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

The effect of backbone flexibility on site-selective modification of macrocycles

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List of Abbreviations

Ac- Acetyl
ACN- Acetonitrile
Cma- (2S,3S)-3-methylaziridine-2-carboxylic acid
COSY- Correlation Spectroscopy
DCM- Dichloromethane
DMAP- 4-(Dimethylamino)pyridine
EtOAc- Ethyl Acetate
HATU- O-(7-Azabenzotriazol-1-yl)-N,N,N′,N′-tetramethyluronium hexafluorophosphate
TEA- Triethylamine
TMS- Tetramethylsilane
Trt- Triphenylmethyl

General Experimental Information:

Dichloromethane (DCM) was of reagent grade quality and acetonitrile (MeCN) was HPLC grade. Triethylamine, 4-dimethylaminopyridine, triethylsilane and acetic anhydride were sourced from Sigma Aldrich (Oakville, ON, Canada). Trifluoroacetic acid was sourced from Caledon Laboratories Ltd. (Georgetown, ON, Canada).

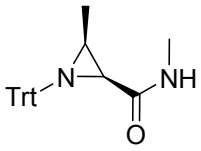
Deuterated chloroform was sourced from Cambridge Isotope Laboratories (Andover, Mass., USA). Peptide grade NMP and DMF were sourced from Caledon Laboratories Ltd., Georgetown, Ontario, Canada. Purifications were carried out on a Teledyne Isco Combiflash, running in normal phase mode with high performance 43 um silica or reverse phase mode with high performance C18 silica columns.

Nuclear magnetic resonance spectra: ^{1}H and ^{13}C NMR spectra were recorded on an Agilent O500 500 MHz NMR equipped with a OneNMR probe. ^{1}H NMR spectra were referenced to DMSO-d_6 (δ 2.50 ppm) or TMS (0 ppm). ^{13}C NMR spectra were referenced to DMSO-d_6 (δ 39.52 ppm) or TMS (0 ppm). Peak multiplicities are designated by the following abbreviations: s, singlet; bs, broad singlet; d, doublet; t, triplet; q, quartet; m, multiplet; ds, doublet of singlets; dd, doublet of doublets; dt, doublet of triplets; ddd, doublet of doublet of doublets; bt, broad triplet; td, triplet of doublets; tdd, triplet of doublets of doublets.

Mass Spectrometry: High-resolution mass spectra were obtained on a VG 70-250S (double focusing) mass spectrometer at 70 eV on a QStar XL (AB Sciex, Concord, ON, Canada) mass spectrometer with electrospray ionization (ESI) source, MS/MS and accurate mass capabilities.

Synthesis and Characterization

Trt-Cma-OH ((2S,3S)-3-methyl-1-tritylaziridine-2-carboxylic acid) was synthesized according to the literature procedure of Galonic *et al*.[1]



Trt-Cma-NHMe: Trt-Cma-OH (1.58 g, 4.6 mmol) was added to a round-bottom flask equipped with stir bar, followed by DCM (10 mL). HATU (4.6 mmol,1.75 g) and TEA (2.56 mL, 18.4 mmol) were added. Methylamine hydrochloride (0.311 g, 4.6 mmol) was added after five minutes. The reaction was then sealed and stirred for 16 h.

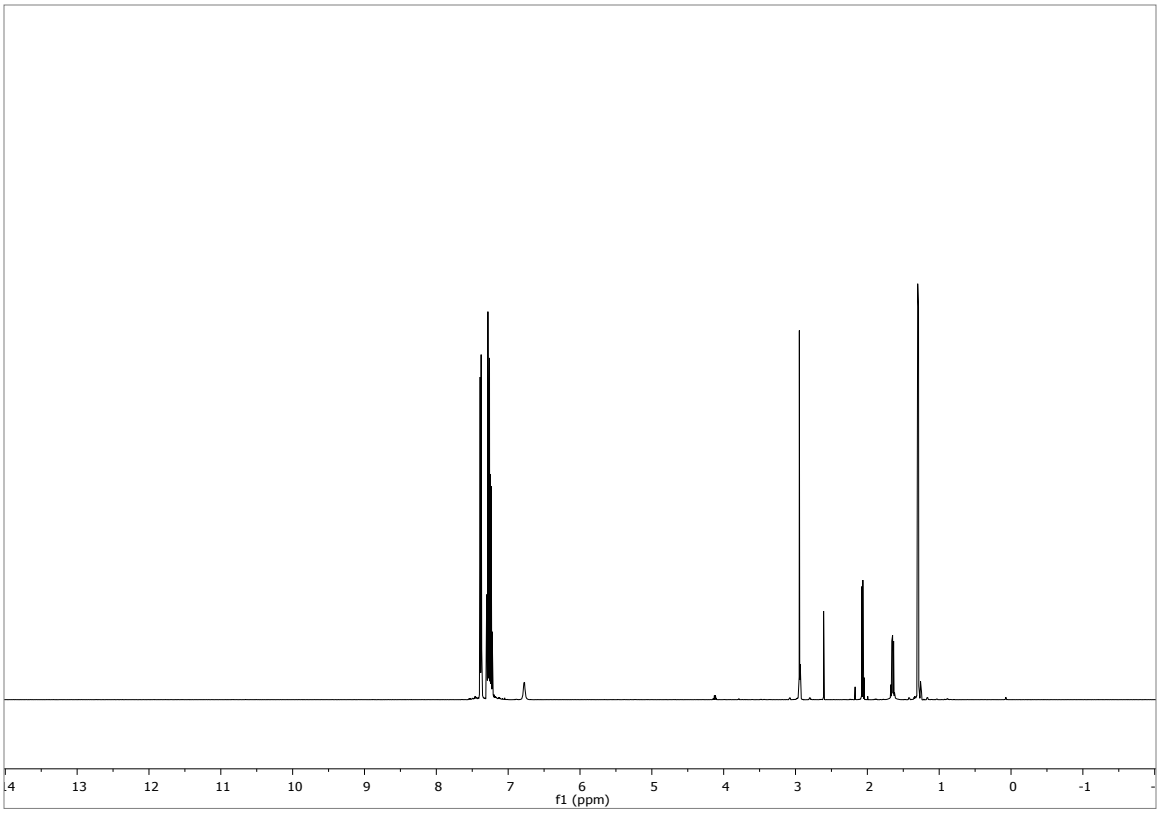
The solvent was removed in vacuo and the residue was redissolved in EtOAc (20 mL). The organic solution was washed sequentially with 5 mL each of water, saturated citric acid solution (aq.), water, sodium bicarbonate solution (aq.), water and brine. The organic part was dried with anhydrous sodium sulfate, filtered, and the solvent was removed by rotary evaporation.

The white crude solid was purified using flash chromatography (Hexane/EtOAc, 100% hexane to 0% hexane in 25 minutes, 30g silica column at 35 mL/min). The fractions containing product (R_f = 0.6 EtOAc:Hexane - 1:1) were dried to give a white foam (1.26 g, 77%)

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 – 7.33 (m, 6H), 7.34 – 7.18 (m, 9H), 6.78 (d, J = 5.5 Hz, 1H), 2.94 (d, J = 5.0 Hz, 3H), 2.07 (d, J = 7.0 Hz, 1H), 1.65 (dq, J = 7.0, 5.6 Hz, 1H), 1.29 (d, J = 5.6 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 170.0, 143.5, 129.4, 127.7, 127.1, 75.2, 39.1, 34.3, 25.7, 13.3.

HRMS: [M-H$^+$] - 355.18159 (found 355.18104, $C_{24}H_{23}N_2O$, ESI-)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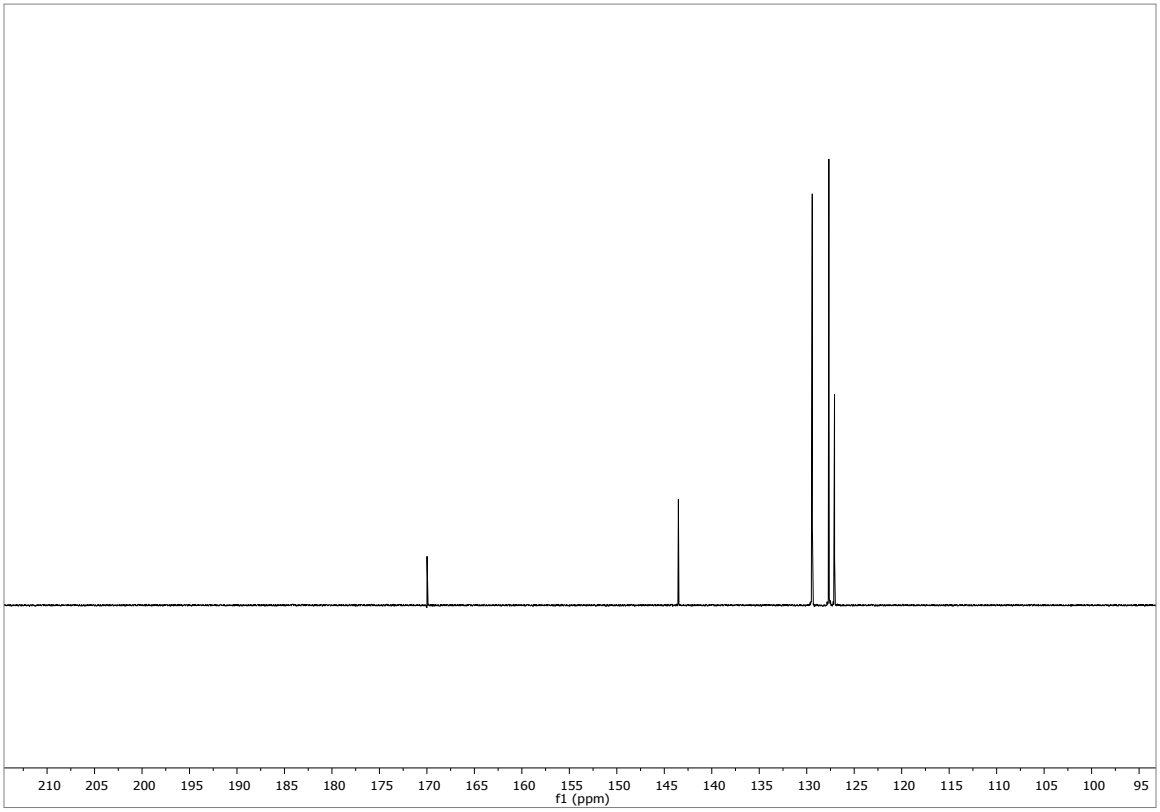
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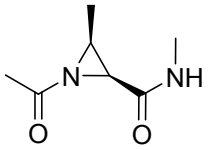


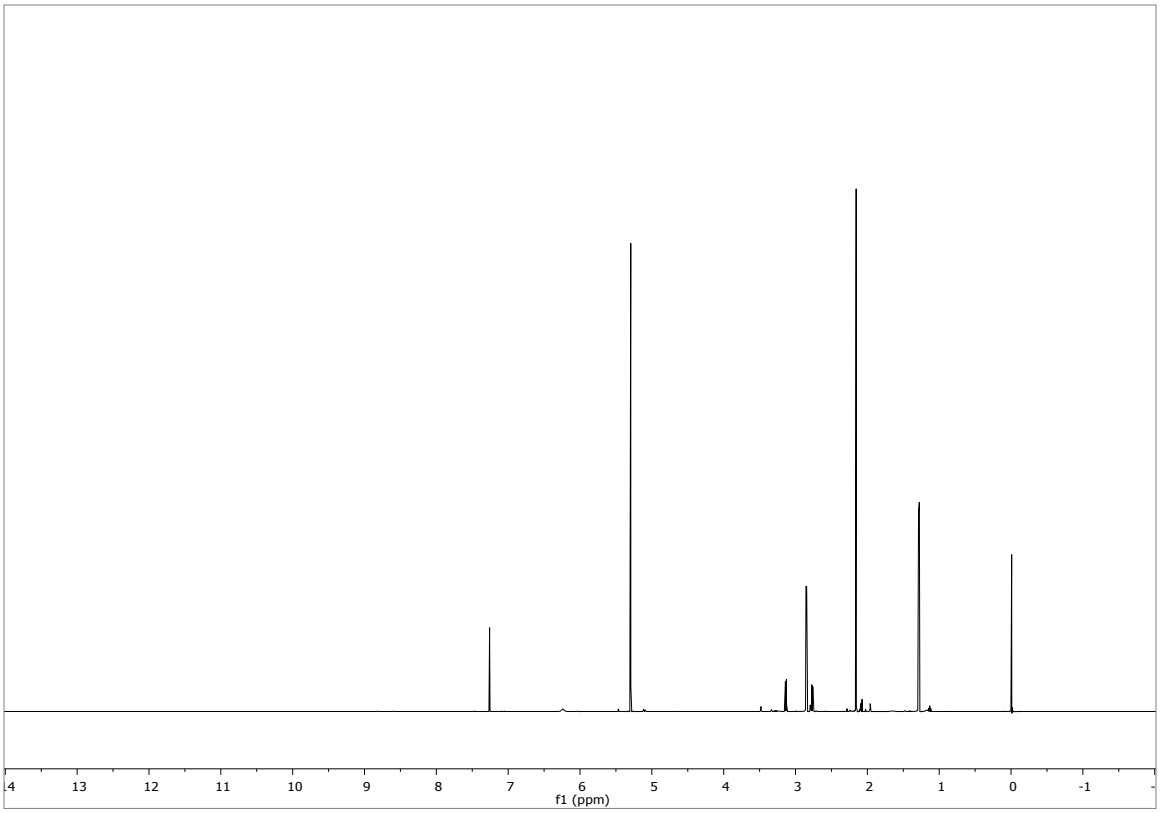
Ac-Cma-NHMe (3): Trt-Cma-NHMe (0.348 mmol, 124 mg) was dissolved in DCM (5 mL) and cooled to 0 °C. Triethylsilane (83 μL, 0.522 mmol, 1.5 eq) was added followed by dropwise addition of trifluoroacetic acid (80 μL, 1.04 mmol, 3 eq). The reaction was stirred for 30 mins at 0 °C after which time the reaction was observed to be complete by consumption of starting material (Rf = 0.6, EtOAc/Hexane -1:1). The solvent was removed by rotary evaporation, and the residue was partitioned between ether (10 mL) and water (10 mL). The aqueous part was adjusted to pH 10 with saturated sodium bicarbonate solution, and then extracted with EtOAc (4 x 20 mL). The organic part was dried with anhydrous sodium sulfate and the solvent removed by rotary evaporation.

