454997	0.879144
H	3.822005	1.058231	0.000552
H	4.184648	-0.453290	-0.881494
H	1.697676	1.542090	0.000433
H	0.152470	-1.944145	0.000426
H	-2.299150	-2.340439	0.000010
H	-3.870014	-0.416745	-0.000458
H	-2.985227	1.905341	-0.000072
H	-0.533341	2.294896	0.000175

12a (in MeCN)

N	0.717674	1.640959	-0.060273
C	1.484159	2.891812	-0.077958
C	-0.570433	1.658884	-0.055457
C	-1.512446	0.540776	-0.088894
C	-1.223958	-0.769249	-0.515184
C	-2.234535	-1.723355	-0.534312
C	-3.528725	-1.397173	-0.120281
C	-3.824635	-0.099253	0.293873
C	-2.825001	0.867953	0.293373
C	1.533048	0.417901	-0.015305
C	2.231181	0.061886	-1.171775
C	2.944411	-1.149005	-0.984869
C	2.956815	-1.884669	0.206224
C	2.243949	-1.431911	1.320668
C	1.516302	-0.250096	1.213032
H	2.082773	2.937539	0.834480
H	0.807822	3.743562	-0.140483
H	2.146884	2.863676	-0.944571
H	-1.020823	2.649248	-0.016165
H	-0.229381	-1.039068	-0.848493
H	-2.010762	-2.729374	-0.874394
H	-4.307138	-2.154249	-0.131592
H	-4.830940	0.162470	0.604238
H	-3.053665	1.886453	0.594974
H	3.527490	-1.553897	-1.814319
H	3.526611	-2.809352	0.272398
H	2.255586	-1.986085	2.254503
H	0.941033	0.135351	2.052528

12b (in MeCN)

N	-0.745819	-1.058684	-0.493294
N	-3.424285	-2.355553	1.189819
C	-2.706235	-2.205631	0.297996
C	-1.797567	-2.022782	-0.843353
C	0.481771	-1.455899	-0.411760
C	1.684800	-0.663740	-0.196364
C	1.805370	0.721933	-0.417558
C	3.032598	1.341177	-0.220205
C	4.138875	0.603781	0.212532
C	4.029227	-0.770020	0.423613
C	2.811898	-1.404245	0.201600
C	-1.219893	0.315188	-0.255644
C	-1.768952	0.997112	-1.341575
C	-2.157745	2.310107	-0.973914
C	-2.024155	2.840514	0.313971
C	-1.488075	2.063121	1.346469
C	-1.076830	0.765549	1.061214
H	-1.361227	-2.982445	-1.124736

H	-2.361427	-1.606596	-1.683481
H	0.636515	-2.527903	-0.522385
H	0.960024	1.306118	-0.760820
H	3.128257	2.406380	-0.403697
H	5.089766	1.102620	0.373963
H	4.889761	-1.346741	0.746123
H	2.722692	-2.478063	0.340931
H	-2.591963	2.966232	-1.730331
H	-2.345959	3.858912	0.521728
H	-1.396627	2.458076	2.353740
H	-0.649589	0.126070	1.831178

13a (in MeCN)

N	0.748618	1.724545	-0.050999
C	1.475078	2.816561	-0.271608
C	-0.593853	1.715680	0.153391
C	-1.503824	0.609356	-0.017167
C	-1.235084	-0.624375	-0.659612
C	-2.217910	-1.605858	-0.772459
C	-3.505633	-1.404079	-0.273822
C	-3.799068	-0.182172	0.340988
C	-2.824073	0.798251	0.466375
C	1.500568	0.486014	0.068179
C	2.313354	0.079389	-0.983593
C	3.024692	-1.114508	-0.861316
C	2.921085	-1.875624	0.302869
C	2.110607	-1.441354	1.354524
C	1.392185	-0.253665	1.241418
H	2.548466	2.749063	-0.179053
H	0.957040	3.753860	-0.425334
H	-1.012203	2.694808	0.355483
H	-0.261735	-0.817834	-1.096138
H	-1.971054	-2.538460	-1.273241
H	-4.264858	-2.173830	-0.370190
H	-4.796325	0.006570	0.729582
H	-3.070503	1.739534	0.952263
H	2.364428	0.676920	-1.888712
H	3.652955	-1.450792	-1.680106
H	3.473579	-2.805760	0.393350
H	2.039054	-2.026906	2.265661
H	0.752082	0.099319	2.044425

13b (in MeCN)

N	-1.035612	0.947237	-0.092898
N	-1.928967	4.276128	0.238402
C	-2.042951	3.119774	0.091954
C	-2.163281	1.742972	-0.068351
C	0.206830	1.386592	-0.133821
C	1.441377	0.626162	0.030601
C	1.575949	-0.589805	0.729007
C	2.822648	-1.196320	0.849401
C	3.959140	-0.611266	0.287018
C	3.842191	0.604149	-0.388366
C	2.599943	1.218718	-0.507593
C	-1.323514	-0.476920	-0.127173
C	-1.990073	-1.060498	0.943586
C	-2.246746	-2.430336	0.901787
C	-1.849608	-3.184838	-0.202950
C	-1.200556	-2.572232	-1.276627
C	-0.933293	-1.205372	-1.245171
H	-3.114427	1.269574	-0.247692
H	0.308748	2.455791	-0.295475
H	0.717620	-1.057227	1.198262
H	2.906724	-2.130689	1.396228
H	4.927046	-1.093071	0.385310
H	4.718900	1.076892	-0.820574
H	2.513782	2.168709	-1.028407
H	-2.279032	-0.456128	1.797998
H	-2.753664	-2.906187	1.735077
H	-2.051603	-4.251073	-0.230434
H	-0.904003	-3.156596	-2.141751
H	-0.426379	-0.708235	-2.066880

14a (in MeCN)

N	-1.500140	2.961374	0.733015
N	0.870714	1.156838	-1.035087
C	-1.724784	2.062820	1.427499
C	-2.000651	0.919707	2.289667
C	1.432716	2.434496	-1.484191
C	-0.366897	0.874017	-1.250003
C	-1.160157	-0.278954	-0.825699
C	-0.719541	-1.379494	-0.064737
C	-1.625087	-2.367396	0.307013
C	-2.969449	-2.278112	-0.060621
C	-3.416112	-1.193039	-0.814414
C	-2.517032	-0.202800	-1.193979
C	1.806062	0.301042	-0.291914
C	1.950556	0.544527	1.075946
C	2.861566	-0.368781	1.663539
C	3.534565	-1.376222	0.961056
C	3.341596	-1.524999	-0.415622
C	2.460755	-0.662491	-1.063769
H	-1.056895	0.435459	2.553048
H	-2.639475	0.210297	1.755832
H	-2.505965	1.259180	3.196235
H	1.778409	2.973717	-0.598926
H	0.673339	3.012067	-2.010226
H	2.282521	2.226719	-2.137952
H	-0.915497	1.625162	-1.815273
H	0.313071	-1.472548	0.243250
H	-1.277680	-3.211555	0.894015
H	-3.666247	-3.054385	0.240947
H	-4.459247	-1.116104	-1.103313
H	-2.866128	0.647846	-1.773326
H	3.064498	-0.301072	2.734061
H	4.216078	-2.045145	1.482819
H	3.865012	-2.296023	-0.973230
H	2.271553	-0.747042	-2.132085

