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Polymer Chemistry

Thiol-Maleimide "Click" Chemistry: Evaluating the Influence of Solvent, Initiator, and Thiol on the Reaction Mechanism, Kinetics, and Selectivity.

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SUPPORTING INFORMATION

(44 pages)

I. General Methods. Chemicals were purchased from Aldrich, Acros, TCI America, or Cambridge Isotope Labs and used as received. All ^{1}H NMR spectra were recorded with a Varian Mercury (300 MHz) or Varian Unity Plus (400 MHz) spectrometer using residual solvent as the internal standard. All chemical shifts are quoted using the δ scale and all coupling constants are expressed in Hertz (Hz).

General procedure for ternary thiol-maleimide reactions in $CDCl_3$. Ternary reactions between thiophenol (**7**), 1-hexanethiol (HT), and *N*-methyl maleimide (NMM) were carried out in $CDCl_3$ in the presence of three different initiators: Et_3N, DBU, or DMPP. In each case **7** (30 mg, 0.27 mmol), HT (32 mg, 0.27 mmol), and NMM (30 mg, 0.27 mmol) were added to a 2-dram vial. To each vial was added 0.2 mL of a stock solution of Et_3N (0.135 M), DBU (0.135 M or 0.0135 M), or DMPP (0.0135 M) in $CDCl_3$ to initiate the reaction. Each mixture was stirred at ambient temperature for a minimum of 30 minutes and then diluted with additional $CDCl_3$ and used directly for ^{1}H NMR spectroscopic analysis to determine the percent formation of thiophenol addition product versus 1-hexanthiol addition product. Spectra of ternary reactions were compared to ^{1}H NMR spectra of pure thiophenol addition product (Figure S1) and 1-hexanethiol addition product (Figure S2). The chiral methine signals and the *N*-methyl signals of the two different addition products were well isolated and therefore used to calculate the relative percentages of the two addition products.

General procedure for ternary thiol-maleimide reactions in DMF. Ternary reactions of **7**, HT, and NMM were similarly run in anhydrous DMF under three different scenarios: initiator free, 0.1 equiv Et_3N, and 0.1 equiv DBU. Stock solutions of Et_3N (0.135 M) and DBU (0.135 M) in anhydrous DMF were prepared so that both the initiator and DMF would be introduced at the same time to avoid preemptive DMF-catalyzed initiation of thiol-maleimide reactions prior to addition of the initiator. Equimolar quantities of 1-hexanethiol, thiophenol, and *N*-methyl maleimide were added to a 2-dram vial followed by the addition of DMF either with or without an initiator as described. The ternary reactions were stirred at ambient temperature for at least 30 minutes to ensure complete reactions. Mixtures were then concentrated under reduced pressure and the resulting residue was placed under high vacuum for 30 minutes. The reaction mixtures were diluted with $CDCl_3$ and used for ^{1}H NMR spectroscopic analysis to determine the percent formation of thiophenol addition product versus 1-hexanthiol addition product.

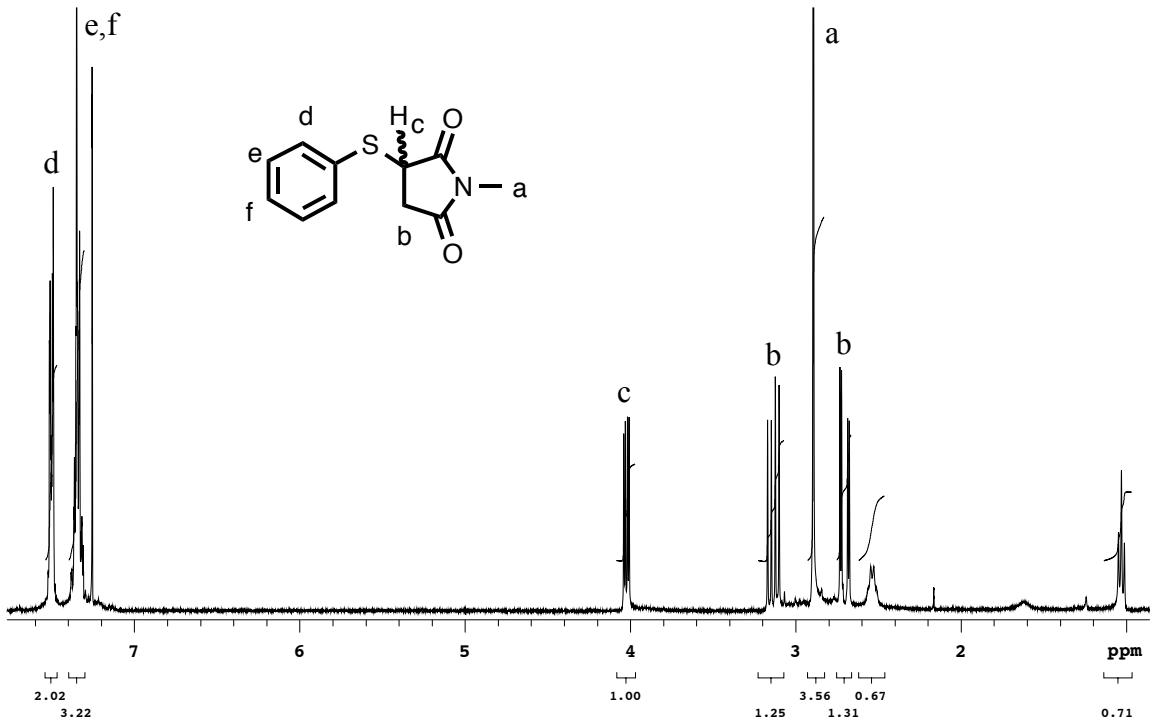


Figure S1. Thiophenol addition product obtained upon reaction of **7** with NMM in $CDCl_3$ in the presence of 0.1 equiv Et_3N.

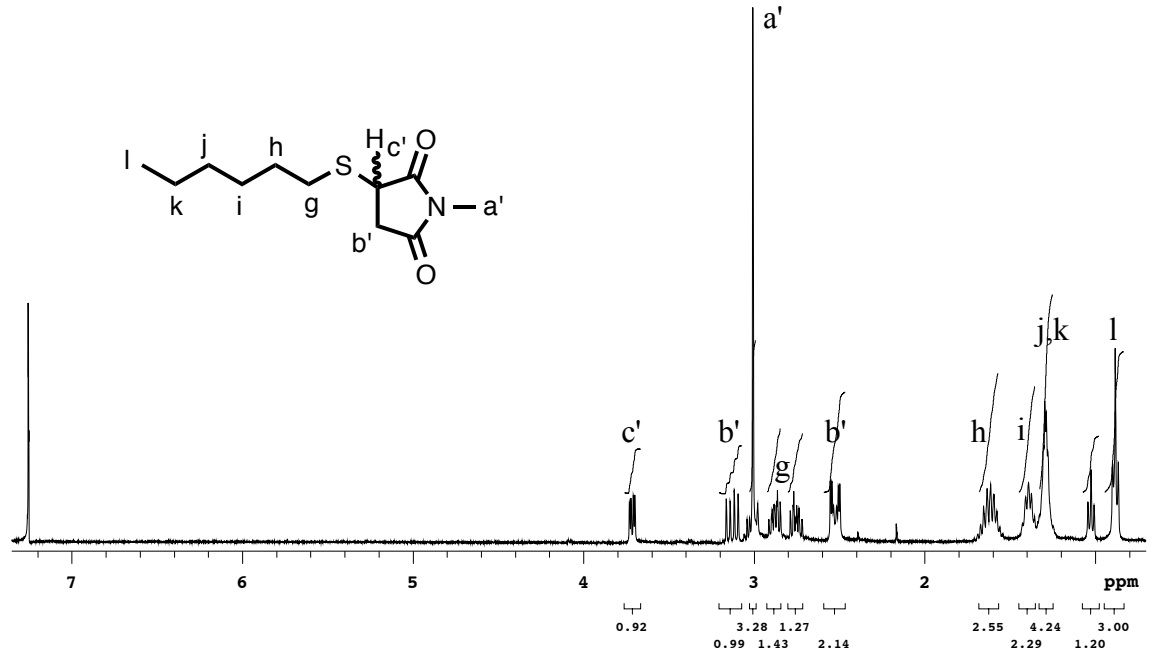


Figure S2. 1-Hexanethiol (HT) addition product obtained upon reaction of HT with NMM in $CDCl_3$ in the presence of 0.1 equiv Et_3N.

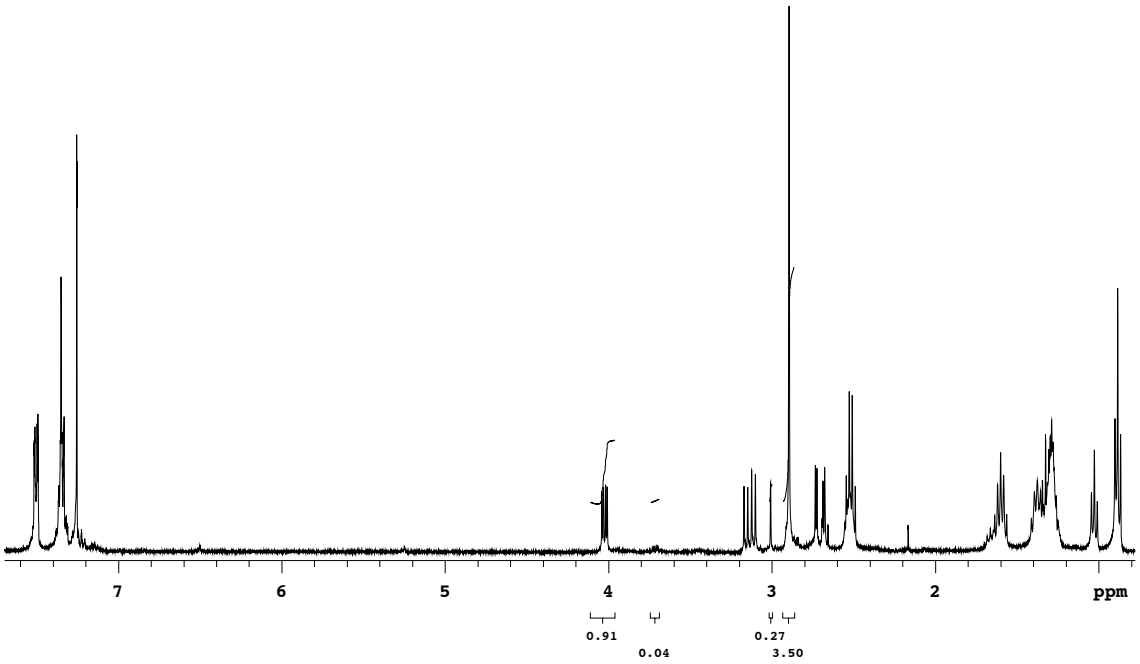


Figure S3. ^{1}H NMR spectrum following the ternary reaction of **7**, HT, and NMM initiated by 0.1 equiv Et_3N in $CDCl_3$.

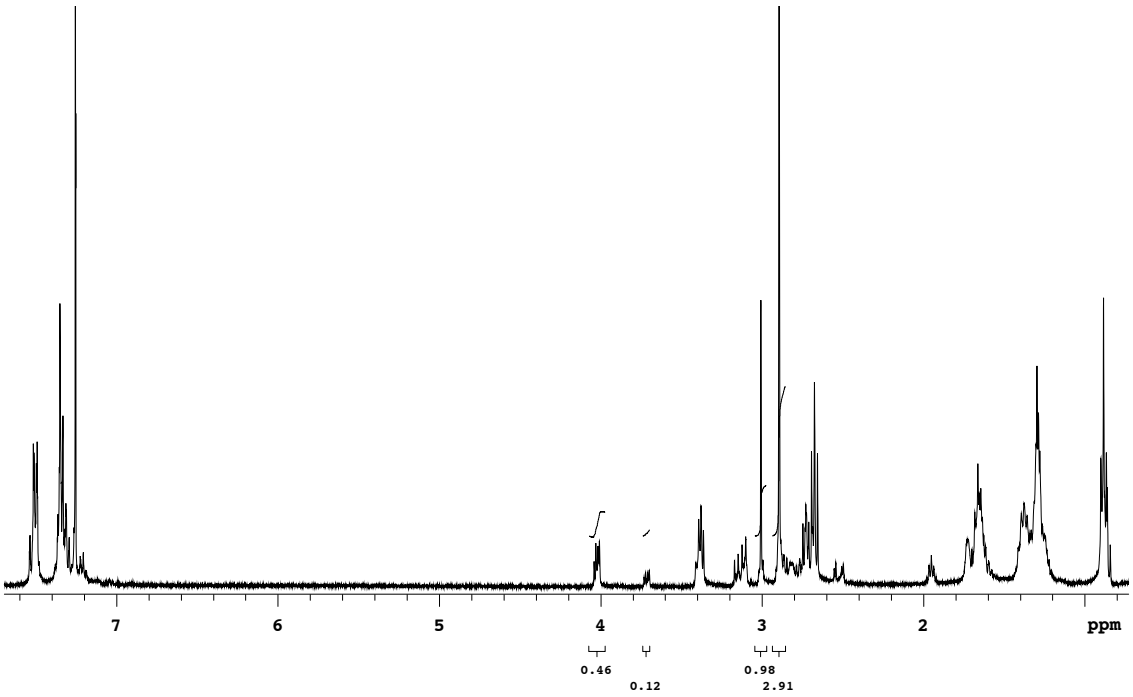


Figure S4. ^{1}H NMR spectrum following the ternary reaction of **7**, HT, and NMM initiated by 0.1 equiv DBU in $CDCl_3$.

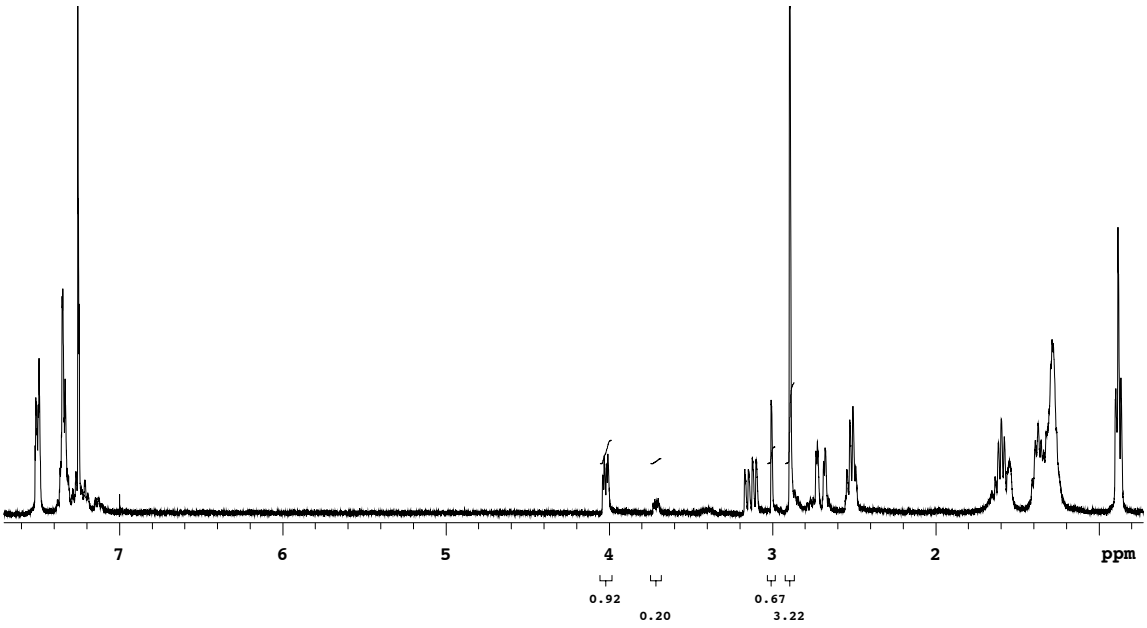


Figure S5. ^{1}H NMR spectrum following the ternary reaction of **7**, HT, and NMM initiated by 0.01 equiv DBU in $CDCl_3$.

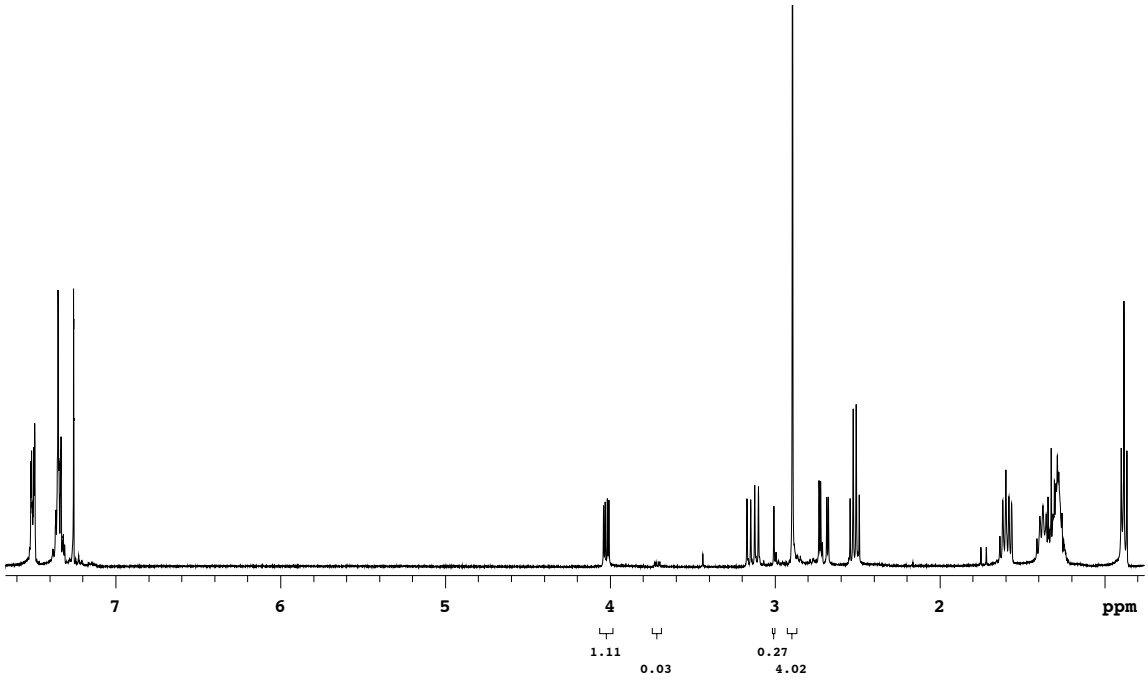


Figure S6. ^{1}H NMR spectrum following the ternary reaction of **7**, HT, and NMM initiated by 0.01 equiv DMPP in $CDCl_3$.

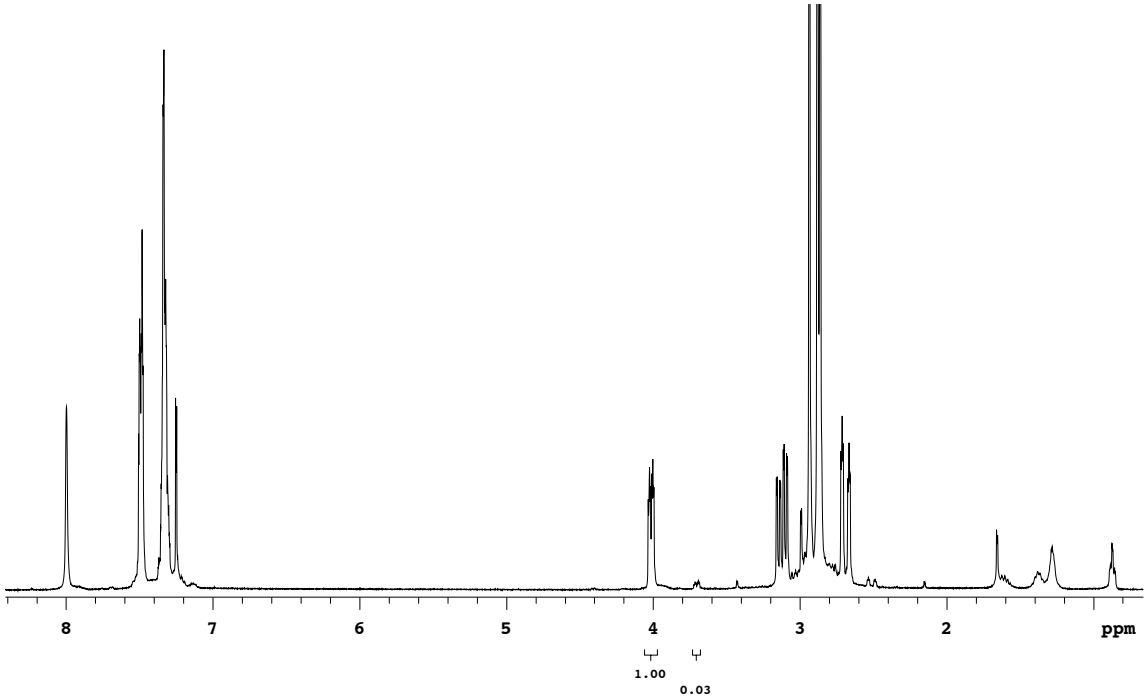


Figure S7. Ternary reaction between NMM, HT, and **7** in DMF in the absence of an initiator. Reaction conditions: *N*-methyl maleimide (150 mg, 1.35 mmol), 1-hexanethiol (160 mg, 1.35 mmol), thiophenol (150 mg, 1.35 mmol), and 1.0 mL of anhydrous DMF. Residual DMF is present in the spectrum.

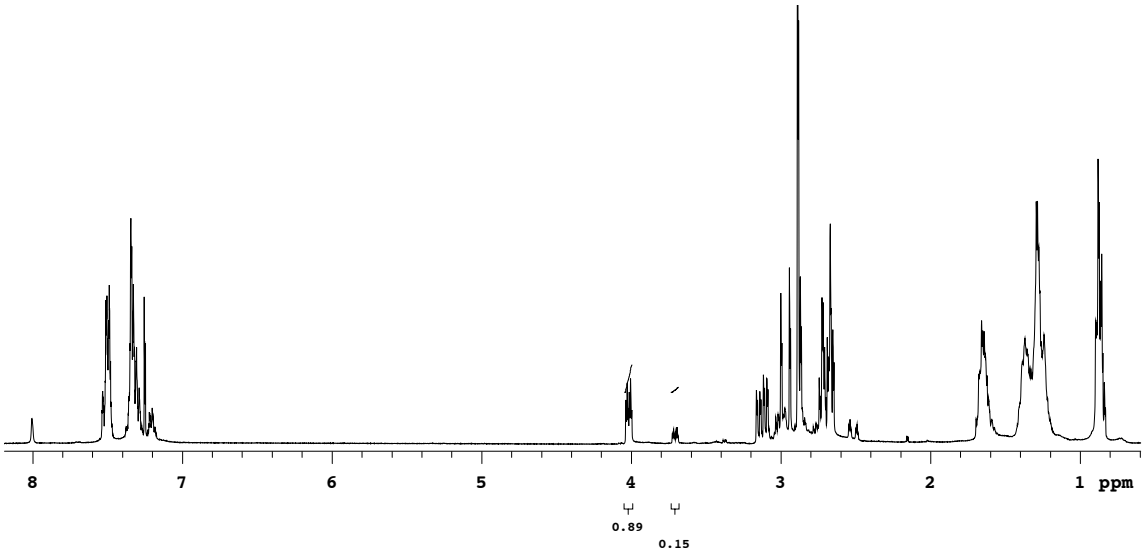


Figure S8. Ternary reaction between NMM, HT, and **7** in DMF in the presence of 0.1 equiv Et_3N. Reaction conditions: *N*-methyl maleimide (150 mg, 1.35 mmol), 1-hexanethiol (160 mg, 1.35 mmol), thiophenol (150 mg 1.35 mmol), and 1.0 mL of the Et_3N stock solution.

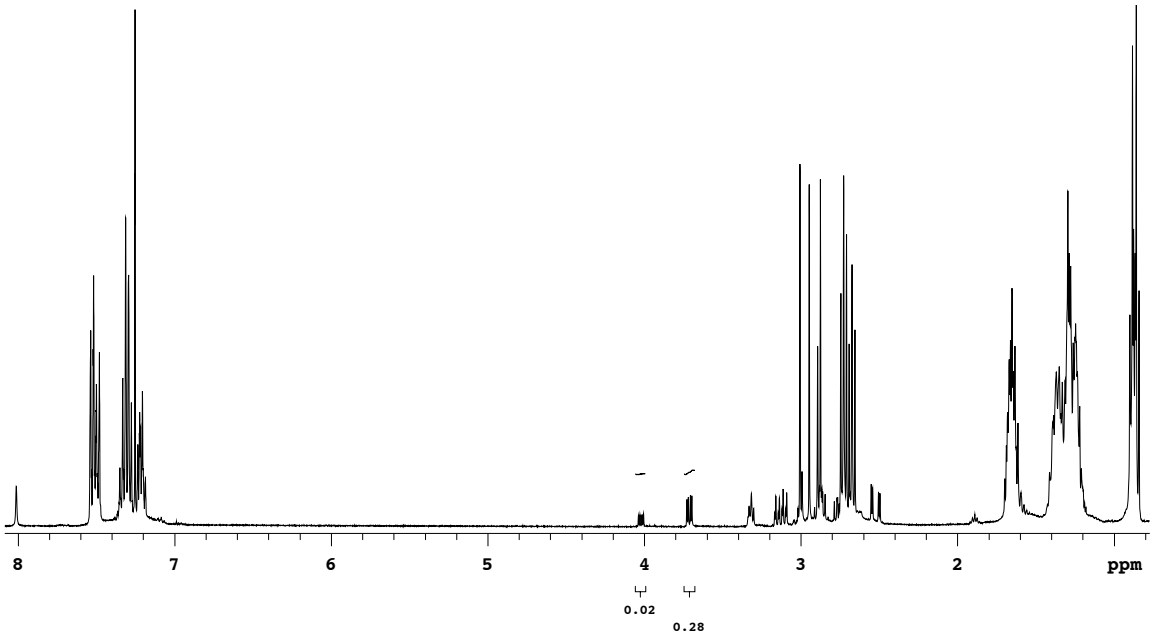
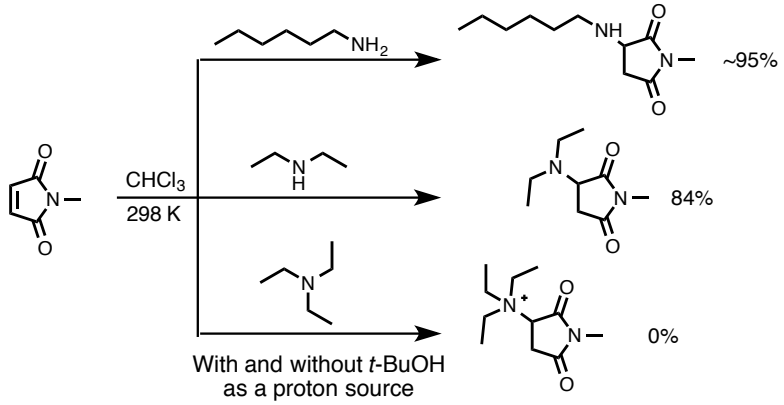


Figure S9. Ternary reaction between NMM, HT, and **7** in DMF in the presence of 0.1 equiv DBU. Reaction conditions: *N*-methyl maleimide (30 mg, 0.27 mmol), 1-hexanethiol (32 mg, 0.27 mmol), thiophenol (30 mg 0.27 mmol), and 0.2 mL the DBU stock solution.