The oil obtained was dissolved in DCM (10 mL). Triethylamine (121 μL, 0.87) and acetic anhydride (66 μL, 0.696 mmol) and DMAP (4.3 mg, 0.035 mmol) were added. The reaction was stirred for 4 hours. The organic solution was washed with water (10 mL), dried (MgSO4), and filtered. The solvent was removed in vacuo to give a clear oil. Yield: 57 mg, 37%

^{1}H NMR (500 MHz, $CDCl_3$) δ 6.24 (s, 1H), 3.13 (d, J = 6.9 Hz, 1H), 2.85 (d, J = 5.0 Hz, 3H), 2.77 (dq, J = 6.8, 5.7 Hz, 1H), 2.16 (s, 3H), 1.28 (d, J = 5.7 Hz, 3H).

^{13}C NMR (126 MHz, $CDCl_3$) δ 182.0, 166.9, 41.9, 38.3, 25.8, 23.3, 13.4.

HRMS: [M+H$^+$] - 157.09715 (found 157.09770, $C_7H_{13}N_2O_2$, ESI+)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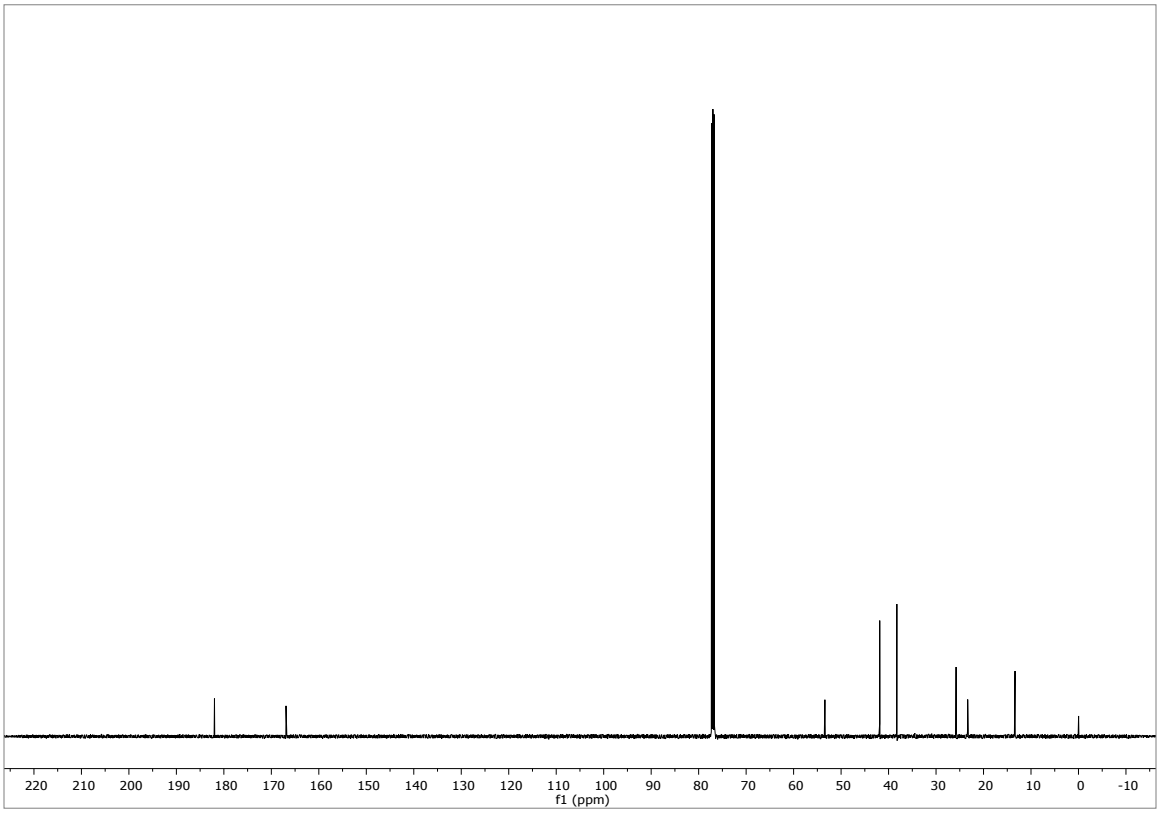
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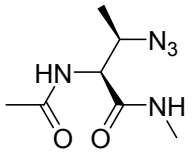


(2S,3R)-2-acetamido-3-azido-N-methylbutanamide (6): Ac-Cma-NHMe (50 mg, 0.32 mmol) was dissolved in DMF (3 mL). Sodium azide (0.208 g, 3.2 mmol) was added, the vial was flushed with argon, sealed and heated to 60 °C overnight. The solvent was removed by rotary evaporation, and the residue was dissolved in water/ACN. The sample was purified by reverse phase flash chromatography (0% ACN, 10 mins-50%, 13 mins-50%).

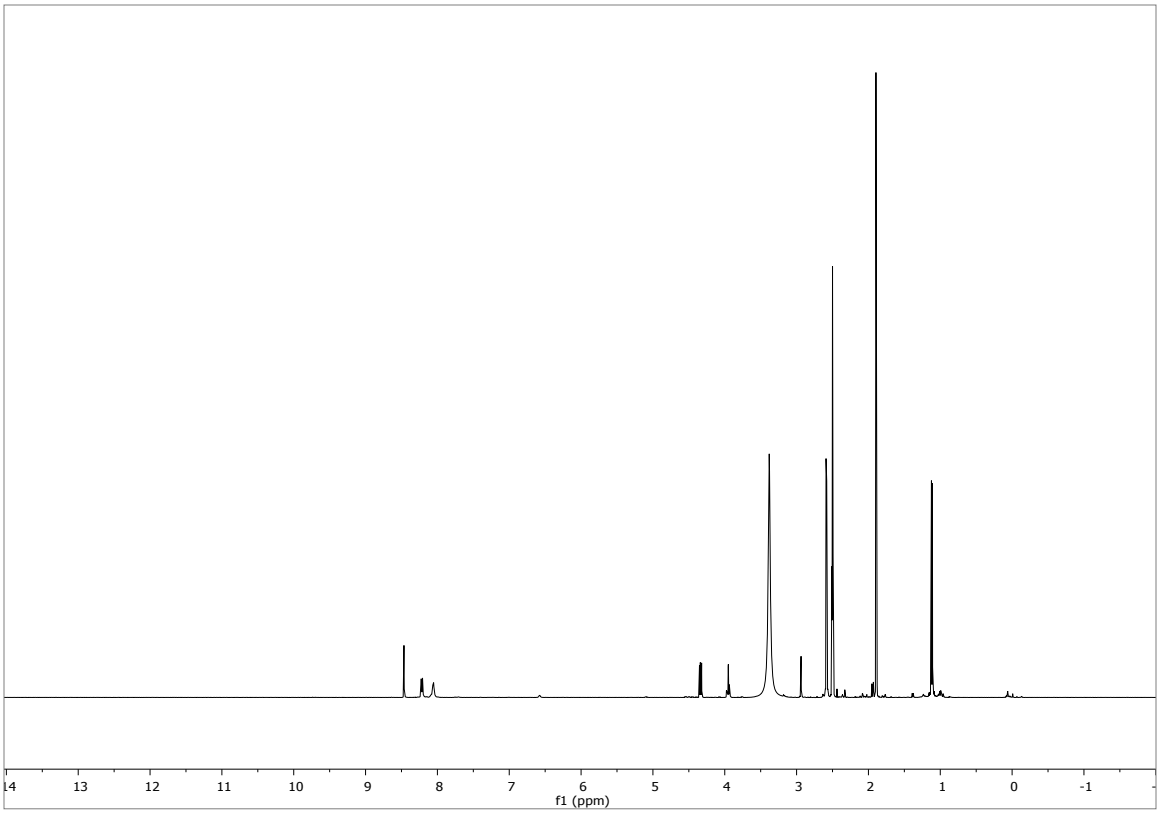
Yield: 41 mg, 64%.

The purified compound was analyzed by NMR. The 2D-COSY coupling pattern was consistent with attack of azide at the beta position of the Cma residue.

^{1}H NMR (500 MHz, DMSO-d6) δ 8.22 (d, J = 9.1 Hz, 1H), 8.06 (d, J = 4.9 Hz, 1H), 4.34 (dd, J = 9.1, 5.7 Hz, 1H), 3.95 (qd, J = 6.6, 5.6 Hz, 1H), 2.59 (d, J = 4.6 Hz, 3H), 1.90 (s, 3H), 1.12 (d, J = 6.7 Hz, 3H).

^{13}C NMR (126 MHz, DMSO-d6) δ 170.2, 169.8, 58.6, 56.7, 26.1, 22.9, 16.6.

HRMS: [M+H^{+}] - 200.11420 (found 200.11475, $C_7H_{14}N_5O_2$, ESI+)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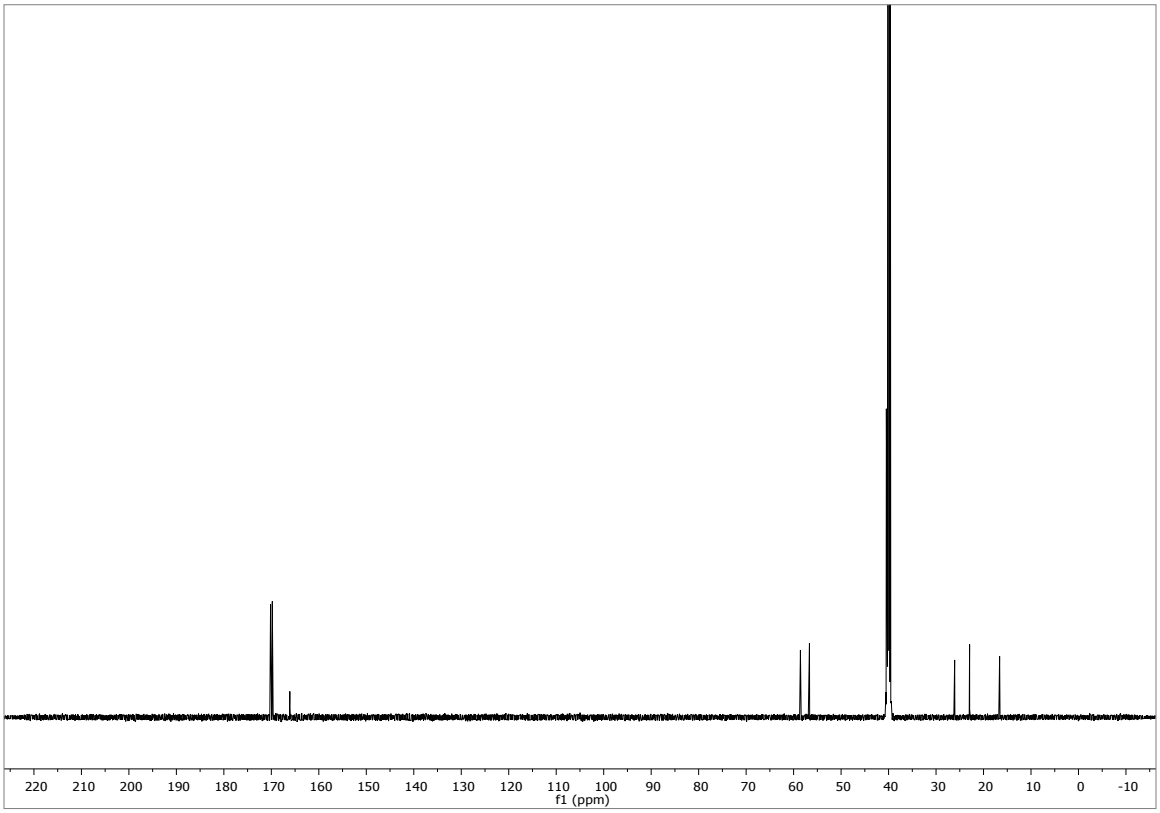
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f1 (ppm)

Computational Methodology

Software

Molecular mechanics modeling was carried out using Schrodinger Small Molecule Drug Discovery Suite (v2015-4). All *ab initio* structures and energies were calculated using Gaussian09.[2] NBO calculations were carried out using NBO6[3] contained in Gaussian09. Figures were generated using PyMol (v1.7).[4] Figures depicting NBOs were generated using VMD (v1.9).[5]

Conformational Searching

Geometry optimizations of ground states for **1**, **2** and **3** were carried out using a strategy involving molecular mechanics-driven conformational searches followed by Hartree-Fock energy re-ranking of conformers, followed by DFT-based geometry optimization.