14b (in MeCN)

N	1.004370	-2.739627	1.647778
N	-0.909239	-0.925394	-0.346422
N	-3.913423	-1.858718	-1.699008
C	1.648777	-1.839077	1.985390
C	2.451398	-0.693285	2.396288
C	-2.965909	-1.964739	-1.047558
C	-1.763213	-2.112031	-0.214628
C	0.296519	-1.061810	-0.790870
C	1.381900	-0.093031	-0.853714
C	1.379950	1.214211	-0.325561
C	2.535049	1.983233	-0.394159
C	3.696495	1.474560	-0.981399
C	3.710166	0.181058	-1.502665
C	2.561761	-0.598509	-1.433779
C	-1.502373	0.329544	0.141920
C	-1.609945	0.483459	1.524458
C	-2.163644	1.746424	1.853463
C	-2.564169	2.700886	0.911113
C	-2.440575	2.439533	-0.457553
C	-1.898752	1.222097	-0.858645
H	1.788955	0.148218	2.613900
H	3.135144	-0.421463	1.587338
H	3.023573	-0.950513	3.290138
H	-2.064052	-2.189803	0.835459
H	-1.221502	-3.012587	-0.510196
H	0.549420	-2.061511	-1.138601
H	0.499204	1.629062	0.146225
H	2.530183	2.986985	0.018093

H	4.591596	2.087535	-1.027448
H	4.611019	-0.220787	-1.954366
H	2.571626	-1.612037	-1.825170
H	-2.294385	2.011489	2.904089
H	-2.980804	3.650834	1.239658
H	-2.760222	3.167899	-1.196646
H	-1.772321	0.977718	-1.911519

15a (in MeCN)

N	-1.180728	2.723329	0.674153
N	0.870753	1.098938	-1.119539
C	-1.517349	2.001047	1.555941
C	-1.886893	1.119219	2.537834
C	1.512705	2.330520	-1.601621
C	-0.411119	0.935685	-1.244156
C	-1.240781	-0.197125	-0.851241
C	-0.784144	-1.476242	-0.485021
C	-1.702210	-2.471909	-0.166668
C	-3.072865	-2.208951	-0.194457
C	-3.534814	-0.944101	-0.559260
C	-2.624375	0.050558	-0.895171
C	1.728245	0.233467	-0.346468
C	1.579146	0.204614	1.037521
C	2.411496	-0.628697	1.782382
C	3.379727	-1.405185	1.143898
C	3.526925	-1.345975	-0.242976
C	2.701368	-0.516088	-1.000035
H	-2.938132	0.915840	2.704597
H	-1.163039	0.822734	3.288119
H	1.844336	2.903956	-0.732026
H	0.797864	2.907173	-2.186546
H	2.374371	2.062352	-2.215043
H	-0.924188	1.735849	-1.767884
H	0.271717	-1.716108	-0.471756
H	-1.343140	-3.459669	0.103624
H	-3.779340	-2.992110	0.063402
H	-4.599232	-0.735034	-0.587892
H	-2.976151	1.036928	-1.184578
H	0.813061	0.812338	1.509997
H	2.301463	-0.669523	2.861401
H	4.023731	-2.054726	1.728548
H	4.282460	-1.947325	-0.738383
H	2.793675	-0.463562	-2.080897

16 (in MeCN)

N	0.707484	-0.029309	-0.014730
C	1.384740	-1.094123	0.459450
C	2.767833	-1.098596	0.478920
C	3.459327	0.012729	0.002847
C	2.741234	1.102023	-0.485408
C	1.359151	1.053164	-0.486903
C	-0.768698	-0.070408	-0.027862
C	-1.376699	-1.214912	-0.548614
C	-2.789068	-1.112964	-0.508699
C	-3.488793	-0.007896	-0.011602
C	-2.792014	1.089237	0.502385
C	-1.400544	1.061995	0.499215
H	0.776467	-1.914370	0.817963
H	3.285648	-1.964857	0.872890
H	4.544121	0.029434	0.010679
H	3.237011	1.982023	-0.877048
H	0.741747	1.853453	-0.876102
H	-3.389714	-1.939941	-0.892005
H	-4.576811	0.000676	-0.017743
H	-3.319613	1.946848	0.908793
H	-0.830068	1.890402	0.913302

17 (in MeCN)

N	-0.752574	-0.074342	-0.024394
C	-1.365185	-1.153914	-0.610198
C	-2.779012	-1.060561	-0.568505
C	-3.470438	0.002930	-0.011329
C	-2.752258	1.057916	0.569660
C	-1.382273	0.990826	0.552461
C	0.695422	-0.041144	-0.018658
C	1.401558	-1.127744	0.491303
C	2.794324	-1.089846	0.498619
C	3.471510	0.023579	-0.002389
C	2.751809	1.104415	-0.510784
C	1.357176	1.077242	-0.519652
H	-3.346977	-1.874036	-1.012626
H	-4.557032	0.025688	-0.016307
H	-3.242609	1.905579	1.033295
H	-0.750022	1.751331	0.996112
H	0.860904	-1.985034	0.878724
H	3.350154	-1.931286	0.900527
H	4.556859	0.047365	0.003088
H	3.272225	1.969842	-0.908983
H	0.788718	1.908752	-0.926238

18 (in MeCN)

N	-1.769181	1.272203	-1.804616
N	-0.123365	-0.751640	0.221184
C	-2.010137	1.907772	-0.867700
C	-2.311262	2.706419	0.315123
C	-0.906497	-0.369382	1.250055
C	-2.219181	-0.797728	1.335178
C	-2.727389	-1.638053	0.346866
C	-1.902440	-2.021669	-0.707043
C	-0.600729	-1.555296	-0.750374
C	1.263075	-0.248668	0.154270
C	1.465493	1.114061	0.384908
C	2.834218	1.461831	0.275721
C	3.857869	0.556896	-0.025423
C	3.561063	-0.794339	-0.224593
C	2.237015	-1.212754	-0.131274
H	-1.449289	2.687729	0.986999
H	-3.183584	2.290177	0.823522
H	-2.518689	3.735978	0.016363
H	-0.436684	0.276070	1.981085
H	-2.822967	-0.478057	2.176371
H	-3.753545	-1.986709	0.396437
H	-2.258443	-2.660935	-1.506000
H	0.080049	-1.786778	-1.560221
H	3.129171	2.501652	0.428242
H	4.888389	0.898244	-0.098661
H	4.346089	-1.513450	-0.438168
H	1.980731	-2.262402	-0.256237

19 (in MeCN)