II. Nucleophilic addition of amine bases to NMM in $CDCl_3$. To a 0.1 M $CDCl_3$ solution of *N*-methyl maleimide (50 mg, 0.45 mmol) was added either hexylamine (46 mg, 0.45 mmol), diethylamine (33 mg, 0.45 mmol) or triethylamine (46 mg, 0.45 mmmol) and the reaction mixtures were stirred overnight at ambient temperature. Separately, to a 0.1 $CDCl_3$ solution of *N*-methyl maleimide (50 mg, 0.45 mmol) was added triethylamine (46 mg, 0.45 mmmol) and *tert*-butanol (33 mg, 0.45 mmol) and the reaction mixture stirred overnight at ambient temperature. Each reaction mixture was then diluted with $CDCl_3$ and used for ^{1}H NMR spectroscopic analysis to determine the extent of nucleophilic addition of each amine to NMM.

Scheme S1. Spectroscopic investigation of the ability of hexylamine, diethylamine, and triethylamine to nucleophilically add to NMM in $CHCl_3$.



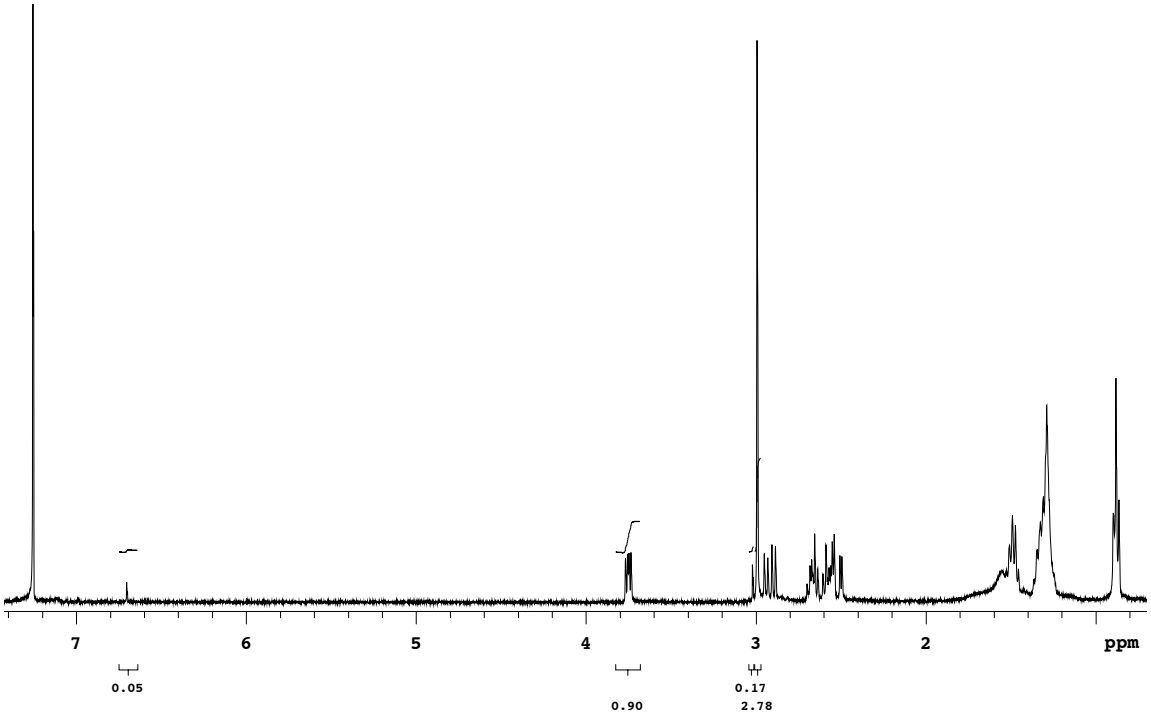


Figure S10. ^{1}H NMR spectrum of indicating approximately 95% addition of hexylamine to NMM in $CDCl_3$.

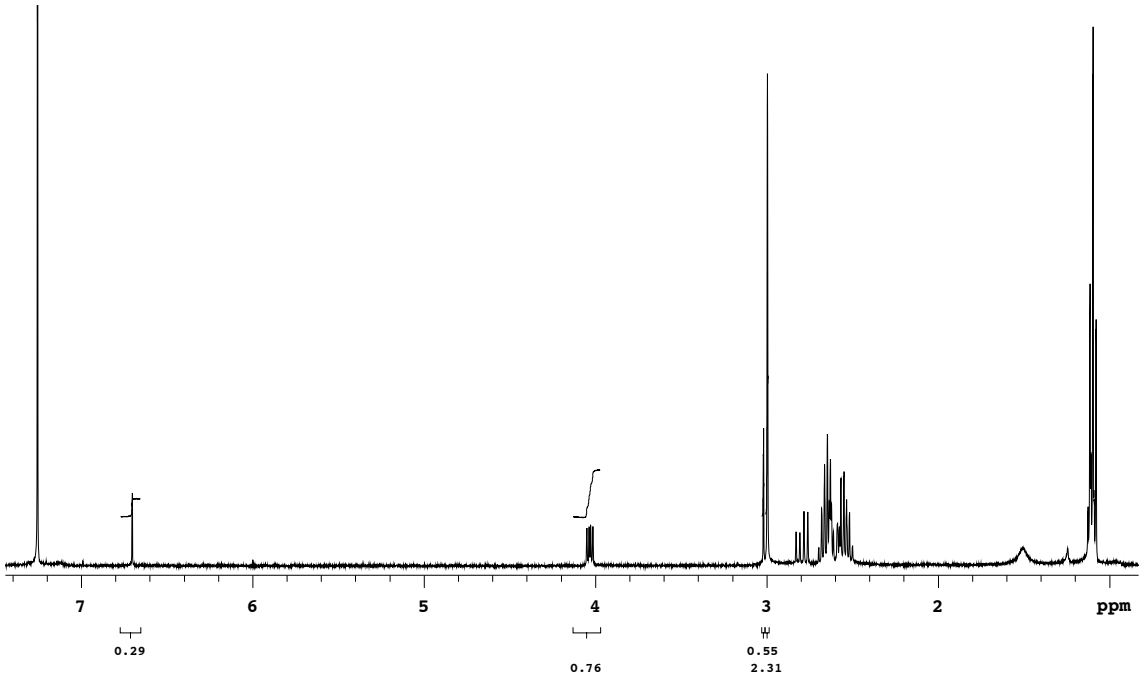


Figure S11. ^{1}H NMR spectrum indicating approximately 84% addition diethylamine to NMM in $CDCl_3$.

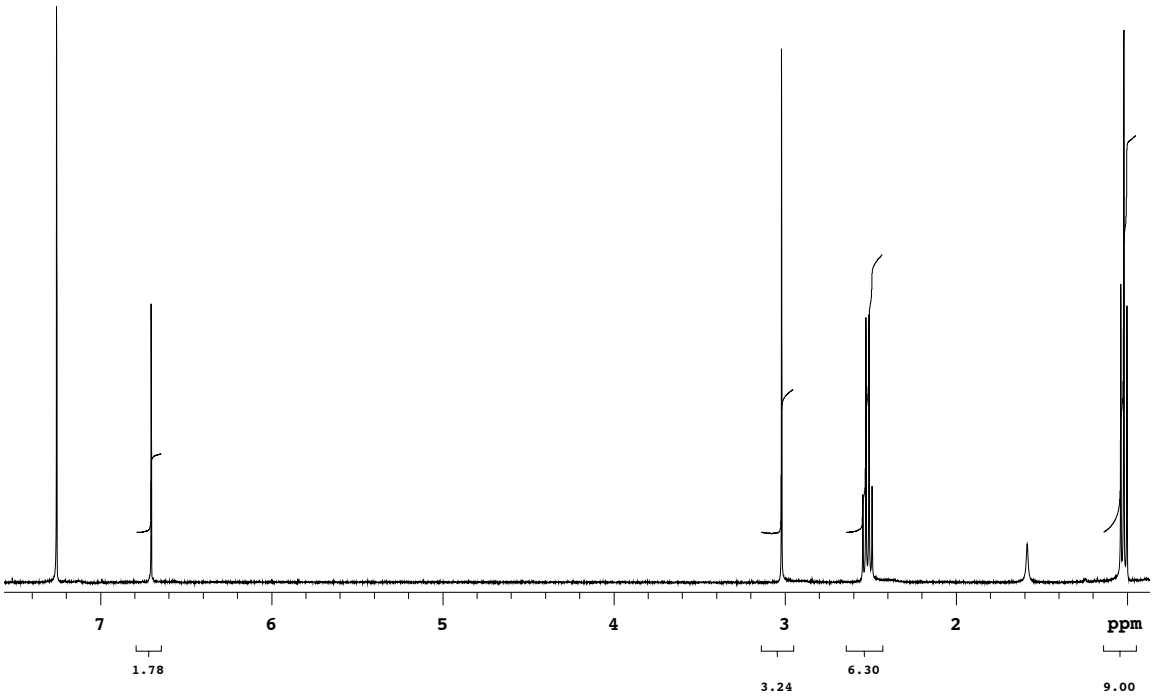


Figure S12. ^{1}H NMR spectrum indicating no addition of triethylamine to NMM in $CDCl_3$.

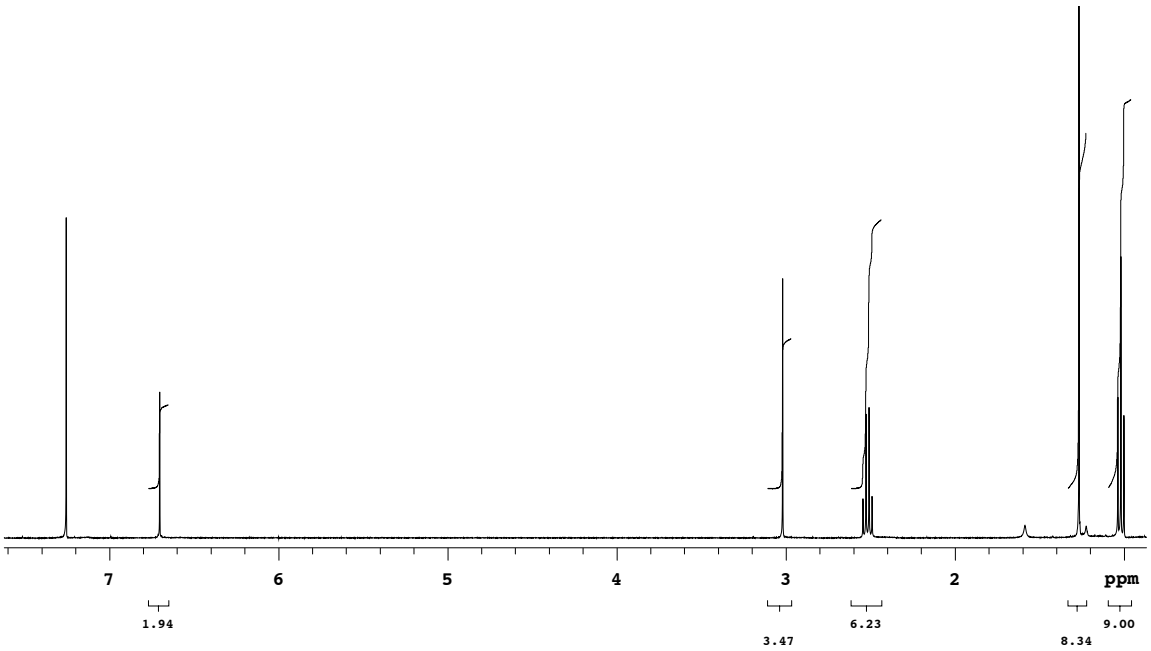


Figure S13. ^{1}H NMR spectrum indicating no addition of triethylamine to NMM in $CDCl_3$ in the presence of 1.0 equiv *tert*-butanol (a non-nucleophilic proton source).

III. Calculation of Nucleophilicity *N* Indices. The nucleophilicity of each thiolate anion was calculated using the formula:

$$N = E_{\mathrm{HOMO(Nu)}}\,(\mathrm{e}V) - E_{\mathrm{HOMO(TCE)}}\,(\mathrm{e}V) \qquad (1)$$

where tetracyanoethylene (TCE) was taken as a reference. Nucleophiliciy *N* indices calculated using equation (1) have shown good general agreement with the nucleophilicity scales developed by Mayr and co workers based on experimentally measured rate constants of various nucleophiles.[S1] To keep consistent with all other computational results presented in the current work, E_{HOMO} values for each thiol and TCE were calculated at the M06-2X/6-311G(2D,P)//B3LYP/6-31+G(D) level.

Table S1. Calculated values of E_{HOMO} for TCE and thiolates of **1**-**7** used to calculate nucleophilicity *N* indices.

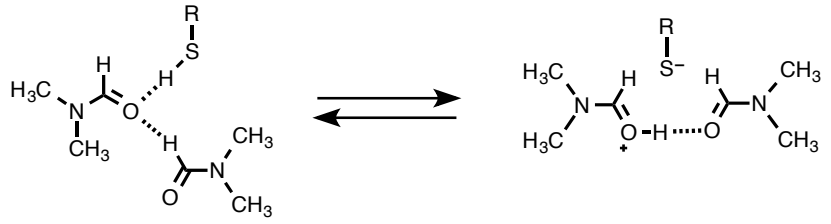
	TCE	**1**	**2**	**3**	**4**	**5**	**6**	**7**
E_{HOMO}[a]	-0.38278	-0.18627	-0.19497	-0.21007	-0.19689	-0.19050	-0.19452	-0.18496
N (eV)	–	5.35	5.11	4.70	5.06	5.23	5.12	5.38

[a] E_{HOMO} values are given in Hartrees.

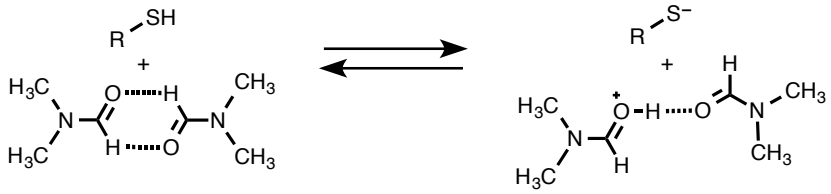
IV. Model for the Deprotonation of 1 and 7 by DMF. As discussed in the text highly polar solvents such as DMF are capable of initiating thiol-Michael reactions in the absence of an initiator. In such cases it is DMF itself that deprotonates the thiol to give a reactive thiolate and a solvated proton. The energetics of this process was modeled according to the reaction scheme summarized below:

Scheme S2. General model for transfer of a proton from a thiol to a dimer of DMF.

(a) Formation of an ion pair:



(b) Formation of isolated thiolate anion and solvated proton:



The free energy required to form an ion pair between a given thiol and DMF (Scheme S2a) was calculated by first optimizing a complex between the starting thiol along with two explicit DMF molecules, all in a solvent model for DMF. The suprastructure of the complex was fully conformationally searched using the program Maestro[S2] and the global energy minimum was optimized to full convergence using the program Gaussian09.[S3] Similarly, the ion pair complex between a thiolate and a proton solvated by two molecules of DMF was conformationally searched and optimized in a solvent model for DMF. Two molecules of DMF were found to be necessary to form a stable ion pair complex. The inclusion of a third molecule of DMF did not influence the free energies calculated. If the three species are not optimized together then a large entropic penalty is incurred upon bring together three separate molecules (the thiol and two equivalents of DMF) into one ion pair complex. It is therefore necessary to optimize all three species together in both their neutral and ion pair arrangements. The model is justified because there should not be an entropic cost associated with bringing molecules of DMF near the thiol when DMF is present throughout as the solvent medium.

The free energy required to form a free thiolate anion and a solvated proton in DMF was calculated as shown in Scheme S2b. The primary difference between the two models being that in the ion pair the thiolate anion is stabilized by the nearby protonated DMF dimer whereas in Scheme S2b the thiolate is modeled as infinitely separated from the protonated DMF dimer, though both species are in an implicit solvent model for DMF.

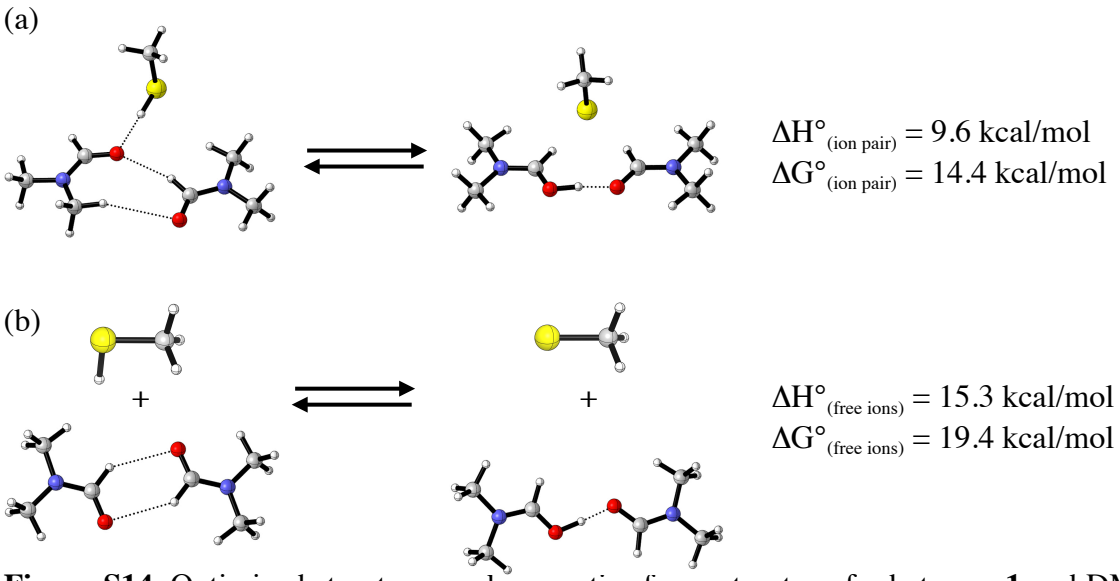


Figure S14. Optimized structures and energetics for proton transfer between **1** and DMF to give (a) an ion pair and (b) free ions as described above.

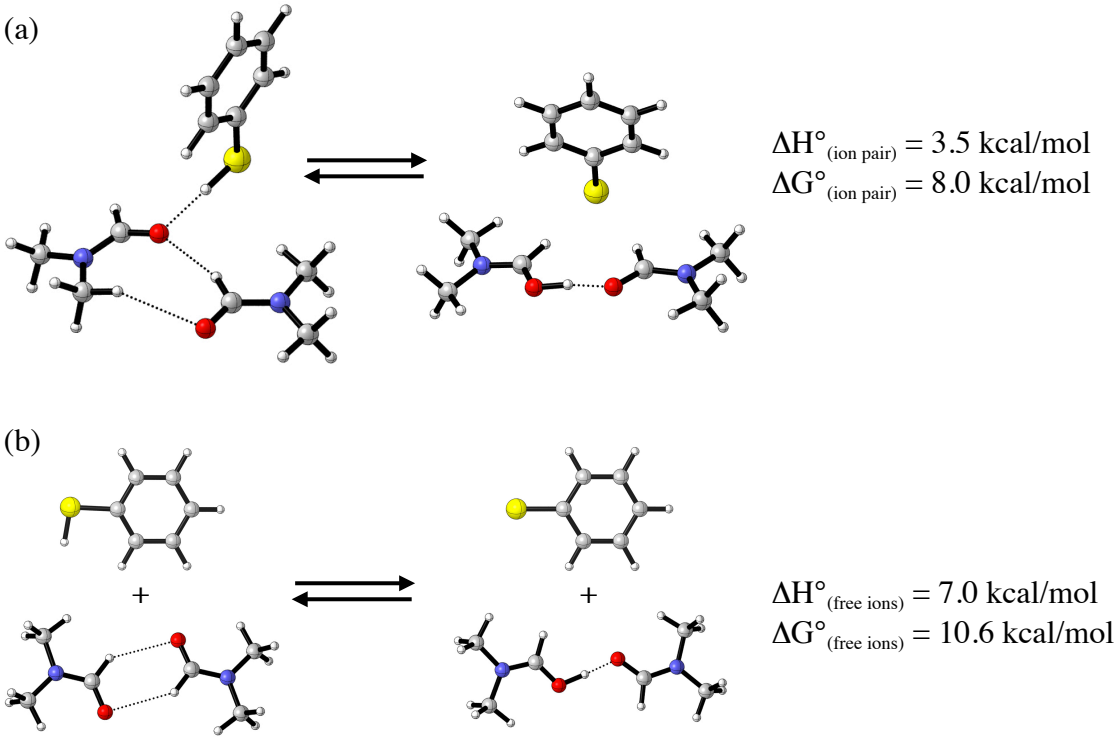


Figure S15. Optimized structures and energetics for proton transfer between **7** and DMF to give (a) an ion pair and (b) free ions as described above.

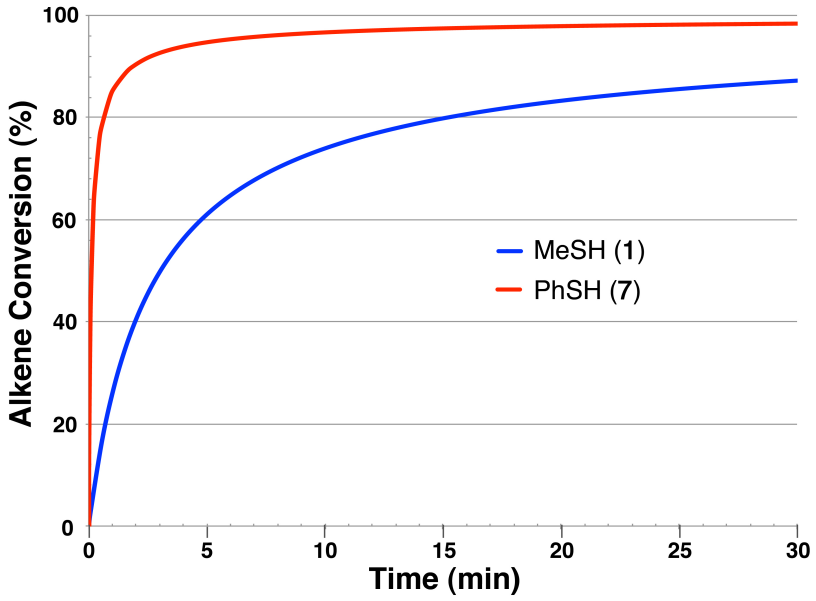


Figure S16. Comparison of the DMF-catalyzed addition of methyl mercaptan (**1**) to NMM versus the DMF-catalyzed addition of phenylthiol (**7**) to NMM in the absence of an initiator. The difference in predicted kinetics reflects the difference in the calculated free energy required for DMF to deprotonate **1** versus **7** (Figures S14 and S15 on the previous page).

V. Ion Pair Free Energies vs. S•••H Distances. The free energy of forming an ion pair between thiols **1**-**7** and Et_3N was found to correlate approximately with the S•••H hydrogen bond distance in each ion pair (Figure S17). Two notable outliers are methyl mercaptan (**1**) and cysteine methyl ester (**6**): the S•••H distance observed in the ion pair $\mathbf{1}^-/Et_3NH^+$ was found to be shorter than the trend (1.98 Å) while the S•••H distance in the ion pair $\mathbf{6}^-/Et_3NH^+$ was found to be longer than the trend (2.03 Å). The likely explanation for methyl mercaptan as an outlier is its size, as **1** represents the smallest thiol possible. Cysteine methyl ester has a notably long S•••H distance because the sulfur anion is able to hydrogen bond with the NH_2 moiety of $\mathbf{6}^-$ as shown in Figure S18 below. With the two outliers the correlation has an R^2 value of 0.816, if thiols **1** and **6** are excluded from the set the correlation increases to $R^2 = 0.992$.