Conformational searches of molecules were performed using Prime Macrocycle Sampling module (v4.3)[6] operating in diversity mode using the OPLS2005 force field and an implicit GBSA aqueous solvent model within Schrödinger Small Molecule Drug Discovery Suite (v2015-4).

The energy of the fifty lowest energy conformers were calculated using HF/3-21G* (in vacuo), the 20 lowest of which were then passed for single point energy calculations using B3LYP/6-31G+(d,p) (in vacuo).

Ground State Energy calculations

The lowest energy conformer from the second round of calculations was optimized to a minimum using B3LYP/6-31G+(d,p) and the IEFPCM continuum solvent model (DMF, ε=37.219).

Vibrational frequency analysis was carried out at a temperature of 333 K using the same level of theory to provide Gibbs free energy values for optimized complexes incorporating zero-point and thermal corrections. Absence of imaginary frequencies confirmed a local energetic minimum had been reached.

Energy values for ground states were recalculated using M06-2X/6-311++G(2d,p) which were then corrected using zero-point and thermal energy corrections from the previously run frequency calculations.

Transition State Energy Calculations

The structure of the azide anion was optimized using B3LYP/6-31G+(d,p). For each scenario involving azide attack at the alpha and beta positions, the azide anion was placed approximately 2.2 Å from the relevant electrophilic carbon of the aziridine ring. The scissile aziridine C-N bond was lengthened to 1.8

Å. These two interatomic distances were then frozen using redundant internal coordinates and the complex was optimized to a minimum using B3LYP/6-31G+(d,p). The resultant structure was optimized to a transition state using the QST3 algorithm at the B3LYP/6-31G+(d,p) level of theory. Vibrational frequency analysis was carried out was carried out at a temperature of 333 K to provide Gibbs Free Energy values for optimized complexes incorporating zero-point and thermal corrections and to confirm a single negative vibration had been obtained for each transition state. Energy values for transition states were recalculated using M06-2X/6-311++G(2d,p) which were then corrected using zero-point and thermal energy corrections from the previously run frequency calculations.

Stationary Point Energies and 3D Coordinates

1: GS-3

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (*N,N*-dimethylformamide)
Electronic Energy:	-533.8705297 hartrees
Thermal Free Energy Correction (333 K):	0.143054 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.097434	1.030338	0.257430
2	1	0	1.742778	1.642281	0.893304
3	6	0	0.355940	0.054305	1.084721
4	1	0	0.877549	-0.273876	1.972290
5	7	0	1.752298	-0.182012	-0.248852
6	6	0	2.940569	-0.512736	0.353270
7	8	0	3.506811	0.131851	1.261988
8	6	0	3.597924	-1.768301	-0.194827
9	1	0	3.845922	-2.442745	0.631335
10	1	0	2.957768	-2.285567	-0.911382
11	1	0	4.539342	-1.497618	-0.686238
12	6	0	-0.712437	-0.918503	0.657902
13	8	0	-0.727847	-2.059707	1.145999
14	7	0	-1.632124	-0.505898	-0.241065
15	1	0	-1.662321	0.466895	-0.506924
16	6	0	-2.728450	-1.366756	-0.667255
17	1	0	-3.385497	-1.621294	0.171296
18	1	0	-3.305866	-0.838820	-1.426659
19	1	0	-2.339267	-2.294679	-1.094520
20	6	0	0.447357	1.877787	-0.826818
21	1	0	-0.261262	2.595962	-0.401372
22	1	0	1.229168	2.444516	-1.342682
23	1	0	-0.059208	1.268029	-1.579522
24	7	0	-1.828358	1.714982	1.919359
25	7	0	-2.691129	2.290072	1.369533
26	7	0	-0.948750	1.122122	2.477460

2: GS-3-OH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-534.2821435 hartrees
Thermal Free Energy Correction (333 K):	0.162965 hartree/particle
Charge/Multiplicity	1/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.097434	1.030338	0.257430
2	1	0	1.742778	1.642281	0.893304
3	6	0	0.355940	0.054305	1.084721
4	1	0	0.877549	-0.273876	1.972290
5	7	0	1.752298	-0.182012	-0.248852
6	6	0	2.940569	-0.512736	0.353270
7	8	0	3.506811	0.131851	1.261988
8	6	0	3.597924	-1.768301	-0.194827
9	1	0	3.845922	-2.442745	0.631335
10	1	0	2.957768	-2.285567	-0.911382
11	1	0	4.539342	-1.497618	-0.686238
12	6	0	-0.712437	-0.918503	0.657902
13	8	0	-0.727847	-2.059707	1.145999
14	7	0	-1.632124	-0.505898	-0.241065
15	1	0	-1.662321	0.466895	-0.506924
16	6	0	-2.728450	-1.366756	-0.667255
17	1	0	-3.385497	-1.621294	0.171296
18	1	0	-3.305866	-0.838820	-1.426659
19	1	0	-2.339267	-2.294679	-1.094520
20	6	0	0.447357	1.877787	-0.826818
21	1	0	-0.261262	2.595962	-0.401372
22	1	0	1.229168	2.444516	-1.342682
23	1	0	-0.059208	1.268029	-1.579522
24	7	0	-1.828358	1.714982	1.919359
25	7	0	-2.691129	2.290072	1.369533
26	7	0	-0.948750	1.122122	2.477460

3: GS-3-NH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-534.2930602 hartrees
Thermal Free Energy Correction (333 K):	0.163517 hartree/particle
Charge/Multiplicity	1/1

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4	1	0	0.632546	-0.282975	2.073214
5	7	0	1.641610	-0.473369	0.165898
6	6	0	2.989943	-0.620717	0.790301
7	8	0	3.186420	-0.049331	1.827011
8	6	0	3.920597	-1.475368	0.000076
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17	1	0	-2.727310	-3.086970	0.854969
18	1	0	-3.714343	-1.899486	1.742651
19	1	0	-3.388797	-1.670332	0.006814
20	6	0	0.274335	1.368915	-1.058157
21	1	0	-0.437571	2.154193	-0.786184
22	1	0	1.041922	1.811871	-1.697073
23	1	0	-0.255859	0.589512	-1.607056
24	1	0	1.428851	-1.050627	-0.659129

4: TS-3a

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-698.1455922 hartrees
Thermal Free Energy Correction (333 K):	0.147094 hartree/particle
Charge/Multiplicity	-1/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.097434	1.030338	0.257430
2	1	0	1.742778	1.642281	0.893304
3	6	0	0.355940	0.054305	1.084721
4	1	0	0.877549	-0.273876	1.972290
5	7	0	1.752298	-0.182012	-0.248852
6	6	0	2.940569	-0.512736	0.353270
7	8	0	3.506811	0.131851	1.261988
8	6	0	3.597924	-1.768301	-0.194827
9	1	0	3.845922	-2.442745	0.631335
10	1	0	2.957768	-2.285567	-0.911382
11	1	0	4.539342	-1.497618	-0.686238
12	6	0	-0.712437	-0.918503	0.657902
13	8	0	-0.727847	-2.059707	1.145999
14	7	0	-1.632124	-0.505898	-0.241065
15	1	0	-1.662321	0.466895	-0.506924
16	6	0	-2.728450	-1.366756	-0.667255
17	1	0	-3.385497	-1.621294	0.171296
18	1	0	-3.305866	-0.838820	-1.426659
19	1	0	-2.339267	-2.294679	-1.094520
20	6	0	0.447357	1.877787	-0.826818
21	1	0	-0.261262	2.595962	-0.401372
22	1	0	1.229168	2.444516	-1.342682
23	1	0	-0.059208	1.268029	-1.579522
24	7	0	-1.828358	1.714982	1.919359
25	7	0	-2.691129	2.290072	1.369533
26	7	0	-0.948750	1.122122	2.477460

5: TS-3b

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-698.1511928 hartrees
Thermal Free Energy Correction (333 K):	0.145475 hartree/particle
Charge/Multiplicity	-1/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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4	1	0	0.585053	0.183250	-1.132046
5	7	0	-0.247346	1.450969	0.422206
6	6	0	0.638902	2.430865	0.055867
7	8	0	1.573212	2.297451	-0.761448
8	6	0	0.408145	3.774855	0.724786
9	1	0	1.322470	4.085746	1.241468
10	1	0	0.196316	4.528480	-0.041372
11	1	0	-0.418518	3.742726	1.436379
12	6	0	-1.347453	-0.588261	-0.550634
13	8	0	-1.333296	-1.681715	-1.138321
14	7	0	-2.471771	0.032283	-0.154090
15	1	0	-2.340455	0.926190	0.307320
16	6	0	-3.803220	-0.508618	-0.378852
17	1	0	-4.535683	0.192870	0.021909
18	1	0	-3.992559	-0.649838	-1.447807
19	1	0	-3.924303	-1.474665	0.121563
20	6	0	0.008239	-0.674878	2.246726
21	1	0	0.766703	-1.035556	2.942897
22	1	0	-0.559483	0.122747	2.734107
23	1	0	-0.677528	-1.495336	2.019042
24	7	0	2.411298	-2.023878	-0.378509
25	7	0	3.020443	-1.900422	-1.378626
26	7	0	1.790575	-2.142400	0.635608

6: TS-3a-OH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-698.5826058 hartrees
Thermal Free Energy Correction (333 K):	0.161623 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.035431	1.050357	0.504962
2	1	0	1.569930	1.669437	1.227970
3	6	0	0.276353	-0.058800	1.165365
4	1	0	0.630162	-0.369528	2.137186
5	7	0	1.715310	-0.187674	0.160557
6	6	0	2.974445	-0.453068	0.296539
7	8	0	3.825641	0.568050	0.398935
8	6	0	3.501690	-1.849061	0.284931
9	1	0	4.081501	-2.034310	1.195540
10	1	0	2.679295	-2.560225	0.223999
11	1	0	4.168577	-1.991072	-0.572664
12	6	0	-0.779631	-0.984055	0.594736
13	8	0	-0.770446	-2.169110	0.949686
14	7	0	-1.663296	-0.481237	-0.289426
15	1	0	-1.744260	0.520984	-0.395502
16	6	0	-2.739201	-1.303248	-0.835079
17	1	0	-3.440109	-1.613527	-0.052860
18	1	0	-3.271876	-0.717275	-1.584187
19	1	0	-2.324232	-2.197145	-1.305764
20	6	0	0.501261	1.867005	-0.658921
21	1	0	-0.269077	2.562587	-0.314226
22	1	0	1.321914	2.453979	-1.080083
23	1	0	0.096884	1.234757	-1.452009
24	7	0	-2.030876	1.649911	1.872451
25	7	0	-2.805626	2.248051	1.220629
26	7	0	-1.240750	1.028011	2.519945
27	1	0	4.749502	0.269200	0.427015

7: TS-3b-OH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-698.5844931 hartrees
Thermal Free Energy Correction (333 K):	0.157824 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.644776	-0.175297	1.144995
2	1	0	1.696306	0.054655	1.243151
3	6	0	0.059563	0.033603	-0.212497
4	1	0	0.759886	-0.045306	-1.043835
5	7	0	-0.026393	1.324105	0.450597
6	6	0	0.497500	2.416735	-0.025277
7	8	0	0.831056	2.454572	-1.311045
8	6	0	0.684931	3.632650	0.817533
9	1	0	1.738741	3.932163	0.805540
10	1	0	0.096434	4.463842	0.413135
11	1	0	0.373101	3.432563	1.841345
12	6	0	-1.264748	-0.642309	-0.572991
13	8	0	-1.255634	-1.742204	-1.135769
14	7	0	-2.383125	0.032408	-0.253858
15	1	0	-2.286005	0.935925	0.190203
16	6	0	-3.716459	-0.480733	-0.547658
17	1	0	-4.450289	0.233798	-0.175141
18	1	0	-3.854036	-0.608507	-1.625479
19	1	0	-3.874405	-1.446516	-0.059497
20	6	0	-0.116660	-0.591830	2.358430
21	1	0	0.198304	-1.605303	2.618200
22	1	0	0.125660	0.064207	3.198407
23	1	0	-1.194871	-0.586298	2.192800
24	7	0	2.469806	-2.188275	-0.184763
25	7	0	3.129821	-2.068169	-1.154006
26	7	0	1.798278	-2.299049	0.796130
27	1	0	1.151849	3.331191	-1.581110

8: TS-3a-NH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-698.6079475 hartrees
Thermal Free Energy Correction (333 K):	0.159805 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.920462	0.920909	0.236433
2	1	0	1.513474	1.643461	0.793635
3	6	0	0.297203	-0.095187	1.099596
4	1	0	0.692056	-0.220094	2.097644
5	7	0	1.730393	-0.308873	0.030644
6	6	0	3.020998	-0.489102	0.608753
7	8	0	3.419853	0.295243	1.447120
8	6	0	3.768652	-1.686043	0.094146
9	1	0	4.703731	-1.786825	0.643850
10	1	0	3.167562	-2.593387	0.211531
11	1	0	3.982504	-1.563711	-0.973127
12	6	0	-0.726833	-1.096129	0.552008
13	8	0	-0.500579	-1.687454	-0.517849
14	7	0	-1.807488	-1.283574	1.310537
15	1	0	-1.949399	-0.603845	2.059329
16	6	0	-2.873151	-2.200415	0.922317
17	1	0	-2.461136	-3.191351	0.718135
18	1	0	-3.582352	-2.267804	1.747307
19	1	0	-3.394235	-1.846980	0.026463
20	6	0	0.239547	1.492553	-0.987097
21	1	0	-0.450352	2.277016	-0.664847
22	1	0	0.988202	1.939475	-1.646144
23	1	0	-0.319622	0.735730	-1.540361
24	7	0	-1.410014	2.224420	2.183531
25	7	0	-1.636596	3.310213	1.802465
26	7	0	-1.174568	1.119822	2.582949
27	1	0	1.407168	-0.943798	-0.704518