N	-1.393218	1.414611	-1.731708
N	-0.254454	-0.745314	0.194850
C	-1.702096	2.045464	-0.776348
C	-1.998993	2.771896	0.357144
C	-1.013211	-0.314643	1.226070
C	-2.355345	-0.642059	1.287443
C	-2.912114	-1.425954	0.281027
C	-2.109283	-1.859834	-0.772649
C	-0.778323	-1.495087	-0.800243
C	1.142371	-0.364790	0.136679
C	1.472510	0.981679	0.256748
C	2.817524	1.342129	0.203602
C	3.801203	0.368232	0.027135
C	3.445543	-0.975497	-0.094301
C	2.105456	-1.353721	-0.038276
H	-2.552816	2.292627	1.156322
H	-2.034555	3.853275	0.282855
H	-0.507730	0.269155	1.985656

H	-2.943583	-0.286309	2.124760
H	-3.962572	-1.694850	0.315212
H	-2.505669	-2.461593	-1.581351
H	-0.103949	-1.764637	-1.603821
H	0.689764	1.727388	0.377607
H	3.092964	2.388229	0.290644
H	4.846796	0.656618	-0.015371
H	4.209799	-1.734838	-0.224278
H	1.813811	-2.397039	-0.114411

20 (in benzene)

N	-1.564746	-1.464024	0.138693
C	-0.863045	-1.924370	-1.115441
C	-2.704987	-2.385659	0.411082
C	-0.589891	-1.552269	1.285388
C	-1.995694	-0.039434	-0.024038
C	-1.002876	0.880809	-0.352695
C	-1.356534	2.219028	-0.499556
C	-2.676914	2.630567	-0.319074
C	-3.652142	1.694428	0.010184
C	-3.319350	0.346636	0.161857
C	2.096850	-0.178633	-0.405336
C	2.378332	0.764633	0.610541
C	3.665287	1.140851	1.017659
C	4.778611	0.567999	0.402543
C	4.571977	-0.371456	-0.609575
C	3.268856	-0.720003	-0.986356
H	-1.536354	-1.764931	-1.958424
H	-0.639852	-2.985899	-0.994174
H	0.072994	-1.357448	-1.211646
H	-3.178942	-2.111869	1.354027
H	-2.299273	-3.394004	0.484955
H	-3.417926	-2.333798	-0.412431
H	0.316095	-1.006803	1.003488
H	-0.350086	-2.606290	1.438123
H	-1.066543	-1.131241	2.171122
H	0.039121	0.551292	-0.502138
H	-0.584684	2.937959	-0.756430
H	-2.944407	3.676187	-0.434169
H	-4.682885	2.002486	0.152687
H	-4.100744	-0.357425	0.417820
H	1.544400	1.254272	1.132386
H	3.801985	1.877935	1.808332
H	5.785150	0.848373	0.703016
H	5.428433	-0.829180	-1.103568
H	3.175865	-1.460196	-1.786923

21 (in *n*-hexane)

N	2.547149	-1.267567	-0.298112
C	2.464745	-1.934933	1.052627
C	3.740582	-1.782740	-1.024124
C	1.300788	-1.637497	-1.067502
C	2.579618	0.217541	-0.108123
C	1.481664	0.781699	0.537675
C	1.471119	2.159708	0.736486
C	2.531447	2.954162	0.299084
C	3.616363	2.365815	-0.343274
C	3.650921	0.985559	-0.553347
C	-0.917931	-1.248315	1.321469
C	-1.867709	-0.431966	0.443315
C	-3.381627	-0.633010	0.635457
C	-4.253067	0.223456	-0.283964
C	-5.753750	0.010649	-0.086853
C	-6.605859	0.875271	-1.013479
H	3.293929	-1.575888	1.663107
H	2.539966	-3.012458	0.892265
H	1.479154	-1.690160	1.480601
H	3.787079	-1.327814	-2.014251
H	3.625912	-2.861923	-1.120888
H	4.641250	-1.560236	-0.451009
H	0.444067	-1.450520	-0.393041
H	1.363753	-2.702245	-1.301873
H	1.272933	-1.041273	-1.979964
H	0.650325	0.125176	0.889382
H	0.621344	2.611260	1.239280
H	2.511971	4.027869	0.457753
H	4.446460	2.973899	-0.687892
H	4.507551	0.554612	-1.056495
H	-1.183266	-2.320458	1.220175
H	-1.120712	-0.999892	2.380664
H	-1.656680	-0.619323	-0.629058
H	-1.666121	0.647086	0.578076
H	-3.617038	-1.695903	0.477859
H	-3.632793	-0.418583	1.684415
H	-3.995067	0.009933	-1.332240
H	-4.016754	1.285873	-0.122498
H	-5.991030	-1.048794	-0.250567
H	-6.012784	0.225317	0.958223
H	-7.676115	0.707244	-0.855949
H	-6.384499	0.657855	-2.064466
H	-6.406698	1.939933	-0.847500

TS1 (in THF)

N	1.425159	0.030626	-0.012017
C	1.850464	1.464376	-0.222703
C	1.981073	-0.882559	-1.052217
C	1.877473	-0.430534	1.334193
C	-0.105678	-0.016063	-0.030517
C	-0.697450	1.229030	-0.021794
C	-2.100419	1.245367	-0.004427
C	-2.836634	0.057855	0.000140
C	-2.180862	-1.178000	-0.001314
C	-0.787109	-1.231252	-0.012113
H	2.105046	1.572050	-1.281356
H	2.737427	1.636339	0.390082
H	0.470913	1.923562	-0.033016
H	1.692080	-1.914141	-0.845395
H	3.067727	-0.791449	-1.034760
H	1.593398	-0.571888	-2.022634
H	1.504581	0.275123	2.077308
H	2.968356	-0.451642	1.345267
H	1.477477	-1.426581	1.528516
H	-2.639260	2.191718	0.005137
H	-3.923506	0.086814	0.008262
H	-2.753430	-2.100692	0.009467
H	-0.282065	-2.192921	0.001748

TS2 (in THF)

O	-1.727166	-0.982409	-1.410321
N	-0.454065	1.025683	0.233902
C	-3.503423	-1.336530	0.153557
C	-2.191974	-0.733853	-0.299551
C	-1.490958	0.053079	0.710414
C	-0.838260	1.755873	-1.014764
C	-0.258990	2.037538	1.323858
C	0.863395	0.255292	0.090673
C	0.895903	-0.920282	0.814691
C	2.108316	-1.625533	0.739932
C	3.187317	-1.160675	-0.019824
C	3.087570	0.045214	-0.718168
C	1.905549	0.785792	-0.663740
H	-3.486518	-1.589319	1.217257
H	-3.723839	-2.226125	-0.438703
H	-4.301562	-0.601427	-0.002570
H	-2.121377	0.501910	1.473815
H	-0.614241	-0.781962	1.160724
H	-0.145666	2.583210	-1.165761
H	-1.846537	2.148048	-0.874311

H	-0.809475	1.064787	-1.852402
H	-0.028698	1.505945	2.247457
H	-1.179087	2.615087	1.430774
H	0.571717	2.687357	1.047057
H	2.227095	-2.566432	1.276534
H	4.108753	-1.735902	-0.071358
H	3.924040	0.411475	-1.305854
H	1.834499	1.727347	-1.199880