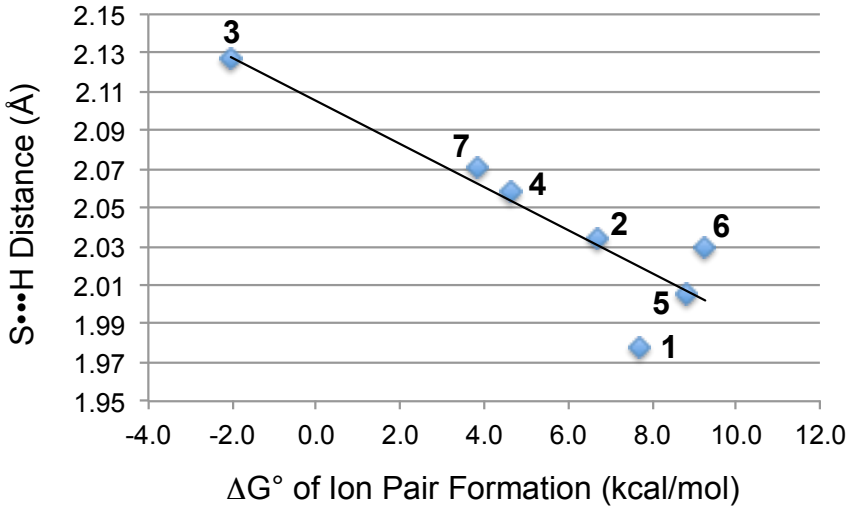


Figure S17. General correlation between the free energy of ion pair formation between thiols **1**-**7** and Et_3N and the S•••H hydrogen bond distances in each ion pair.

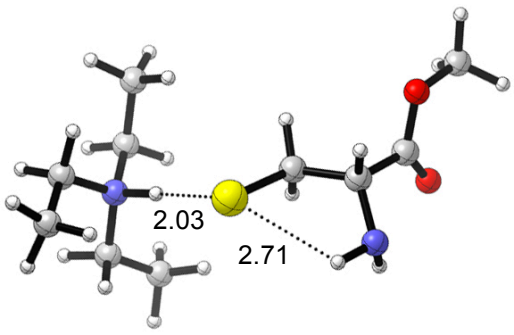
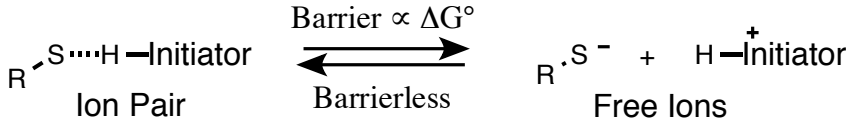


Figure S18. Global free energy minimized structure of the $\mathbf{6}^-/Et_3NH^+$ ion pair with hydrogen bonding interactions between $S•••H_{ammonium}$ and $S•••H_{amide}$ indicated by dotted lines. Distances are given in Å.

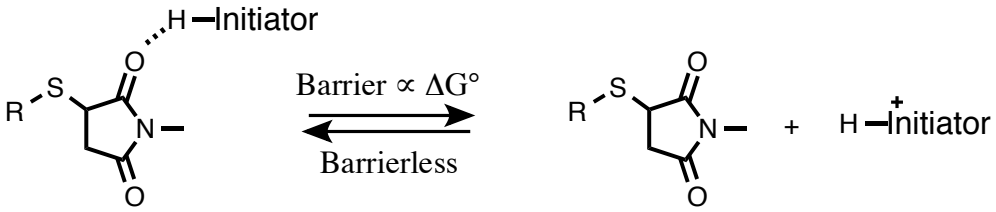
VI. Calculated Rate Constants. Rate constants were calculated at 298.15 K using the transition state free energies ($\Delta G^{\ddagger}$) for every elementary step of each reaction mechanism according to conventional activated complex theory: $k_{(T)} = (k_B T/h)e^{(-{}_A G^{\ddagger}/RT)}$. Two general classes of reactions were considered to be barrierless: (i) the association of free thiolate and a protonated base to give an ion pair, and (ii) the association of a protonated base and thiol-maleimide addition product (Scheme S3).

Scheme S3. Generic examples of the two classes of reactions that were considered be barrierless in all kinetic models.

(i)



(ii)



The rate constant for the above barrierless processes was taken to be $k = 6.21\text{x}10^{12}$ M^{-1} s^{-1} (i.e. $k_B T/h$). All other calculated rate constants are summarized in the Tables below.

Table S2. Calculated rate constants for all forward and reverse elementary steps of every mechanism discussed in the main text.

Process	solvent	initiator	thiol	$k_{forward}$	$k_{reverse}$
Formation of a thiolate/initiator ion pair (e.g. $\mathbf{1}^{-}$•••Et_3NH^{+})	$CHCl_3$	Et_3N	**1**	$4.32\text{x}10^{6}$	$1.87\text{x}10^{12}$
	$CHCl_3$	Et_3N	**2**	$4.83\text{x}10^{7}$	$4.05\text{x}10^{12}$
	$CHCl_3$	Et_3N	**3**	$2.90\text{x}10^{10}$	$9.33\text{x}10^{8}$
	$CHCl_3$	Et_3N	**4**	$7.89\text{x}10^{7}$	$2.00\text{x}10^{11}$
	$CHCl_3$	Et_3N	**5**	$1.55\text{x}10^{5}$	$4.52\text{x}10^{11}$
	$CHCl_3$	Et_3N	**6**	$1.96\text{x}10^{5}$	$1.19\text{x}10^{12}$
	$CHCl_3$	Et_3N	**7**	$6.46\text{x}10^{8}$	$4.15\text{x}10^{11}$
	$CHCl_3$	$EtNH_2$	**1**	$3.61\text{x}10^{4}$	$5.45\text{x}10^{12}$
	$CHCl_3$	Et_2NH	**1**	$1.85\text{x}10^{5}$	$5.38\text{x}10^{12}$
	$CHCl_3$	DBU	**1**	$2.72\text{x}10^{8}$	$2.26\text{x}10^{11}$
	DMF	$EtNH_2$	**1**	$5.28\text{x}10^{4}$	$9.02\text{x}10^{11}$
	DMF	Et_2NH	**1**	$9.47\text{x}10^{5}$	$5.05\text{x}10^{11}$
	DMF	Et_3N	**1**	$2.38\text{x}10^{7}$	$3.62\text{x}10^{11}$
	DMF	DBU	**1**	$1.08\text{x}10^{11}$	$2.54\text{x}10^{12}$
	DMF	DMF	**1**	$1.70\text{x}10^{2}$	$1.19\text{x}10^{12}$
	DMF	DMF	**7**	$8.91\text{x}10^{6}$	$1.09\text{x}10^{5}$

Separation of thiolate/initiator into free ions (e.g. **1**$^-$ and Et_3NH^+)	$CHCl_3$	Et_3N	**1**	$8.93x10^{-7}$	$6.21x10^{12}$
	$CHCl_3$	Et_3N	**2**	$3.80x10^{-4}$	$6.21x10^{12}$
	$CHCl_3$	Et_3N	**3**	$3.07x10^{-5}$	$6.21x10^{12}$
	$CHCl_3$	Et_3N	**4**	$3.33x10^{-5}$	$6.21x10^{12}$
	$CHCl_3$	Et_3N	**5**	$3.63x10^{-5}$	$6.21x10^{12}$
	$CHCl_3$	Et_3N	**6**	$3.36x10^{-5}$	$6.21x10^{12}$
	$CHCl_3$	Et_3N	**7**	$7.54x10^{-3}$	$6.21x10^{12}$
	$CHCl_3$	$EtNH_2$	**1**	$1.96x10^{-8}$	$6.21x10^{12}$
	$CHCl_3$	Et_2NH	**1**	$4.04x10^{-7}$	$6.21x10^{12}$
	$CHCl_3$	DBU	**1**	$2.00x10^{-1}$	$6.21x10^{12}$
	DMF	$EtNH_2$	**1**	$3.21x10^{8}$	$6.21x10^{12}$
	DMF	Et_2NH	**1**	$3.45x10^{8}$	$6.21x10^{12}$
	DMF	Et_3N	**1**	$2.46x10^{7}$	$6.21x10^{12}$
	DMF	DBU	**1**	$5.09x10^{12}$	$6.21x10^{12}$
	DMF	DMF	**1**	$1.50x10^{9}$	$6.21x10^{12}$
	DMF	DMF	**7**	$7.58x10^{10}$	$6.21x10^{12}$
Propagation Step thiolate/initiator ion pair adding to NMM π-bond (e.g. **TS13**)	$CHCl_3$	Et_3N	**1**	$5.39x10^{1}$	$2.20x10^{10}$
	EtSH	Et_3N	**1**	$6.43x10^{1}$	$7.05x10^{9}$
	DMF	Et_3N	**1**	$2.54x10^{2}$	$2.38x10^{10}$
	$CHCl_3$	$EtNH_2$	**1**	$5.75x10^{1}$	$5.21x10^{9}$
	$CHCl_3$	Et_2NH	**1**	$4.77x10^{3}$	$5.00x10^{9}$
	$CHCl_3$	DBU	**1**	$1.41x10^{3}$	$1.30x10^{9}$
Chain Transfer Step proton abstraction from the thiol (e.g. **TS17**)	$CHCl_3$	Et_3N	**1**	$1.68x10^{7}$	–
	EtSH	Et_3N	**1**	$2.82x10^{6}$	–
	DMF	Et_3N	**1**	$3.39x10^{7}$	–
	$CHCl_3$	$EtNH_2$	**1**	$1.34x10^{7}$	–
	$CHCl_3$	Et_2NH	**1**	$5.35x10^{6}$	–
	$CHCl_3$	DBU	**1**	$6.87x10^{7}$	–
Chain Transfer Step proton abstraction from initiator conjugate acid (e.g. **TS15**)	$CHCl_3$	Et_3N	**1**	$9.38x10^{8}$	–
	EtSH	Et_3N	**1**	$9.04x10^{8}$	–
	DMF	Et_3N	**1**	$9.63x10^{9}$	–
	$CHCl_3$	$EtNH_2$	**1**	$1.57x10^{9}$	–
	$CHCl_3$	Et_2NH	**1**	$4.04x10^{9}$	–
	$CHCl_3$	DBU	**1**	$2.45x10^{11}$	–
Separation of ammonium ion from thiol-maleimide addition product (e.g. **11**•••Et_3NH^+ –> **11** + Et_3NH^+)	$CHCl_3$	Et_3N	**1**	$3.27x10^{14}$	$6.21x10^{12}$
	EtSH	Et_3N	**1**	$2.51x10^{14}$	$6.21x10^{12}$
	DMF	Et_3N	**1**	$5.95x10^{13}$	$6.21x10^{12}$
	$CHCl_3$	$EtNH_2$	**1**	$6.00x10^{12}$	$6.21x10^{12}$
	$CHCl_3$	Et_2NH	**1**	$1.79x10^{14}$	$6.21x10^{12}$
	$CHCl_3$	DBU	**1**	$1.04x10^{15}$	$6.21x10^{12}$
Propagation Step free thiolate adding to the NMM π-bond (e.g. **TS8**)	$CHCl_3$	–	**1**	$7.61x10^{6}$	$3.94x10^{9}$
	EtSH	–	**1**	$2.61x10^{6}$	$3.56x10^{9}$
	DMF	–	**1**	$4.07x10^{4}$	$1.95x10^{10}$

Nucleophilic addition of initiator to the π-bond of NMM (e.g. **TS19**)	$CHCl_3$	$EtNH_2$	–	$8.37x10^{-5}$	$1.33x10^{11}$
	$CHCl_3$	Et_2NH	–	$2.80x10^{-4}$	$1.78x10^{11}$
	$CHCl_3$	Et_3N	–	$6.92x10^{-6}$	$1.88x10^{12}$
	$CHCl_3$	DBU	–	$1.12x10^{-3}$	$1.19x10^{9}$
	$CHCl_3$	DMPP	–	$7.73x10^{-4}$	$6.88x10^{7}$
	EtSH	Et_3N	–	$1.17x10^{-5}$	$9.37x10^{11}$
	DMF	Et_3N	–	$3.80x10^{-5}$	$2.91x10^{11}$
Chain transfer step proton abstraction from **1** by the zwitterionic intermediate (e.g. **TS21**)	$CHCl_3$	$EtNH_2$	**1**	$4.16x10^{3}$	–
	$CHCl_3$	Et_2NH	**1**	$1.24x10^{4}$	–
	$CHCl_3$	Et_3N	**1**	$6.81x10^{4}$	–
	$CHCl_3$	DBU	**1**	$1.29x10^{7}$	–
	$CHCl_3$	DMPP	**1**	$6.15x10^{5}$	–
	EtSH	Et_3N	**1**	$8.12x10^{4}$	–
	DMF	Et_3N	**1**	$1.57x10^{5}$	–

VII. Kinetic Comparison of Initiators in DMF.

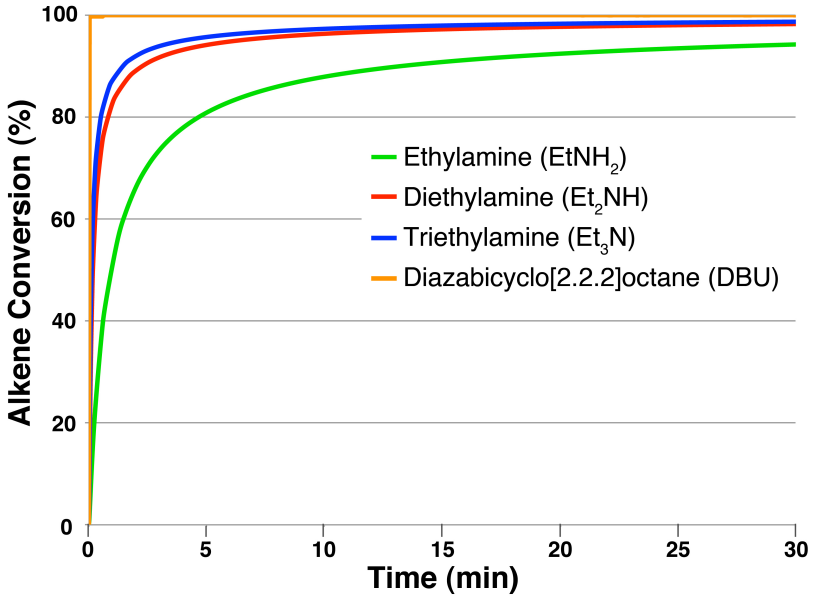


Figure S19. Plot of alkene conversion versus time for the addition of methyl mercaptan (**1**) to NMM as catalyzed by ethylamine (green trace), diethylaine (red trace), triethylamine (blue trace), and DBU (orange trace) in DMF. In each case the only pathway available for initial thiolate formation is through the direct deprotonation of **1** by each N-centered base. Kinetic modeling indicates that, in DMF, all four N-centered bases are able to directly deprotonate enough of **1** to initiate the catalytic thiol-maleimide cycle. Inclusion of the ion pair addition, nucleophile-initiated, and DMF-catalyzed pathways would further increase the rate of alkene conversion for each initiator.

VIII. Stationary Point Coordinates and Free Energies. Stationary points were optimized and frequencies calculated at the B3LYP/6-31+G(D) level of theory while single point electronic energies were calculated at the M06-2X/6-311G(2D,P) level on B3LYP-optimized geometries as described in the text. Geometries of all stationary points are given in Cartesian coordinates below. Atoms are given either by atomic number of atomic symbol. Free energies are given in Hartrees. For structures that were optimized in multiple solvents the free energy of each optimized structure in each solvent is given.

N-methyl maleimide (NMM)

C	1.13741600	-0.22522500	-0.00000500
C	0.63904400	-1.64177600	0.00001600
C	-1.14826700	-0.18496400	-0.00001300
N	0.01011800	0.59471400	-0.00006500
H	1.31213400	-2.48968400	0.00002800
O	-2.29142400	0.23949400	0.00000000
O	2.29296600	0.16596100	0.00001100
C	0.04695500	2.05001100	0.00003100
H	-0.98290100	2.40951900	-0.00168200
H	0.56181100	2.41651200	0.89244200
H	0.56477700	2.41640200	-0.89068900
C	-0.69806700	-1.61781600	0.00001300
H	-1.40147300	-2.44076100	0.00002200

G_{CHCl3}: -398.6424917
G_{EtSH}: -398.6432037
G_{DMF}: -398.644714

Methyl mercaptan (**1**)

C	-0.04781100	1.16216400	0.00000000
H	-1.09556300	1.46309200	0.00000000
H	0.43082600	1.55738100	0.89506100
H	0.43082600	1.55738100	-0.89506100
S	-0.04781100	-0.66970400	0.00000000
H	1.28575000	-0.83557700	0.00000000

G_{CHCl3}: -438.6584536
G_{EtSH}: -438.6587668
G_{DMF}: -438.6594546

Methane thiolate (**1**$^-$)

C	0.00002500	1.14053700	0.00000000
H	-1.02263200	1.53956200	0.00000000
H	0.51103600	1.54036400	0.88534000
H	0.51103600	1.54036400	-0.88534000
S	0.00002500	-0.71646900	0.00000000

G_{CHCl3}: -438.1745793
G_{EtSH}: -438.1805391
G_{DMF}: -438.1946726

TS8

C	1.18470900	-1.06274700	0.34137500
C	0.08691400	-1.00504100	1.25521000
C	0.42779300	1.12085700	0.36051100
N	1.31423200	0.25137400	-0.23675300
H	-0.24043200	-1.85452800	1.84043500
O	0.45667800	2.34797900	0.25072000
O	1.96772700	-1.98049100	0.04338700
C	2.39984500	0.66007000	-1.10246500
H	2.01230300	1.16276700	-1.99477300
H	3.08519700	1.34401900	-0.58654900
H	2.94360500	-0.23968100	-1.39762200
C	-0.49773600	0.27055000	1.19502600
H	-1.03034200	0.74573500	2.00879800
S	-2.34803800	0.40088500	-0.21728700
C	-2.17354700	-1.23641600	-0.99404800
H	-1.33535200	-1.75832300	-0.50030700
H	-3.07792200	-1.83928000	-0.85943800
H	-1.95119400	-1.15802400	-2.06319000

G_{CHCl3}: -836.8042187
G_{EtSH}: -836.8098784
G_{DMF}: -836.8215943

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C	1.65326100	-0.93571800	0.08702600
C	0.47964800	-1.49710500	0.56310300
C	0.14874600	0.84688800	0.33961500
N	1.39751900	0.51816700	-0.05958900
H	0.33771400	-2.55482700	0.74552200
O	-0.31439400	1.99606300	0.42067600
O	2.79590200	-1.38019300	-0.19790600
C	2.39859700	1.47197600	-0.48035100
H	2.08889600	1.99303700	-1.39455700
H	2.58125200	2.22194400	0.29910600
H	3.31713200	0.91272600	-0.67230100
C	-0.57916100	-0.46218000	0.68211900
H	-1.08365700	-0.36877300	1.65273500
S	-1.96958700	-0.75942900	-0.56098800
C	-3.24065300	0.46084700	-0.04997200
H	-4.12926600	0.27386500	-0.66107300
H	-3.50379600	0.32778500	1.00503800
H	-2.89221100	1.48272400	-0.21292700

G_{CHCl3}: -836.8111697
G_{EtSH}: -836.8169276
G_{DMF}: -836.8289265

TS10

C	-0.53225400	1.09823500	0.90907700
C	-0.35720600	-0.30740400	0.90800500
C	1.02843800	0.66329800	-0.76962900
N	0.27851000	1.63142800	-0.17494900
H	-0.55652700	-0.87850000	1.81013500
O	1.75581900	0.82117100	-1.75610700
O	-1.24749900	1.85891500	1.58878200
C	0.24453500	3.01126400	-0.61376800

H	1.24265400	3.45968700	-0.55972800
H	-0.11461200	3.08318600	-1.64693300
H	-0.43578400	3.54976700	0.04867200
C	0.79669300	-0.63841600	0.00587300
H	0.63542500	-1.46830600	-0.69534800
S	2.32587700	-1.07494800	0.98926500
C	3.47671100	-1.65491600	-0.31458800
H	4.39397900	-1.97106200	0.19153600
H	3.05521100	-2.51002800	-0.85314100
H	3.70559500	-0.85308600	-1.01965000
S	-2.74122900	-1.51260700	-0.82602000
C	-4.08412100	-0.71801300	0.15264100
H	-3.98406200	-0.95486200	1.21606000
H	-4.07176800	0.36834200	0.02769200
H	-5.04408000	-1.10341300	-0.20260200
H	-1.63332300	-0.90581500	-0.03102400

G_{CHCl3}: -1275.461973
G_{EtSH}: -1275.467882
G_{DMF}: -1275.479187

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C	1.68714800	-0.84473900	0.03617000
C	0.44164100	-1.54609800	0.55353500
C	0.12756800	0.84570400	0.35427000
N	1.41823600	0.51919100	-0.04204900
H	0.17524700	-2.36267800	-0.12459900
O	-0.29665200	1.98719600	0.42995000
O	2.75338000	-1.35929400	-0.25358800
C	2.38986600	1.52030100	-0.46649900
H	2.03292800	2.02873100	-1.36616500
H	2.53409600	2.25754700	0.32750100
H	3.32880500	1.00754100	-0.67630600
C	-0.62872500	-0.44572600	0.66140400
H	-1.07279700	-0.37887800	1.65858700
S	-1.98197500	-0.73964100	-0.55942300
C	-3.20686500	0.52535700	-0.06584800
H	-4.07195300	0.37740100	-0.71828200
H	-3.51511900	0.38061600	0.97378500
H	-2.81187300	1.53286300	-0.20500100
H	0.66700800	-1.99522500	1.52648200

G_{CHCl3}: -837.3195539
G_{EtSH}: -837.3195809
G_{DMF}: -837.3197703

Et_3N

C	2.27101300	-0.98452800	-0.41954500
C	1.40336200	-0.05541700	0.42956900
N	-0.00014500	-0.00015000	-0.00560200
C	-0.75016100	-1.18760500	0.42950400
C	-1.98744300	-1.47391900	-0.42159400
C	-0.65314400	1.24305900	0.43059100
C	-0.28320100	2.45851600	-0.41974400
H	1.47012100	-0.34578500	1.49465800
H	1.81630700	0.95321700	0.36347800
H	2.26320500	-0.66603500	-1.46509600
H	3.30431300	-0.96460800	-0.06040400
H	1.93084000	-2.02233800	-0.37990100
H	-0.08316500	-2.04963500	0.36505000
H	-1.03683000	-1.09887400	1.49395600
H	-2.71323500	-0.65761600	-0.38664600
H	-1.70586800	-1.63089300	-1.46597400
H	-2.49051000	-2.37576500	-0.06021600
H	-1.73331600	1.09687400	0.36693400
H	-0.43202000	1.44599900	1.49508100
H	-0.80919500	3.34579700	-0.05488200
H	0.78724900	2.67642700	-0.38888400
H	-0.56465600	2.29573500	-1.46325000

G_{CHCl3}: -292.1735718
G_{EtSH}: -292.1736304
G_{DMF}: -292.1744282

Et_3NH^+

C	-2.65027900	0.21448700	0.02801500
C	-1.40320200	-0.63672800	-0.17496500
N	-0.14158600	0.02372800	0.36627800
C	0.34128700	1.15144300	-0.53166500
C	1.44682400	1.99213700	0.09387900
C	0.93585300	-0.99852400	0.71530700
C	1.45414500	-1.79323800	-0.47430900
H	-1.49913400	-1.58654000	0.35503000
H	-1.22271500	-0.84642000	-1.23072400
H	-2.62636200	1.15061600	-0.53635600
H	-3.51331800	-0.35893500	-0.32454700
H	-2.81536400	0.44164400	1.08716300
H	0.65616500	0.69131400	-1.46968800
H	-0.53539900	1.76778000	-0.73406000
H	1.15470800	2.38198600	1.07573100
H	2.39044500	1.44943000	0.19431700
H	1.62881900	2.85028200	-0.56071800
H	1.73726900	-0.44488000	1.20682400
H	0.47747000	-1.65579600	1.45769900
H	2.19530200	-2.50545200	-0.09789400
H	0.66525600	-2.36877200	-0.96673600
H	1.95329100	-1.16538500	-1.21764900
H	-0.40309900	0.45557100	1.26008700

G_{CHCl3}: -292.6042296
G_{EtSH}: -292.6082804
G_{DMF}: -292.6183707

TS12

S	1.80011814	1.17328652	0.08280840
C	2.96007214	-0.26042548	0.01346940
H	2.79795514	-0.94929048	0.84943040
H	2.85761214	-0.81622948	-0.92487460
H	3.98665814	0.11264552	0.07641640
N	-0.83250386	-0.24049048	-0.01753860
C	-1.29562886	-0.46496448	1.38268940
H	-1.31767586	0.51389652	1.86529340
H	-2.32763886	-0.84701948	1.35325440
C	-1.73566786	0.69396152	-0.75220560
H	-2.69560186	0.18651452	-0.93240360
H	-1.26923286	0.87689652	-1.72216360
C	-0.66716886	-1.52916348	-0.75246560
H	0.08037914	-2.10744948	-0.20567760
H	-1.61620186	-2.08471048	-0.70339260
H	0.36831714	0.36596852	0.03602940
C	-0.21054086	-1.38349248	-2.20472860
H	0.06847714	-2.37385148	-2.58110560

H	-0.99624286	-0.99471348	-2.85918060
H	0.66495314	-0.73062648	-2.28495060
C	-1.96342686	2.03899352	-0.06064960
H	-2.47443186	2.70582252	-0.76379360
H	-2.59270486	1.95924552	0.83061940
H	-1.01643286	2.51183052	0.21960540
C	-0.40496486	-1.39223948	2.20944540
H	-0.74080786	-1.35464248	3.25160740
H	-0.45724286	-2.43631648	1.88663440
H	0.63915014	-1.06373648	2.18336040