9: TS-3b-NH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-698.6140977 hartrees
Thermal Free Energy Correction (333 K):	0.160645 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.889075	-0.012921	1.163275
2	1	0	1.905139	0.354147	1.093844
3	6	0	0.098893	0.105639	-0.075649
4	1	0	0.678406	0.160778	-0.995013
5	7	0	-0.070812	1.428602	0.548316
6	6	0	0.625768	2.580311	0.081020
7	8	0	1.572178	2.444586	-0.669129
8	6	0	0.097615	3.882386	0.610692
9	1	0	0.023510	3.852292	1.701997
10	1	0	0.762638	4.688659	0.303646
11	1	0	-0.906112	4.066809	0.212583
12	6	0	-1.252632	-0.610179	-0.193507
13	8	0	-2.239394	-0.139660	0.393170
14	7	0	-1.252112	-1.719178	-0.935713
15	1	0	-0.372421	-2.040023	-1.354585
16	6	0	-2.455114	-2.527257	-1.112814
17	1	0	-3.246744	-1.940515	-1.587076
18	1	0	-2.205534	-3.374917	-1.750604
19	1	0	-2.821483	-2.895507	-0.150143
20	6	0	0.383143	-0.492144	2.479096
21	1	0	0.936064	-1.406714	2.713255
22	1	0	0.606587	0.237617	3.262122
23	1	0	-0.684275	-0.715741	2.467893
24	7	0	1.918135	-2.314389	-0.538290
25	7	0	1.559038	-2.539205	-1.644986
26	7	0	2.242109	-2.064632	0.576088
27	1	0	-0.976737	1.535400	1.011155

10: GS-1

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1336.921629 hartrees
Thermal Free Energy Correction (333 K):	0.40698 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.323914	-0.917452	0.524778
2	6	0	-2.336635	-1.546620	-0.307287
3	6	0	-1.821850	-1.744557	-1.753620
4	8	0	-2.518884	-1.482544	-2.727451
5	6	0	-3.709933	-0.827844	-0.263153
6	6	0	-3.679002	0.684351	-0.396744
7	6	0	-3.852509	1.488752	0.740437
8	6	0	-3.506462	1.318382	-1.639175
9	6	0	-3.842551	2.883635	0.649150
10	6	0	-3.492871	2.712690	-1.732240
11	6	0	-3.657837	3.501278	-0.589780
12	1	0	-0.897468	-0.047635	0.230374
13	1	0	-2.482203	-2.546826	0.120927
14	1	0	-4.332032	-1.264885	-1.049240
15	1	0	-4.163906	-1.085282	0.698813
16	1	0	-4.013062	1.016606	1.706856
17	1	0	-3.390825	0.711273	-2.530816
18	1	0	-3.985781	3.484211	1.543171
19	1	0	-3.363201	3.183349	-2.703002
20	1	0	-3.652693	4.584798	-0.666164
21	7	0	-0.535868	-2.215445	-1.941691
22	6	0	0.299371	-2.991251	-1.026679
23	6	0	1.518011	-2.276025	-0.421032
24	8	0	2.262447	-2.892212	0.337805
25	1	0	-0.353508	-2.352073	-2.929953
26	1	0	-0.284055	-3.376050	-0.186567
27	1	0	0.683262	-3.869134	-1.555640
28	7	0	1.690493	-0.969923	-0.749887
29	6	0	2.722462	-0.129755	-0.156940
30	6	0	3.165277	0.933460	-1.194356
31	6	0	4.452870	1.728678	-0.897954
32	6	0	5.684897	0.819278	-0.772107
33	6	0	4.662313	2.777970	-2.002369
34	1	0	1.001517	-0.548887	-1.359395
35	1	0	3.561468	-0.787467	0.087724
36	1	0	3.298847	0.396153	-2.143278
37	1	0	2.335317	1.638314	-1.346999
38	1	0	4.321540	2.253974	0.053699
39	1	0	5.834649	0.225884	-1.683699
40	1	0	6.588063	1.418741	-0.615291
41	1	0	5.605248	0.129653	0.073990

42	1	0	3.804455	3.455785	-2.081226
43	1	0	5.549575	3.386412	-1.797480
44	1	0	4.805239	2.301933	-2.981155
45	6	0	2.293831	0.519032	1.176700
46	8	0	3.069573	1.197444	1.825912
47	7	0	0.943833	0.365168	1.544119
48	6	0	0.430471	-0.845715	2.204337
49	6	0	-0.815060	-1.497029	1.647801
50	8	0	-1.253083	-2.534196	2.141261
51	6	0	0.513376	0.473518	2.931014
52	1	0	1.159308	-1.597596	2.501631
53	1	0	1.328805	0.529606	3.652155
54	6	0	-0.681474	1.338557	3.250490
55	1	0	-1.455436	1.263495	2.483316
56	1	0	-1.111999	1.040029	4.212081
57	1	0	-0.373538	2.386535	3.324761

11: GS-1-OH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1337.330964 hartrees
Thermal Free Energy Correction (333 K):	0.429176 hartree/particle
Charge/Multiplicity	1/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.708976	-1.623826	-0.721784
2	6	0	0.386472	-2.351147	-0.070462
3	6	0	1.365428	-1.375151	0.628813
4	8	0	2.578894	-1.457209	0.457207
5	6	0	1.105595	-3.326942	-1.031725
6	6	0	1.818690	-4.474860	-0.340770
7	6	0	1.082579	-5.477923	0.311500
8	6	0	3.216179	-4.585464	-0.367456
9	6	0	1.724523	-6.554440	0.930089
10	6	0	3.863117	-5.663806	0.244580
11	6	0	3.119707	-6.650929	0.898765
12	1	0	-1.650271	-1.963025	-0.568138
13	1	0	-0.090473	-2.938390	0.721366
14	1	0	0.329304	-3.735314	-1.688110
15	1	0	1.803114	-2.765112	-1.655559
16	1	0	-0.003939	-5.425680	0.329025
17	1	0	3.800362	-3.817632	-0.865701
18	1	0	1.135676	-7.319704	1.427891
19	1	0	4.946952	-5.730765	0.210914
20	1	0	3.620903	-7.488485	1.375262
21	7	0	0.848890	-0.428887	1.477447
22	6	0	-0.498833	-0.296071	2.010829
23	6	0	-1.376070	0.806043	1.397522
24	8	0	-2.550797	0.920736	1.748543
25	1	0	1.575473	0.092941	1.955731
26	1	0	-1.054447	-1.231375	1.933626
27	1	0	-0.429425	-0.070996	3.079656
28	7	0	-0.782678	1.618511	0.481213
29	6	0	-1.417095	2.807441	-0.056678
30	6	0	-0.609176	4.090150	0.257308
31	6	0	-0.476572	4.399925	1.762071
32	6	0	0.521033	5.553718	1.955212
33	6	0	-1.827561	4.734110	2.414788
34	1	0	0.206878	1.480472	0.305536
35	1	0	-2.411205	2.870554	0.405449
36	1	0	0.388898	3.986699	-0.186404
37	1	0	-1.092273	4.935657	-0.240993
38	1	0	-0.061018	3.515242	2.262712
39	1	0	0.658947	5.771390	3.019447
40	1	0	1.501144	5.310111	1.530651
41	1	0	0.160950	6.469366	1.470134

42	1	0	-1.689533	4.972967	3.474607
43	1	0	-2.288267	5.605480	1.932917
44	1	0	-2.537764	3.902407	2.361162
45	6	0	-1.688684	2.666032	-1.551177
46	8	0	-1.878282	3.796238	-2.190167
47	7	0	-1.740690	1.528586	-2.157147
48	6	0	-1.809039	0.101098	-1.986151
49	6	0	-0.516963	-0.582082	-1.562676
50	8	0	0.589270	-0.155213	-1.889982
51	6	0	-2.009968	0.745529	-3.355519
52	1	0	-2.716569	-0.237039	-1.491223
53	1	0	-3.053559	0.799110	-3.662095
54	6	0	-0.995960	0.698004	-4.471975
55	1	0	-1.181893	-0.205394	-5.060197
56	1	0	-1.124302	1.562093	-5.128805
57	1	0	0.024130	0.672970	-4.090358
58	1	0	-2.126538	3.680581	-3.125056

12: GS-1-NH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1337.331366 hartrees
Thermal Free Energy Correction (333 K):	0.40698 hartree/particle
Charge/Multiplicity	1/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.526137	-2.206230	-0.827786
2	6	0	-0.473878	-3.340141	0.110737
3	6	0	-1.609178	-3.310034	1.176342
4	8	0	-2.277064	-4.342370	1.304329
5	6	0	0.907463	-3.664397	0.729058
6	6	0	1.920015	-4.157530	-0.289997
7	6	0	3.034762	-3.382376	-0.638218
8	6	0	1.767918	-5.420519	-0.885432
9	6	0	3.972861	-3.853554	-1.563546
10	6	0	2.700378	-5.892790	-1.812093
11	6	0	3.807512	-5.108660	-2.155452
12	1	0	-1.288997	-2.263786	-1.491978
13	1	0	-0.761338	-4.204700	-0.489878
14	1	0	1.306360	-2.808744	1.272992
15	1	0	0.718829	-4.458811	1.459915
16	1	0	3.165135	-2.404081	-0.185908
17	1	0	0.919631	-6.045823	-0.616200
18	1	0	4.831567	-3.239225	-1.819319
19	1	0	2.567014	-6.873842	-2.258976
20	1	0	4.535476	-5.475709	-2.873072
21	7	0	-1.875888	-2.229217	1.957176
22	6	0	-1.200104	-0.960201	2.110449
23	6	0	-1.780882	0.160837	1.230890
24	8	0	-2.632317	-0.031680	0.363228
25	1	0	-2.673916	-2.384995	2.562478
26	1	0	-1.263304	-0.663375	3.161662
27	1	0	-0.136558	-1.052350	1.877628
28	7	0	-1.211450	1.389098	1.401785
29	6	0	-1.614184	2.529336	0.587241
30	6	0	-0.924848	3.817433	1.104318
31	6	0	-1.362242	5.137097	0.436810
32	6	0	-2.846626	5.456485	0.676238
33	6	0	-0.469887	6.278528	0.952274
34	1	0	-0.561949	1.546781	2.163370
35	1	0	-2.701132	2.643841	0.623443
36	1	0	-1.149516	3.867567	2.177210
37	1	0	0.161740	3.700859	1.011722
38	1	0	-1.199453	5.054329	-0.645735
39	1	0	-3.105205	6.417474	0.219803
40	1	0	-3.513791	4.703310	0.245026
41	1	0	-3.061940	5.526344	1.749594

42	1	0	-0.736872	7.223263	0.467884
43	1	0	0.588625	6.082315	0.749580
44	1	0	-0.588565	6.411598	2.034547
45	6	0	-1.303410	2.283442	-0.890741
46	8	0	-1.887186	2.731496	-1.834324
47	7	0	-0.142880	1.376291	-1.126083
48	6	0	-0.387387	0.018412	-1.751063
49	6	0	0.163563	-1.055280	-0.816700
50	8	0	1.095307	-0.759127	-0.060393
51	6	0	0.437339	1.024396	-2.473354
52	1	0	-1.409930	-0.098450	-2.095162
53	1	0	-0.112912	1.537768	-3.257649
54	6	0	1.934931	1.001825	-2.615209
55	1	0	2.172229	0.459834	-3.535163
56	1	0	2.312061	2.022525	-2.713901
57	1	0	2.426917	0.504867	-1.778965
58	1	0	0.518240	1.267464	-0.344856

13: TS-1a

Calculation Method M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation IEFPCM (N,N-dimethylformamide)
Electronic Energy: -1501.202254 hartrees
Thermal Free Energy Correction (333 K): 0.408981 hartree/particle
Charge/Multiplicity -1/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.083320	-0.343067	-0.844423
2	6	0	1.871397	-1.551117	-1.054434
3	6	0	1.112144	-2.815669	-0.587292
4	8	0	1.622620	-3.625118	0.191381
5	6	0	3.303750	-1.454900	-0.463807
6	6	0	3.453617	-0.839017	0.916816
7	6	0	4.083008	0.408935	1.050702
8	6	0	3.020392	-1.490932	2.084684
9	6	0	4.275477	0.993461	2.306860
10	6	0	3.205134	-0.906719	3.341466
11	6	0	3.834531	0.337309	3.459168
12	1	0	0.564375	-0.204992	0.018217
13	1	0	1.989443	-1.645346	-2.140095
14	1	0	3.726694	-2.463974	-0.474718
15	1	0	3.886913	-0.854627	-1.168176
16	1	0	4.429242	0.928975	0.161070
17	1	0	2.541432	-2.460459	2.001117
18	1	0	4.767925	1.959005	2.382102
19	1	0	2.862994	-1.428754	4.231063
20	1	0	3.981454	0.787145	4.437001
21	7	0	-0.148475	-3.038300	-1.070501
22	6	0	-0.824671	-2.415781	-2.201070
23	6	0	-1.960580	-1.439478	-1.865998
24	8	0	-2.533911	-0.849913	-2.791723
25	1	0	-0.529346	-3.922883	-0.751805
26	1	0	-0.116578	-1.867613	-2.825662
27	1	0	-1.250336	-3.202642	-2.831075
28	7	0	-2.273627	-1.280432	-0.564371
29	6	0	-3.138843	-0.203560	-0.087553
30	6	0	-3.576644	-0.527648	1.357138
31	6	0	-4.619578	0.417082	1.985973
32	6	0	-5.977745	0.348535	1.269291
33	6	0	-4.780062	0.088031	3.479247
34	1	0	-1.664670	-1.729147	0.108703
35	1	0	-4.008569	-0.161447	-0.746306
36	1	0	-3.980240	-1.549456	1.355072
37	1	0	-2.678613	-0.542398	1.989254
38	1	0	-4.245494	1.445915	1.907039
39	1	0	-6.386255	-0.669650	1.307247
40	1	0	-6.701384	1.016296	1.749922
41	1	0	-5.905427	0.644479	0.218259