TS3 (in THF)

O	3.170792	-0.436915	-0.472884
O	1.654863	-0.695390	1.174413
N	-0.067156	1.207264	-0.195119
C	4.060685	-1.276256	0.268007
C	1.959351	-0.233459	0.086646
C	1.073714	0.477013	-0.831922
C	0.273274	1.881201	1.097553
C	-0.507105	2.263066	-1.166589
C	-1.227592	0.211250	-0.058170
C	-1.115949	-0.875852	-0.901463
C	-2.188839	-1.780118	-0.846450
C	-3.275069	-1.581138	0.012488
C	-3.324821	-0.452983	0.835300
C	-2.286240	0.479278	0.803785
H	4.970926	-1.338491	-0.327218
H	3.629165	-2.270757	0.402974
H	4.278369	-0.839237	1.245344
H	1.581536	1.102203	-1.559638
H	0.291046	-0.463000	-1.310824
H	-0.531272	2.567667	1.359766
H	1.195551	2.443991	0.946344
H	0.406747	1.127006	1.868412
H	-0.699437	1.785374	-2.127512
H	0.288362	3.004751	-1.257498
H	-1.419389	2.722328	-0.785818
H	-2.188886	-2.668208	-1.477540
H	-4.086488	-2.304347	0.045094
H	-4.167914	-0.294933	1.501129
H	-2.331917	1.361228	1.435478

TS4 (in THF)

N	-0.805841	0.552895	-0.089157
N	-3.889377	-1.086503	0.351669
C	-1.027796	1.769399	-0.928374
C	-1.224181	0.842761	1.320806
C	-1.545688	-0.626149	-0.653667
C	-2.846293	-0.837564	-0.097705
C	0.676713	0.136921	-0.055841
C	0.879192	-1.223850	-0.140111
C	2.224242	-1.627766	-0.069335
C	3.262166	-0.703054	0.070904
C	2.981310	0.664351	0.160303
C	1.661442	1.109568	0.104492
H	-0.540622	2.626035	-0.464453
H	-2.102857	1.945185	-0.988759
H	-0.613454	1.584366	-1.919465
H	-1.126982	-0.073534	1.904093
H	-2.255967	1.196454	1.322799
H	-0.561134	1.611412	1.717042
H	-0.598203	-1.475363	-0.395401
H	-1.585518	-0.534688	-1.739411
H	2.480388	-2.685009	-0.125037
H	4.294571	-1.041383	0.114034
H	3.785954	1.384077	0.276304
H	1.443712	2.170009	0.191841

TS5 (in THF)

O	-1.729870	-1.048547	-1.379786
N	-3.419318	-1.254030	0.122862
N	-0.486059	1.004088	0.227970
C	-2.199178	-0.766883	-0.273402
C	-1.490716	0.019903	0.743199
C	-0.893815	1.706433	-1.029532
C	-0.295979	2.040464	1.295719
C	0.848979	0.261378	0.083191
C	0.909847	-0.901102	0.825140
C	2.133724	-1.585412	0.760272
C	3.199505	-1.112215	-0.013038
C	3.072121	0.078540	-0.732597
C	1.876500	0.798144	-0.685532
H	-3.782785	-2.039136	-0.401532
H	-3.689036	-1.200021	1.095706
H	-2.125276	0.487236	1.492036
H	-0.542842	-0.801539	1.185207
H	-0.213969	2.540093	-1.203350
H	-1.905983	2.086693	-0.884176
H	-0.866241	0.999239	-1.853591
H	-0.049411	1.531119	2.227566
H	-1.223550	2.606327	1.399813
H	0.522094	2.697037	0.998439
H	2.272344	-2.513547	1.313767
H	4.132158	-1.669447	-0.059060
H	3.898589	0.449914	-1.331158
H	1.784578	1.728508	-1.237722

TS6 (in THF)

N	-0.597387	1.370661	0.073868
C	1.660278	0.261745	-0.328734
C	1.497110	-0.897030	0.458764
C	2.594676	-1.670801	0.837610
C	3.884174	-1.327931	0.433994
C	4.063570	-0.188985	-0.355898
C	2.973329	0.592411	-0.723343
C	0.539184	1.044981	-0.869866
C	-0.172934	1.667248	1.474573
C	-1.285550	2.587682	-0.465587
C	-1.603914	0.221844	-0.000570
C	-1.445364	-0.557335	-1.129214
C	-2.363686	-1.605756	-1.278349
C	-3.360309	-1.838067	-0.323801
C	-3.470345	-1.011232	0.797422
C	-2.583247	0.053173	0.972561
H	0.505660	-1.201809	0.781756
H	2.434323	-2.554469	1.449527
H	4.734865	-1.934389	0.729323
H	5.060799	0.098444	-0.678221
H	3.130578	1.479950	-1.332285
H	0.859233	1.976617	-1.333269
H	-0.278210	0.129570	-1.550536
H	-1.020718	2.067720	2.030908
H	0.622886	2.411833	1.431142
H	0.190196	0.758543	1.949756
H	-1.535774	2.401730	-1.510266
H	-0.605790	3.437017	-0.380144
H	-2.192418	2.763732	0.113811
H	-2.307946	-2.267073	-2.141701
H	-4.053768	-2.666265	-0.448008
H	-4.246058	-1.189973	1.535960
H	-2.677981	0.702524	1.837793

TS7 (in THF)

Si	-2.227610	-0.404135	-0.070305
N	0.249639	1.171178	0.327127
C	-3.295618	-1.271002	1.220511
C	-1.576012	-1.691460	-1.289852
C	-3.362794	0.760386	-1.046970
C	-0.839436	0.321554	0.925006
C	-0.138666	1.808072	-0.966253

C	0.623165	2.255816	1.286566
C	1.496519	0.288964	0.115019
C	1.379217	-0.968708	0.661777
C	2.494654	-1.808721	0.516844
C	3.645433	-1.376024	-0.147162
C	3.710466	-0.080690	-0.671717
C	2.622882	0.782899	-0.540584
H	-2.709050	-1.997564	1.793596
H	-4.123740	-1.806349	0.741888
H	-3.726404	-0.552151	1.927176
H	-0.887682	-1.260710	-2.026618
H	-2.406818	-2.148676	-1.840894
H	-1.038328	-2.488181	-0.763313
H	-3.695295	1.606293	-0.433816
H	-4.256885	0.213194	-1.371950
H	-2.880090	1.160698	-1.945208
H	-1.169688	0.783296	1.856855
H	0.078149	-0.763902	1.109241
H	0.672912	2.440936	-1.327016
H	-1.030072	2.411760	-0.794305
H	-0.342415	1.024100	-1.696532
H	0.914199	1.790407	2.228440
H	-0.245068	2.900267	1.432341
H	1.456494	2.828897	0.877398
H	2.478494	-2.819495	0.922556
H	4.498145	-2.041696	-0.256890
H	4.607635	0.259478	-1.180402
H	2.685719	1.792533	-0.937280

TS8 (in THF)