G_{CHCl3}: -730.8186382
G_{EtSH}: -730.8194571
G_{DMF}: -730.8221059

1^{-}/Et_3NH^+ ion pair

C	0.20351100	-1.24305700	2.25661500
C	0.68395200	-1.46077200	0.82362800
N	0.84183200	-0.19325300	0.02499800
C	1.73646500	0.79814000	0.72231200
C	1.92190600	2.11496200	-0.02813200
C	1.30134300	-0.47034200	-1.38228200
C	0.41858200	-1.45088500	-2.14996800
H	1.64578100	-1.98599800	0.79832100
H	-0.04770700	-2.06628500	0.28770900
H	-0.68286900	-0.60078800	2.28198600
H	-0.06867800	-2.21732900	2.67646400
H	0.97306100	-0.81092700	2.90224600
H	1.26792900	0.99957900	1.68596500
H	2.69684700	0.30136300	0.90294800
H	2.54223000	2.01373700	-0.92297100
H	0.95880400	2.55257800	-0.30940000
H	2.42593300	2.81857100	0.64297700
H	1.29533000	0.49119600	-1.89618200
H	2.33750400	-0.82364100	-1.32417300
H	0.73094100	-1.43829000	-3.19962300
H	0.51047500	-2.48043600	-1.79271800
H	-0.63249600	-1.14754800	-2.11024600
H	-0.16284700	0.27646300	-0.04230400
S	-1.91993800	1.18034900	-0.13784500
C	-3.08799100	-0.24949300	-0.00929800
H	-2.97001000	-0.78295700	0.94194200
H	-4.12285700	0.10497200	-0.06575300
H	-2.93779100	-0.96838700	-0.82390100

G_{CHCl3}: -730.8197732
G_{EtSH}: -730.8212996
G_{DMF}: -730.8247893

TS13

C	3.58627200	0.31231200	0.02882600
C	2.96395300	1.19602200	0.93338400
C	1.59753200	-0.70039000	0.67540400
N	2.67510300	-0.82631700	-0.14287600
H	3.41229200	2.12240700	1.26778500
O	0.73336700	-1.56337700	0.87394300
O	4.68307800	0.32279600	-0.55853800
C	3.00762200	-2.02230700	-0.88842800
H	3.16501800	-2.87673200	-0.21879300
H	2.20850100	-2.27471600	-1.59349900
H	3.92971900	-1.81972800	-1.43687700
C	1.67157500	0.69435200	1.29157900
H	1.29841100	0.75785400	2.31203200
S	0.03395700	1.71584600	0.41777700
C	0.77099400	2.16773800	-1.18663900
H	0.49918700	1.46777300	-1.98213800
H	0.45601400	3.17699100	-1.46420900
H	1.86310700	2.16205800	-1.05580900
N	-2.54897700	-0.30086000	-0.12184000
C	-3.22048000	-0.47501800	1.22577400
H	-3.32494600	0.52970800	1.63647800
H	-4.22094100	-0.87058000	1.02434100
H	-1.66679400	0.24983800	0.04161000
C	-2.45385800	-1.35888300	2.20387400
H	-1.40001500	-1.07365200	2.26926700
H	-2.90929100	-1.23684400	3.19229900
H	-2.50764200	-2.41919800	1.94240500
C	-3.40480400	0.51524900	-1.06781700
H	-2.78985800	0.69240500	-1.95038500
H	-4.24533600	-0.12342900	-1.35671900
C	-3.88413700	1.84753400	-0.49955900
H	-4.64347600	1.72993000	0.27814100
H	-3.05330500	2.43863000	-0.10070600
H	-4.33653000	2.41712100	-1.31810700
C	-2.14288200	-1.62977100	-0.72705900
H	-1.42610900	-2.06250500	-0.03034500
H	-3.04592300	-2.24789400	-0.75445500
C	-1.50035600	-1.51821300	-2.10554300
H	-0.66065900	-0.81544100	-2.10389300
H	-1.10128200	-2.50381300	-2.36646500
H	-2.20648100	-1.23058900	-2.88939600

G_{CHCl3}: -1129.438216
G_{EtSH}: -1129.437814
G_{DMF}: -1129.445227

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C	3.49093700	0.56092300	-0.44974200
C	3.01868700	-0.56456900	-1.10152000
C	1.15905700	0.60540900	-0.20991400
N	2.28296600	1.25170600	0.11260800
H	3.64513600	-1.27868600	-1.61973800
O	-0.00046600	0.99432000	0.06560100
O	4.61265100	1.08724200	-0.26638400
C	2.34164800	2.50564400	0.83394400
H	1.83922100	3.30487300	0.27642900
H	1.86593000	2.41203400	1.81636300
H	3.39727100	2.75601900	0.95687000
C	1.55031200	-0.67165300	-0.96520500
H	0.97469200	-0.73916300	-1.89719400
S	0.87721300	-2.20024700	-0.04303400
C	1.88878000	-2.17053200	1.47734700
H	1.50047700	-1.45964700	2.21316100
H	1.87347900	-3.17653400	1.90508200
H	2.91753300	-1.90516500	1.21239100
N	-2.61573800	0.17027600	-0.02477200
C	-3.29205600	1.23365000	-0.86330000
H	-2.89509500	1.11725400	-1.87187800
H	-4.35892000	0.98891500	-0.88376900
H	-1.57807800	0.34903100	-0.07728900
C	-3.04979900	2.66124100	-0.38243800
H	-1.98254100	2.85727800	-0.23936000
H	-3.41706100	3.34321900	-1.15649900

H	-3.58456300	2.89653600	0.54177800
C	-2.87835700	-1.22127700	-0.55944700
H	-2.25052700	-1.88848600	0.03092400
H	-3.92945400	-1.44563300	-0.35132600
C	-2.55258200	-1.40021400	-2.03874500
H	-3.26218400	-0.89430300	-2.69896800
H	-1.53984900	-1.05656100	-2.27415900
H	-2.59673400	-2.47065900	-2.26453100
C	-2.99375100	0.28571900	1.43693100
H	-2.68259900	1.28297500	1.74742500
H	-4.08609900	0.23265100	1.48734000
C	-2.33769100	-0.75803600	2.33528500
H	-1.25615200	-0.80135800	2.17325800
H	-2.51342900	-0.46556000	3.37582500
H	-2.75506500	-1.75927000	2.19864800

G_{CHCl3}: -1129.443546
G_{EtSH}: -1129.447024
G_{DMF}: -1129.452172

TS15

C	1.69849900	-0.89193700	1.12243400
O	1.62497100	-2.07059100	1.55330700
C	3.22454000	-1.62986000	-0.82866700
H	2.91264800	-1.69856700	-1.87687800
H	4.29418600	-1.39045800	-0.80278600
H	3.05384900	-2.58585300	-0.32958200
C	1.19251600	0.32815400	1.54881900
C	1.59031300	1.40577200	0.61442100
H	2.15327000	2.24691500	1.03727000
H	-1.20622300	0.04400400	-0.07631000
N	-1.94378400	-0.66513500	-0.26714800
C	-1.23580800	-1.97793600	-0.56561400
H	-0.56315300	-2.15558200	0.27465500
H	-2.01382000	-2.74714600	-0.56990400
C	-0.44612000	-1.98271400	-1.86922000
H	0.25686400	-1.14593300	-1.92247800
H	0.14102400	-2.90628800	-1.89312100
H	-1.08379300	-1.97364000	-2.75728000
C	-2.73593100	-0.16824700	-1.46247300
H	-2.00637800	0.01277200	-2.25166400
H	-3.37967500	-0.99845500	-1.76797500
C	-2.81788800	-0.77224200	0.97099500
H	-3.12119100	0.24745300	1.21135300
H	-3.70719100	-1.33226800	0.66586400
C	-2.14365200	-1.41821700	2.17578800
H	-1.99795400	-2.49371600	2.04998800
H	-1.17623500	-0.95856200	2.39515900
H	-2.79901500	-1.27057100	3.04080300
C	-3.54544500	1.09878500	-1.21048000
H	-3.94998500	1.43007500	-2.17260900
H	-4.39052700	0.93988900	-0.53572600
H	-2.91989200	1.90711700	-0.82000900
S	0.16388600	2.25059900	-0.31896500
C	-0.62263100	3.07574100	1.11086500
H	0.06479100	3.79847800	1.56142400
H	-1.50192300	3.61191800	0.74295400
H	-0.93347000	2.34714300	1.86589800
H	0.69850300	0.47931400	2.49959200
C	2.45396500	0.68800600	-0.43911000
N	2.45489200	-0.62812300	-0.12137000
O	3.03768100	1.20850900	-1.39732000

G_{CHCl3}: -1129.435239
G_{EtSH}: -1129.438682
G_{DMF}: -1129.446062

TS16

C	-0.50515500	-1.69866600	-0.78690500
O	0.15577300	-2.72277800	-1.01293900
C	-2.22519800	-2.96293600	0.61004900
H	-3.21899300	-3.21375900	0.22651100
H	-1.52909900	-3.77314000	0.38787300
H	-2.29440000	-2.81842000	1.69340300
C	-0.25258500	-0.31929800	-1.12593500
C	-1.55876000	0.42029000	-0.86515100
H	-2.11461700	0.63159900	-1.78979500
H	1.05464000	0.05613300	-0.28196200
N	2.12424100	0.27393700	0.25330100
C	2.13963600	-0.51294700	1.53201000
H	1.94228200	-1.54946700	1.25422600
H	3.15488900	-0.46097600	1.94625500
C	1.11295200	-0.06316600	2.57030700
H	0.10607400	0.00079000	2.14653200
H	1.09273200	-0.80698300	3.37417000
H	1.36064100	0.90198500	3.02118200
C	2.23592900	1.74809100	0.51756900
H	1.34909200	2.03140900	1.08589000
H	3.11404500	1.90386000	1.15806900
C	3.21003200	-0.17792700	-0.68658200
H	2.98462300	0.28091000	-1.65182600
H	4.15408200	0.24987900	-0.32515300
C	3.34231200	-1.68889800	-0.86311600
H	3.75814400	-2.17829800	0.02314900
H	2.38416300	-2.15701300	-1.10951800
H	4.03714100	-1.86900100	-1.69138500
C	2.32514300	2.61566900	-0.73668000
H	2.24099300	3.66412500	-0.43087100
H	3.27579900	2.50118200	-1.26496400
H	1.50304700	2.40838500	-1.42801700
S	-1.34599700	2.05292200	-0.01936600
C	-2.99496600	2.81853100	-0.23737100
H	-3.76064100	2.26291900	0.30608000
H	-2.92242600	3.83426900	0.16230700
H	-3.25598700	2.87424500	-1.29923400
H	0.19435000	-0.17338200	-2.11114600
C	-2.39169000	-0.56795000	-0.03807900
N	-1.72286400	-1.76244300	-0.03467000
O	-3.46954300	-0.36387200	0.51756100

G_{CHCl3}: -1129.451809

TS17

C	2.67362700	-1.12107100	0.72911700
C	2.45862300	-0.59309200	-0.57142900
C	0.42918800	-0.49729500	0.67151700
N	1.41645200	-0.95063300	1.46700200
H	3.07816700	-0.93724800	-1.39438700
O	-0.72539900	-0.22918000	1.05698100
O	3.66389700	-1.59515200	1.30172600
C	1.27974000	-1.18849000	2.89237200
H	1.05268700	-0.25577200	3.41963500

H	0.47931500	-1.90929800	3.08635000
H	2.23114000	-1.58832900	3.24677700
C	0.98246300	-0.37539500	-0.75167600
H	0.71660900	0.61380600	-1.15019300
S	0.08411000	-1.50615100	-1.93578300
C	0.53634900	-3.15975700	-1.30249100
H	0.06375200	-3.36995400	-0.33850200
H	0.17707600	-3.88298900	-2.03991400
H	1.62183400	-3.25152300	-1.21221300
N	-3.14930600	0.65970700	0.04829300
C	-3.42988400	1.90987200	0.85648700
H	-2.67578300	2.63721900	0.55649500
H	-4.41028500	2.27713400	0.53730500
H	-2.17867600	0.34427400	0.29703200
C	-3.36649700	1.70416900	2.36686700
H	-2.43435800	1.21246300	2.66298100
H	-3.39034000	2.69087900	2.84103800
H	-4.21330000	1.13285100	2.75650500
C	-3.18288600	0.92716600	-1.44287000
H	-2.83629200	0.00819600	-1.91639400
H	-4.23286700	1.08444500	-1.70896100
C	-2.31468200	2.09571900	-1.89816300
H	-2.71710400	3.06828000	-1.60309000
H	-1.28713500	2.01119500	-1.52961000
H	-2.27345200	2.07466600	-2.99204700
C	-4.08410200	-0.46958000	0.42943300
H	-3.93170800	-0.63871300	1.49528500
H	-5.10233500	-0.09645000	0.28075100
C	-3.84254100	-1.76671800	-0.33548900
H	-2.78872900	-2.06074000	-0.30348700
H	-4.42932400	-2.55579600	0.14636300
H	-4.16076700	-1.71042500	-1.37990700
H	2.91557200	0.92225400	-0.51092300
S	3.27425000	2.42218200	-0.57929500
C	5.07390800	2.16508400	-0.27955500
H	5.58789900	3.12287200	-0.40000100
H	5.25643600	1.79347300	0.73283500
H	5.49036300	1.45418500	-0.99990500

G_{CHCl3}: -1568.089895
G_{EtSH}: -1568.092001
G_{DMF}: -1568.100185

Product **11**•••Et_3NH^+

C	-3.52984100	0.72622400	0.28643700
C	-3.22933700	-0.60686100	0.94660300
C	-1.22300200	0.50961200	0.16657800
N	-2.31289400	1.29013300	-0.13369900
H	-3.77006100	-1.39879400	0.42024700
O	-0.06749200	0.82593900	-0.10520600
O	-4.61269300	1.25133200	0.12602600
C	-2.20811400	2.58252000	-0.80610500
H	-1.57701500	3.25489900	-0.21985600
H	-1.77171800	2.45051100	-1.79937200
H	-3.21339700	2.99438000	-0.89279300
C	-1.69782100	-0.75722900	0.88030500
H	-1.25738900	-0.75541400	1.88298800
S	-1.03675000	-2.30156900	0.13632500
C	-1.69075000	-2.22039900	-1.57068900
H	-1.28520000	-1.36525400	-2.11854200
H	-1.35907500	-3.14079400	-2.05856800
H	-2.78340700	-2.19627800	-1.58690500
N	2.74090900	0.19118600	0.05366500
C	3.27761300	1.51746200	0.56147900
H	2.84146800	1.65753500	1.55033500
H	4.35799800	1.39039800	0.67618400
H	1.70628000	0.27743600	0.02336400
C	2.93747100	2.71295900	-0.32242100
H	1.86416300	2.76479000	-0.53212600
H	3.21509900	3.62038000	0.22371200
H	3.48824700	2.71904200	-1.26637600
C	3.07383700	-0.94891000	0.99859300
H	2.58835100	-1.83255800	0.58455900
H	4.15714300	-1.08947000	0.94383400
C	2.60686100	-0.72978200	2.43336700
H	3.18560700	0.03273200	2.96032500
H	1.54493400	-0.46549400	2.47753700
H	2.73555600	-1.67258800	2.97464200
C	3.21111300	-0.10001200	-1.36010500
H	2.87899900	0.74215400	-1.96677000
H	4.30471700	-0.09415000	-1.33197800
C	2.66862500	-1.40092600	-1.94140900
H	1.58092900	-1.46810200	-1.83443200
H	2.90109000	-1.41284800	-3.01111900
H	3.12360300	-2.28979300	-1.49714700
H	-3.60347200	-0.59294900	1.97493800

G_{CHCl3}: -1129.920042
G_{EtSH}: -1129.924371
G_{DMF}: -1129.93601

TS19

C	-1.14293800	1.10415800	0.05942200
C	-0.11825200	0.37402500	-0.83881900
C	-2.14710700	-0.77901800	-0.87498400
N	-2.26801200	0.36080100	0.05931500
O	-3.13601600	-1.50291800	-1.08124400
O	-0.95748300	2.16425100	0.66721700
C	-3.48407400	0.70760400	0.76646500
H	-4.22060200	-0.06605800	0.54188400
H	-3.30836000	0.74869200	1.84690400
H	-3.86390800	1.68086600	0.43604400
C	-0.84262200	-0.75498600	-1.38231700
H	-0.52353400	-1.37222100	-2.21121900
H	0.36583800	1.05508900	-1.53720300
N	1.26604000	0.02446800	0.12359900
C	2.02866800	-1.02962400	-0.63411000
H	1.34323500	-1.86897600	-0.75574000
H	2.21037500	-0.62109800	-1.63086800
C	3.33876900	-1.48427500	0.00603800
H	3.80317900	-2.21531900	-0.66463900
H	4.05224000	-0.66623600	0.14511100
H	3.18602800	-1.97718000	0.97061200
C	0.91262800	-0.43503200	1.52835300
H	1.85313800	-0.45632300	2.08704300
H	0.30879400	0.36564600	1.95964600
C	0.20670500	-1.78103500	1.67009000
H	0.01762500	-1.93207700	2.73921600
H	-0.74727700	-1.81722800	1.14553900
H	0.82205500	-2.61760200	1.32642700
C	2.06326600	1.31256000	0.28222800
H	2.81050900	1.12474600	1.05839200

C	2.75934400	1.85499000	-0.96447000
H	3.24123400	2.79645300	-0.67819600
H	3.54158700	1.18963700	-1.34097500
H	2.07269300	2.08301200	-1.78434700
H	1.35062600	2.04242400	0.67080900

G_{CHCl3}: -690.7770326
G_{EtSH}: -690.7782957
G_{DMF}: -690.7817198

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C	-1.13714700	1.08983500	0.07787600
C	-0.10102200	0.34425100	-0.80103100
C	-2.14690500	-0.79255000	-0.86572400
N	-2.27125800	0.36576200	0.05150700
O	-3.14842900	-1.49935300	-1.08411400
O	-0.94811500	2.14796000	0.69043500
C	-3.49547800	0.73203700	0.73402800
H	-4.23784800	-0.03241700	0.49733700
H	-3.34001000	0.77483000	1.81759600
H	-3.85480200	1.70944500	0.39320700
C	-0.83282100	-0.80195600	-1.33277400
H	-0.50769600	-1.42616900	-2.15422900
H	0.34195800	1.02258200	-1.53157300
N	1.25277900	0.02385700	0.11457200
C	2.03341400	-1.02263500	-0.64574600
H	1.36479300	-1.87717900	-0.74838300
H	2.19120000	-0.61782600	-1.64786600
C	3.36106400	-1.43981700	-0.01866900
H	3.82506600	-2.17636200	-0.68349700
H	4.06326100	-0.60782800	0.08985600
H	3.23415500	-1.91641700	0.95770600
C	0.92120800	-0.44304000	1.52762000
H	1.86861400	-0.44175400	2.07316800
H	0.30529200	0.34638400	1.96159200
C	0.24647900	-1.80327400	1.67858500
H	0.06725600	-1.95240700	2.74975300
H	-0.70801900	-1.86161200	1.15720800
H	0.87907600	-2.62721800	1.33572300
C	2.04482700	1.32142300	0.27264000
H	2.81005700	1.12458500	1.02754900
C	2.70573000	1.88632500	-0.98252400
H	3.20241300	2.81781900	-0.68892200
H	3.47172900	1.22556200	-1.39824900
H	1.99507200	2.13837300	-1.77426500
H	1.33405100	2.03782300	0.68748600

G_{CHCl3}: -690.7781623
G_{EtSH}: -690.7800823
G_{DMF}: -690.7846087

TS21

C	0.11731100	1.22383100	1.10812000
C	-0.18931800	-0.08515200	0.33102300
C	1.47068600	1.19825500	-0.78640900
N	1.06891800	1.89819100	0.41724900
O	2.27337200	1.70367900	-1.57468400
O	-0.39877200	1.58166600	2.16633900
C	1.64655100	3.15532400	0.86221300
H	2.35781300	3.47654600	0.10017600
H	0.86584200	3.91222100	0.98402300
H	2.16244400	3.02128100	1.81829000
C	0.83709000	-0.08468400	-0.76513300
H	1.80315600	-1.05850400	-0.13633400
H	-0.06310600	-0.93046900	1.01529600
N	-1.70979700	-0.19031200	-0.05129600
C	-1.86523600	-1.41541400	-0.94527900
H	-1.29327800	-1.20900500	-1.84705500
H	-1.36590900	-2.23431200	-0.42487400
C	-3.29876000	-1.79083400	-1.30426800
H	-3.24679200	-2.63979100	-1.99407200
H	-3.88832300	-2.10864500	-0.44046300
H	-3.83291100	-0.98632700	-1.81843400
C	-2.24441400	1.07502800	-0.73390300
H	-3.33168900	0.98471200	-0.70287500
H	-1.97560200	1.90074600	-0.07277100
C	-1.79904000	1.35519000	-2.16529200
H	-2.27900700	2.29413300	-2.46361600
H	-0.72115600	1.48344200	-2.26449400
H	-2.13053000	0.58573800	-2.86842800
C	-2.54659200	-0.35048000	1.23346700
H	-3.58669100	-0.33669500	0.90523800
C	-2.27994000	-1.59059500	2.07897800
H	-3.00446900	-1.56965900	2.90076700
H	-2.43078600	-2.52815500	1.53666500
H	-1.28514900	-1.59786500	2.53067300
H	-2.35475600	0.55027000	1.81508700
H	0.69658800	-0.60332500	-1.70617600
S	2.63984900	-2.21471700	0.56236600
C	4.02224300	-2.15105700	-0.65566200
H	4.57726700	-1.21186000	-0.57403500
H	4.70703300	-2.97960500	-0.45308200
H	3.64829200	-2.25379500	-1.67938900

G_{CHCl3}: -1129.41931
G_{EtSH}: -1129.421709
G_{DMF}: -1129.427544

22$^+$

C	2.22130700	1.07545100	-0.21796100
C	0.76273500	1.50436800	-0.14615300
C	1.01032500	-0.90422200	-0.21677200
N	2.26042500	-0.31796800	-0.20424500
H	0.58908200	1.85459000	0.87453300
O	0.80719100	-2.09621100	-0.09594200
O	3.19233000	1.80160600	-0.24533600
C	3.49423200	-1.10103800	-0.14352700
H	3.58964800	-1.57409600	0.83718000
H	3.47407900	-1.87108100	-0.91712700
H	4.32772400	-0.41914700	-0.31055600
C	-0.01784700	0.22326600	-0.50016700
H	-0.17649300	0.20666900	-1.58209200
C	-2.33114600	-0.75458900	-0.86924200
H	-3.33911600	-0.60704100	-0.47530800
H	-2.26055000	-0.23000000	-1.82198400
H	0.58201100	2.34011200	-0.82348800
N	-1.42171800	0.03778000	0.10541600
C	-2.06528700	-2.23877300	-1.07401100
H	-2.17736800	-2.82722200	-0.16076300
H	-2.83053500	-2.58077300	-1.78012900
H	-1.08725300	-2.44642600	-1.50821600
C	-2.10870300	1.40676100	0.29807100
H	-1.46573400	1.99153700	0.95011600

H	-3.02305000	1.18507800	0.85261000
C	-2.43251100	2.18558700	-0.97307400
H	-2.75472600	3.18395600	-0.65945800
H	-1.57074100	2.31688800	-1.63280000
H	-3.25064000	1.74323600	-1.54488000
C	-1.42124900	-0.69425900	1.45937200
H	-0.99156500	-1.67416400	1.26964100
H	-2.47857500	-0.82248200	1.70103000
C	-0.69241600	-0.01020800	2.60933000
H	0.38461500	0.08223400	2.44549800
H	-1.10409900	0.96825500	2.86861900
H	-0.82046700	-0.65602800	3.48441200

G_{CHCl3}: -691.2341141
G_{EtSH}: -691.2394261
G_{DMF}: -691.2509546

$EtNH_2$

C	0.04692300	0.55958800	0.05438300
H	0.07421900	1.30378900	-0.75078000
H	0.07277400	1.11698300	1.00641400
N	1.21464000	-0.32287300	-0.12107900
H	2.07508300	0.22235800	-0.08538700
H	1.26720300	-0.98447600	0.65364900
C	-1.25292400	-0.23820500	-0.02756300
H	-2.12129900	0.42256600	0.08090100
H	-1.33005100	-0.75910200	-0.98902600
H	-1.30440600	-0.99031400	0.77086300

G_{CHCl3}: -135.075223
G_{DMF}: -135.0764422

$EtNH_2^+$

C	0.05381000	0.60520100	0.00047700
H	-0.01182600	1.23747500	0.88737200
H	-0.00723200	1.23483100	-0.88860300
N	-1.20412200	-0.24436700	-0.00014200
H	-2.05216000	0.32883100	-0.07034400
H	-1.21435200	-0.90102600	-0.78821300
C	1.29901000	-0.26706900	0.00035200
H	2.17821500	0.38383500	0.02330000
H	1.34187200	-0.91952000	0.87923100
H	1.36105700	-0.88156700	-0.90448500
H	-1.28363500	-0.80108600	0.85776300

G_{CHCl3}: -135.4967436
G_{DMF}: -135.5161797

TS12 between $EtNH_2$ and **1**

N	-0.99577300	0.98207700	-0.50864400
H	-1.30626200	0.91070600	-1.48056100
H	-0.69674400	1.94803600	-0.35823500
C	-2.08059800	0.59385700	0.44136000
H	-1.63519800	0.60855300	1.44011200
H	-2.87193500	1.34909600	0.40658200
C	-2.62096600	-0.79062900	0.10486000
H	-1.82763900	-1.54388200	0.14427900
H	-3.39348800	-1.06864500	0.82912700
H	-3.07360700	-0.81004400	-0.89396600
S	1.41961900	-0.72669000	-0.13125000
C	2.60503700	0.62035400	0.31700000
H	2.28343100	1.15506600	1.21808100
H	3.59016300	0.18744900	0.51788600
H	2.71675200	1.34524000	-0.49736000
H	-0.02263800	0.28297400	-0.37313700