42	1	0	-3.828027	0.182582	4.013838
43	1	0	-5.501001	0.763429	3.952961
44	1	0	-5.142835	-0.938477	3.618622
45	6	0	-2.439160	1.171999	-0.192593
46	8	0	-3.122426	2.184271	-0.423860
47	7	0	-1.089282	1.127935	0.026430
48	6	0	-0.085042	1.718483	-1.497821
49	6	0	0.796431	0.532480	-1.842114
50	8	0	1.176556	0.367722	-3.007623
51	6	0	-0.331985	2.357278	-0.183210
52	1	0	-0.832080	1.912078	-2.256310
53	1	0	-0.955068	3.247165	-0.303375
54	6	0	0.797755	2.607508	0.799835
55	1	0	1.451979	1.741700	0.921137
56	1	0	1.403885	3.452648	0.460077
57	1	0	0.374706	2.859126	1.777869
58	7	0	1.057536	3.341055	-2.511516
59	7	0	2.241643	3.170630	-2.533307
60	7	0	3.405805	3.014021	-2.561747

14: TS-1b

Calculation Method M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation IEFPCM (N,N-dimethylformamide)
Electronic Energy: -1501.194538 hartrees
Thermal Free Energy Correction (333 K): 0.408601 hartree/particle
Charge/Multiplicity -1/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.420902	-0.711727	0.416305
2	6	0	-2.350220	-1.539765	-0.336447
3	6	0	-1.882596	-1.664185	-1.808688
4	8	0	-2.632362	-1.400793	-2.750482
5	6	0	-3.827681	-1.084055	-0.206267
6	6	0	-4.097941	0.407734	-0.302452
7	6	0	-4.310909	1.154116	0.867876
8	6	0	-4.177512	1.074430	-1.537150
9	6	0	-4.583001	2.525028	0.813679
10	6	0	-4.448999	2.444656	-1.595578
11	6	0	-4.651055	3.176826	-0.420829
12	1	0	-1.190003	0.222618	0.090312
13	1	0	-2.287742	-2.539999	0.107500
14	1	0	-4.403721	-1.623205	-0.963426
15	1	0	-4.171371	-1.433335	0.772058
16	1	0	-4.272969	0.654947	1.832868
17	1	0	-4.021616	0.511296	-2.450663
18	1	0	-4.745767	3.079116	1.733912
19	1	0	-4.507850	2.939414	-2.561290
20	1	0	-4.865043	4.240776	-0.467880
21	7	0	-0.593201	-2.064474	-2.052019
22	6	0	0.319023	-2.789733	-1.174782
23	6	0	1.485023	-2.001458	-0.561257
24	8	0	2.261816	-2.591419	0.201421
25	1	0	-0.403861	-2.141003	-3.045607
26	1	0	-0.219088	-3.230841	-0.332525
27	1	0	0.751618	-3.622708	-1.735826
28	7	0	1.566540	-0.688521	-0.855483
29	6	0	2.457874	0.252952	-0.168423
30	6	0	3.571498	0.761406	-1.098300
31	6	0	4.778469	1.411478	-0.388340
32	6	0	5.619034	0.386567	0.391485
33	6	0	5.653296	2.151071	-1.413052
34	1	0	0.881680	-0.320074	-1.504324
35	1	0	2.906280	-0.318857	0.649296
36	1	0	3.927826	-0.096282	-1.683978
37	1	0	3.135400	1.476862	-1.804273
38	1	0	4.393677	2.154512	0.320924
39	1	0	6.037526	-0.369497	-0.285328
40	1	0	6.455917	0.879169	0.899346
41	1	0	5.037280	-0.137575	1.157301

42	1	0	5.083522	2.926969	-1.936731
43	1	0	6.509502	2.632004	-0.926543
44	1	0	6.045896	1.456378	-2.167199
45	6	0	1.577911	1.395414	0.439504
46	8	0	1.828295	2.574957	0.138982
47	7	0	0.487758	1.058243	1.180608
48	6	0	0.400090	-0.178559	1.921998
49	6	0	-0.739731	-1.122305	1.511892
50	8	0	-0.931554	-2.203938	2.078197
51	6	0	0.245418	0.756253	3.069734
52	1	0	1.303041	-0.793689	1.999839
53	1	0	1.170818	1.177439	3.438327
54	6	0	-1.041836	1.420183	3.456670
55	1	0	-1.079344	2.436019	3.056012
56	1	0	-1.909975	0.868367	3.089294
57	1	0	-1.097972	1.480505	4.545016
58	7	0	0.367405	-0.543626	4.864726
59	7	0	1.376327	-1.185840	4.812828
60	7	0	2.368782	-1.812761	4.757822

15: TS-1a-OH+

Calculation Method M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation IEFPCM (N,N-dimethylformamide)
Electronic Energy: -1501.635898 hartrees
Thermal Free Energy Correction (333 K): 0.420947 hartree/particle
Charge/Multiplicity 0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.633831	-1.663788	-0.826894
2	6	0	0.457967	-2.387915	-0.169095
3	6	0	1.481411	-1.394779	0.436335
4	8	0	2.680507	-1.458552	0.173393
5	6	0	1.125812	-3.455149	-1.069720
6	6	0	1.788247	-4.579528	-0.295119
7	6	0	1.004706	-5.555602	0.343433
8	6	0	3.184018	-4.688982	-0.213934
9	6	0	1.597477	-6.605451	1.050389
10	6	0	3.782304	-5.740650	0.488071
11	6	0	2.991180	-6.701371	1.125365
12	1	0	-1.576569	-1.960506	-0.604584
13	1	0	-0.013907	-2.907806	0.670936
14	1	0	0.328542	-3.873689	-1.692859
15	1	0	1.844603	-2.968801	-1.730331
16	1	0	-0.079880	-5.501108	0.279366
17	1	0	3.803602	-3.940854	-0.698828
18	1	0	0.972403	-7.350703	1.534341
19	1	0	4.865619	-5.808185	0.536342
20	1	0	3.454563	-7.518681	1.670497
21	7	0	1.011472	-0.439538	1.302189
22	6	0	-0.289262	-0.357007	1.951611
23	6	0	-1.254629	0.723285	1.443323
24	8	0	-2.415382	0.741642	1.864141
25	1	0	1.760682	0.100566	1.721601
26	1	0	-0.819462	-1.307977	1.901445
27	1	0	-0.133946	-0.150966	3.015599
28	7	0	-0.750923	1.635108	0.578936
29	6	0	-1.505905	2.765490	0.073720
30	6	0	-0.744602	4.099817	0.281311
31	6	0	-0.518709	4.484715	1.757058
32	6	0	0.457473	5.670050	1.833603
33	6	0	-1.832123	4.815177	2.483529
34	1	0	0.210707	1.521568	0.280828
35	1	0	-2.453400	2.787147	0.622380
36	1	0	0.223343	4.021651	-0.230271
37	1	0	-1.304370	4.896933	-0.218773
38	1	0	-0.049074	3.632073	2.265673
39	1	0	0.652261	5.945467	2.875612
40	1	0	1.417050	5.428679	1.363154
41	1	0	0.045379	6.551292	1.326204

42	1	0	-1.634178	5.092180	3.524520
43	1	0	-2.340569	5.660405	2.002913
44	1	0	-2.526465	3.968668	2.499669
45	6	0	-1.865546	2.573732	-1.392175
46	8	0	-2.576828	3.580281	-1.890714
47	7	0	-1.441377	1.565317	-2.069125
48	6	0	-1.716992	-0.132005	-2.313022
49	6	0	-0.443916	-0.819900	-1.879225
50	8	0	0.661398	-0.566565	-2.354685
51	6	0	-1.829968	0.950626	-3.330919
52	1	0	-2.614287	-0.333112	-1.741607
53	1	0	-2.867614	1.133244	-3.623473
54	6	0	-0.866989	1.080105	-4.496303
55	1	0	-1.117490	0.320921	-5.241886
56	1	0	-0.981714	2.066018	-4.955904
57	1	0	0.164744	0.939277	-4.177649
58	1	0	-2.814979	3.445374	-2.823932
59	7	0	-2.308628	-1.951308	-3.559569
60	7	0	-2.745122	-2.771273	-2.804085
61	7	0	-3.158410	-3.563804	-2.041353

16: TS-1b-OH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1501.634838 hartrees
Thermal Free Energy Correction (333 K):	0.418483 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.592472	-1.499774	-0.748864
2	6	0	0.488417	-2.257856	-0.112563
3	6	0	1.485278	-1.305027	0.591670
4	8	0	2.698486	-1.407961	0.424494
5	6	0	1.186705	-3.241534	-1.081280
6	6	0	1.875132	-4.409520	-0.399357
7	6	0	1.118188	-5.401264	0.246573
8	6	0	3.269999	-4.550103	-0.427233
9	6	0	1.737224	-6.495429	0.857542
10	6	0	3.894141	-5.646211	0.176921
11	6	0	3.130046	-6.621699	0.824807
12	1	0	-1.540556	-1.828777	-0.615831
13	1	0	0.003451	-2.842246	0.676805
14	1	0	0.401674	-3.628024	-1.740410
15	1	0	1.895785	-2.690535	-1.701584
16	1	0	0.033028	-5.325953	0.264590
17	1	0	3.869957	-3.791455	-0.920809
18	1	0	1.132286	-7.251374	1.350358
19	1	0	4.976313	-5.736194	0.141968
20	1	0	3.613337	-7.473162	1.295181
21	7	0	0.981495	-0.350813	1.439104
22	6	0	-0.365548	-0.209466	1.973000
23	6	0	-1.256418	0.868932	1.337217
24	8	0	-2.443831	0.943377	1.661527
25	1	0	1.713577	0.161604	1.918680
26	1	0	-0.916123	-1.149653	1.923466
27	1	0	-0.290313	0.044029	3.035157
28	7	0	-0.667969	1.703275	0.441774
29	6	0	-1.323834	2.879013	-0.111106
30	6	0	-0.593018	4.180196	0.295012
31	6	0	-0.560402	4.452250	1.812540
32	6	0	0.384433	5.631040	2.098192
33	6	0	-1.958361	4.725701	2.390895
34	1	0	0.327216	1.590213	0.282170
35	1	0	-2.343872	2.882477	0.292402
36	1	0	0.433184	4.130491	-0.091007
37	1	0	-1.078608	5.021387	-0.207915
38	1	0	-0.147494	3.567359	2.315343
39	1	0	0.446549	5.827157	3.173966
40	1	0	1.397616	5.429732	1.732702
41	1	0	0.026396	6.546784	1.611416
42	1	0	-1.893436	4.933866	3.464318
43	1	0	-2.415101	5.598855	1.908160

44	1	0	-2.636592	3.875715	2.265207
45	6	0	-1.490211	2.758192	-1.629212
46	8	0	-1.635759	3.929973	-2.241021
47	7	0	-1.489057	1.674090	-2.311713
48	6	0	-1.659952	0.283819	-1.984019
49	6	0	-0.381786	-0.461838	-1.590866
50	8	0	0.734813	-0.081522	-1.942657
51	6	0	-2.068888	0.385826	-3.414596
52	1	0	-2.489747	0.080498	-1.306608
53	1	0	-3.103877	0.658077	-3.578519
54	6	0	-1.149744	0.263859	-4.586002
55	1	0	-1.408870	-0.656678	-5.114743
56	1	0	-1.301997	1.102436	-5.270005
57	1	0	-0.104631	0.221428	-4.278842
58	1	0	-1.797118	3.792968	-3.191731
59	7	0	-2.954288	-1.827027	-3.472460
60	7	0	-4.131732	-1.794140	-3.268012
61	7	0	-5.291486	-1.757440	-3.067796

17: TS-1a-NH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1501.653408 hartrees
Thermal Free Energy Correction (333 K):	0.408981 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.530893	-2.255824	-0.919507
2	6	0	-0.476737	-3.349188	0.058760
3	6	0	-1.651220	-3.314436	1.080967
4	8	0	-2.359706	-4.326242	1.156706
5	6	0	0.890875	-3.619897	0.736468
6	6	0	1.941279	-4.135180	-0.231477
7	6	0	3.012396	-3.327565	-0.638521
8	6	0	1.862472	-5.446324	-0.728750
9	6	0	3.979892	-3.815174	-1.524037
10	6	0	2.825027	-5.935971	-1.614937
11	6	0	3.888502	-5.119829	-2.016656
12	1	0	-1.103352	-2.419140	-1.746863
13	1	0	-0.720884	-4.242094	-0.518591
14	1	0	1.257750	-2.732448	1.251342
15	1	0	0.698172	-4.385268	1.496966
16	1	0	3.082657	-2.310594	-0.264987
17	1	0	1.046608	-6.093649	-0.414793
18	1	0	4.803218	-3.174586	-1.827522
19	1	0	2.748516	-6.954135	-1.985803
20	1	0	4.639323	-5.499447	-2.703596
21	7	0	-1.902033	-2.253398	1.892720
22	6	0	-1.217938	-0.991413	2.061990
23	6	0	-1.816409	0.151318	1.222751
24	8	0	-2.710726	-0.017933	0.394236
25	1	0	-2.724602	-2.397077	2.467264
26	1	0	-1.253968	-0.718633	3.121322
27	1	0	-0.163169	-1.082565	1.795394
28	7	0	-1.225662	1.366568	1.400250
29	6	0	-1.607231	2.525769	0.599649
30	6	0	-0.894615	3.788563	1.138950
31	6	0	-1.297456	5.126948	0.486912
32	6	0	-2.771278	5.484574	0.737332
33	6	0	-0.372924	6.239837	1.007550
34	1	0	-0.520198	1.483756	2.117827
35	1	0	-2.691589	2.655852	0.646267
36	1	0	-1.117087	3.834695	2.212800
37	1	0	0.189680	3.649775	1.044615
38	1	0	-1.143890	5.048409	-0.597303
39	1	0	-3.007430	6.456313	0.291135
40	1	0	-3.459539	4.752091	0.304100
41	1	0	-2.978377	5.550442	1.812749
42	1	0	-0.617332	7.196985	0.535343