N	-1.401626	0.130367	-0.050950
C	-2.042773	1.358262	-0.544538
C	-2.094074	-0.636217	1.007628
C	-1.963073	-1.218845	-0.351618
C	0.090534	0.101815	-0.026373
C	0.602638	-1.167279	-0.238401
C	2.000419	-1.262945	-0.217754
C	2.805129	-0.137750	0.001406
C	2.225123	1.115601	0.211500
C	0.834717	1.253324	0.204113
H	-3.118160	1.188314	-0.597745
H	-1.650558	1.579755	-1.538717
H	-1.837416	2.184365	0.138259
H	-3.013595	-0.171458	1.357053
H	-1.419428	-0.986639	1.787596
H	-2.837821	-1.132598	-0.994169
H	-0.669249	-1.764563	-0.452633
H	2.488671	-2.223408	-0.377741
H	3.888136	-0.234201	0.008561
H	2.850538	1.987129	0.380658
H	0.378418	2.224945	0.369750

TS9 (in THF)

N	-0.772143	0.549872	0.235257
N	-3.821527	-0.834418	-0.935685
C	-1.274124	1.752035	-0.457295
C	-1.374747	0.189605	1.538181
C	-1.588632	-0.681487	0.358791
C	-2.826305	-0.724117	-0.349329
C	0.677624	0.188049	0.048224
C	0.909774	-1.174185	0.074543
C	2.257143	-1.540324	-0.072402
C	3.265704	-0.584274	-0.238459
C	2.954153	0.777882	-0.252036
C	1.629615	1.191192	-0.100312
H	-2.349836	1.829683	-0.297780
H	-1.053427	1.652965	-1.520840
H	-0.781936	2.629769	-0.039487
H	-2.151872	0.870864	1.872272
H	-0.649087	-0.143464	2.275604
H	-0.599484	-1.492579	0.220053
H	2.542064	-2.591567	-0.065030
H	4.299925	-0.897590	-0.358565
H	3.737011	1.519339	-0.379394
H	1.381102	2.248142	-0.103272

TS9' (in THF)

N	-0.778876	0.069855	0.479255
N	-3.999032	0.251098	-0.964387
C	-1.329975	1.262612	1.151696
C	-1.234712	-1.301594	0.804767
C	-1.609345	-0.677542	-0.497883
C	-2.934377	-0.150551	-0.758456
C	0.692967	0.084079	0.163376
C	1.260304	-1.173530	0.234236
C	2.631698	-1.220607	-0.057532
C	3.346617	-0.064474	-0.390853
C	2.703863	1.175603	-0.449301
C	1.338790	1.268388	-0.172313
H	-2.350063	1.052515	1.471880
H	-1.322675	2.109661	0.464570
H	-0.703488	1.466882	2.020349
H	-2.000333	-1.298322	1.576574
H	0.021049	-1.820040	0.652866
H	-1.064068	-0.975640	-1.393107
H	3.168165	-2.167749	-0.024986
H	4.410163	-0.125029	-0.608176
H	3.261367	2.070027	-0.710237
H	0.830264	2.226721	-0.220231

TS10 (in $CHCl_3$)

N	-1.187447	-0.465708	0.124476
C	-1.715020	-0.162939	1.484869
C	-1.585516	-1.845169	-0.241051
C	-1.910188	0.528593	-0.914654
C	-1.654324	1.960584	-0.620193
C	0.287303	-0.241885	0.086143
C	0.685607	1.058009	0.417000
C	2.063644	1.306768	0.331262
C	2.980536	0.308348	-0.008036
C	2.528692	-0.973895	-0.321710
C	1.162635	-1.260417	-0.292406
H	-1.226886	-0.822756	2.204604
H	-2.794021	-0.333458	1.480916
H	-1.498850	0.875966	1.723744
H	-1.251507	-2.064898	-1.255406
H	-2.673543	-1.905872	-0.197297
H	-1.151454	-2.554815	0.465000
H	-2.950125	0.192055	-0.831707
H	-1.502266	0.191379	-1.871200
H	-0.404999	1.823529	0.156566
H	-2.489167	2.457286	-0.119000
H	-1.352709	2.513708	-1.511636
H	2.441551	2.306843	0.541595
H	4.045819	0.525176	-0.033476
H	3.231885	-1.754623	-0.595613
H	0.828191	-2.257542	-0.555756

TS11 (in $CHCl_3$)

Cl	2.565720	-1.534010	-0.736369
Cl	2.445578	0.078429	1.706732
Cl	3.053987	1.344031	-0.866238
N	-1.843501	-1.199829	-0.434156
C	2.085479	0.068225	-0.054723
C	-1.175709	-1.509227	-1.740586
C	-3.204475	-1.809404	-0.472852
C	-1.036646	-1.862070	0.670116
C	-1.557845	-1.585253	2.065457

C	-1.851764	0.308505	-0.242116
C	-0.602040	0.919762	-0.175523
C	-0.646629	2.310811	0.013035
C	-1.840148	3.031208	0.118343
C	-3.057057	2.358652	0.039504
C	-3.073194	0.973825	-0.140483
H	0.814991	0.349873	-0.187077
H	-1.761762	-1.054604	-2.539945
H	-1.134232	-2.593469	-1.859379
H	-0.173267	-1.086164	-1.727172
H	-3.741595	-1.585764	0.446648
H	-3.080160	-2.887774	-0.578519
H	-3.747700	-1.415494	-1.331605
H	-0.018981	-1.489318	0.559058
H	-1.047050	-2.930782	0.438015
H	-2.549920	-2.009235	2.237866
H	-1.579441	-0.513530	2.277794
H	-0.868589	-2.052979	2.773781
H	0.292739	2.860264	0.086672
H	-1.823705	4.108459	0.263859
H	-3.996163	2.897530	0.120380
H	-4.030331	0.467957	-0.192445

TS12 (in $CHCl_3$)

O	3.293771	-1.187808	-0.411228
O	2.915757	0.857079	0.446220
N	-0.648694	1.285039	0.064998
C	4.576129	-1.162575	0.214850
C	2.518768	-0.094672	-0.216257
C	-0.005365	1.388465	1.412438
C	-1.273649	2.600361	-0.240487
C	0.438111	1.045295	-1.009744
C	1.199351	-0.239531	-0.821770
C	-1.634510	0.136670	0.070944
C	-1.079428	-1.109126	0.373801
C	-1.994948	-2.174599	0.353257
C	-3.356626	-1.997113	0.089119
C	-3.847936	-0.724911	-0.201207
C	-2.979117	0.367917	-0.221773
H	5.049885	-2.109557	-0.043042
H	4.475741	-1.075685	1.299601
H	5.174406	-0.328334	-0.160207
H	-0.790109	1.589385	2.143513
H	0.724523	2.197847	1.383118
H	0.486204	0.447548	1.644823
H	-1.713275	2.573571	-1.237558
H	-0.490596	3.358738	-0.205703
H	-2.033761	2.823426	0.508343
H	1.080124	1.929078	-0.946845
H	-0.111252	1.057801	-1.952812
H	1.220890	-0.865036	-1.713463
H	0.382884	-0.907101	-0.059608
H	-1.642133	-3.185764	0.556223
H	-4.035551	-2.846675	0.104186
H	-4.901727	-0.573840	-0.415039
H	-3.376301	1.348067	-0.459467