G_{CHCl3}: -573.7157714
G_{DMF}: -573.7183512

1$^-$/$EtNH_3^+$ ion pair

N	-0.97513900	1.02032200	-0.37960600
C	-2.10464600	0.49771000	0.45522700
C	-2.57264600	-0.85698900	-0.06031100
H	-1.72155500	0.42454300	1.47622500
H	-2.91229700	1.23452000	0.43900900
H	-2.95026400	-0.78409800	-1.08706000
H	-1.76234000	-1.59235600	-0.03646500
H	-3.38695100	-1.22431000	0.57235700
H	-0.05120900	0.36472100	-0.27592500
S	1.47589600	-0.75233000	-0.04929100
C	2.79379900	0.53411200	0.14776300
H	2.61875900	1.15540900	1.03359300
H	3.76964000	0.05123000	0.26506900
H	2.84811300	1.19071300	-0.72820200
H	-1.22931900	1.05806800	-1.37033600
H	-0.70998700	1.96758300	-0.09845000

G_{CHCl3}: -573.7158945
G_{DMF}: -573.7201735

Et_2NH

C	-1.22484400	0.51504000	0.02199900
H	-1.23262200	1.22141700	-0.81866400
H	-1.24070500	1.12543200	0.94591300
N	0.00000100	-0.28442200	-0.08106800
H	-0.00000200	-0.97981600	0.66638600
C	-2.47269900	-0.36448500	-0.03069700
H	-3.37942000	0.24795100	0.03685700
H	-2.50952300	-0.93541800	-0.96558900
H	-2.48961800	-1.07731900	0.80419700
C	1.22484500	0.51503800	0.02200800
H	1.23262200	1.22141200	-0.81865600
H	1.24070200	1.12543100	0.94592200
C	2.47269900	-0.36448600	-0.03069900
H	3.37941600	0.24795600	0.03685700
H	2.48962200	-1.07732700	0.80418600
H	2.50952100	-0.93540500	-0.96560100

G_{CHCl3}: -213.6257696
G_{DMF}: -213.6266772

$Et_2NH_2^+$

C	1.27585400	0.54539800	-0.04369100
H	1.22882300	1.23293900	0.80325500
H	1.23560200	1.12388300	-0.96891400
N	0.00000100	-0.26878600	0.00055300
H	-0.02592100	-0.89175900	-0.81449300
C	2.50425500	-0.35101900	0.01857900
H	3.39856700	0.27722300	-0.03398500
H	2.54679300	-0.91477300	0.95715900
H	2.53881300	-1.05374900	-0.82104600
C	-1.27590100	0.54544900	0.04363300

H	-1.23628500	1.12421000	0.96871600
H	-1.22831600	1.23266300	-0.80352800
C	-2.50421600	-0.35104500	-0.01912200
H	-3.39860800	0.27710600	0.03308000
H	-2.54627500	-0.91485400	-0.95768800
H	-2.53904400	-1.05375300	0.82050300
H	0.02588900	-0.89033500	0.81667800

G_{CHCl3}: -214.0517048
G_{DMF}: -214.069757

TS12 between Et_2NH and **1**

N	1.02774000	0.09798800	0.22673700
C	1.50061300	1.40725800	-0.30053300
H	2.58872300	1.46499300	-0.18108400
H	1.27570400	1.41130300	-1.37192300
C	0.80731600	2.56783500	0.40392200
H	1.03637700	2.57749400	1.47678800
H	1.15438700	3.51569700	-0.02028700
H	-0.27816400	2.51197900	0.27501300
C	1.80012900	-1.07604100	-0.26460700
H	1.57069000	-1.17576900	-1.33055100
H	2.87061400	-0.86187000	-0.16656200
C	1.42064500	-2.34354700	0.49281400
H	0.35081800	-2.55263800	0.39445200
H	1.97580500	-3.19494500	0.08559100
H	1.66835000	-2.26145400	1.55844400
H	1.04438800	0.11518100	1.24966800
S	-1.76337200	-0.25569100	-0.73804300
C	-2.59880700	-0.09803400	0.90235800
H	-2.40415900	0.87842600	1.36104500
H	-3.68085300	-0.19670400	0.77022000
H	-2.27270700	-0.88048900	1.59742700
H	-0.12460800	-0.04819700	-0.12755500

G_{CHCl3}: -652.2678631
G_{DMF}: -652.2713113

1$^-$/$Et_2NH_2^+$ ion pair

N	-0.88499200	0.23005400	0.58387100
C	-1.81517700	-0.93117000	0.79306800
C	-2.10371300	-1.69568200	-0.49369800
C	-1.37038700	1.30247600	-0.34281700
C	-0.47461900	2.53307100	-0.26489500
H	-1.31972700	-1.57870100	1.52156300
H	-2.73353800	-0.54333900	1.24502400
H	-2.66951700	-1.09726400	-1.21433200
H	-1.17847400	-2.03827600	-0.96755600
H	-2.70610500	-2.57659800	-0.24892600
H	-1.36314900	0.88028400	-1.34954700
H	-2.40401200	1.54011800	-0.07125400
H	-0.83937300	3.29138700	-0.96499800
H	-0.48118400	2.97242400	0.73973100
H	0.55677900	2.28661200	-0.53618400
H	0.09423200	-0.16127500	0.22391800
S	1.78892600	-0.92599800	-0.40908900
C	3.01065800	0.18113400	0.43447700
H	3.12896200	-0.08493200	1.49103600
H	3.99131400	0.09463500	-0.04546600
H	2.70537600	1.23321200	0.38027400
H	-0.69001700	0.64833700	1.49822600

G_{CHCl3}: -652.2679983
G_{DMF}: -652.2736812

DBU

N	0.32885100	0.63826300	-0.05266900
C	0.36775400	-0.73727400	-0.17798900
N	1.45562700	-1.43622800	-0.31507700
C	2.72211000	-0.71485800	-0.38164300
C	2.73187200	0.48202800	0.56812300
C	1.56698900	1.39498400	0.20610600
C	-0.85224300	1.51847500	-0.02130700
C	-2.12885500	1.01316500	-0.69649300
C	-2.92856600	0.00747500	0.14569200
C	-2.03151000	-1.06371300	0.78649600
C	-0.92371500	-1.55081700	-0.16060100
H	2.90397900	-0.36665500	-1.41298000
H	3.53219800	-1.41303200	-0.14018600
H	2.62496200	0.12364200	1.60020700
H	3.67162900	1.04354400	0.50846600
H	1.80973200	1.99615600	-0.68326600
H	1.36706100	2.10088500	1.02405400
H	-1.06967100	1.80331300	1.02197900
H	-0.54044600	2.43965000	-0.53056600
H	-1.87180800	0.58589200	-1.67385200
H	-2.75545800	1.88929400	-0.90611100
H	-3.67892200	-0.47328200	-0.49658600
H	-3.48457800	0.53976300	0.92932700
H	-2.64587000	-1.91959000	1.09223000
H	-1.57524500	-0.67453600	1.70665400
H	-1.31565200	-1.62513900	-1.18512500
H	-0.60627000	-2.56093900	0.10967000

G_{CHCl3}: -461.8056765
G_{DMF}: -461.8003929

DBUH$^+$

N	0.29504800	0.65714900	-0.01334300
C	0.31043100	-0.66356700	-0.15440700
N	1.46740200	-1.31789700	-0.28903300
C	2.79474400	-0.69464700	-0.30164900
C	2.72917000	0.56483800	0.55219000
C	1.56112100	1.42828100	0.09455000
C	-0.90861300	1.53323300	0.04950600
C	-2.16515700	1.03554200	-0.66449800
C	-2.96811400	-0.01439000	0.11680900
C	-2.07574700	-1.09214500	0.75013600
C	-0.92919300	-1.53653100	-0.17322300
H	1.41448500	-2.32462600	-0.37468700
H	3.08128400	-0.46274600	-1.33449900
H	3.50703200	-1.41997300	0.09740500
H	2.60679700	0.29153200	1.60630100
H	3.65671400	1.13655600	0.45966500
H	1.76085400	1.88507600	-0.88205000
H	1.38104200	2.23449500	0.81036200
H	-1.11042400	1.75479200	1.10527000
H	-0.58783200	2.46811400	-0.41838200
H	-1.88723800	0.66131600	-1.65769700
H	-2.79457400	1.91477900	-0.84459800
H	-3.68880600	-0.48305200	-0.56489800
H	-3.55433900	0.47543200	0.90401800

H	-2.67725000	-1.97412700	0.99440000
H	-1.65846600	-0.73887400	1.70127600
H	-1.27682300	-1.61563500	-1.21161500
H	-0.60145100	-2.54150100	0.10987500

G_{CHCl3}: -462.2538717
G_{DMF}: -462.2620057

TS12 between DBH and **1**

C	2.71239700	-2.11204400	-0.27859800
C	3.34736700	-0.71634500	-0.21903100
C	2.70459500	0.21437000	0.82119500
C	0.27697900	0.10807600	0.30288300
N	-0.88880000	0.64158000	0.04776100
C	-1.01193500	2.08301100	-0.14627500
C	0.25926800	2.66333800	-0.76461000
C	1.46079100	2.25929300	0.08494400
N	1.43249800	0.81868400	0.39304000
C	1.20372200	-2.13123700	-0.56454700
C	0.33365200	-1.39529100	0.48010800
H	2.55944900	-0.31836800	1.76955600
H	3.37721800	1.04879900	1.03758000
H	4.41121200	-0.82221500	0.03261000
H	3.30211000	-0.23063600	-1.20367800
H	2.89418700	-2.62136200	0.68010200
H	3.22775800	-2.70684700	-1.04411000
H	2.39386200	2.47054300	-0.44900600
H	1.48232700	2.83059700	1.02410800
H	0.37763500	2.27722200	-1.78463000
H	0.20465400	3.75560700	-0.82712500
H	-1.88277500	2.25902100	-0.78763800
H	-1.22029200	2.56758700	0.81936400
H	0.87097500	-3.17609500	-0.59471500
H	0.99977000	-1.71511600	-1.56084600
H	-0.69616300	-1.75413800	0.41572300
H	0.68928900	-1.63225300	1.49273800
H	-2.03255200	-0.10638000	-0.26728300
S	-3.37210500	-0.85117300	-0.62294800
C	-4.21977700	-0.52738700	0.98244700
H	-4.43224000	0.53883700	1.11226100
H	-5.16890400	-1.07123800	0.99934400
H	-3.61208400	-0.87135800	1.82610600

G_{CHCl3}: -900.4546528
G_{DMF}: -900.4560229

1^{-}/DBUH^{+} ion pair

N	-1.47379100	0.88625100	0.00377500
C	-0.39901400	0.11330400	-0.20499800
N	0.79549900	0.64506200	-0.41929900
C	1.05465500	2.08202500	-0.45939100
C	0.08301200	2.78092600	0.48348900
C	-1.33887400	2.35713000	0.13688900
C	-2.88232400	0.43715700	0.14350400
C	-3.26600300	-0.86879400	-0.55262600
C	-2.85755500	-2.13514800	0.21458000
C	-1.42678500	-2.05232000	0.76894200
C	-0.44149700	-1.40271000	-0.21504900
H	1.63856800	0.00651000	-0.48377500
H	0.93748900	2.45018100	-1.48683000
H	2.09633500	2.23474900	-0.16632800
H	0.31597000	2.51016400	1.51999500
H	0.16725800	3.86822800	0.39412700
H	-1.66890600	2.81729100	-0.80333300
H	-2.03280700	2.67358800	0.92176100
H	-3.12841600	0.39694100	1.21350300
H	-3.47557800	1.24940800	-0.28781600
H	-2.84550600	-0.86967000	-1.56594600
H	-4.35503300	-0.85539300	-0.68057500
H	-2.94544600	-2.99798500	-0.45811000
H	-3.55805100	-2.31008900	1.04112300
H	-1.06353400	-3.05847700	1.00591300
H	-1.41363900	-1.49705700	1.71574900
H	-0.65105400	-1.73236600	-1.24164200
H	0.58196200	-1.73080900	-0.00589600
S	3.43706700	-1.13281900	-0.54155300
C	4.37684500	-0.44943200	0.90287100
H	3.73837600	-0.35892500	1.79026500
H	5.21517500	-1.10589600	1.16254200
H	4.78704500	0.54269900	0.67952200

G_{CHCl3}: -900.4577839
G_{DMF}: -900.4568667

DMPP

C	2.26759600	-1.42175700	0.44766000
H	3.36300700	-1.39099200	0.45629600
H	1.90163300	-1.37346000	1.48008800
H	1.97096700	-2.37850500	0.00715100
C	2.26759700	1.42175800	0.44765800
H	3.36300700	1.39099200	0.45629400
H	1.97096800	2.37850500	0.00714700
H	1.90163300	1.37346300	1.48008500
C	-0.15322300	0.00000000	-0.20856300
C	-0.87353800	-1.20557700	-0.11506600
C	-0.87353700	1.20557700	-0.11506500
C	-2.25788900	-1.20638400	0.08065600
H	-0.35753100	-2.15891600	-0.19309500
C	-2.25788800	1.20638500	0.08065700
H	-0.35753000	2.15891600	-0.19309300
C	-2.95727800	0.00000000	0.18113300
H	-2.78841300	-2.15265700	0.15567900
H	-2.78841200	2.15265800	0.15568100
H	-4.03346500	0.00000000	0.33357300
P	1.65887300	-0.00000100	-0.59601500

G_{CHCl3}: -652.6320165
G_{DMF}: -652.6323182

DMPPH^{+}

C	2.35237500	-0.17894900	1.51385600
H	3.41502100	-0.42497400	1.42888700
H	2.24757900	0.85299600	1.86001400
H	1.87467000	-0.85178500	2.23109300
C	2.34948700	0.72129900	-1.33114000
H	3.41845100	0.49476600	-1.38388900
H	1.88964600	0.55900500	-2.30946500
H	2.21603600	1.76634300	-1.03685500
C	-0.22241300	-0.13391400	-0.04725200
C	-1.06679300	-1.23612400	-0.26214900
C	-0.76723600	1.13499200	0.21967300
C	-2.45170900	-1.06705400	-0.20787900

H	-0.65552700	-2.21942400	-0.47206300
C	-2.15222700	1.29152800	0.27059700
H	-0.12957100	1.99904300	0.38543400
C	-2.99299400	0.19333500	0.05782300
H	-3.10310600	-1.91952500	-0.37512300
H	-2.57435800	2.27088600	0.47472500
H	-4.07071400	0.32217300	0.09764900
P	1.56124600	-0.36734900	-0.11054400
H	1.76224100	-1.68993700	-0.52340800

G_{CHCl3}: -653.0481804
G_{DMF}: -653.0488312

1^{-}/DMPPH^{+} ion pair [approximate energy where the distance between PH•••S is fixed, otherwise the proton transfers back to **1**]

C	0.50745800	2.20923500	1.44389300
H	1.44049300	2.78063900	1.42302900
H	-0.33426200	2.90510900	1.51002800
H	0.50956600	1.55697000	2.32126800
C	0.33996200	2.32044300	-1.50563700
H	1.24819900	2.93114100	-1.52551100
H	0.29090300	1.72711600	-2.42312700
H	-0.53698900	2.97160100	-1.44789000
C	-1.07174600	0.14951600	-0.03053300
C	-0.94698700	-1.18777300	-0.44436500
C	-2.31958200	0.64141000	0.38880500
C	-2.06834300	-2.02171700	-0.44313900
H	0.02097000	-1.57227100	-0.75827500
C	-3.43328100	-0.19982100	0.39073300
H	-2.42883700	1.67253600	0.71439400
C	-3.30842200	-1.52992300	-0.02649500
H	-1.96893100	-3.05515500	-0.76282800
H	-4.39647100	0.18219900	0.71745000
H	-4.17793600	-2.18164600	-0.02367700
P	0.40736700	1.19469800	-0.07044300
H	1.54751400	0.35231200	-0.24194600
S	3.14209800	-0.96894700	-0.54652200
C	2.92799400	-1.61758100	1.17201900
H	2.80906500	-2.70693800	1.17085900
H	3.79324300	-1.37345000	1.79868700
H	2.03709400	-1.19020400	1.65683700

G_{CHCl3}: -1091.246429
G_{DMF}: -1091.24599

TS23 (EtNH$_2$ analogue of **TS13**)

C	-2.79731600	-0.28409200	-0.36182600
C	-2.17931200	0.66109400	-1.21446100
C	-0.53579600	-0.78350700	-0.38312500
N	-1.71932200	-1.13541100	0.16431900
H	-2.72738000	1.41174800	-1.76778100
O	0.52784300	-1.42174200	-0.24655100
O	-3.97534200	-0.51251800	-0.05399000
C	-1.93724700	-2.30381600	0.99399600
H	-1.67481800	-3.22152500	0.45572700
H	-1.33652800	-2.24770700	1.90771000
H	-2.99712500	-2.32609800	1.25351400
C	-0.77302500	0.48274300	-1.19036400
H	-0.14409100	0.61747400	-2.06533800
S	0.31437600	2.01756000	-0.02018500
C	-0.89508500	2.24873900	1.32316900
H	-0.64221200	1.67003900	2.21611100
H	-0.95680400	3.30924900	1.58152600
H	-1.87632600	1.92633500	0.94391900
N	2.73197000	-0.03388700	0.62575100
C	3.95655400	0.10573900	-0.22970800
H	3.60467400	0.38744900	-1.22493300
H	4.53934400	0.93563800	0.17709200
H	2.14641900	0.83610700	0.63304200
H	2.96875300	-0.27699900	1.59132400
H	2.05736700	-0.74393400	0.25556500
C	4.75878300	-1.18774900	-0.26038600
H	4.17176500	-2.01314600	-0.67724500
H	5.64392700	-1.05001700	-0.88933300
H	5.09913400	-1.47131500	0.74213900

G_{CHCl3}: -972.3343988

EtNH$_3^+$ analogue of **14**

C	-2.75183300	-0.33115500	-0.54398500
C	-2.05944500	0.66854900	-1.20640100
C	-0.48495900	-0.69453100	-0.07172300
N	-1.71463700	-1.15115800	0.16863300
H	-2.52191700	1.41815100	-1.83467200
O	0.57456500	-1.22425800	0.34668900
O	-3.94970000	-0.67540800	-0.44446100
C	-2.02321800	-2.32962900	0.95273300
H	-1.55008400	-3.21946400	0.52280300
H	-1.67687400	-2.21310200	1.98561400
H	-3.10832600	-2.44891800	0.93927800
C	-0.61174800	0.56455200	-0.94536000
H	0.04578700	0.47702100	-1.81975600
S	0.19906700	2.07421500	-0.07593100
C	-0.86530000	2.24444700	1.39896100
H	-0.59128300	1.53501400	2.18505100
H	-0.75407600	3.26497800	1.77387200
H	-1.90450100	2.08187500	1.09449400
N	2.87980300	0.16485900	0.58869400
C	3.92473400	-0.03722400	-0.47086400
H	3.43003100	0.14649500	-1.42741700
H	4.68920700	0.72962400	-0.32470100
H	2.04018600	-0.47612600	0.46562700
C	4.51141000	-1.44066700	-0.40421500
H	3.73958900	-2.20444700	-0.54598200
H	5.25428400	-1.55776100	-1.19950600
H	5.01396600	-1.62223400	0.55282400
H	2.45454700	1.10560000	0.54414400
H	3.26146900	0.03122300	1.52922600

G_{CHCl3}: -972.3410868

EtNH$_3^+$ analogue of **TS15**

C	-0.73744400	1.24913300	-0.91515900
C	-0.11998100	0.09493800	-1.45544000
C	1.31821400	1.11028800	0.16712500
N	0.12648600	1.77853000	0.11135400
H	-0.30876900	-0.17353700	-2.49251400
O	2.24565700	1.37797900	0.93244000
O	-1.85982200	1.75521700	-1.13183500
C	-0.21580400	2.89399900	0.97410500
H	-0.24347100	2.58049200	2.02354400
H	0.52006200	3.69772300	0.86992600

H	-1.19998800	3.25509700	0.67084400
C	1.26700700	-0.01171900	-0.88078700
H	2.07742300	0.13875900	-1.60633700
S	1.54258300	-1.68411800	-0.11578700
C	3.33620100	-1.67344700	0.26049100
H	3.58026700	-2.66393400	0.65584700
H	3.92087600	-1.50098700	-0.64884600
H	3.57357400	-0.91144900	1.00454600
N	-2.53617200	-1.24563900	-0.71951100
H	-1.50224800	-0.86838100	-0.88813900
H	-3.12827300	-0.41113100	-0.78862000
C	-2.70457200	-1.95374100	0.59137300
H	-3.69724700	-2.41188600	0.59811700
H	-1.95490400	-2.74900000	0.61158000
C	-2.52843500	-0.99280000	1.75964500
H	-2.65268900	-1.54221000	2.69827600
H	-1.53132300	-0.54170100	1.76112900
H	-3.27659600	-0.19250400	1.73480200
H	-2.76801500	-1.85517100	-1.50741800

G_{CHCl3}: -972.3227391

$EtNH_3^+$ analogue of **TS17**

C	1.94411000	-1.16343100	0.41635200
C	1.55810100	-0.42809000	-0.73850500
C	-0.27877300	-0.56816600	0.77497200
N	0.80483400	-1.12424300	1.34209400
H	2.03848200	1.03340500	-0.50762400
O	-1.37281100	-0.39461600	1.35159400
O	2.99582300	-1.71608400	0.75707600
C	0.86192800	-1.59725700	2.71430300
H	0.70143400	-0.76916600	3.41215600
H	0.09846900	-2.36168000	2.88844700
H	1.85423200	-2.02332600	2.86955800
C	0.07519800	-0.19185300	-0.66957600
H	-0.22100900	0.85273600	-0.84320500
S	-0.99139000	-1.09225700	-1.91417300
C	-0.61021200	-2.84299200	-1.55089400
H	-1.00514200	-3.15062800	-0.57868200
H	-1.08629500	-3.43591000	-2.33634500
H	0.46995100	-3.00641900	-1.58573900
N	-3.60599100	0.19339700	-0.08926100
C	-3.93545800	1.65358700	-0.24010900
H	-3.04027200	2.12914400	-0.64753000
H	-4.73612500	1.72953400	-0.97952600
H	-2.77115800	0.03063500	0.54438500
C	-4.33725700	2.26079400	1.09652500
H	-3.52968600	2.18109100	1.83166200
H	-4.56206600	3.32242500	0.95478900
H	-5.23370100	1.77926200	1.50396300
H	-3.32490200	-0.23605300	-0.98244200
H	-4.40224900	-0.33580500	0.27744400
H	2.04461200	-0.63875700	-1.68643900
S	2.40002600	2.54578400	-0.38805200
C	4.22200200	2.27145700	-0.41477000
H	4.51554700	1.68739300	-1.29260500
H	4.72143100	3.24332400	-0.46218300
H	4.55643200	1.74957400	0.48653600

G_{CHCl3}: -1410.987221

$EtNH_2$ analogue of **TS19**

C	-0.73971400	0.99092500	-0.41092200
C	0.28136500	-0.01784600	-0.95388500
C	-1.50715300	-1.16689100	-0.04811900
N	-1.73852000	0.26746100	0.15045400
O	-2.34067500	-1.99070800	0.34091300
O	-0.62715200	2.21777000	-0.43522400
C	-2.90032000	0.82702000	0.81374100
H	-3.50722500	-0.00765300	1.16903100
H	-2.59949000	1.45134100	1.66177200
H	-3.48928900	1.43589300	0.11951000
C	-0.27793700	-1.29857700	-0.74846800
H	0.08813200	-2.24076600	-1.13263800
H	0.79826600	0.26759700	-1.86877300
N	1.68133400	0.39314900	0.15165400
H	1.83688500	1.40370300	0.09785100
C	2.90440000	-0.37684000	-0.17884400
H	2.60983700	-1.43067200	-0.20082200
H	3.19929500	-0.08651900	-1.19212200
C	4.04373600	-0.14567900	0.81165900
H	4.91553600	-0.73823500	0.51257900
H	4.34430900	0.90784200	0.83921200
H	3.75959500	-0.45257000	1.82486100
H	1.36078800	0.17659200	1.09829000

G_{CHCl3}: -533.6810372

$EtNH_2$ analogue of **20**

C	-0.82272000	-1.15750200	0.56833800
C	-0.52584900	-1.54717500	-0.89612600
C	-1.48912400	0.58337200	-0.84048100
N	-1.32564100	0.08486400	0.55523100
O	-1.91565100	1.73724500	-1.01652600
O	-0.66998600	-1.92177700	1.53046800
C	-1.78347400	0.80434600	1.72759500
H	-2.06023100	1.80931700	1.40368100
H	-2.65379200	0.31215300	2.17799000
H	-0.98626700	0.86215700	2.47482900
C	-1.07009900	-0.44066400	-1.69602700
H	-0.85014600	-0.27044400	-2.74217200
H	0.53640500	-1.79834500	-1.01965200
N	-1.23289600	-2.92083100	-1.08495500
H	-1.03411900	-3.49335300	-0.25214600
C	-0.85100800	-3.65160400	-2.34028400
H	-1.06215700	-2.96786700	-3.16567800
H	0.22867800	-3.81244500	-2.28603100
C	-1.61177000	-4.96333500	-2.48390400
H	-1.29912800	-5.45591700	-3.41020500
H	-1.40319400	-5.64677800	-1.65332000
H	-2.69327100	-4.79815600	-2.54146000
H	-2.24317200	-2.73721800	-1.09168000

G_{CHCl3}: -533.6846662

$EtNH_2$ analogue of **TS21**

C	0.67528500	1.39223600	-0.78876600
C	0.75358800	-0.09103400	-0.37258900
C	-0.76453100	1.07903300	1.01022300
N	-0.25105700	1.98888900	-0.00543800
O	-1.51894500	1.48506100	1.89238900
O	1.38657700	1.90569900	-1.65142700
C	-0.61737300	3.39276000	-0.09926500