43	1	0	0.679019	6.018124	0.796482
44	1	0	-0.481098	6.364349	2.092146
45	6	0	-1.307187	2.292067	-0.888532
46	8	0	-1.955792	2.748621	-1.801762
47	7	0	-0.179797	1.448234	-1.149590
48	6	0	-0.466893	-0.063801	-1.918434
49	6	0	0.105212	-1.077355	-0.923437
50	8	0	0.993843	-0.719599	-0.135234
51	6	0	0.296777	1.050612	-2.507268
52	1	0	-1.529150	-0.097002	-2.116713
53	1	0	-0.265891	1.597447	-3.260898
54	6	0	1.788542	1.026413	-2.735586
55	1	0	1.976816	0.512898	-3.682269
56	1	0	2.165331	2.048911	-2.817757
57	1	0	2.321231	0.502978	-1.940928
58	1	0	0.465412	1.237534	-0.381634
59	7	0	-0.682506	-1.748470	-3.695516
60	7	0	-1.226509	-1.196859	-4.607698
61	7	0	-1.755090	-0.651649	-5.503948

18: TS-1b-NH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1501.647615 hartrees
Thermal Free Energy Correction (333 K):	0.408601 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.536179	-2.151121	-0.964338
2	6	0	-0.501465	-3.292181	-0.039381
3	6	0	-1.680796	-3.298177	0.979944
4	8	0	-2.385952	-4.314931	1.008498
5	6	0	0.857601	-3.603997	0.636279
6	6	0	1.926809	-4.047512	-0.346213
7	6	0	3.018464	-3.222122	-0.650338
8	6	0	1.850548	-5.310637	-0.955664
9	6	0	4.008757	-3.644938	-1.543916
10	6	0	2.835681	-5.735211	-1.850609
11	6	0	3.919783	-4.901864	-2.148442
12	1	0	-1.157189	-2.261675	-1.773315
13	1	0	-0.749727	-4.154031	-0.660815
14	1	0	1.211910	-2.751657	1.214935
15	1	0	0.656829	-4.419562	1.340556
16	1	0	3.088638	-2.242093	-0.188187
17	1	0	1.019087	-5.972168	-0.722888
18	1	0	4.848027	-2.991661	-1.765715
19	1	0	2.760621	-6.717091	-2.309245
20	1	0	4.688130	-5.231532	-2.841758
21	7	0	-1.941664	-2.278171	1.842227
22	6	0	-1.286244	-1.010240	2.079501
23	6	0	-1.879816	0.149225	1.259401
24	8	0	-2.720856	-0.021984	0.374959
25	1	0	-2.768282	-2.460153	2.400081
26	1	0	-1.361708	-0.778936	3.146258
27	1	0	-0.221942	-1.071805	1.843220
28	7	0	-1.348417	1.378612	1.502789
29	6	0	-1.698829	2.534168	0.675704
30	6	0	-0.885533	3.766530	1.128512
31	6	0	-1.196019	5.084645	0.390160
32	6	0	-2.647328	5.549234	0.592763
33	6	0	-0.209496	6.168262	0.854873
34	1	0	-0.661672	1.496826	2.237757
35	1	0	-2.769913	2.734907	0.761784
36	1	0	-1.087698	3.899886	2.199210
37	1	0	0.185163	3.544156	1.035516
38	1	0	-1.033352	4.928197	-0.685158
39	1	0	-2.812846	6.508332	0.090836
40	1	0	-3.375101	4.839717	0.186903
41	1	0	-2.865697	5.687411	1.659026
42	1	0	-0.384621	7.106054	0.317589
43	1	0	0.829126	5.867231	0.679092

44	1	0	-0.326391	6.369308	1.926964
45	6	0	-1.492572	2.196301	-0.814168
46	8	0	-2.251449	2.512766	-1.699748
47	7	0	-0.314280	1.430811	-1.092431
48	6	0	-0.450705	0.127442	-1.795582
49	6	0	0.091089	-0.972846	-0.864667
50	8	0	0.953294	-0.662075	-0.030998
51	6	0	0.387226	0.887487	-2.728487
52	1	0	-1.471702	-0.039136	-2.130467
53	1	0	-0.166372	1.500528	-3.429026
54	6	0	1.873002	0.964854	-2.724825
55	1	0	2.208538	0.558011	-3.683529
56	1	0	2.197010	2.008252	-2.680657
57	1	0	2.325351	0.392535	-1.915260
58	1	0	0.364824	1.326511	-0.333024
59	7	0	0.121955	-0.767051	-4.604706
60	7	0	-0.752991	-1.473394	-4.221281
61	7	0	-1.622294	-2.157271	-3.797129

19: GS-2

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1544.922423 hartrees
Thermal Free Energy Correction (333 K):	0.45271 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.335827	-0.650317	4.844605
2	6	0	-1.715244	-0.084840	6.132762
3	6	0	-2.501386	1.238644	5.967622
4	8	0	-2.629040	2.020909	6.910927
5	6	0	-0.536747	0.053889	7.131618
6	6	0	0.669185	0.838900	6.649933
7	6	0	0.652376	2.242951	6.570201
8	6	0	1.853241	0.169563	6.303108
9	6	0	1.779583	2.949661	6.141325
10	6	0	2.984361	0.873537	5.876188
11	6	0	2.949869	2.267926	5.790092
12	1	0	-0.837155	-0.076166	4.174154
13	1	0	-2.423154	-0.795829	6.574142
14	1	0	-0.946350	0.510250	8.037364
15	1	0	-0.223509	-0.961339	7.391698
16	1	0	-0.245018	2.782516	6.856038
17	1	0	1.894613	-0.913848	6.380733
18	1	0	1.746429	4.034507	6.091291
19	1	0	3.889896	0.332278	5.616898
20	1	0	3.826813	2.818544	5.462181
21	7	0	-3.040299	1.461377	4.737807
22	6	0	-3.870942	2.610237	4.416889
23	6	0	-3.486939	3.302778	3.101707
24	8	0	-4.330057	3.955271	2.479922
25	1	0	-3.042428	0.686716	4.086546
26	1	0	-4.923465	2.325849	4.326485
27	1	0	-3.786068	3.328392	5.237122
28	7	0	-2.196377	3.156649	2.709068
29	6	0	-1.663075	3.616517	1.424802
30	6	0	-1.609706	2.408078	0.457730
31	8	0	-2.422721	2.296629	-0.462894
32	6	0	-0.328949	4.358506	1.619117
33	6	0	0.317923	4.901695	0.328124
34	6	0	-0.551979	5.967102	-0.359237
35	6	0	1.714378	5.461203	0.643098
36	1	0	-1.591836	2.623117	3.320732
37	1	0	-2.413988	4.285612	1.005279
38	1	0	-0.520527	5.190229	2.308932
39	1	0	0.387394	3.700834	2.130354
40	1	0	0.446547	4.063243	-0.371165
41	1	0	-0.051864	6.349867	-1.255346
42	1	0	-1.524938	5.573812	-0.670710
43	1	0	-0.729787	6.815407	0.313592

44	1	0	2.359394	4.697524	1.092031
45	1	0	2.203908	5.823442	-0.267257
46	1	0	1.648466	6.301715	1.345233
47	7	0	-0.653805	1.473665	0.717464
48	6	0	-0.640685	0.149103	0.101288
49	6	0	-1.454676	-0.816049	0.969902
50	8	0	-2.603935	-1.136446	0.707905
51	1	0	-0.025135	1.617599	1.495677
52	1	0	-1.098856	0.212312	-0.884577
53	1	0	0.393932	-0.189851	0.008937
54	7	0	-0.826048	-1.152025	2.175621
55	6	0	-1.288121	-2.244860	3.010166
56	6	0	-1.609599	-1.924163	4.455655
57	8	0	-2.140723	-2.770105	5.180488
58	6	0	0.097863	-2.277433	2.401139
59	1	0	-2.013827	-2.931363	2.579864
60	1	0	0.172419	-2.970945	1.563791
61	6	0	1.386938	-2.047683	3.144658
62	1	0	2.143127	-1.641293	2.465528
63	1	0	1.265373	-1.356358	3.980037
64	1	0	1.758560	-3.001645	3.532515

20: GS-2-OH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1545.345593 hartrees
Thermal Free Energy Correction (333 K):	0.480531 hartree/particle
Charge/Multiplicity	1/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.010094	0.206128	4.367430
2	6	0	-1.202407	1.035985	5.566799
3	6	0	-2.076325	2.249192	5.166262
4	8	0	-1.620442	3.399078	5.138927
5	6	0	0.120935	1.518863	6.200970
6	6	0	0.942769	0.427703	6.854628
7	6	0	2.093168	-0.081783	6.236281
8	6	0	0.579764	-0.080603	8.112681
9	6	0	2.854084	-1.084649	6.847759
10	6	0	1.335025	-1.081651	8.727234
11	6	0	2.475004	-1.590635	8.093991
12	1	0	-0.863878	0.697001	3.486557
13	1	0	-1.749970	0.420258	6.286568
14	1	0	0.709174	2.031428	5.434772
15	1	0	-0.145133	2.273356	6.947970
16	1	0	2.402386	0.314365	5.272728
17	1	0	-0.299602	0.313448	8.616942
18	1	0	3.742900	-1.464708	6.351957
19	1	0	1.038336	-1.460430	9.701273
20	1	0	3.065034	-2.367180	8.572068
21	7	0	-3.353765	1.973481	4.815146
22	6	0	-4.259616	2.995794	4.289687
23	6	0	-4.036331	3.197064	2.780438
24	8	0	-4.848884	2.796456	1.942644
25	1	0	-3.667985	1.011912	4.804598
26	1	0	-5.286249	2.666937	4.443900
27	1	0	-4.091624	3.927067	4.836388
28	7	0	-2.861881	3.805851	2.460986
29	6	0	-2.281146	3.734215	1.121091
30	6	0	-1.626121	2.346918	0.986179
31	8	0	-0.839803	1.923599	1.846340
32	6	0	-1.247416	4.862092	0.940435
33	6	0	-0.661835	5.010937	-0.479042
34	6	0	-1.703376	5.516060	-1.491292
35	6	0	0.552460	5.952957	-0.441963
36	1	0	-2.221748	3.987544	3.231324
37	1	0	-3.095513	3.834193	0.401418
38	1	0	-1.736564	5.799900	1.231185
39	1	0	-0.432970	4.690490	1.655113
40	1	0	-0.304802	4.026792	-0.815737
41	1	0	-2.570465	4.852589	-1.573647
42	1	0	-2.069187	6.509426	-1.203043
43	1	0	-1.260750	5.599294	-2.489667

44	1	0	0.993705	6.059594	-1.438724
45	1	0	0.260514	6.952703	-0.096817
46	1	0	1.328794	5.576927	0.233390
47	7	0	-1.964781	1.578467	-0.076050
48	6	0	-1.469764	0.213891	-0.165349
49	6	0	-1.899670	-0.566381	1.060019
50	8	0	-3.181665	-0.496834	1.328908
51	1	0	-2.694591	1.872362	-0.711121
52	1	0	-1.899806	-0.260057	-1.050189
53	1	0	-0.382120	0.190848	-0.242784
54	7	0	-1.070800	-1.212243	1.806282
55	6	0	-0.903277	-1.898763	3.069104
56	6	0	-1.066355	-1.146149	4.391572
57	8	0	-1.258370	-1.824946	5.399706
58	6	0	0.262580	-1.705837	2.092845
59	1	0	-1.330578	-2.896273	3.124337
60	1	0	0.479475	-2.604342	1.517184
61	6	0	1.439199	-0.783293	2.285474
62	1	0	1.193356	0.124436	2.834284
63	1	0	2.209273	-1.332227	2.834568
64	1	0	1.852292	-0.506290	1.312018
65	1	0	-3.459063	-1.033808	2.092859