TS13 (in $CHCl_3$)

Cl	-2.615587	-2.039304	1.177401
Cl	-2.334739	-1.635783	-1.710834
Cl	-4.322740	-0.106345	-0.196341
O	4.069960	-0.932882	-1.395707
O	3.669412	-1.765298	0.648044
N	0.959830	0.563553	1.338659
C	-2.672999	-0.812935	-0.147393
C	5.435245	-1.361219	-1.280723
C	3.280012	-1.210711	-0.357451
C	0.073950	0.417675	2.541181
C	2.335059	0.877263	1.827701
C	0.975372	-0.769023	0.615143
C	1.854823	-0.782253	-0.622462
C	0.369918	1.641976	0.439452
C	-0.879562	1.365170	-0.108987
C	-1.390601	2.382377	-0.931575
C	-0.712937	3.579745	-1.177659
C	0.530754	3.798258	-0.589996
C	1.090344	2.818317	0.232395
H	-1.793423	0.154790	-0.016805
H	5.915583	-1.059084	-2.209672
H	5.481447	-2.445469	-1.160646
H	5.912366	-0.874900	-0.427379
H	0.055041	1.373267	3.065925
H	0.483639	-0.366868	3.180002
H	-0.927728	0.157014	2.204166
H	3.000417	1.055134	0.982728
H	2.687833	0.023728	2.406411
H	2.291707	1.764967	2.458383
H	-0.058277	-0.973417	0.347739
H	1.312580	-1.511586	1.342309
H	1.844631	0.175661	-1.151332
H	1.442621	-1.514842	-1.326460
H	-2.361624	2.234185	-1.405453
H	-1.149159	4.338133	-1.822864
H	1.074091	4.721588	-0.765925
H	2.060327	3.004777	0.677990

TS14 (in $CHCl_3$)

S	-1.134666	2.736922	-0.094819
O	-1.384532	2.081162	-1.378498
O	-1.148439	4.201113	-0.054950
O	-4.232474	-0.177930	-0.732242
O	-3.944135	-2.134763	0.341589
N	0.356421	2.292250	0.539156
N	-0.343037	-2.569166	0.285704
C	-2.297989	2.126249	1.098826
C	-5.541324	-0.114119	-0.169791
C	-3.489543	-1.256518	-0.384703
C	-1.096489	-2.493971	1.582801
C	0.218015	-3.947676	0.227358
C	-1.350625	-2.459590	-0.898418
C	-2.133524	-1.179233	-0.907423
C	0.650276	-1.410143	0.229342
C	-0.022821	-0.197812	0.428235
C	0.780078	0.926055	0.384195
C	2.159962	0.888163	0.243292
C	2.789236	-0.339969	0.037744
C	2.032757	-1.547817	-0.025500
C	1.495127	3.158357	0.108961
C	2.731546	2.275165	0.355933
C	4.219690	-0.326516	-0.121823
C	5.424296	-0.251593	-0.239798
C	6.877703	-0.176724	-0.387256
C	2.799337	-2.796502	-0.417339
H	-3.286383	2.400134	0.722102
H	-2.089760	2.615478	2.050928
H	-2.192449	1.043666	1.172032
H	-5.983151	0.806243	-0.551697
H	-5.493640	-0.083819	0.922401
H	-6.141224	-0.974060	-0.478237
H	-0.376495	-2.619404	2.393222
H	-1.841058	-3.289734	1.589038
H	-1.584399	-1.528793	1.668337
H	0.674458	-4.129094	-0.740724
H	-0.611982	-4.642223	0.363061
H	0.934242	-4.081300	1.035597
H	-1.987098	-3.342190	-0.785909
H	-0.725741	-2.566598	-1.787247
H	-2.061205	-0.605031	-1.828636

H	-1.375980	-0.454379	-0.121765
H	1.494416	4.085002	0.680737
H	1.409160	3.392115	-0.959230
H	3.135965	2.437341	1.362548
H	3.526697	2.479274	-0.364794
H	7.332226	0.292992	0.489548
H	7.147706	0.411920	-1.268575
H	7.304952	-1.176950	-0.499970
H	3.828247	-2.525104	-0.650972
H	2.385727	-3.259944	-1.315771
H	2.840131	-3.549380	0.372046

TS15 (in $CHCl_3$)

Cl	2.474106	-1.670592	-0.096979
Cl	2.658840	0.765730	1.512679
Cl	2.681766	0.932773	-1.414200
N	-1.877100	-1.410918	-0.000111
C	1.988562	0.068122	-0.000624
C	-1.156631	-1.859215	-1.235963
C	-3.208692	-2.083425	0.024241
C	-1.113931	-1.862303	1.209250
C	-1.960124	0.109696	0.001173
C	-0.741977	0.782692	0.002812
C	-0.853129	2.182604	0.003681
C	-2.080505	2.851340	0.001202
C	-3.263894	2.116569	-0.003493
C	-3.213953	0.721201	-0.003664
H	0.693655	0.270333	-0.001378
H	-1.741021	-1.548503	-2.102660
H	-1.059387	-2.945956	-1.203330
H	-0.176632	-1.387799	-1.259509
H	-3.742286	-1.792953	0.929011
H	-3.036533	-3.159917	0.026812
H	-3.771185	-1.803612	-0.865952
H	-0.127711	-1.404160	1.194212
H	-1.031574	-2.950274	1.177282
H	-1.660786	-1.541361	2.096464
H	0.058447	2.781845	0.006231
H	-2.116945	3.937867	0.002055
H	-4.227871	2.616029	-0.007069
H	-4.144926	0.166716	-0.008585

TS16 (in $CHCl_3$)

Cl	-2.566921	1.940609	-1.939257
Cl	-4.102021	0.841093	0.305159
Cl	-3.059278	-0.918237	-1.780659
S	-0.687928	-2.733573	1.169088
O	0.304835	-2.519877	2.228676
O	-1.057665	-4.114197	0.849597
N	-0.208987	-2.016985	-0.290589
N	0.265246	2.786267	0.982664
C	-2.694930	0.536279	-0.794856
C	-2.154072	-1.834960	1.595530
C	0.258910	3.866595	-0.059760
C	1.003808	3.209009	2.221181
C	-1.163293	2.623379	1.419012
C	0.836365	1.481668	0.422827
C	-0.086004	0.442182	0.239046
C	0.500487	-0.762272	-0.127658
C	1.850900	-0.943791	-0.399073
C	2.713405	0.142081	-0.281317
C	2.218529	1.403142	0.146452
C	0.706572	-2.877301	-1.098381
C	2.128709	-2.364664	-0.804930
C	4.107555	-0.052041	-0.571840
C	5.276637	-0.256051	-0.819768
C	6.687364	-0.500291	-1.117029
C	3.269467	2.491818	0.236697
H	-1.479856	0.480752	-0.127925
H	-2.504365	-2.271128	2.534163
H	-2.886977	-1.975651	0.801547
H	-1.895814	-0.783998	1.730898
H	1.266138	4.070392	-0.407901
H	-0.175899	4.765307	0.380408
H	-0.352681	3.515770	-0.891221
H	0.940252	2.390356	2.938779
H	0.513527	4.099369	2.616964
H	2.041293	3.432095	2.004106
H	-1.786791	2.441806	0.550601
H	-1.460090	3.559457	1.892301
H	-1.232149	1.796067	2.122855
H	0.443495	-2.699824	-2.144912
H	0.547878	-3.930299	-0.869960
H	2.778858	-2.437035	-1.680471
H	2.602976	-2.912869	0.018664
H	7.289486	0.381008	-0.880047
H	6.823630	-0.734869	-2.176487
H	7.063905	-1.342142	-0.529347
H	3.905810	2.333474	1.115494
H	2.891338	3.507888	0.279366
H	3.919003	2.431279	-0.639924