H	-1.37860500	3.58343900	0.65837700
H	0.25319300	4.03088700	0.08294800
H	-1.01832100	3.61216400	-1.09305800
C	-0.28533300	-0.23963300	0.69217200
H	-1.33572300	-0.93567000	-0.09743700
H	0.61230300	-0.72839500	-1.25553000
N	2.20326000	-0.34823500	0.04388600
H	2.81180300	0.07983100	-0.66840400
C	2.56576200	-1.80439800	0.21456200
H	1.88751300	-2.20511400	0.96999300
H	2.34805800	-2.28659100	-0.74078400
C	4.02528200	-1.96574500	0.61464800
H	4.24602300	-3.03308500	0.71357500
H	4.70107200	-1.55235100	-0.14198700
H	4.23843800	-1.48973400	1.57809800
H	2.38840000	0.15091900	0.92188600
H	-0.17874300	-0.96159400	1.49759700
S	-2.32264500	-1.82280100	-0.99796400
C	-3.59271300	-2.01598500	0.32446500
H	-4.07580400	-1.06089700	0.55108200
H	-4.35632700	-2.71916500	-0.02056200
H	-3.14723700	-2.41390100	1.24210600

G_{CHCl3}: -972.3231753

TS24 (Et_2NH analogue of **TS13**)

C	3.08868200	-0.12080000	-0.30372000
C	2.47270500	-1.38809000	-0.44832500
C	0.88363000	0.27143100	-0.89010900
N	2.04166500	0.87982300	-0.54445600
H	3.00530300	-2.32411400	-0.34706700
O	-0.13137600	0.86157200	-1.30878300
O	4.25200400	0.23795400	-0.07374800
C	2.28605200	2.30679100	-0.61609400
H	2.14732100	2.67837400	-1.63778400
H	1.60965500	2.85026900	0.05133900
H	3.31894400	2.47543600	-0.30630400
C	1.08906600	-1.22195000	-0.69900000
H	0.52087900	-1.87449400	-1.35401800
S	-0.21152400	-1.66498000	1.05629000
C	0.88368800	-1.03327600	2.36682500
H	0.62194400	-0.01595200	2.67288000
H	0.84088700	-1.69692400	3.23473400
H	1.91177700	-1.04140700	1.97419400
N	-2.56875500	0.33382000	-0.06717800
C	-3.63689400	-0.36780000	-0.85601300
H	-4.39299400	-0.70100600	-0.13979500
H	-4.09003900	0.38322300	-1.50901000
H	-2.07453600	-0.34406200	0.55579100
H	-1.78841800	0.63132600	-0.69485200
C	-3.07900500	-1.53637500	-1.65963600
H	-2.63678900	-2.29832000	-1.00975500
H	-3.89617700	-2.00278600	-2.21927800
H	-2.32174000	-1.20510700	-2.37726200
C	-3.07143200	1.49941900	0.73426100
H	-3.85399600	1.11569100	1.39481000
H	-3.53042400	2.19499100	0.02640800
C	-1.95556200	2.17004100	1.52648100
H	-2.37575500	3.01083200	2.08774600
H	-1.49983400	1.47902500	2.24322000
H	-1.17259200	2.55663100	0.86704000

G_{CHCl3}: -1050.890674

$Et_2NH_2^+$ analogue of **14**

C	3.16081100	-0.02073200	-0.39325900
C	2.49413500	-1.21766400	-0.59039400
C	0.88385500	0.52299700	-0.51847500
N	2.10019000	1.04061900	-0.33831200
H	2.98155400	-2.17750200	-0.69875700
O	-0.18119200	1.18616800	-0.57411600
O	4.35641000	0.33213400	-0.28455900
C	2.38761400	2.45133300	-0.17995200
H	2.06667700	3.01762500	-1.06160100
H	1.87878300	2.85727800	0.70130900
H	3.46846700	2.54556200	-0.05817200
C	1.03475200	-1.00166200	-0.64902400
H	0.52353700	-1.34705000	-1.55643000
S	-0.01799400	-1.89401300	0.68025900
C	0.84208700	-1.38676600	2.20940800
H	0.55416800	-0.38008700	2.52615600
H	0.57923100	-2.10315300	2.99203000
H	1.92155800	-1.42593600	2.03012200
N	-2.68301500	0.21593200	-0.10162600
C	-3.48918500	0.03219300	-1.35586500
H	-4.46886700	-0.34999100	-1.05579400
H	-3.62483700	1.02866600	-1.78443000
H	-1.71882700	0.58922900	-0.33868400
C	-2.80269000	-0.90573700	-2.34091800
H	-2.66892300	-1.90794700	-1.91933900
H	-3.42633200	-0.99865400	-3.23575500
H	-1.82579100	-0.51939500	-2.64768500
C	-3.33678600	1.11051900	0.91336900
H	-3.44731800	2.08850800	0.43778900
H	-4.33434000	0.70491400	1.10439400
C	-2.51728100	1.20398200	2.19421000
H	-1.51722800	1.60253200	1.99878400
H	-3.02419900	1.87793000	2.89226200
H	-2.41874500	0.22697700	2.67977500
H	-2.47651800	-0.69835900	0.32426500

G_{CHCl3}: -1050.897401

$Et_2NH_2^+$ analogue of **TS15**

C	-0.04224900	1.36422600	-0.87872500
C	0.02247600	0.00320800	-1.24084800
C	2.09671400	0.67692600	-0.25808600
N	1.20090500	1.70662800	-0.21841300
H	-0.54480100	-0.36650500	-2.08993100
O	3.24263800	0.71287200	0.19523700
O	-0.96634300	2.20429500	-0.96834600
C	1.48146800	2.99937800	0.37659200
H	1.73171500	2.89216500	1.43761600
H	2.32192900	3.48450100	-0.13143500
H	0.58586100	3.61338400	0.26714800
C	1.40667400	-0.50614900	-0.95452200
H	1.98800300	-0.78984500	-1.84195900
S	1.35226700	-2.01179700	0.13980200
C	3.08504000	-2.60927300	0.10493900
H	3.10623000	-3.54674800	0.66864600
H	3.40360900	-2.80747000	-0.92361500
H	3.75838600	-1.88640500	0.56850800
N	-2.42114100	-0.20032200	0.40928100
C	-3.40442600	-1.12340700	-0.24958500
H	-2.93040600	-2.10852300	-0.28008900
H	-4.27970600	-1.18363500	0.40345900

H	-1.47276100	-0.24506500	-0.11673500
H	-2.72199200	0.77364100	0.29242900
C	-3.79462100	-0.64413000	-1.64233800
H	-2.93028700	-0.58193500	-2.30921200
H	-4.50757200	-1.35360500	-2.07470700
H	-4.27710300	0.33915700	-1.60698200
C	-2.18889100	-0.49576400	1.86296500
H	-3.17016100	-0.59883800	2.33477200
H	-1.68103500	-1.46346900	1.90223500
C	-1.36439200	0.59316100	2.53725600
H	-1.21711700	0.32700200	3.58890300
H	-0.37921000	0.69840000	2.07437900
H	-1.87531900	1.56201600	2.50264800

G_{CHCl3}: -1050.874861

$Et_2NH_2^+$ analogue of **TS17**

C	-2.11928600	-1.48377700	-0.13165200
C	-1.92579800	-0.42518000	0.79723100
C	-0.06356700	-0.53936200	-0.68863100
N	-0.99390300	-1.43168300	-1.07288800
H	-2.71385300	0.79901900	0.23210300
O	0.98626700	-0.29005000	-1.31540700
O	-3.02132000	-2.31401000	-0.29458700
C	-0.91582900	-2.23145600	-2.28264600
H	-0.93034500	-1.58941300	-3.16942900
H	0.00250600	-2.82663400	-2.29054500
H	-1.78435700	-2.89187200	-2.29202400
C	-0.52679400	0.09746200	0.62771100
H	-0.46604100	1.19070900	0.53094200
S	0.68186000	-0.22069300	2.01822200
C	0.62126600	-2.04141100	2.16672700
H	1.08449200	-2.53476600	1.30763200
H	1.17778800	-2.30041400	3.07148000
H	-0.41348100	-2.37595500	2.27655600
N	3.24541900	0.83861100	-0.20927300
C	3.45519000	2.28309300	-0.57368500
H	4.39030700	2.59761600	-0.10233500
H	3.58938100	2.31061600	-1.65799800
H	2.36023600	0.47417400	-0.65354300
C	2.28683200	3.15602400	-0.13388200
H	2.14688000	3.12881800	0.95234300
H	2.49289500	4.19258200	-0.41875800
H	1.35283000	2.85423600	-0.61763900
C	4.39488700	-0.05674700	-0.58478000
H	4.49653600	0.01303000	-1.67072800
H	5.29254800	0.36630600	-0.12580500
C	4.16177200	-1.49407700	-0.13739800
H	3.26132300	-1.91423300	-0.59556300
H	5.01766900	-2.10348900	-0.44468100
H	4.07059800	-1.56747600	0.95175800
H	3.05994300	0.75599500	0.79909400
H	-2.37956400	-0.49575700	1.78155400
S	-3.41151900	2.11222900	-0.22434700
C	-5.11811900	1.48885100	0.08272600
H	-5.82086200	2.31892300	-0.03309900
H	-5.38516800	0.70170900	-0.62839000
H	-5.21123000	1.09516200	1.09983500

G_{CHCl3}: -1489.542670

Et_2NH analogue of **TS19**

C	-0.86401800	0.50353600	-0.98138800
C	0.04446400	-0.72969300	-0.85904600
C	-1.91603900	-1.10273600	0.32360000
N	-1.97431000	0.25165100	-0.25564400
O	-2.87940300	-1.53768000	0.96621600
O	-0.58049700	1.53949100	-1.59067300
C	-3.08886600	1.16388500	-0.09173700
H	-3.83882000	0.65563800	0.51701000
H	-2.77122100	2.08499100	0.40931700
H	-3.52179000	1.42380900	-1.06342400
C	-0.67652300	-1.66412900	-0.05913300
H	-0.42537700	-2.70397000	0.10197100
H	0.51069800	-1.02760200	-1.79884100
N	1.50163200	-0.02037500	-0.13706300
H	1.58347400	0.86626200	-0.64569800
C	1.33218600	0.24015100	1.32638600
H	0.50932500	-0.41114400	1.64915400
H	2.23465400	-0.09515000	1.84233200
C	1.04983900	1.70544300	1.64669400
H	0.89350800	1.81055900	2.72553700
H	1.89079100	2.34969300	1.36418500
H	0.15037800	2.07020100	1.14199000
C	2.67913100	-0.87785900	-0.46934700
H	2.59016900	-1.78545800	0.13523600
H	2.57930100	-1.16539000	-1.52002600
C	4.02093700	-0.18181300	-0.25159400
H	4.82688200	-0.86475800	-0.54158000
H	4.10456500	0.71772000	-0.87224100
H	4.18474500	0.10046400	0.79306900

G_{CHCl3}: -612.2327219

Et_2NH analogue of **20**

C	0.51045600	-0.81207800	-0.59470200
C	-0.88492600	-0.60942500	-1.22158300
C	-1.03375000	-0.34239200	1.09484400
N	0.38581100	-0.62077300	0.72634400
O	-1.30398700	-0.09665400	2.28361800
O	1.51612800	-1.14575500	-1.23632900
C	1.46126800	-0.74746300	1.68949400
H	1.05271600	-0.48151200	2.66616700
H	1.84520800	-1.77388100	1.71872500
H	2.28435800	-0.07132400	1.43733200
C	-1.78156300	-0.40204200	-0.08330200
H	-2.80142300	-0.04601100	-0.15003500
H	-0.84452500	0.17803000	-1.98529500
N	-1.11215600	-1.90527300	-2.11618000
H	-0.22740700	-1.99081200	-2.63474900
C	-1.28949200	-3.16939700	-1.29539300
H	-1.15099400	-2.88363900	-0.25092400
H	-2.32991700	-3.48200400	-1.39877400
C	-0.32320700	-4.27250800	-1.71322700
H	-0.49359200	-5.14883400	-1.07888800
H	-0.46744000	-4.57912400	-2.75456000
H	0.71758700	-3.95885100	-1.58013300
C	-2.22152700	-1.66433800	-3.10651100
H	-3.13503000	-1.54722100	-2.51743200
H	-1.99905100	-0.70702000	-3.58567900
C	-2.36097100	-2.76008200	-4.15641300
H	-3.15231500	-2.46721400	-4.85440000
H	-1.43829300	-2.88670800	-4.73356500

H	-2.64285700	-3.72507700	-3.72535000

G_{CHCl3}: -612.2360789

Et_2NH analogue of **TS21**

C	0.40331500	1.23506300	-0.97395700
C	0.27432200	-0.21956300	-0.48153500
C	-0.99593100	1.23379900	0.88471600
N	-0.39573100	2.00309100	-0.19860900
O	-1.65349500	1.79351300	1.76131100
O	1.13815500	1.59383000	-1.89384700
C	-0.56910000	3.43571200	-0.37347600
H	-1.24136000	3.78254200	0.41240300
H	0.39273200	3.95157400	-0.29234900
H	-1.00472400	3.64703500	-1.35464000
C	-0.71746500	-0.15349500	0.63523600
H	-1.90284800	-0.74030800	-0.06129700
H	-0.03715600	-0.84741900	-1.32783900
N	1.69427300	-0.73066700	-0.16420000
H	2.23361000	-0.51325700	-1.01301700
C	2.36868400	-0.00275100	0.99658900
H	1.67956900	0.77420000	1.32867600
H	2.46407100	-0.72101000	1.81249500
C	3.71583500	0.58888100	0.59889500
H	4.13509700	1.11398300	1.46324400
H	4.43296300	-0.17960900	0.29359300
H	3.60741500	1.31435900	-0.21430700
C	1.69410900	-2.23879500	-0.00591000
H	1.15086000	-2.45031600	0.91765900
H	1.11170200	-2.63134000	-0.84241500
C	3.09252900	-2.84053800	0.00419000
H	2.99312100	-3.92874400	0.07011500
H	3.63754600	-2.61229400	-0.91872700
H	3.68923000	-2.51174900	0.85998000
H	-0.67929700	-0.83488500	1.48020500
S	-3.05188400	-1.54123000	-0.82731800
C	-4.18674100	-1.57144500	0.62537600
H	-5.00211300	-2.27198100	0.42327100
H	-3.66018300	-1.90573800	1.52548200
H	-4.61450500	-0.58229700	0.81376900

G_{CHCl3}: -1050.875621

TS25 (DBU analogue of **TS13**)

C	-4.24084800	-1.08364800	-0.31371500
C	-3.38067100	-0.86313100	-1.43318700
C	-2.15493300	-0.56506000	0.52357800
N	-3.44305500	-0.83435400	0.87447700
H	-3.69905600	-0.98773600	-2.45947300
O	-1.20348100	-0.50783300	1.32364800
O	-5.41964800	-1.44959000	-0.22461200
C	-3.90674400	-1.05260000	2.23001400
H	-3.44197500	-1.94253600	2.67094400
H	-3.67437300	-0.18613100	2.85655300
H	-4.98795800	-1.19569000	2.18728900
C	-2.13030700	-0.42397700	-0.97473700
H	-1.19326400	-0.57976900	-1.49379800
S	-1.85252400	1.89847500	-1.00595900
C	-3.59827400	2.33826600	-1.27120700
H	-4.02974200	2.83639400	-0.39759500
H	-3.71076500	2.98401600	-2.14777200
H	-4.15756300	1.40537800	-1.45733400
H	0.36601900	0.26259200	1.03444800
C	2.32705600	-0.08121100	0.65123600
N	1.29703400	0.70261200	0.93003700
C	1.38527700	2.16180100	1.03492400
H	1.55725700	2.43801800	2.08297000
H	0.41879600	2.56789200	0.72628200
C	2.51904100	2.65452100	0.14232300
H	2.69945100	3.72033600	0.31041300
H	2.23982800	2.52570900	-0.90963100
C	3.79522200	1.87317000	0.44090300
H	4.21351600	2.15470600	1.41581700
H	4.55393700	2.07667900	-0.31976300
N	3.54855000	0.41406400	0.43833700
C	4.72253900	-0.45986800	0.22501400
H	5.59404000	0.19476500	0.29121200
H	4.79998400	-1.16962900	1.05701600
C	4.71753200	-1.19959400	-1.12048600
H	4.43660800	-0.49418200	-1.91418100
H	5.74846700	-1.51322000	-1.32861000
C	3.81082500	-2.43757000	-1.14898300
H	3.88317300	-2.90914100	-2.13692700
H	4.19689800	-3.17266500	-0.42742800
C	2.33192700	-2.17157300	-0.83532100
H	1.78768400	-3.12178700	-0.88322400
H	1.88809600	-1.52193800	-1.60146800
C	2.06980200	-1.56549900	0.56361200
H	1.02833000	-1.73150800	0.84849200
H	2.68566500	-2.07718700	1.31505300

G_{CHCl3}: -1299.079309

$DBUH^+$ analogue of **14**

C	-4.29941700	-1.06174600	-0.41098500
C	-3.61346100	-0.48674000	-1.46680800
C	-2.19475400	-0.46691000	0.43434000
N	-3.37349100	-1.00672500	0.76584800
H	-4.01512500	-0.37015200	-2.46494900
O	-1.20571700	-0.36510800	1.19528600
O	-5.42488300	-1.59133100	-0.25684900
C	-3.69543900	-1.55964200	2.06453200
H	-3.01605000	-2.38067700	2.32198500
H	-3.62706700	-0.79289600	2.84441700
H	-4.71847300	-1.93699500	2.00756400
C	-2.28284300	-0.01247700	-1.03031900
H	-1.41621400	-0.39234000	-1.58658200
S	-1.95634500	1.86505400	-1.15036600
C	-3.42523700	2.53426800	-0.29551600
H	-3.30868500	2.51172500	0.79212600
H	-3.55767300	3.56886500	-0.62330500
H	-4.30182100	1.94680500	-0.58811500
H	0.34334800	0.38295300	0.88242300
C	2.30627600	-0.05866500	0.59721500
N	1.30087800	0.77718400	0.80355800
C	1.45371200	2.23144900	0.88300100
H	1.58157000	2.52539100	1.93263700
H	0.52533200	2.67326200	0.51314100
C	2.65502800	2.65284800	0.04361100
H	2.87640000	3.71263700	0.20064600
H	2.42707500	2.51389400	-1.01954200
C	3.87558200	1.81996700	0.42479100
H	4.25631200	2.10392700	1.41439400
H	4.68119800	1.97184000	-0.29897200

N	3.55988700	0.37484800	0.43768300
C	4.70092400	-0.55738300	0.30758000
H	5.59752700	0.05777200	0.40764400
H	4.69919900	-1.24980900	1.15759300
C	4.73408000	-1.32813000	-1.02000900
H	4.53256200	-0.62909500	-1.84295300
H	5.75834300	-1.69549000	-1.16294300
C	3.77015900	-2.52125800	-1.07445300
H	3.87254600	-3.01742900	-2.04760200
H	4.07953800	-3.25814500	-0.31860400
C	2.29179300	-2.17667200	-0.84725600
H	1.70351200	-3.09938400	-0.90916600
H	1.92344600	-1.52105100	-1.64759400
C	1.98595300	-1.53120900	0.52512300
H	0.92499500	-1.64384000	0.75939600
H	2.53947200	-2.05446600	1.31600400

G_{CHCl3}: -1299.087305

DBUH$^+$ analogue of **TS15**

C	2.25649600	1.66510400	-0.17230300
C	2.64046200	0.86153600	0.89331700
C	3.05967700	-0.31734000	-1.13410900
N	2.49600100	0.88442800	-1.40262100
H	2.70641900	1.21177500	1.91556100
O	3.40180200	-1.16436300	-1.96872300
O	1.77501800	2.82296800	-0.26819500
C	2.25177000	1.38425400	-2.73886000
H	3.18882900	1.48132900	-3.30006800
H	1.58739300	0.71145700	-3.29302100
H	1.78558200	2.36669800	-2.63942600
C	3.17898900	-0.42947800	0.39685100
H	4.21664000	-0.66042700	0.66892100
S	2.21444000	-1.98719100	0.89620300
C	2.42647700	-1.87301500	2.70814100
H	2.01067100	-0.93829300	3.09600300
H	1.88960700	-2.71576400	3.15280500
H	3.48439600	-1.94510100	2.98018500
H	0.21347100	0.01686200	0.88741400
C	-1.63709400	0.07390400	0.06757300
N	-0.68466200	0.50676100	0.88241800
C	-0.74869100	1.76047400	1.64151100
H	-0.24153200	2.54291900	1.06566700
H	-0.18803400	1.61130200	2.56735800
C	-2.21002400	2.08857300	1.92171500
H	-2.29428500	3.09287700	2.34715700
H	-2.61920100	1.38142600	2.65315100
C	-3.02087700	2.01855600	0.63085700
H	-2.77242900	2.85234900	-0.03786300
H	-4.09075200	2.06981400	0.84975100
N	-2.77722800	0.74927900	-0.08981800
C	-3.81014800	0.32618400	-1.06160400
H	-4.51189200	1.15998700	-1.12534700
H	-3.35269500	0.22550200	-2.05281300
C	-4.55367900	-0.95868100	-0.67164500
H	-4.83005200	-0.90272200	0.39003100
H	-5.49213200	-0.98044100	-1.24015100
C	-3.77172900	-2.24655200	-0.96131900
H	-4.38118900	-3.10860900	-0.66245700
H	-3.62656600	-2.33433600	-2.04813000
C	-2.40307300	-2.34644600	-0.27332000
H	-1.93979500	-3.29997500	-0.55155100
H	-2.52278700	-2.36730300	0.81825200
C	-1.40465400	-1.22821600	-0.65580600
H	-0.38799900	-1.55465500	-0.42330000
H	-1.43946900	-1.04686700	-1.73788300

G_{CHCl3}: -1299.084252

DBUH$^+$ analogue of **TS17**

C	3.89261800	-0.29356400	0.43021700
C	3.21891400	-0.08043300	-0.80097100
C	1.64793000	-0.74945500	0.85921600
N	2.86543500	-0.61751800	1.42392400
H	3.76184600	-0.19894800	-1.73402000
O	0.59425000	-0.97418600	1.48256400
O	5.07881100	-0.19973800	0.77707700
C	3.12269100	-0.71572000	2.84882200
H	2.61640900	0.09055200	3.39086300
H	2.77073500	-1.67685800	3.23608300
H	4.20128100	-0.63118400	2.99107500
C	1.80640300	-0.57082400	-0.65535200
H	1.03988200	0.13192800	-1.01188100
S	1.33863300	-2.13025500	-1.57547000
C	2.61300400	-3.30616900	-0.99766600
H	2.47251900	-3.56972400	0.05460400
H	2.50538100	-4.20712200	-1.60810000
H	3.61291900	-2.89066700	-1.14738800
H	-1.04796200	-1.13199600	0.81712700
C	-2.83433000	-0.18747700	0.62229500
N	-2.02924100	-1.23333200	0.50558700
C	-2.42974300	-2.51077500	-0.08967100
H	-2.77198200	-3.18869000	0.70245300
H	-1.54027800	-2.94551400	-0.55210900
C	-3.53224200	-2.25828100	-1.11259300
H	-3.94908900	-3.20663900	-1.46425800
H	-3.11496500	-1.73501000	-1.98060900
C	-4.64268000	-1.42025300	-0.48578500
H	-5.21980800	-2.00637100	0.24103900
H	-5.33491900	-1.06888600	-1.25580700
N	-4.09881400	-0.22583700	0.19682900
C	-5.03407700	0.90003100	0.41532300
H	-6.02425300	0.51219200	0.16712800
H	-5.05335400	1.14844900	1.48278100
C	-4.72662700	2.14418700	-0.42948200
H	-4.51855000	1.83033200	-1.46140200
H	-5.63898400	2.75319500	-0.46375700
C	-3.57858700	3.00433200	0.11657200
H	-3.43829900	3.86998600	-0.54233100
H	-3.87515300	3.40737500	1.09634700
C	-2.23535300	2.27793900	0.26944400
H	-1.49522700	2.98532700	0.65947700
H	-1.86158700	1.95284000	-0.71033200
C	-2.26412800	1.06813300	1.23373700
H	-1.24962800	0.83749900	1.56675100
H	-2.84030600	1.31908200	2.13421300
H	2.91032200	1.48821800	-0.87129900
S	2.49937000	2.95837900	-1.03649600
C	4.21590100	3.61798700	-0.92301500
H	4.19164800	4.69021500	-1.13721200
H	4.63039100	3.46919000	0.07812900
H	4.86864500	3.13149400	-1.65416800

G_{CHCl3}: -1737.734984

DBU analogue of **TS19**

C	-1.95428800	-1.17625500	0.16704400
C	-1.42985600	-0.07796100	1.09846800
C	-3.51435100	0.53022300	0.28914600
N	-3.10986900	-0.70216900	-0.37881800
O	-4.60320700	1.05807400	0.02969500
O	-1.44018000	-2.27175700	-0.05340100
C	-3.95472400	-1.45177800	-1.28739100
H	-4.35495000	-2.35259800	-0.80645500
H	-4.78234400	-0.80358600	-1.58094700
H	-3.38778300	-1.75088800	-2.17429200
C	-2.48207600	0.86224500	1.20671500
H	-2.53423800	1.70684600	1.88095000
H	-0.87431400	-0.40506800	1.96941100
C	-0.28742500	1.73843700	-0.64962900
C	0.67998800	2.86049300	-0.28606500
H	-0.21155100	1.49435100	-1.71832000
H	0.52751200	3.14763600	0.76137000
N	-0.00349300	0.54303200	0.13145400
N	2.29429900	1.00990000	0.05337500
C	1.24812800	0.21615800	0.39159100
C	2.10413800	2.36627000	-0.49772200
H	-1.32470700	2.02185200	-0.43878100
H	0.50300700	3.74690800	-0.90423800
H	2.35788000	2.35179800	-1.56646000
H	2.81883100	3.02905500	0.00160800
C	3.70036000	0.57036300	0.17342500
H	3.92985800	0.34446700	1.22302800
H	4.30216100	1.44134400	-0.09440200
C	1.55142300	-1.11838000	1.03802400
H	0.61966900	-1.53938500	1.40656600
H	2.21537400	-0.97577500	1.89990300
C	4.09084600	-0.61049600	-0.72756500
H	5.18261500	-0.59093400	-0.84167500
H	3.66687600	-0.45050300	-1.72856900
C	2.17050300	-2.14577900	0.05655600
C	3.67614000	-1.98006400	-0.17706100
H	1.98563800	-3.14378700	0.47086100
H	1.62467400	-2.10382300	-0.89438500
H	4.01936600	-2.76412300	-0.86428800
H	4.20411600	-2.15053000	0.77347500