21: GS-2-NH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1545.345593 hartrees
Thermal Free Energy Correction (333 K):	0.466903 hartree/particle
Charge/Multiplicity	1/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.601850	-0.101700	4.068646
2	6	0	-0.448486	0.548479	5.382968
3	6	0	-0.789998	2.026229	5.129422
4	8	0	0.055743	2.800323	4.660046
5	6	0	0.964513	0.354231	5.971099
6	6	0	1.073321	0.845802	7.401309
7	6	0	1.634328	2.096977	7.698384
8	6	0	0.600043	0.054648	8.461081
9	6	0	1.717987	2.548633	9.019580
10	6	0	0.680067	0.503350	9.782052
11	6	0	1.239118	1.754177	10.065511
12	1	0	-0.391653	0.460058	3.249472
13	1	0	-1.185324	0.090213	6.046793
14	1	0	1.186097	-0.716589	5.925767
15	1	0	1.682757	0.872219	5.329754
16	1	0	2.008629	2.719639	6.890663
17	1	0	0.173667	-0.923677	8.251853
18	1	0	2.158982	3.518874	9.230047
19	1	0	0.312113	-0.124734	10.588373
20	1	0	1.305257	2.103129	11.091922
21	7	0	-2.076040	2.382480	5.332026
22	6	0	-2.616074	3.663427	4.877616
23	6	0	-2.930023	3.635192	3.369210
24	8	0	-4.089220	3.653968	2.946545
25	1	0	-2.731693	1.686120	5.661844
26	1	0	-3.543087	3.860673	5.413320
27	1	0	-1.894291	4.452298	5.104582
28	7	0	-1.831112	3.569699	2.572978
29	6	0	-1.886535	3.396261	1.129397
30	6	0	-1.524697	1.946359	0.778137
31	8	0	-0.484086	1.416744	1.225789
32	6	0	-0.903076	4.370538	0.438180
33	6	0	-0.929180	4.387318	-1.103743
34	6	0	-2.249646	4.944700	-1.660490
35	6	0	0.263040	5.203865	-1.628623
36	1	0	-0.922088	3.531954	3.029265
37	1	0	-2.913596	3.605846	0.825201
38	1	0	-1.138112	5.372725	0.816496
39	1	0	0.108544	4.126404	0.784459
40	1	0	-0.808063	3.357703	-1.470115
41	1	0	-2.235710	4.944817	-2.755480
42	1	0	-3.122508	4.362814	-1.346493
43	1	0	-2.401721	5.978444	-1.326523

44	1	0	1.215476	4.787830	-1.282293
45	1	0	0.276270	5.213507	-2.723697
46	1	0	0.204203	6.244197	-1.285231
47	7	0	-2.354227	1.285120	-0.051829
48	6	0	-2.021588	0.020287	-0.703269
49	6	0	-2.104846	-1.199340	0.208361
50	8	0	-2.845966	-2.133685	0.090262
51	1	0	-3.226254	1.720600	-0.323461
52	1	0	-2.721548	-0.142608	-1.520647
53	1	0	-1.005148	0.070677	-1.112015
54	7	0	-1.101403	-1.186898	1.290386
55	6	0	-1.382814	-1.933876	2.575905
56	6	0	-1.119543	-1.341469	3.952404
57	8	0	-1.414611	-2.066518	4.902519
58	6	0	-0.348482	-2.473800	1.666894
59	1	0	-2.350506	-2.425250	2.533034
60	1	0	-0.687318	-3.292964	1.038341
61	6	0	1.133283	-2.367285	1.887927
62	1	0	1.655335	-2.306805	0.930367
63	1	0	1.412338	-1.514321	2.509343
64	1	0	1.456435	-3.281285	2.395747
65	1	0	-0.591852	-0.269472	1.324909

22: TS-2a

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1709.208251 hartrees
Thermal Free Energy Correction (333 K):	0.466938 hartree/particle
Charge/Multiplicity	-1/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-5.125400	-2.692000	-5.897400
2	6	0	-5.696100	-2.094600	-4.675900
3	6	0	-6.362500	-0.705200	-4.905500
4	8	0	-6.152700	0.255600	-4.159900
5	6	0	-4.639600	-2.081600	-3.542600
6	6	0	-3.247900	-1.559900	-3.881300
7	6	0	-2.969800	-0.183300	-3.981800
8	6	0	-2.184800	-2.464600	-4.049900
9	6	0	-1.674000	0.268800	-4.248900
10	6	0	-0.886100	-2.013200	-4.318400
11	6	0	-0.626500	-0.643900	-4.420900
12	1	0	-4.114800	-2.702700	-5.959300
13	1	0	-6.518200	-2.747000	-4.351400
14	1	0	-5.066100	-1.495300	-2.724200
15	1	0	-4.547900	-3.112100	-3.185300
16	1	0	-3.771900	0.533100	-3.836700
17	1	0	-2.369800	-3.532100	-3.953500
18	1	0	-1.480000	1.337300	-4.314100
19	1	0	-0.079100	-2.732300	-4.438500
20	1	0	0.381700	-0.289900	-4.623600
21	7	0	-7.226000	-0.653600	-5.959000
22	6	0	-8.024000	0.524100	-6.274000
23	6	0	-7.608600	1.269900	-7.553200
24	8	0	-8.262800	2.252200	-7.936200
25	1	0	-7.505100	-1.550800	-6.358000
26	1	0	-9.075800	0.241000	-6.389100
27	1	0	-7.957100	1.237100	-5.447400
28	7	0	-6.519800	0.781600	-8.183900
29	6	0	-5.893500	1.332300	-9.390500
30	6	0	-6.008800	0.293800	-10.536900
31	8	0	-6.712100	0.515100	-11.538500
32	6	0	-4.448100	1.770800	-9.059600
33	6	0	-3.629600	2.389400	-10.211100
34	6	0	-4.227000	3.718200	-10.700800
35	6	0	-2.172400	2.587500	-9.759000
36	1	0	-6.073900	-0.006500	-7.728700
37	1	0	-6.499400	2.185900	-9.696400
38	1	0	-4.514700	2.494500	-8.235900
39	1	0	-3.898200	0.905900	-8.660400
40	1	0	-3.624100	1.684200	-11.054700
41	1	0	-3.618400	4.139200	-11.508900
42	1	0	-5.245400	3.599000	-11.084400
43	1	0	-4.257100	4.453500	-9.886500

44	1	0	-1.714400	1.640400	-9.451100
45	1	0	-1.564200	3.006900	-10.568800
46	1	0	-2.117100	3.278400	-8.907800
47	7	0	-5.326600	-0.850500	-10.350500
48	6	0	-5.437400	-2.047700	-11.175800
49	6	0	-4.904300	-3.283600	-10.435300
50	8	0	-4.886000	-4.372800	-11.041400
51	1	0	-4.795400	-1.011600	-9.498700
52	1	0	-6.482800	-2.223900	-11.456900
53	1	0	-4.863500	-1.946800	-12.106900
54	7	0	-4.452000	-3.028100	-9.169900
55	6	0	-5.137400	-4.243200	-7.838400
56	6	0	-5.841900	-3.418100	-6.787700
57	8	0	-7.087300	-3.443500	-6.761700
58	6	0	-3.797300	-4.128800	-8.451500
59	1	0	-5.848700	-4.826400	-8.411900
60	1	0	-3.604600	-5.005000	-9.077500
61	6	0	-2.531300	-3.715100	-7.716100
62	1	0	-1.724000	-3.623400	-8.450900
63	1	0	-2.621600	-2.741800	-7.225000
64	1	0	-2.232800	-4.467400	-6.980900
65	7	0	-5.130800	-5.988000	-6.433000
66	7	0	-4.223200	-5.959400	-5.650500
67	7	0	-3.339600	-5.941300	-4.879600

23: TS-2b

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1709.204625 hartrees
Thermal Free Energy Correction (333 K):	0.464009 hartree/particle
Charge/Multiplicity	-1/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.421100	-1.108300	5.104500
2	6	0	-1.741800	-0.435800	6.361800
3	6	0	-2.503300	0.891100	6.103800
4	8	0	-2.445100	1.831900	6.902000
5	6	0	-0.518800	-0.258600	7.303400
6	6	0	0.732900	0.384300	6.724200
7	6	0	0.838500	1.774600	6.530200
8	6	0	1.857600	-0.408100	6.436900
9	6	0	2.026200	2.346700	6.060500
10	6	0	3.046900	0.160200	5.966300
11	6	0	3.135300	1.542500	5.774600
12	1	0	-0.959200	-0.598200	4.359500
13	1	0	-2.454200	-1.084000	6.888900
14	1	0	-0.868200	0.316000	8.166800
15	1	0	-0.262100	-1.258800	7.668300
16	1	0	-0.003500	2.415100	6.776200
17	1	0	1.811600	-1.481000	6.609300
18	1	0	2.090800	3.425400	5.937200
19	1	0	3.906900	-0.474700	5.764000
20	1	0	4.062500	1.988900	5.422700
21	7	0	-3.231500	0.941200	4.951500
22	6	0	-4.033100	2.088600	4.544100
23	6	0	-3.603200	2.703300	3.199700
24	8	0	-4.405000	3.373600	2.535100
25	1	0	-3.408500	0.065300	4.468400
26	1	0	-5.085300	1.806300	4.447700
27	1	0	-3.957600	2.863800	5.312900
28	7	0	-2.319100	2.474300	2.833500
29	6	0	-1.683900	2.913200	1.587600
30	6	0	-1.593900	1.751200	0.562900
31	8	0	-1.955100	1.916200	-0.613400
32	6	0	-0.304800	3.536000	1.917400
33	6	0	0.510400	4.086600	0.729000
34	6	0	-0.173900	5.291200	0.062800
35	6	0	1.925900	4.464500	1.201200
36	1	0	-1.755800	1.973100	3.507600
37	1	0	-2.347200	3.650900	1.133300
38	1	0	-0.480000	4.343800	2.641200
39	1	0	0.301000	2.778100	2.436300
40	1	0	0.613700	3.292300	-0.024200
41	1	0	0.420100	5.650800	-0.784900
42	1	0	-1.169900	5.041600	-0.316200
43	1	0	-0.278600	6.121600	0.773400

44	1	0	2.454700	3.602300	1.624200
45	1	0	2.523500	4.847500	0.366000
46	1	0	1.889500	5.246800	1.970500
47	7	0	-1.103100	0.581400	1.027200
48	6	0	-1.098500	-0.674200	0.283800
49	6	0	-1.351400	-1.891400	1.186300
50	8	0	-1.860200	-2.906700	0.673600
51	1	0	-0.822600	0.492600	1.994800
52	1	0	-1.879700	-0.643400	-0.478600
53	1	0	-0.138700	-0.826200	-0.232600
54	7	0	-0.949300	-1.745300	2.485800
55	6	0	-1.330100	-2.847400	3.392700
56	6	0	-1.648300	-2.416600	4.832400
57	8	0	-2.121100	-3.221400	5.643300
58	6	0	0.004900	-3.358000	3.047400
59	1	0	-2.152800	-3.469100	3.028800
60	6	0	1.274900	-3.008600	3.754800
61	1	0	1.477400	-1.935900	3.671500
62	1	0	1.215900	-3.265300	4.817000
63	1	0	2.113700	-3.547800	3.309000
64	7	0	-2.142800	-6.461600	3.375100
65	7	0	-1.074600	-6.034100	3.626500
66	7	0	0.004300	-5.592800	3.877300
67	1	0	0.223700	-3.973700	2.174900

24: TS-2a-OH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1709.635725 hartrees
Thermal Free Energy Correction (333 K):	0.467744 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.640228	0.326942	4.548292
2	6	0	-0.821788	1.135647	5.761814
3	6	0	-1.460994	2.492265	5.385942
4	8	0	-0.779022	3.502629	5.163028
5	6	0	0.509352	1.343481	6.501190
6	6	0	1.133434	0.071486	7.041272
7	6	0	2.382420	-0.366378	6.578375
8	6	0	0.492008	-0.676802	8.042326
9	6	0	2.975478	-1.524222	7.094579
10	6	0	1.078057	-1.835243	8.557530
11	6	0	2.323577	-2.264119	8.084202
12	1	0	0.203059	0.457595	4.003079
13	1	0	-1.519918	0.585698	6.397629
14	1	0	1.210815	1.859399	5.838876
15	1	0	0.306145	2.033745	7.327614
16	1	0	2.899779	0.205278	5.811713
17	1	0	-0.469482	-0.349067	8.430462
18	1	0	3.944658	-1.844487	6.722797
19	1	0	0.566173	-2.399132	9.332121
20	1	0	2.781245	-3.163020	8.486807
21	7	0	-2.808946	2.473317	5.288286
22	6	0	-3.578500	3.613574	4.799821
23	6	0	-3.607927	3.666625	3.263762
24	8	0	-4.654763	3.500584	2.627234
25	1	0	-3.259408	1.562377	5.302918
26	1	0	-4.604565	3.522494	5.154238
27	1	0	-3.139912	4.529984	5.203672
28	7	0	-2.398569	3.872400	2.689191
29	6	0	-2.170611	3.782450	1.249106
30	6	0	-0.893891	2.949753	1.046634
31	8	0	0.205248	3.369583	1.415273
32	6	0	-2.024575	5.180496	0.612791
33	6	0	-1.877449	5.205760	-0.922328
34	6	0	-3.157919	4.751975	-1.643095
35	6	0	-1.472113	6.615006	-1.383590
36	1	0	-1.598037	4.026803	3.298575
37	1	0	-3.037114	3.266471	0.830489
38	1	0	-2.908490	5.761622	0.904071
39	1	0	-1.154904	5.663725	1.072679
40	1	0	-1.064271	4.520755	-1.204227
41	1	0	-3.453766	3.732365	-1.375766
42	1	0	-3.994825	5.417587	-1.397406
43	1	0	-3.018749	4.777051	-2.729440