TS17a (in MeCN)

N	0.710563	1.584560	0.084192
C	1.582522	2.678122	-0.242394
C	-0.584283	1.693308	0.148655
C	-1.575245	0.626556	-0.019824
C	-1.384187	-0.471727	-0.875031
C	-2.392367	-1.416964	-1.028267
C	-3.598374	-1.282412	-0.334359
C	-3.803176	-0.182273	0.498312
C	-2.802186	0.775298	0.643636
C	1.476241	0.338228	0.135101
C	2.603139	0.375548	-0.679864
C	3.427770	-0.759338	-0.619490
C	3.107641	-1.849632	0.196328
C	1.971182	-1.815124	1.015155
C	1.138182	-0.699722	1.001776
H	2.219385	2.939965	0.606942
H	1.025720	3.520002	-0.650347
H	2.418023	1.793670	-0.930856
H	-0.960200	2.702412	0.296569
H	-0.456736	-0.575891	-1.429361
H	-2.240670	-2.258906	-1.696646
H	-4.379870	-2.026521	-0.455028
H	-4.743744	-0.064199	1.027281
H	-2.962722	1.642049	1.279443
H	4.335241	-0.812557	-1.219298
H	3.750561	-2.726508	0.212325
H	1.747923	-2.647505	1.675652
H	0.271998	-0.637137	1.655571

TS17b (in MeCN)

N	-0.793459	0.942439	-0.387566
N	-1.296401	4.210207	0.720673
C	-1.520387	3.188855	0.214837
C	-1.874868	1.924281	-0.359664
C	0.457954	1.271121	-0.449792
C	1.616439	0.439457	-0.125826
C	1.601971	-0.516500	0.903200
C	2.762703	-1.216166	1.207508
C	3.937253	-0.980842	0.485910
C	3.959815	-0.019683	-0.524094
C	2.807508	0.705599	-0.815749
C	-1.365252	-0.403092	-0.229036
C	-2.573048	-0.401303	0.459453
C	-3.180309	-1.664398	0.583813
C	-2.607502	-2.815227	0.036077

C	-1.410002	-2.735920	-0.688081
C	-0.770706	-1.510391	-0.838145
H	-2.636627	1.143807	0.341210
H	-2.356776	2.015588	-1.334320
H	0.662958	2.299738	-0.741912
H	0.694670	-0.695817	1.471322
H	2.754804	-1.945223	2.011513
H	4.838191	-1.538114	0.724074
H	4.875041	0.176361	-1.073327
H	2.821354	1.474522	-1.583622
H	-4.127556	-1.764829	1.112058
H	-3.100411	-3.777851	0.149185
H	-0.987162	-3.623827	-1.147939
H	0.141125	-1.427623	-1.422467

TS18a (in MeCN)

N	-1.349939	3.224395	0.685605
N	0.748586	1.048062	-1.114488
C	-1.220348	2.336389	1.433427
C	-0.919902	1.202889	2.244736
C	1.365860	2.282966	-1.617265
C	-0.516037	0.842299	-1.260194
C	-1.322984	-0.288286	-0.809617
C	-0.843549	-1.571698	-0.491776
C	-1.733914	-2.550398	-0.066388
C	-3.096039	-2.263860	0.061490
C	-3.580360	-0.998312	-0.267192
C	-2.699276	-0.020576	-0.717704
C	1.644384	0.178415	-0.347609
C	1.460669	0.125242	1.033833
C	2.367673	-0.730954	1.686411
C	3.359623	-1.452478	1.013269
C	3.491031	-1.338077	-0.373490
C	2.623683	-0.501106	-1.073459
H	0.211620	0.714634	1.711681
H	-1.710623	0.449649	2.184767
H	-0.728814	1.492195	3.281062
H	1.754194	2.836041	-0.758600
H	0.625678	2.876698	-2.152041
H	2.189891	2.015602	-2.281158
H	-1.061384	1.635142	-1.768060
H	0.207638	-1.813748	-0.589941
H	-1.363377	-3.542778	0.169473
H	-3.779585	-3.033443	0.407265
H	-4.638930	-0.775650	-0.181904
H	-3.068730	0.965600	-0.986381
H	2.300452	-0.849160	2.769158
H	4.033842	-2.103726	1.564783
H	4.258156	-1.892877	-0.905159
H	2.696362	-0.396105	-2.153610

TS18b (in MeCN)

N	0.244538	-3.306075	0.514888
N	-0.748663	-0.471415	-1.089651
N	-3.244246	-2.361224	0.312107
C	0.401091	-2.491893	1.338209
C	0.499134	-1.388085	2.235388
C	-2.575375	-1.937696	-0.528429
C	-1.752988	-1.402912	-1.625684
C	0.507489	-0.758320	-1.209653
C	1.663067	-0.002221	-0.753230
C	1.684267	1.369579	-0.438112
C	2.868341	1.952984	-0.007042
C	4.028291	1.184706	0.132581
C	4.017589	-0.171892	-0.189692
C	2.843858	-0.759018	-0.648890
C	-1.282601	0.678204	-0.349400
C	-1.123605	0.669777	1.034884
C	-1.667708	1.805241	1.664703
C	-2.305561	2.834483	0.964293
C	-2.436634	2.765134	-0.426024
C	-1.922163	1.662242	-1.104357
H	-0.277998	-0.424659	1.707478
H	1.527869	-1.022017	2.301048
H	0.109949	-1.642413	3.224386
H	-1.266449	-2.228250	-2.148136
H	-2.403683	-0.864989	-2.321177
H	0.725873	-1.705176	-1.699349
H	0.796811	1.980519	-0.546675
H	2.888046	3.012822	0.224728
H	4.944110	1.650761	0.483408
H	4.919781	-0.766804	-0.094136
H	2.826802	-1.812594	-0.914707
H	-1.591955	1.899281	2.748826
H	-2.706037	3.693375	1.497807
H	-2.931850	3.559317	-0.976108
H	-2.001622	1.579943	-2.186065

TS19 (in MeCN)