G_{CHCl3}: -860.4139366

DBU analogue of **20**

C	-0.59869300	-1.19053100	0.08234800
C	-0.34620000	-0.85931400	-1.41570000
C	-1.81744100	0.73563200	-0.49233100
N	-1.41896800	-0.24067200	0.56338800
O	-2.55275900	1.69531500	-0.17052700
O	-0.11988700	-2.15515700	0.69187200
C	-1.88343100	-0.17614400	1.93356200
H	-1.03713400	-0.14587900	2.62844300
H	-2.47377700	0.73695000	2.03173900
H	-2.50636000	-1.04420600	2.18067600
C	-1.21655800	0.31845000	-1.67107200
H	-1.21050100	0.89831400	-2.58571300
H	0.72597000	-0.67639600	-1.50634600
C	-1.99575300	-2.64226900	-2.00982900
C	-2.46544000	-3.41587100	-3.22851100
H	-1.96722300	-3.28307400	-1.12075000
H	-2.62332100	-2.73181700	-4.07073600
N	-0.64611000	-2.08924700	-2.23287700
N	-0.08509400	-3.83160500	-3.68693500
C	0.21607000	-2.68172100	-3.05608800
C	-1.41842500	-4.45688600	-3.58832800
H	-2.64330200	-1.78503900	-1.80681400
H	-3.41899400	-3.90784500	-3.01411500
H	-1.38593900	-5.26119900	-2.84153600
H	-1.63822300	-4.90925400	-4.55954000
C	0.94442100	-4.62370800	-4.40079500
H	1.31631000	-4.06101600	-5.26590200
H	0.41343400	-5.48983600	-4.79910600
C	1.57532400	-2.07778700	-3.33665200
H	1.55632900	-1.01539700	-3.10303100
H	1.74947000	-2.13621300	-4.41677000
C	2.10604800	-5.10597500	-3.51565800
H	2.55403500	-5.97480500	-4.01461800
H	1.69734700	-5.46863500	-2.56279300
C	2.73556700	-2.77556500	-2.58580900
C	3.20713500	-4.06443900	-3.27209200
H	3.57428400	-2.07171100	-2.53677000
H	2.43563400	-2.97729200	-1.55002000
H	4.00374400	-4.51990400	-2.67095200
H	3.66053000	-3.80264600	-4.23957300

G_{CHCl3}: -860.4220172

DBU analogue of **TS21**

C	-2.18699600	-0.66871200	-0.94033600
C	-1.38502100	-0.19968400	0.30225900
C	-3.59795300	0.66254100	0.36375900
N	-3.44721600	-0.18594200	-0.81405700
O	-4.65537300	1.27481200	0.55842000
O	-1.75167500	-1.37047300	-1.85284900
C	-4.51647400	-0.45748800	-1.75756800
H	-4.70316800	-1.53411700	-1.82354100
H	-5.40985900	0.05213200	-1.39348600
H	-4.25861500	-0.08254800	-2.75358800
C	-2.40231100	0.54339400	1.12813600
H	-2.64693200	-0.55702500	2.23765000
H	-1.02390800	-1.12013600	0.76929600
C	-0.43888200	1.59333100	-1.16154700
C	0.61507300	2.68563600	-1.12305300
H	-0.45461100	1.09110100	-2.13510900
H	0.49330100	3.29914900	-0.22283200
N	-0.18751900	0.57949000	-0.11519700
N	2.09983400	1.05433100	-0.04676900
C	1.02474800	0.39968200	0.41754600
C	1.99473700	2.04848000	-1.13217500
H	-1.43278900	2.00564900	-0.96974900
H	0.50047800	3.33985400	-1.99224200
H	2.20240700	1.55967800	-2.09311700
H	2.76901500	2.80063100	-0.96286600
C	3.47365000	0.72068800	0.40267700
H	3.57279600	0.93096300	1.47438400
H	4.12373000	1.42778000	-0.11450200
C	1.22870700	-0.54682100	1.57934800
H	0.27907400	-0.72807900	2.07996000
H	1.85337600	-0.03353900	2.31919300
C	3.92143800	-0.71344500	0.07630400
H	5.01882100	-0.71776700	0.08345400
H	3.61471600	-0.95479200	-0.95041300
C	1.89736300	-1.88557900	1.18018200

C	3.42303000	-1.78412400	1.05692900
H	1.64938200	-2.62296500	1.95160000
H	1.45925100	-2.25416400	0.24385500
H	3.82428400	-2.75933400	0.75485100
H	3.84249500	-1.57177000	2.05123200
H	-2.10123900	1.36084900	1.77746400
S	-2.65675900	-1.62187600	3.35311100
C	-3.57695600	-0.57114600	4.55424900
H	-3.58638300	-1.07679500	5.52384200
H	-3.09157100	0.40253200	4.67545100
H	-4.60974900	-0.41551100	4.22960200

G_{CHCl3}: -1299.068113

DMPP analogue of **TS19**

C	1.57211500	-0.92055400	-0.84853000
C	1.32100900	0.54350900	-1.18914000
C	3.31945600	0.36895900	-0.03966600
N	2.70184200	-0.94154300	-0.07683900
O	4.40373600	0.55212800	0.52508700
O	0.90320100	-1.89555800	-1.18623100
C	3.32273600	-2.15032800	0.43203900
H	4.17121200	-1.85152700	1.04978100
H	2.60915700	-2.71974500	1.03489100
H	3.67727300	-2.78586800	-0.38762400
C	2.46536900	1.25119000	-0.77195500
H	2.69728300	2.29312500	-0.94584400
H	0.77456500	0.74747600	-2.10569500
C	0.21921700	0.83679200	1.90613600
H	1.25911700	1.17993800	1.91782800
H	-0.36999000	1.45903500	2.58704700
H	0.18580700	-0.20083300	2.24714900
C	-0.65999600	2.77377100	-0.07533400
H	0.31025100	3.26571000	0.04442400
H	-1.02238600	2.97164000	-1.08840000
H	-1.36265200	3.19266600	0.65173500
C	-2.06030700	0.18574400	0.14568300
C	-2.20431400	-1.13152000	0.62369400
C	-3.16658600	0.81720100	-0.45223600
C	-3.43260600	-1.78636000	0.53142300
H	-1.35914100	-1.65306500	1.06352300
C	-4.39278000	0.15412900	-0.54681500
H	-3.08416300	1.82849200	-0.83813700
C	-4.53067800	-1.14621000	-0.05340100
H	-3.52947300	-2.79995200	0.91084700
H	-5.24029200	0.65820500	-1.00368500
H	-5.48547700	-1.65962500	-0.12704900
P	-0.41568600	0.97564200	0.18965600

G_{CHCl3}: -1051.23993

DMPP analogue of **20**

C	1.54463100	-1.05078900	-0.22979700
C	0.93169500	0.24065800	-0.82695600
C	3.25289700	0.54092800	-0.50018700
N	2.85879400	-0.82288400	-0.06478900
O	4.45672700	0.87056400	-0.44132700
O	0.92942600	-2.08724000	0.05939000
C	3.79021400	-1.79736900	0.46753700
H	4.78292500	-1.34420000	0.43638800
H	3.53558700	-2.06008000	1.50072600
H	3.78164300	-2.71041600	-0.13714700
C	2.09063600	1.17511100	-0.92030600
H	2.07680400	2.12709900	-1.43304200
H	0.41380200	-0.00615700	-1.76619300
C	0.10787700	0.65587000	2.04039600
H	1.12152200	1.05090900	2.16171300
H	-0.57515900	1.19156900	2.70562500
H	0.09631400	-0.40893000	2.28660300
C	-0.54734300	2.68835600	0.02928000
H	0.44516500	3.12397500	0.16699800
H	-0.89141500	2.89359300	-0.98841300
H	-1.23836700	3.13442000	0.74934800
C	-2.04422600	0.14102200	0.03761300
C	-2.15614000	-1.25860800	-0.05269200
C	-3.19480300	0.94030900	-0.08301000
C	-3.40847800	-1.84350600	-0.25025600
H	-1.26612500	-1.87812500	0.01992500
C	-4.44253100	0.34500100	-0.28230100
H	-3.13327600	2.02189700	-0.02322100
C	-4.55134700	-1.04598400	-0.36385900
H	-3.48800200	-2.92485000	-0.31941600
H	-5.32615600	0.97033200	-0.37427700
H	-5.52318800	-1.50651300	-0.51961900
P	-0.41009000	0.89553900	0.31001700

G_{CHCl3}: -1051.250704

DMPP analogue of **TS21**

C	0.77107500	-1.26732900	-0.86595100
C	0.46255800	-0.01570900	-0.01047700
C	2.58669500	-0.92456900	0.55969100
N	1.99207300	-1.72389800	-0.49440900
O	3.65885900	-1.25474500	1.07614400
O	0.03691500	-1.76650100	-1.71986400
C	2.63644900	-2.87710000	-1.10035100
H	3.58949100	-3.02376500	-0.59007300
H	2.01266600	-3.76897700	-0.98612000
H	2.80979900	-2.70017700	-2.16639500
C	1.75423100	0.22397800	0.74243100
H	2.32031700	1.33935600	-0.12606300
H	0.18161700	0.80753900	-0.68642300
C	-1.13630100	-2.04476100	1.54657600
H	-0.21013700	-2.33390200	2.05268000
H	-1.98090800	-2.18031900	2.22841000
H	-1.28122900	-2.67169600	0.66300200
C	-0.89245000	0.70439100	2.56230000
H	0.00269100	0.39075300	3.10407700
H	-0.81027700	1.76615900	2.31389100
H	-1.76264600	0.54078600	3.20339600
C	-2.56455500	0.17857400	0.17669600
C	-2.78327300	-0.29082900	-1.13123000
C	-3.52606200	0.99448800	0.79740200
C	-3.95884200	0.05095900	-1.80160800
H	-2.03481100	-0.90638600	-1.62290900
C	-4.69812500	1.33079200	0.11637000
H	-3.37459000	1.37570900	1.80168100
C	-4.91640900	0.85877000	-1.18068300
H	-4.12169600	-0.31138400	-2.81261600
H	-5.43597900	1.96384200	0.60081000
H	-5.82837300	1.12421300	-1.70834300
P	-1.04325400	-0.29398800	1.04946300
H	1.77816200	0.72877400	1.70228900
S	2.74124900	2.57758000	-1.00316100

C	4.33623900	2.83807100	-0.11658000
H	5.01999500	2.00029700	-0.28173800
H	4.80368300	3.75073600	-0.49727000
H	4.17296900	2.95589500	0.95945500

G_{CHCl3}: -1489.89393

2

S	2.48763000	0.04773700	-1.22976700
C	3.23865600	-0.19754700	0.43958700
H	3.21317000	0.79175000	0.90664400
H	2.60713500	-0.87048700	1.02750400
C	4.67383200	-0.71825500	0.38430400
H	5.06384100	-0.80116600	1.40436600
H	4.69585000	-1.72033500	-0.06952600
O	5.55981500	0.16225900	-0.30135700
H	5.19036000	0.31714900	-1.18900900
H	2.40111400	-1.25810600	-1.56471900

G_{CHCl3}: -553.1510762

2^{-}

S	2.58338600	0.09267300	-1.27378700
C	3.24376000	-0.18133300	0.43853200
H	3.23391500	0.76724600	0.99233700
H	2.61033600	-0.89004400	0.98822600
C	4.67376200	-0.72742700	0.40895900
H	5.11488300	-0.73092000	1.41482500
H	4.66534400	-1.76221800	0.03021900
O	5.53022100	0.07864200	-0.40706000
H	4.95312400	0.31621400	-1.17149400

G_{CHCl3}: -552.6744648

Proton transfer TS from **2** to Et_3N

C	1.84043700	2.20354200	-0.83940600
C	2.31306700	0.99361400	-0.03249900
N	1.43564000	-0.20653100	-0.13611900
C	1.25157300	-0.62464700	-1.55556400
C	0.34628000	-1.84081700	-1.75711600
C	1.95497400	-1.33510500	0.68929100
C	2.20261600	-0.99937900	2.16120000
H	3.33596400	0.71143900	-0.32852400
H	2.34049600	1.27185700	1.02291700
H	0.79285400	2.43896100	-0.62360900
H	2.44425900	3.07068900	-0.54975300
H	1.95747200	2.07061600	-1.91907500
H	0.81749100	0.22660800	-2.08358500
H	2.24350200	-0.81285100	-1.99710500
H	0.80499800	-2.77337500	-1.41519800
H	-0.61536400	-1.71601400	-1.24883500
H	0.14640100	-1.94937800	-2.82894700
H	1.20784000	-2.12958000	0.63489300
H	2.87886800	-1.71595600	0.22592200
H	2.39841000	-1.93349800	2.69921800
H	3.06959000	-0.34892100	2.31009400
H	1.32842700	-0.52724500	2.62154700
S	-1.15813900	0.52103700	1.18820500
C	-2.18845100	1.09499500	-0.24105500
H	-2.34908100	2.17616700	-0.16625400
H	-1.65241600	0.89566900	-1.17523000
C	-3.54233400	0.38452900	-0.26365000
H	-4.12606400	0.66668600	0.62562900
H	-4.10892000	0.68431000	-1.15251700
O	-3.41080200	-1.03574100	-0.33640000
H	-2.75951100	-1.27251700	0.35355000
H	0.19041600	0.13834200	0.43232300

G_{CHCl3}: -845.3139885

2^{-}/Et_3NH^{+}

C	2.13617000	2.20499300	-0.86457800
C	2.45120600	0.98801800	0.00028600
N	1.48538300	-0.16071700	-0.16165600
C	1.30323100	-0.54402100	-1.60965300
C	0.34187000	-1.70750800	-1.83836900
C	1.87868200	-1.34618300	0.68499400
C	2.08824300	-1.02358300	2.16203200
H	3.45396600	0.59886300	-0.20839300
H	2.40469100	1.27129900	1.05219800
H	1.09748900	2.52544100	-0.73555600
H	2.78268100	3.02664900	-0.53840800
H	2.33189000	2.03447100	-1.92680500
H	0.92160100	0.34605300	-2.11074700
H	2.29801900	-0.76289100	-2.01365700
H	0.75394000	-2.66850500	-1.51814300
H	-0.61518800	-1.54463400	-1.33245800
H	0.14560900	-1.77681100	-2.91368000
H	1.06641000	-2.06672400	0.58638600
H	2.78076700	-1.77798200	0.23734700
H	2.19539200	-1.97056600	2.70161300
H	2.99173800	-0.43588100	2.34659700
H	1.22563800	-0.49617400	2.58136600
S	-1.21001500	0.81171200	1.08093700
C	-2.41197800	1.05557200	-0.31142400
H	-2.72671800	2.10537000	-0.35164500
H	-1.93030900	0.81781700	-1.26860500
C	-3.65080400	0.17455100	-0.13847700
H	-4.23123700	0.51958000	0.73105200
H	-4.29329200	0.23230900	-1.02572400
O	-3.30818200	-1.20488600	0.02030500
H	-2.56305000	-1.19370500	0.65936900
H	0.51826600	0.18170700	0.21319000

G_{CHCl3}: -845.3139437

3

S	2.46480000	1.02557100	0.08439800
C	3.17138100	-0.63737300	-0.04436300
C	4.67848700	-0.64620200	-0.15682600
H	5.13712700	0.13133500	0.46101500
H	5.05525800	-1.63007000	0.13278000
H	4.95512900	-0.45530500	-1.20125700
O	2.47980200	-1.63421400	-0.06223400
H	1.18210600	0.60902600	0.08426000

G_{CHCl3}: -551.9845989

3^{-}

S	2.40998300	0.95378100	-0.11673900
C	3.16979700	-0.62257000	-0.02396100
C	4.69569200	-0.65947600	-0.16684700
H	5.16654500	-0.00587900	0.57554000
H	5.06454900	-1.68382200	-0.04260200

H	4.98881800	-0.28637200	-1.15508100
O	2.56555000	-1.69502000	0.14133700

G_{CHCl3}: -551.5195621

Proton transfer TS from **3** to Et_3NH^+

C	-0.86691400	-1.44261600	2.17188600
C	-1.77192000	-0.46738000	1.41632700
N	-1.36315200	-0.19145100	0.01589200
C	-1.25003100	-1.44729900	-0.76978900
C	-0.83228600	-1.25608900	-2.22911400
C	-2.28953800	0.76978900	-0.63398300
C	-2.45931200	2.10318900	0.09918700
H	-2.81265400	-0.83680900	1.42369000
H	-1.76496400	0.48856900	1.94567000
H	0.18571100	-1.15204900	2.09531900
H	-1.14732600	-1.42949900	3.23132300
H	-0.96558000	-2.47382800	1.81983200
H	-0.49387400	-2.06048500	-0.27772200
H	-2.21002700	-1.99097700	-0.72211900
H	-1.61934800	-0.81093300	-2.84581100
H	0.06731900	-0.63663400	-2.30754800
H	-0.59846400	-2.23799100	-2.65574000
H	-1.89003800	0.97432600	-1.63004500
H	-3.27495400	0.29058400	-0.76992000
H	-3.00820000	2.79229300	-0.55249400
H	-3.02909200	2.00985900	1.02860100
H	-1.49282000	2.56428700	0.33075000
S	1.34290600	1.28208100	0.10859100
C	2.48645500	-0.08684800	-0.02283900
C	3.94852200	0.31797400	-0.06914400
H	4.17117700	1.09716900	0.66605300
H	4.57612500	-0.55929200	0.10933700
H	4.17824700	0.72386100	-1.06215000
O	2.13258800	-1.25502100	-0.09186100
H	0.06331800	0.50671500	0.05820200

G_{CHCl3}: -844.1531037

3$^-$/Et_3NH^+

C	-0.48326500	-1.34322200	2.20044200
C	-1.22497200	-0.22585900	1.47307300
N	-0.86180200	-0.08365400	0.01318400
C	-0.95961700	-1.40184300	-0.72180700
C	-0.65920300	-1.31231400	-2.21461700
C	-1.66318000	1.00508200	-0.65998700
C	-1.61149600	2.35625600	0.04862900
H	-2.31014900	-0.36768500	1.51875700
H	-0.98432500	0.73199900	1.93535300
H	0.59553900	-1.28279700	2.03115700
H	-0.67111700	-1.22846500	3.27336200
H	-0.82846700	-2.33886800	1.90855500
H	-0.22449500	-2.05198700	-0.24970900
H	-1.96510800	-1.79496700	-0.53725000
H	-1.44383800	-0.80322100	-2.78172700
H	0.29832800	-0.81509900	-2.39845100
H	-0.58239100	-2.33388000	-2.60172200
H	-1.24727100	1.10630200	-1.66282300
H	-2.69152400	0.63873400	-0.74858000
H	-2.06959900	3.10037800	-0.61150200
H	-2.16729000	2.36560400	0.99018600
H	-0.58032700	2.66933900	0.24040500
S	2.15965200	0.95639000	-0.09848500
C	2.90774600	-0.63836100	-0.08675600
C	4.43137500	-0.67793700	-0.14771400
H	4.85717200	-0.14947700	0.71277600
H	4.78109800	-1.71522400	-0.15033900
H	4.78880000	-0.16649000	-1.04828800
O	2.27004000	-1.69849900	-0.03060600
H	0.16418500	0.22487200	-0.02427000

G_{CHCl3}: -844.1614157

4

S	-2.13265800	-0.35470000	-0.36307800
C	-0.86422000	0.09174700	0.89941900
H	-0.79401800	-0.76998600	1.56527000
H	-1.19811200	0.96431800	1.46368600
C	0.47342500	0.38981000	0.25654300
O	0.76790900	1.46213300	-0.24173900
O	1.29154100	-0.67353300	0.28725600
H	-2.18534100	0.85487600	-0.95978700
C	2.58165900	-0.51588400	-0.34623800
H	2.45246700	-0.28871800	-1.40700500
H	3.14317100	0.28562800	0.13925500
H	3.08357900	-1.47375400	-0.21464500

G_{CHCl3}: -666.4823385

4$^-$

S	2.12111700	-0.43741200	-0.35207500
C	0.93633200	0.41964200	0.80438000
H	1.26973900	1.44253900	1.00123100
H	0.87130200	-0.12491000	1.75139500
C	-0.42491300	0.49593500	0.17651500
O	-0.84906600	1.41758300	-0.50823800
O	-1.17481700	-0.60447600	0.44153900
C	-2.44587400	-0.68995900	-0.22201500
H	-3.07662600	0.16611900	0.03400900
H	-2.30618900	-0.72688100	-1.30642800
H	-2.89831000	-1.61682800	0.13330200

G_{CHCl3}: -666.0067349

Proton transfer TS from **4** to Et_3N

C	1.62667400	0.13199800	2.57711700
C	2.48460700	-0.02086800	1.32120000
N	1.81359600	0.35621100	0.04685900
C	1.22839900	1.72599600	0.12334100
C	0.58893500	2.22416800	-1.17343300
C	2.74672900	0.22727400	-1.10803900
C	3.41881200	-1.14061000	-1.24535700
H	3.40664200	0.57408700	1.42413900
H	2.77860600	-1.06852600	1.22570200
H	0.66940600	-0.38940200	2.47857900
H	2.16495900	-0.31565800	3.42003000
H	1.42623800	1.17663300	2.83203600
H	0.45866000	1.69607200	0.89624700
H	2.01250400	2.42734500	0.45197000
H	1.32474400	2.46958300	-1.94546200
H	-0.11497300	1.48976500	-1.57792400
H	0.02800100	3.13857600	-0.95122800
H	2.15975400	0.41770500	-2.00927800
H	3.50979300	1.01896800	-1.03753100

H	3.92624100	-1.18088200	-2.21561100
H	4.17296400	-1.32366700	-0.47401500
H	2.68697000	-1.95484400	-1.21624400
S	-0.32933200	-1.64864200	-0.64136000
C	-1.63736700	-1.40744800	0.64732200
H	-1.18750900	-1.35110500	1.64065200
H	-2.29654300	-2.27700400	0.60333500
C	-2.42840000	-0.14515700	0.40747800
O	-2.15301700	0.94984200	0.87270600
O	-3.48511800	-0.35711400	-0.40092500
H	0.74588000	-0.57107900	-0.20802700
C	-4.27312800	0.79853600	-0.75177100
H	-5.06167600	0.42236500	-1.40327000
H	-4.69981900	1.25426400	0.14531100
H	-3.65581800	1.53060500	-1.27849200

G_{CHCl3}: -958.6452655

4^{-}/Et_3NH^{+}

C	1.55376900	0.17648500	2.55420500
C	2.47137100	0.03139400	1.34381700
N	1.82527300	0.37538800	0.02524200
C	1.16280400	1.73339700	0.06182800
C	0.55869200	2.17301200	-1.26854700
C	2.79930600	0.24731800	-1.11974000
C	3.49022100	-1.11127200	-1.20937900
H	3.36001800	0.66513400	1.43984100
H	2.79629300	-1.00603100	1.25851800
H	0.61573300	-0.36834900	2.41364300
H	2.06738700	-0.25448400	3.42026700
H	1.32294600	1.21852500	2.79084600
H	0.36841900	1.65467200	0.80408100
H	1.91371800	2.44816300	0.41598900
H	1.31252900	2.44371000	-2.01350700
H	-0.09278200	1.39615900	-1.68091000
H	-0.05414000	3.06103600	-1.08125100
H	2.21995400	0.41651200	-2.02767600
H	3.52589700	1.06108900	-1.01797600
H	4.02325500	-1.15683700	-2.16500400
H	4.22522000	-1.27008200	-0.41530400
H	2.76402700	-1.93030600	-1.19051900
S	-0.36483000	-1.77142800	-0.65994300
C	-1.72314100	-1.58234200	0.59658000
H	-1.31891900	-1.64560200	1.61083500
H	-2.45304300	-2.38303100	0.45557500
C	-2.39778600	-0.24607400	0.44641600
O	-2.02021700	0.79846600	0.96140300
O	-3.48818200	-0.30948200	-0.34807600
H	1.03810400	-0.35405300	-0.15108300
C	-4.16386100	0.93236700	-0.62144100
H	-5.00488500	0.66857400	-1.26301000
H	-4.51791900	1.38835100	0.30688000
H	-3.49250400	1.62439400	-1.13688900

G_{CHCl3}: -958.6485115

5

S	2.42590600	-0.59359600	-0.40310300
C	1.60489400	0.80539200	0.47473400
H	2.28915800	1.64877500	0.34805800
H	1.55578300	0.57186600	1.54084300
C	0.22967900	1.18733100	-0.06851300
H	0.26768900	1.38314600	-1.14537800
H	-0.09764900	2.12519100	0.40440600
C	-0.84768100	0.15713900	0.20666900
O	-0.73829400	-0.79292600	0.96208700
O	-1.97215900	0.43405100	-0.47751100
H	1.60843700	-1.56798700	0.04670900
C	-3.09369800	-0.45307500	-0.26884500
H	-2.83254300	-1.46883600	-0.57488500
H	-3.38814700	-0.44801000	0.78333000
H	-3.89275300	-0.05633100	-0.89429900

G_{CHCl3}: -705.7658604

5^{-}

S	-3.13534400	-0.25900900	0.00429400
C	-1.47791200	0.56454500	0.05441300
H	-1.36772100	1.12754200	0.98955000
H	-1.39680100	1.29262000	-0.76104400
C	-0.32670000	-0.43828100	-0.05943600
H	-0.41412400	-1.00759100	-0.99533600
H	-0.38851900	-1.18608500	0.74122500
C	1.05646500	0.17613000	-0.02485400
O	1.32527000	1.36581200	-0.03454000
O	2.01911200	-0.78005800	0.01275100
C	3.38364800	-0.31955300	0.03269600
H	3.60455500	0.26120100	-0.86697100
H	3.56614800	0.29602200	0.91762700
H	3.99391700	-1.22265200	0.06365200