44	1	0	-1.342796	6.649057	-2.470896
45	1	0	-2.242349	7.349080	-1.115184
46	1	0	-0.530775	6.930694	-0.920413
47	7	0	-1.053176	1.735905	0.449184
48	6	0	0.074315	0.974495	-0.030277
49	6	0	0.351342	-0.334437	0.668756
50	8	0	1.109609	-1.113933	-0.092747
51	1	0	-1.974316	1.466708	0.129934
52	1	0	-0.042335	0.749139	-1.094451
53	1	0	0.974009	1.590944	0.078214
54	7	0	-0.008855	-0.635746	1.876119
55	6	0	-1.365641	-1.251355	2.792293
56	6	0	-1.658327	-0.383676	4.007938
57	8	0	-2.808147	-0.359492	4.455068
58	6	0	-0.105662	-1.973048	2.463068
59	1	0	-2.187873	-1.323360	2.093146
60	1	0	-0.275503	-2.761455	1.725334
61	6	0	0.900198	-2.395019	3.515254
62	1	0	1.094517	-1.622805	4.259111
63	1	0	0.505377	-3.277170	4.024723
64	1	0	1.846002	-2.664608	3.036907
65	1	0	1.365880	-1.946941	0.338840
66	7	0	-2.354602	-3.223304	3.704522
67	7	0	-2.808605	-3.808461	2.766668
68	7	0	-3.254937	-4.381885	1.839492

25: TS-2b-OH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1709.637907 hartrees
Thermal Free Energy Correction (333 K):	0.468025 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.719567	0.155820	4.472067
2	6	0	-1.014892	0.982929	5.649113
3	6	0	-1.720110	2.255458	5.130305
4	8	0	-1.082129	3.285653	4.872397
5	6	0	0.234847	1.363284	6.472189
6	6	0	0.913476	0.193087	7.152148
7	6	0	2.109168	-0.339393	6.649862
8	6	0	0.366354	-0.373762	8.315061
9	6	0	2.736020	-1.420027	7.280199
10	6	0	0.987801	-1.452580	8.948042
11	6	0	2.175278	-1.982311	8.429954
12	1	0	-0.398022	0.625910	3.632186
13	1	0	-1.700362	0.399110	6.268804
14	1	0	0.937014	1.885746	5.817203
15	1	0	-0.091130	2.087883	7.226918
16	1	0	2.560590	0.099895	5.764124
17	1	0	-0.551820	0.034459	8.731257
18	1	0	3.661740	-1.817704	6.873987
19	1	0	0.548832	-1.876489	9.846812
20	1	0	2.660406	-2.820329	8.921907
21	7	0	-3.051009	2.158094	4.918419
22	6	0	-3.844004	3.256018	4.365684
23	6	0	-3.738909	3.351682	2.831300
24	8	0	-4.685905	3.040667	2.100490
25	1	0	-3.524987	1.289313	5.126752
26	1	0	-4.889346	3.082876	4.616466
27	1	0	-3.515737	4.192652	4.825476
28	7	0	-2.543674	3.803974	2.376544
29	6	0	-2.168491	3.842744	0.962219
30	6	0	-1.289635	2.602652	0.699401
31	8	0	-0.165516	2.494410	1.193747
32	6	0	-1.421742	5.147488	0.641707
33	6	0	-1.029133	5.338714	-0.837507
34	6	0	-2.251228	5.483390	-1.759531
35	6	0	-0.103935	6.558541	-0.975057
36	1	0	-1.809574	3.944342	3.068708
37	1	0	-3.096560	3.777767	0.391667
38	1	0	-2.062468	5.979353	0.960002
39	1	0	-0.517858	5.180602	1.261652
40	1	0	-0.459572	4.454917	-1.160022
41	1	0	-2.898989	4.600749	-1.743483
42	1	0	-2.857830	6.349435	-1.465828
43	1	0	-1.934103	5.634715	-2.797104

44	1	0	0.210126	6.695685	-2.015461
45	1	0	-0.616971	7.474941	-0.657027
46	1	0	0.797072	6.447359	-0.361694
47	7	0	-1.851891	1.626358	-0.065722
48	6	0	-1.232767	0.315998	-0.217383
49	6	0	-1.612676	-0.557810	0.958959
50	8	0	-2.905285	-0.845650	0.994111
51	1	0	-2.807052	1.738595	-0.378602
52	1	0	-1.586080	-0.144395	-1.142208
53	1	0	-0.150033	0.424815	-0.247875
54	7	0	-0.754143	-0.859746	1.879817
55	6	0	-0.902754	-1.788340	2.984611
56	6	0	-1.041512	-1.157109	4.378026
57	8	0	-1.473825	-1.842901	5.302323
58	6	0	0.422949	-2.062780	2.356197
59	1	0	-1.634564	-2.592190	2.883985
60	1	0	0.399416	-2.767151	1.535048
61	6	0	1.735268	-1.467994	2.738819
62	1	0	1.645963	-0.705434	3.511844
63	1	0	2.362545	-2.279895	3.113794
64	1	0	2.220387	-1.041924	1.856890
65	1	0	-3.168842	-1.368266	1.771316
66	7	0	0.793447	-4.248440	3.442986
67	7	0	-0.151154	-4.938942	3.206846
68	7	0	-1.090239	-5.611185	2.968259

26: TS-2a-NH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1709.654249 hartrees
Thermal Free Energy Correction (333 K):	0.469175 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.722886	-0.064747	4.154727
2	6	0	-0.437672	0.653239	5.404940
3	6	0	-1.133614	2.024842	5.246508
4	8	0	-0.498564	3.067604	5.057111
5	6	0	1.071355	0.777797	5.703763
6	6	0	1.370264	1.181570	7.135171
7	6	0	1.772585	2.485975	7.457972
8	6	0	1.255758	0.241218	8.172830
9	6	0	2.052943	2.843187	8.781024
10	6	0	1.530711	0.594957	9.496611
11	6	0	1.931152	1.899446	9.805419
12	1	0	-0.784791	0.486119	3.296502
13	1	0	-0.918750	0.088580	6.210353
14	1	0	1.513716	-0.202696	5.503895
15	1	0	1.510448	1.493577	5.004268
16	1	0	1.862577	3.225120	6.667637
17	1	0	0.957436	-0.778802	7.942074
18	1	0	2.366582	3.857941	9.009776
19	1	0	1.438791	-0.148184	10.283704
20	1	0	2.149357	2.175638	10.833013
21	7	0	-2.488193	1.982612	5.230800
22	6	0	-3.303520	3.107557	4.774731
23	6	0	-3.402638	3.129189	3.236353
24	8	0	-4.454496	2.858195	2.649673
25	1	0	-2.943856	1.082245	5.311682
26	1	0	-4.309185	3.001094	5.178798
27	1	0	-2.861477	4.034651	5.147382
28	7	0	-2.239442	3.439560	2.606654
29	6	0	-2.014110	3.266186	1.177738
30	6	0	-1.197081	1.977275	0.970055
31	8	0	-0.373660	1.595349	1.816402
32	6	0	-1.269939	4.505248	0.617006
33	6	0	-1.088775	4.586704	-0.911754
34	6	0	-2.429285	4.694472	-1.657672
35	6	0	-0.185989	5.783522	-1.254714
36	1	0	-1.419940	3.585082	3.190368
37	1	0	-2.995724	3.162879	0.710670
38	1	0	-1.835862	5.381540	0.956197
39	1	0	-0.286803	4.556643	1.102052
40	1	0	-0.572537	3.680101	-1.255163
41	1	0	-2.264558	4.758936	-2.738384
42	1	0	-3.086713	3.836263	-1.480220
43	1	0	-2.973294	5.594828	-1.346445

44	1	0	0.791064	5.699166	-0.766214
45	1	0	-0.019374	5.848086	-2.335274
46	1	0	-0.645278	6.725404	-0.929664
47	7	0	-1.375368	1.287329	-0.178439
48	6	0	-0.553069	0.123135	-0.484095
49	6	0	-1.096005	-1.130865	0.205615
50	8	0	-2.111265	-1.695816	-0.129348
51	1	0	-2.102428	1.548354	-0.831031
52	1	0	-0.598594	-0.063358	-1.557750
53	1	0	0.480387	0.324725	-0.198489
54	7	0	-0.365812	-1.607957	1.348311
55	6	0	-1.312296	-1.957717	2.764685
56	6	0	-0.750421	-1.411673	4.077993
57	8	0	-0.436878	-2.178584	4.985635
58	6	0	-0.663018	-2.970718	1.933188
59	1	0	-2.296769	-1.621847	2.466233
60	1	0	-1.342614	-3.497908	1.267925
61	6	0	0.535312	-3.770785	2.379268
62	1	0	1.063045	-4.159710	1.505304
63	1	0	1.224531	-3.188709	2.993611
64	1	0	0.178710	-4.614636	2.975304
65	1	0	0.557736	-1.212381	1.519980
66	7	0	-3.145064	-3.332204	3.939360
67	7	0	-4.059437	-3.104289	3.208401
68	7	0	-4.948400	-2.858969	2.470336

27: TS-2b-NH+

Calculation Method	M06-2X/6-311++G(2d,p)//B3LYP/6-31+G(d,p)
Solvation	IEFPCM (N,N-dimethylformamide)
Electronic Energy:	-1709.662753 hartrees
Thermal Free Energy Correction (333 K):	0.46752 hartree/particle
Charge/Multiplicity	0/1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.550257	-0.183810	4.077288
2	6	0	-0.429431	0.487611	5.382539
3	6	0	-0.726697	1.967770	5.093601
4	8	0	0.141470	2.701006	4.598236
5	6	0	0.958933	0.275794	6.023436
6	6	0	1.033770	0.803175	7.442819
7	6	0	1.590749	2.060424	7.721976
8	6	0	0.530539	0.041218	8.510069
9	6	0	1.640905	2.546410	9.032613
10	6	0	0.577465	0.524030	9.820632
11	6	0	1.132417	1.780618	10.085990
12	1	0	-0.306772	0.362490	3.258421
13	1	0	-1.197169	0.057089	6.029873
14	1	0	1.154833	-0.800772	6.013753
15	1	0	1.709970	0.758955	5.392476
16	1	0	1.988318	2.660746	6.908434
17	1	0	0.106962	-0.941102	8.314690
18	1	0	2.079122	3.520826	9.229274
19	1	0	0.186979	-0.082132	10.633123
20	1	0	1.172896	2.156066	11.104372
21	7	0	-1.995123	2.376487	5.303345
22	6	0	-2.482290	3.684407	4.866897
23	6	0	-2.825189	3.697000	3.364252
24	8	0	-3.988165	3.815798	2.967105
25	1	0	-2.673826	1.713088	5.653644
26	1	0	-3.388899	3.920355	5.421587
27	1	0	-1.719909	4.436139	5.088503
28	7	0	-1.751162	3.557705	2.546105
29	6	0	-1.844055	3.400942	1.101069
30	6	0	-1.467938	1.956683	0.740199
31	8	0	-0.412933	1.444229	1.167620
32	6	0	-0.899218	4.399069	0.391779
33	6	0	-0.968936	4.425965	-1.148515
34	6	0	-2.318905	4.952287	-1.663393
35	6	0	0.185954	5.276558	-1.701799
36	1	0	-0.839256	3.441998	2.983583
37	1	0	-2.883186	3.596317	0.830296
38	1	0	-1.141887	5.394413	0.783618
39	1	0	0.126093	4.171856	0.708233
40	1	0	-0.832264	3.402012	-1.525123
41	1	0	-2.336850	4.960075	-2.758356
42	1	0	-3.166510	4.345245	-1.328426

43	1	0	-2.488498	5.979425	-1.317453
44	1	0	1.158497	4.882103	-1.387600
45	1	0	0.166262	5.295354	-2.796760
46	1	0	0.111582	6.312366	-1.347721
47	7	0	-2.311477	1.281803	-0.065429
48	6	0	-2.001845	-0.018542	-0.658413
49	6	0	-2.143541	-1.180608	0.326373
50	8	0	-2.979842	-2.051356	0.263401
51	1	0	-3.192229	1.707576	-0.322791
52	1	0	-2.695927	-0.197845	-1.477377
53	1	0	-0.979401	-0.007898	-1.051817
54	7	0	-1.149994	-1.176316	1.353204
55	6	0	-1.312699	-2.011916	2.573412
56	6	0	-1.072484	-1.425235	3.964717
57	8	0	-1.390441	-2.126856	4.923936
58	6	0	-0.269350	-2.648206	1.757580
59	1	0	-2.273280	-2.522440	2.552960
60	1	0	-0.622129	-3.374752	1.037418
61	6	0	1.197834	-2.407748	1.878070
62	1	0	1.643345	-2.244405	0.893664
63	1	0	1.443077	-1.575328	2.539885
64	1	0	1.625930	-3.322268	2.297313
65	1	0	-0.584488	-0.306614	1.369197
66	7	0	-0.198103	-4.996236	2.865886
67	7	0	-1.324522	-5.369428	2.975686
68	7	0	-2.445039	-5.729175	3.079878

References

[1] Galonic, D. P.; Ide, N. D.; van der Donk, W. A.; Gin, D. Y. *J. Am. Chem. Soc.* **2005**, *127*, 7359.

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

[3] NBO 6.0. E. D. Glendening, J, K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis, and F. Weinhold, Theoretical Chemistry Institute, University of Wisconsin, Madison (2013).

[4] The PyMOL Molecular Graphics System, Version 1.7 Schrödinger, LLC.

[5] Humphrey, W., Dalke, A. and Schulten, K., "VMD - Visual Molecular Dynamics", J. Molec. Graphics, 1996, vol. 14, pp. 33-38. (http://www.ks.uiuc.edu/Research/vmd/)

[6] Prime, version 4.3, Schrödinger, LLC, New York, NY, 2015