N	0.739744	0.083136	-0.002071
C	1.266478	-1.165325	0.027277
C	2.655948	-1.268495	0.030816
C	3.456893	-0.129378	0.008576
C	2.854072	1.130327	-0.026996
C	1.475965	1.212147	-0.034804
C	-0.749100	0.083093	-0.003115
C	-1.271314	-1.204548	-0.029995
C	-2.669451	-1.286239	-0.029273
C	-3.473174	-0.138456	-0.003504
C	-2.885927	1.127655	0.028938
C	-1.494492	1.257316	0.032106
H	0.058740	-1.807701	0.002415
H	3.112268	-2.253187	0.053075
H	4.539706	-0.213224	0.015421
H	3.438394	2.042265	-0.051752
H	0.954733	2.159499	-0.070776
H	-3.162487	-2.257625	-0.049688
H	-4.556758	-0.228139	-0.005447
H	-3.504946	2.019385	0.055044
H	-1.053239	2.248185	0.066048

TS20 (in MeCN)

N	-2.083258	1.734851	-1.570076
N	-0.353326	-0.748274	0.194312
C	-1.476030	2.279221	-0.733917
C	-0.633723	2.821736	0.281789
C	-1.056515	-0.294097	1.253150
C	-2.413369	-0.538686	1.353819
C	-3.049173	-1.271367	0.354135
C	-2.305670	-1.731386	-0.730048
C	-0.954317	-1.446410	-0.791810
C	1.082747	-0.444814	0.114982
C	1.465314	0.870113	0.367195
C	2.851319	1.088072	0.260913
C	3.758353	0.072694	-0.056988
C	3.302181	-1.228742	-0.286124
C	1.939180	-1.502187	-0.200747
H	0.388484	1.937006	0.407844
H	-1.164425	2.905971	1.233875
H	-0.220937	3.787263	-0.021134
H	-0.488641	0.251106	1.997028
H	-2.952610	-0.162134	2.214823
H	-4.112267	-1.478322	0.417372
H	-2.761856	-2.292200	-1.536809
H	-0.325356	-1.742385	-1.622628
H	3.246210	2.091408	0.425258
H	4.821873	0.288852	-0.125517
H	3.999801	-2.026682	-0.521097

H	1.564035	-2.510805	-0.356756

TS21 (in MeCN)

N	0.101728	1.870321	-0.193231
C	0.811141	3.108932	0.071307
C	-1.093719	1.761036	0.227776
C	-1.914298	0.554189	0.013635
C	-1.526108	-0.457111	-0.876784
C	-2.327384	-1.581655	-1.047659
C	-3.521966	-1.708616	-0.332281
C	-3.917542	-0.702660	0.549247
C	-3.118220	0.427331	0.717069
C	1.746920	0.033951	0.085221
C	1.571956	-0.900858	0.912691
C	2.635324	-1.808756	1.073618
C	3.766294	-1.554706	0.280218
C	3.825495	-0.466788	-0.610322
C	2.751865	0.434380	-0.756360
H	1.708912	2.890742	0.658996
H	0.198434	3.843594	0.609873
H	1.140390	3.542049	-0.878527
H	-1.575281	2.574439	0.789219
H	-0.601243	-0.348575	-1.435045
H	-2.024301	-2.360755	-1.740643
H	-4.144602	-2.587960	-0.468051
H	-4.847298	-0.795842	1.102125
H	-3.423413	1.217419	1.398928
H	2.613880	-2.656048	1.753378
H	4.623733	-2.218720	0.352505
H	4.720628	-0.308993	-1.205898
H	2.759520	1.284386	-1.428494

TS22 (in benzene)

N	1.557938	-1.476750	-0.107326
C	0.840645	-1.895568	1.144028
C	2.730445	-2.373535	-0.303873
C	0.624895	-1.649731	-1.270888
C	1.930313	-0.011248	0.008757
C	0.863854	0.854671	0.214290
C	1.195411	2.208975	0.320675
C	2.512322	2.663462	0.223826
C	3.544618	1.750359	0.018274
C	3.262085	0.387110	-0.091669
C	-1.926015	0.230909	0.312902
C	-2.445262	0.691667	-0.911255
C	-3.808113	0.678511	-1.226893
C	-4.725498	0.188687	-0.296115
C	-4.260340	-0.275728	0.935555
C	-2.890344	-0.248114	1.220850
H	1.502710	-1.719121	1.992290
H	0.597824	-2.956490	1.057507
H	-0.071370	-1.303837	1.233228
H	3.239622	-2.105833	-1.229873
H	2.361922	-3.397780	-0.368887
H	3.405810	-2.278005	0.546620
H	-0.280521	-1.073829	-1.076117
H	0.385801	-2.711272	-1.361134
H	1.127071	-1.289108	-2.168988
H	0.393673	2.928417	0.485772
H	2.738081	3.723150	0.308221
H	4.573617	2.087791	-0.057035
H	4.081665	-0.304805	-0.249235
H	-0.415352	0.496140	0.350829
H	-1.751279	1.088992	-1.660636
H	-4.158069	1.049848	-2.188552
H	-5.787874	0.172221	-0.525157
H	-4.967554	-0.655772	1.670859
H	-2.575434	-0.616016	2.200796

TS23 (in *n*-hexane)

N	2.558386	-1.318197	-0.257542
C	2.462977	-1.918924	1.117913
C	3.765162	-1.862684	-0.937432
C	1.339010	-1.726825	-1.036048
C	2.570546	0.189545	-0.126608
C	1.454456	0.735170	0.495026
C	1.452170	2.125654	0.635342
C	2.504615	2.917999	0.172258
C	3.600380	2.321123	-0.447459
C	3.646950	0.934373	-0.603382
C	-0.848191	-0.780652	1.438254
C	-1.854119	-0.140699	0.482262
C	-3.339630	-0.464896	0.696742
C	-4.280068	0.214032	-0.299371
C	-5.755118	-0.119394	-0.078181
C	-6.678025	0.566123	-1.083317
H	3.312189	-1.566155	1.703797
H	2.491298	-3.005742	1.013480
H	1.513917	-1.602419	1.561229
H	3.825155	-1.458527	-1.948270
H	3.664299	-2.947519	-0.979964
H	4.654594	-1.599106	-0.365004
H	0.458511	-1.440169	-0.456099
H	1.370606	-2.810200	-1.169891
H	1.362283	-1.217860	-1.999937
H	0.602661	2.601255	1.122620
H	2.474682	3.997579	0.291941
H	4.425184	2.925306	-0.811827
H	4.510264	0.490239	-1.085922
H	0.496202	0.011042	0.953278
H	-0.988168	-1.879293	1.428838
H	-1.074509	-0.460436	2.470708
H	-1.606986	-0.409401	-0.563210
H	-1.742280	0.956914	0.516618
H	-3.475473	-1.555189	0.642271
H	-3.618422	-0.175007	1.720103
H	-3.995993	-0.074449	-1.322506
H	-4.144820	1.304105	-0.241451
H	-5.890683	-1.207455	-0.136469
H	-6.040342	0.171576	0.941279
H	-7.728742	0.315058	-0.906599
H	-6.430728	0.267751	-2.108296
H	-6.580084	1.655802	-1.023914