G_{CHCl3}: -705.2836836

Proton transfer TS from **5** to Et_3N

C	-2.06386900	-1.43036300	2.19384100
C	-3.07846500	-0.59184500	1.41632000
N	-2.68879500	-0.28327600	0.01081700
C	-2.38148100	-1.52331500	-0.75827000
C	-1.98483600	-1.28945700	-2.21711500
C	-3.72778700	0.53830200	-0.67496500
C	-4.09804600	1.83596400	0.04548900
H	-4.06068100	-1.09002900	1.40934000
H	-3.19798200	0.36675000	1.92535600
H	-1.06236200	-0.99124500	2.14120200
H	-2.36525000	-1.44878000	3.24702700
H	-2.01318600	-2.46773700	1.85001800
H	-1.55223100	-2.01480900	-0.24518000
H	-3.25023800	-2.19807200	-0.70303300
H	-2.83012700	-0.99098100	-2.84436300
H	-1.20256800	-0.52779300	-2.30178400
H	-1.58975300	-2.22693600	-2.62362000
H	-3.32623400	0.79006900	-1.65855500
H	-4.62423800	-0.08236900	-0.82931600
H	-4.72097200	2.43744200	-0.62571300
H	-4.67274400	1.66643200	0.96081500
H	-3.20957600	2.42576300	0.29395400
S	-0.26764100	1.47978300	0.10914200
C	1.07549400	0.21562300	-0.00491100
H	0.97316300	-0.35199700	-0.93485200
H	0.98958900	-0.49368900	0.82436700
C	2.44757900	0.88686800	0.03762900
H	2.56800200	1.46755400	0.96075500
H	2.55104300	1.60867700	-0.78297500
C	3.59912600	-0.09321000	-0.05640300

O	3.50149100	-1.29993600	-0.19883300
O	4.78719400	0.54122200	0.03519100
H	-1.54775000	0.49631900	0.05493500
C	5.96942500	-0.28228200	-0.04793000
H	6.80784300	0.40814500	0.04244800
H	5.98217200	-1.01088900	0.76653900
H	6.00218200	-0.80334500	-1.00800400

G_{CHCl3}: -997.923829

5^{-}/Et_3NH^{+}

C	-2.07549700	-1.45757800	2.16287500
C	-3.10842700	-0.60545800	1.43074600
N	-2.75640000	-0.29711600	-0.00218400
C	-2.46182700	-1.54800700	-0.79021200
C	-2.10951700	-1.30198500	-2.25522700
C	-3.80949300	0.55251600	-0.66739900
C	-4.13480400	1.84598100	0.07560800
H	-4.09407100	-1.08478400	1.42812400
H	-3.19646100	0.35859000	1.93237700
H	-1.07373800	-1.02565700	2.07423500
H	-2.34059700	-1.47192700	3.22539500
H	-2.05200300	-2.49437800	1.81607600
H	-1.61636900	-2.02449200	-0.29278800
H	-3.33161800	-2.20763000	-0.69329000
H	-2.97206400	-0.99951000	-2.85559600
H	-1.32528300	-0.54448200	-2.35255300
H	-1.72938700	-2.23975000	-2.67421700
H	-3.41761300	0.79591700	-1.65529100
H	-4.70117700	-0.07215300	-0.79344200
H	-4.76214300	2.46210600	-0.57730700
H	-4.69058800	1.67825800	1.00230500
H	-3.22735300	2.41456200	0.30199600
S	-0.20501600	1.47522100	0.02872000
C	1.16065900	0.22893400	-0.04902300
H	1.09453900	-0.34029100	-0.98347400
H	1.06002900	-0.49083800	0.77093400
C	2.53511100	0.89363600	0.03754300
H	2.61530600	1.48359600	0.96025100
H	2.67103600	1.61062800	-0.78171800
C	3.69238600	-0.08315900	0.01157000
O	3.60657200	-1.29980000	0.01257900
O	4.88002000	0.56339400	-0.00499100
H	-1.83216500	0.30158100	0.01310600
C	6.06486300	-0.25903600	-0.01153300
H	6.90103000	0.44016700	-0.02200700
H	6.09891400	-0.88446300	0.88430400
H	6.08337900	-0.89259300	-0.90204500

G_{CHCl3}: -997.925379

6

C	-0.92922100	0.45637200	-0.07934600
O	-1.29551800	0.90705700	-1.14827100
O	-1.60767000	-0.48173500	0.60648500
C	0.33954300	0.89836800	0.67183500
H	-0.00476600	1.27367900	1.64599800
N	1.07188300	1.96689500	0.01128400
H	1.39504200	1.64751100	-0.90184300
H	0.45581200	2.75818500	-0.16549100
C	1.26581300	-0.29256300	0.98379600
H	2.11102000	0.07937400	1.56816600
H	0.74291100	-1.04741400	1.57293500
S	2.03242200	-1.09764300	-0.48915200
H	0.94328900	-1.78095700	-0.90197100
C	-2.84453200	-0.94994600	0.02131000
H	-3.54535300	-0.11905000	-0.08861100
H	-2.65285200	-1.40308400	-0.95406400
H	-3.23114600	-1.69017500	0.72103900

G_{CHCl3}: -761.0963565

6^{-}

C	1.15720400	0.32657600	0.01839700
O	1.65019100	1.10627400	0.81837300
O	1.84343500	-0.70881300	-0.51141100
C	-0.28661800	0.34516400	-0.44403000
H	-0.33397600	-0.09274100	-1.44649100
N	-0.74641300	1.73517400	-0.52204400
H	-1.76623300	1.68510000	-0.60302400
H	-0.55544100	2.19062100	0.37217400
C	-1.12704400	-0.56439100	0.50437800
H	-0.69985600	-1.57499200	0.48074900
H	-1.01523600	-0.18220000	1.52897900
S	-2.91357300	-0.61924400	0.03888500
C	3.20107400	-0.88067700	-0.05893800
H	3.79799200	0.00128000	-0.30503500
H	3.22410600	-1.04898200	1.02097100
H	3.57401500	-1.75611800	-0.59071000

G_{CHCl3}: -760.6177558

Proton transfer TS from **6** to Et_3N

C	1.95356400	-0.70958400	2.36883300
C	3.01619300	-0.64428200	1.27191800
N	2.71273300	0.30125200	0.16109400
C	2.45084900	1.67758200	0.67125100
C	2.12135400	2.71044300	-0.40796900
C	3.79900600	0.30609200	-0.86148600
C	4.15532000	-1.06932900	-1.42843600
H	3.99426400	-0.38036100	1.70455200
H	3.11133400	-1.63509300	0.82303300
H	0.95809500	-0.88726900	1.94854700
H	2.19062900	-1.55006400	3.03046700
H	1.91918500	0.19237100	2.98699800
H	1.60401700	1.60626500	1.35672900
H	3.32196700	2.00737500	1.25997200
H	2.99083100	2.98694200	-1.01171800
H	1.33256500	2.35256300	-1.07786500
H	1.76130000	3.62160500	0.08254900
H	3.45330600	0.94007700	-1.68062500
H	4.69200700	0.78182000	-0.42614100
H	4.82339900	-0.92663500	-2.28491000
H	4.67843500	-1.70470600	-0.70770400
H	3.26711800	-1.60186500	-1.78433300
S	0.35212800	-0.75456400	-1.36427900
C	-1.06234700	0.12049100	-0.56162700
H	-1.39176200	0.94155200	-1.20741800
H	-0.73566900	0.54885000	0.39307000
C	-2.25826600	-0.83877400	-0.30091900
H	-2.58882100	-1.23575200	-1.26629600
C	-3.39695800	-0.01869900	0.29015600
O	-3.55974300	0.17508100	1.48277800
O	-4.17764900	0.51734200	-0.66349300

N	-1.97917000	-1.96154500	0.59297500
H	-1.09974900	-2.38747600	0.29826600
H	-1.84128100	-1.61217300	1.54143900
H	1.56622800	-0.17124900	-0.51276800
C	-5.24471900	1.38281700	-0.21633100
H	-5.74906800	1.70936000	-1.12526500
H	-5.93159300	0.83040600	0.42902400
H	-4.83462400	2.23794000	0.32655000

G_{CHCl3}: -1053.255818

6^{-}/Et_3NH^{+}

C	2.28428200	-0.48665900	2.54300900
C	3.27202400	-0.45988800	1.38038900
N	2.81536100	0.35567100	0.19637200
C	2.43729300	1.76089700	0.59351400
C	1.96160500	2.63679900	-0.56278100
C	3.82857100	0.34144000	-0.92144300
C	4.24074800	-1.05576800	-1.37772000
H	4.24614100	-0.06530900	1.69018600
H	3.41436300	-1.47452800	1.00781500
H	1.28378400	-0.77417500	2.20461000
H	2.62476400	-1.24297700	3.25813600
H	2.22502200	0.46604600	3.07647200
H	1.63359900	1.66152800	1.32386700
H	3.30529600	2.19949200	1.09802100
H	2.77080300	2.92928900	-1.23752900
H	1.17790200	2.13884200	-1.14263400
H	1.53876000	3.55438400	-0.13999600
H	3.36274400	0.86752100	-1.75492300
H	4.69212200	0.92516100	-0.58347100
H	4.82310300	-0.95152900	-2.29928700
H	4.86901700	-1.57511800	-0.64891800
H	3.36703000	-1.67563500	-1.60256500
S	0.31696500	-1.09080200	-0.98823700
C	-1.10788100	-0.20721800	-0.21125500
H	-1.16877200	0.81645200	-0.60130900
H	-0.96727600	-0.14426300	0.87632200
C	-2.46087100	-0.92440000	-0.48614200
H	-2.62240700	-0.93042000	-1.56882300
C	-3.57173500	-0.11204500	0.15980700
O	-3.94515800	-0.24118300	1.31399700
O	-4.06770100	0.82023500	-0.67602300
N	-2.54512700	-2.30224100	0.00234400
H	-1.69016600	-2.77775200	-0.29211100
H	-2.53558000	-2.29335500	1.02311200
H	1.91404400	-0.12457100	-0.19306200
C	-5.07719900	1.70013800	-0.13681600
H	-5.34104400	2.37052900	-0.95447500
H	-5.94797800	1.12350600	0.18445800
H	-4.67650700	2.26350700	0.70971700

G_{CHCl3}: -1053.255176

7

S	2.52682100	1.07470900	-0.26485000
C	3.29489500	-0.53541500	-0.11972000
C	3.31088200	-1.35683200	-1.25749700
C	3.87076800	-0.99460400	1.07382600
C	3.89760400	-2.62293200	-1.19738700
H	2.86707800	-1.00990300	-2.18727800
C	4.45570900	-2.26311400	1.12345300
H	3.86586400	-0.36951500	1.96293100
C	4.47284000	-3.08333500	-0.00853300
H	3.90335700	-3.24957600	-2.08557200
H	4.89911900	-2.60734200	2.05441100
H	4.92837700	-4.06872000	0.03479600
H	2.74402700	1.47888600	1.00282600

G_{CHCl3}: -630.3241825

G_{DMF}: -630.325583

7^{-}

S	2.34130200	0.99280300	-0.04488000
C	3.17194000	-0.56910300	-0.03621000
C	3.27572500	-1.36760500	-1.20331300
C	3.77339400	-1.09253800	1.13648600
C	3.93796700	-2.59742600	-1.19951100
H	2.82485300	-1.00389700	-2.12381900
C	4.43551300	-2.32262900	1.13973300
H	3.71370800	-0.51235600	2.05463900
C	4.52793300	-3.09124900	-0.02833400
H	3.99334500	-3.17549600	-2.12100300
H	4.88397700	-2.68417200	2.06415900
H	5.04430900	-4.04839400	-0.02620800

G_{CHCl3}: -629.8549924

G_{DMF}: -629.8747659

Proton transfer TS from **7** to Et_3N

C	0.62739900	0.15076800	2.46607500
C	1.87740700	-0.28540300	1.70066800
N	1.96256500	0.21640000	0.30188400
C	1.82046700	1.69724600	0.24396100
C	1.90622200	2.29480800	-1.16188900
C	3.22183800	-0.22815300	-0.35802000
C	3.47480500	-1.73684100	-0.32010000
H	2.78290700	0.02588900	2.24715900
H	1.88679900	-1.37594100	1.64370000
H	-0.28483200	-0.05805200	1.89780200
H	0.57805900	-0.41847200	3.40107900
H	0.63961200	1.21242300	2.73083900
H	0.84315900	1.93780400	0.66698100
H	2.58324000	2.15489900	0.89572400
H	2.92075500	2.27504900	-1.57134400
H	1.24005600	1.77509200	-1.85863800
H	1.59399600	3.34407100	-1.11409100
H	3.15870200	0.08655300	-1.40230800
H	4.07035600	0.30862100	0.09686800
H	4.31971900	-1.96222300	-0.98028000
H	3.73451800	-2.09967200	0.67899100
H	2.60826400	-2.30100300	-0.68066200
S	-0.19085800	-1.16674900	-1.30878500
C	-1.70393700	-0.49744100	-0.61760000
C	-2.02372800	0.86804900	-0.72864400
C	-2.62244900	-1.34806200	0.02329800
C	-3.21625400	1.36914900	-0.19821700
H	-1.33908800	1.53768700	-1.24193800
C	-3.82075300	-0.84721000	0.54178200
H	-2.39175500	-2.40591400	0.11557400
C	-4.12245400	0.51462200	0.43880000
H	-3.44073900	2.42923000	-0.29305500
H	-4.51681300	-1.52445700	1.03150100

H	-5.05246000	0.90398800	0.84502600
H	0.86994100	-0.40157500	-0.46222900

G_{CHCl3}: -922.4890944

7^{-}/Et_3NH^{+}

C	-0.62188600	-1.20993800	2.36078400
C	-1.33304300	-0.14233200	1.53471800
N	-0.91124300	-0.09625000	0.08535800
C	-1.02420100	-1.44892000	-0.57679000
C	-0.60895100	-1.46810400	-2.04490000
C	-1.65698200	0.96763200	-0.68507300
C	-1.59204700	2.35912000	-0.06160300
H	-2.41968800	-0.27978800	1.54930400
H	-1.10486000	0.84194700	1.94416000
H	0.46397800	-1.14743200	2.23814300
H	-0.85117500	-1.02856000	3.41617100
H	-0.95147300	-2.22488900	2.12225200
H	-0.37630900	-2.11695600	-0.00946200
H	-2.05989300	-1.78191000	-0.44820300
H	-1.32147000	-0.95570500	-2.69713000
H	0.38413100	-1.02898900	-2.18227200
H	-0.56032900	-2.51373100	-2.36677600
H	-1.20067500	0.99407600	-1.67479900
H	-2.69130400	0.62236600	-0.78960500
H	-2.00427300	3.07094200	-0.78454200
H	-2.18107900	2.44414700	0.85573600
H	-0.55963200	2.65651900	0.14770100
S	2.08147000	0.88530500	0.04279900
C	3.01295200	-0.62828700	-0.07666600
C	3.42073100	-1.14531800	-1.32674000
C	3.39288200	-1.35459900	1.07418900
C	4.15759600	-2.32925600	-1.42095700
H	3.15916200	-0.60102600	-2.23084100
C	4.12898500	-2.53916300	0.97940000
H	3.11170300	-0.97315500	2.05275800
C	4.51681500	-3.03920000	-0.26916100
H	4.45658300	-2.69576700	-2.40126400
H	4.40565900	-3.07039600	1.88822300
H	5.09338800	-3.95796500	-0.34274600
H	0.13200900	0.18798500	0.06917300

G_{CHCl3}: -922.4916503

DMF dimer (**26**)

C	1.84068600	0.21798800	-0.01692900
O	1.38105000	1.36738200	-0.08241100
N	3.15080300	-0.10572600	0.01550300
H	1.17435100	-0.65838000	0.01986600
C	3.58858300	-1.49412100	0.09625600
H	4.20717400	-1.74995600	-0.77205700
H	4.17822300	-1.65590200	1.00644200
H	2.71904000	-2.15530200	0.11701500
C	4.18998900	0.91539600	-0.02914900
H	3.72090300	1.89792500	-0.08368100
H	4.81457900	0.85792900	0.87024500
H	4.82802300	0.76581400	-0.90833100
O	-1.38142600	-1.36782400	-0.08238600
C	-1.84064100	-0.21829200	-0.01692600
H	-1.17420600	0.65807500	0.01977200
N	-3.15072400	0.10580000	0.01560400
C	-3.58815400	1.49428100	0.09622400
H	-4.20502700	1.75094600	-0.77308000
H	-4.17942700	1.65571300	1.00540900
H	-2.71842300	2.15515800	0.11913600
C	-4.19019600	-0.91502800	-0.02916600
H	-3.72140600	-1.89761200	-0.08522800
H	-4.81396400	-0.85843700	0.87086000
H	-4.82898200	-0.76429800	-0.90760200

G_{DMF}: -496.8030525

Protonated DMF dimer (**27**)

C	2.05149400	0.32563800	0.00072700
O	1.17644800	-0.58914300	-0.23046700
N	3.33201700	0.07415400	0.05123600
H	1.72940800	1.35415200	0.16064200
C	4.30089600	1.14652800	0.31384700
H	4.87370300	0.89896000	1.21122800
H	4.97939100	1.23393600	-0.53882000
H	3.77795600	2.09158400	0.46384700
C	3.87692400	-1.27517000	-0.14788700
H	3.06826300	-1.97236500	-0.35755300
H	4.57751200	-1.25186100	-0.98685400
H	4.40769200	-1.57957700	0.75846800
H	0.17619300	-0.20677700	-0.22802500
O	-1.11935900	0.34515300	-0.23244000
C	-2.09218700	-0.41841400	0.00855600
H	-1.93188400	-1.48381900	0.20633600
N	-3.35878900	-0.02624600	0.04467900
C	-4.43791300	-0.97205900	0.33199200
H	-4.97517100	-0.65867400	1.23271800
H	-5.13722700	-1.00070700	-0.50951900
H	-4.02494400	-1.97013200	0.48970100
C	-3.74285700	1.36544800	-0.19314800
H	-2.85428700	1.95055800	-0.42527400
H	-4.44567900	1.41049000	-1.03101200
H	-4.22837600	1.76897400	0.70145100

G_{DMF}: -497.2370062

Complex **28** (**1**•••DMF•••DMF)

C	2.14814200	-1.29347100	0.11996300
O	2.12383500	-2.50656600	0.37505100
N	3.26127700	-0.55309100	-0.07108600
H	1.21775600	-0.71183200	0.02730300
C	3.18293600	0.87195700	-0.36900400
H	3.70993500	1.45109600	0.39861300
H	3.64033800	1.08417000	-1.34282100
H	2.13760900	1.18867400	-0.39399400
C	4.59237000	-1.14143900	0.00691400
H	4.49879100	-2.20374100	0.23294400
H	5.11723300	-1.01555400	-0.94770200
H	5.17675400	-0.65032000	0.79420000
O	-1.21611300	-0.03178700	-0.10841700
C	-2.41063800	-0.36275100	-0.17641400
H	-3.19817800	0.38548100	-0.35896000
N	-2.88987100	-1.61293600	-0.04501200
C	-4.31820600	-1.89368900	-0.14242600
H	-4.51310300	-2.58651000	-0.96911900
H	-4.67986400	-2.34590600	0.78818000
H	-4.86658800	-0.96593400	-0.32137400
C	-2.00675800	-2.74789400	0.20113400
H	-0.97523000	-2.39860100	0.24291200

H	-2.26953000	-3.22759000	1.15121800
H	-2.11129500	-3.48446900	-0.60396700
H	-0.89968300	2.00241300	-0.39035500
S	-0.70368800	3.33546300	-0.57410500
C	-0.84878000	3.84613400	1.18676400
H	-0.07950100	3.36836600	1.79769200
H	-0.70353400	4.92863400	1.21565400
H	-1.83891300	3.61014600	1.58328600

G_{DMF}: -935.4508133

Complex **29** (**1**$^{-}$•••DMFH^{+}•••DMF)

C	-1.86616700	-0.64345200	-0.09334400
O	-1.19055000	-1.72885100	0.09856500
N	-3.17303100	-0.64518300	-0.08684400
H	-1.34578500	0.31094900	-0.28318200
C	-3.91311800	0.60589600	-0.30218800
H	-4.55930000	0.49476300	-1.17743600
H	-4.52865400	0.81461900	0.57739400
H	-3.20678700	1.42275800	-0.46397500
C	-3.96851400	-1.85911000	0.13086500
H	-3.30932600	-2.70927500	0.29515800
H	-4.61042100	-1.71104300	1.00377700
H	-4.59332700	-2.03666100	-0.74917000
H	-0.14843100	-1.57656500	0.07451200
O	1.30836400	-1.57986600	0.09035800
C	1.98742800	-0.53561200	-0.09881600
H	1.49381700	0.42840600	-0.29617900
N	3.31791700	-0.50537300	-0.08457800
C	4.04338800	0.74397700	-0.31180000
H	4.65648700	0.98354800	0.56350200
H	4.69626500	0.64187800	-1.18510800
H	3.33386200	1.55500800	-0.48728200
C	4.11949000	-1.70411700	0.15400200
H	3.45734900	-2.55282600	0.32020800
H	4.75836000	-1.89913800	-0.71410300
H	4.75406900	-1.55344700	1.03381200
S	-0.23471000	2.48823900	-0.54247100
C	-0.16725400	2.49437500	1.30968200
H	0.81045300	2.15628600	1.67484700
H	-0.34212300	3.49960700	1.71013400
H	-0.92938500	1.83118900	1.74077900

G_{DMF}: -935.427849

Complex **30** (**7**•••DMF•••DMF)

C	2.31787600	2.08813600	0.33787700
O	3.28365800	2.00736300	1.11107500
N	1.81867000	3.23153800	-0.17882300
H	1.77811400	1.18818100	0.00454600
C	0.67128800	3.22033900	-1.07824300
H	-0.15131500	3.80791600	-0.65351000
H	0.94340100	3.65053500	-2.04950300
H	0.32913700	2.19393400	-1.23005100
C	2.39825900	4.53045400	0.13890200
H	3.24994500	4.38682900	0.80405200
H	2.73133000	5.02891500	-0.77924600
H	1.65307100	5.16696500	0.63109600
O	1.13636300	-1.22161000	-0.39321000
C	1.47785500	-2.41491100	-0.45888300
H	0.86554800	-3.15077100	-1.00284700
N	2.58063700	-2.94691900	0.09456800
C	2.89185000	-4.36593100	-0.04386500
H	3.85646800	-4.49429800	-0.54798800
H	2.94418900	-4.83949700	0.94304200
H	2.11575800	-4.85971400	-0.63308300
C	3.52170300	-2.13397800	0.85837600
H	3.16803200	-1.10349500	0.88568000
H	3.60404500	-2.52076800	1.88065500
H	4.51169900	-2.16899700	0.38914200
H	-0.58158300	-0.80749500	-1.30120200
S	-1.76554900	-0.53858500	-1.92215700
C	-2.76391600	-0.33932200	-0.45036500
C	-2.22333400	-0.43460900	0.84197500
C	-4.13377100	-0.07321700	-0.60756600
C	-3.04858200	-0.26706200	1.95820800
H	-1.16496100	-0.63956800	0.97567200
C	-4.94963700	0.09419700	0.51446000
H	-4.56303800	0.00237100	-1.60366000
C	-4.41311100	-0.00173100	1.80309400
H	-2.61724400	-0.34431200	2.95328600
H	-6.00835300	0.29971200	0.37748600
H	-5.04966100	0.12835800	2.67399700

G_{DMF}: -1127.120883

Complex **31** (**7**$^{-}$•••DMFH^{+}•••DMF)

C	2.13880000	-1.20735100	-0.05587600
O	1.53561600	-1.96801400	-0.90828800
N	3.44275300	-1.13586900	-0.01057200
H	1.55942000	-0.59847000	0.65315900
C	4.10463000	-0.26998500	0.97453800
H	4.72677700	-0.88423400	1.63158500
H	4.73574300	0.45250300	0.44994600
H	3.35162800	0.25689400	1.56293800
C	4.31345900	-1.90005600	-0.91195100
H	3.71035700	-2.51934000	-1.57298500
H	4.91470300	-1.20169800	-1.50101000
H	4.97697900	-2.53022900	-0.31320600
H	0.48733800	-1.95672500	-0.81115100
O	-0.95823500	-2.12763600	-0.83275400
C	-1.72669100	-1.63074200	0.03172200
H	-1.33938900	-0.95894900	0.81032100
N	-3.03639800	-1.86205600	0.07896700
C	-3.87209100	-1.25970200	1.11640500
H	-4.64040100	-0.62877300	0.65723400
H	-4.36087000	-2.04561900	1.70174500
H	-3.25554100	-0.64999400	1.77939800
C	-3.70523000	-2.72927400	-0.88919600
H	-2.97280300	-3.10625700	-1.60171700
H	-4.17766900	-3.56799800	-0.36679400
H	-4.47741400	-2.16173400	-1.41941800
S	0.21585200	1.00262000	2.08662700
C	-0.18734100	1.96784800	0.64962300
C	0.81549800	2.47625400	-0.21004100
C	-1.52821900	2.26249300	0.30624200
C	0.49650600	3.22676900	-1.34560200
H	1.85955100	2.28501300	0.02602700
C	-1.84653200	3.01396800	-0.82850000
H	-2.32698000	1.89764400	0.94738700
C	-0.83782200	3.50284200	-1.66798000
H	1.29803400	3.60070600	-1.98002000
H	-2.89085900	3.21968100	-1.05617600
H	-1.08557400	4.08795700	-2.55000600

G_{DMF}: -1127.108179

IX. Supporting References.

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