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

Supporting Information

The role of proton shuttling mechanisms in solvent-free and catalyst-free acetalization reactions of imines.

V.J. Lillo, J. Mansilla and J.M. Saá*

Supporting information 1 (SI1): Experimental

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Contents:

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Contents:

1. General information

^{1}H NMR spectra were recorded on a Bruker AMX-300 (300 MHz) spectrometer using the deuterated solvent employed as internal standard. Chemical shifts (δ) are reported in ppm, and are qualified either as: s = singlet, d = doublet, dd = double doublet, t = triplet, q = quartet, m = multiplet, or br = broad. Coupling constant(s) J are given in Hz. Proton-decoupled ^{13}C NMR spectra were also recorded on a Bruker AMX-300 (75.5 MHz) spectrometer and their chemical shifts (δ) are reported in ppm using the deuterated solvent as internal standard. Melting points (ºC) were measured on a Sanyo Gallenkamp MPD350 apparatus and are uncorrected. Temperatures (T) are given in Celsius degrees (°C). MS spectra (ESI, ESI-TOF and EI^{+}) were recorded on a Micromass Autospec 3000 mass spectrometer or on a Bruker MicrOTOF mass spectrometer, pertaining to the Mass Spectrometry equipment of the University of Santiago de Compostela (Rede de Infraestruturas de Apoio á Investigación e ao Desenvolvemento Tecnolóxico - RIAIDT) and the University of the Balearic Islands (Serveis Cientificotècnics - SCT).

2. Materials

Solvents were used directly from commercial sources except for the dichloromethane (CH_2Cl_2) employed for the preparation of imine derivatives **1a-d** which was distilled from CaH_2. The MeOH used as reagent was HPLC-grade (water content < 0.02%). Prior to use, the caesium carbonate (Cs_2CO_3) employed for the preparation of imine derivatives **1a-d** was dried with a heat gun under vacuum for 15 minutes. Imine **1a** was prepared following the methodology reported by us.[1] Aryl and heteroaryl *N*-Boc imines **1c** were prepared following the reported methodology.[2] Alkylidene *N*-Boc imines were obtained following the methodology described in the literature.[3] Imine **1d** was prepared following the published methodology.[4] Unless otherwise specified, all other materials were obtained from commercial sources and used without purification. Celite® 521 was used as filtering agent.

3. Experimental procedures. Analytical and spectroscopic data

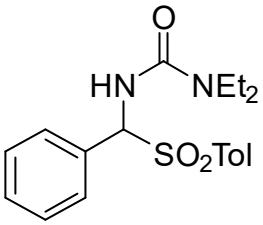
3.1 Preparation of 1,1-diethyl-3-(phenyl(tosyl)methyl)urea:

A procedure similar to that applied to obtain *N*-Boc sulfones (precursors of imine derivatives **1c**) was employed for the preparation of the α-ureidosulfones precursors of imine derivatives **1a** and **1b**.[2] Thus, to a solution of *N,N* diethylurea (5 mmol) and sodium *p*-toluenesulfinate (12 mmol) in deionized water (10 mL), together with methanol (5 mL) and the appropriate aldehyde (10 mmol), formic acid (390 µL, 10 mmol) was added at room temperature. The mixture was stirred for 20 hours after which time an

[1] V. J. Lillo, J. Mansilla, J. M. Saá, *Angew. Chem. Int. Ed.,* **2016,** *55*, 4312.
[2] C. T. Mbofana, S. J. Miller, *J. Am. Chem. Soc*., **2014**, *136*, 3285.
[3] A. J. Neuvonen, P. M. Pihko, *Org. Lett.*, **2014**, *16*, 5152.
[4] B. J. Cowen, L. B. Saunders, S. J. Miller, *J. Am. Chem. Soc*., **2009**, *131*, 6105.

abundant precipitate was formed. The resulting suspension was filtered off, the solid washed with water (100 mL) and pentane (50 mL), and eventually dried over vacuum for 3 hours. The resulting α-ureidosulfone (1,1-diethyl-3-(phenyl(tosyl)methyl)urea) was used without further purification for the preparation of **1b**. Physical, spectroscopic and analytical data follow.

1,1-Diethyl-3-(phenyl(tosyl)methyl)urea:

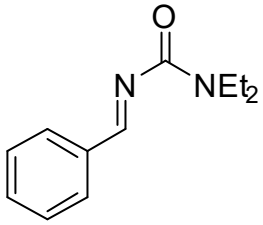


White solid, 49% yield; mp=131ºC (decomposition); ^{1}H NMR (300 MHz, CD_3CN) δ: 0.95 (6H, t, *J* = 7.1, CH_2CH_3), 2.42 (3H, s, $ArCH_3$), 3.00–3.28 (4H, m, 2×CH_2), 5.91 (1H, d, *J* = 10.2, NH), 6.34 (1H, d, *J* = 10.5, CH), 7.34–7.48 (5H, m, 5×ArH), 7.41–7.48 (3H, m, 3×ArH), 7.54–7.62 (2H, m, 2×ArH), 7.71–7.79 (2H, m, 2×ArH); ^{13}C NMR (75.5 MHz, CD_3CN) δ: 14.1 (CH_2CH_3), 21.7 ($ArCCH_3$), 42.0 (CH_2), 74.9 (CH), 129.4, 130.2, 130.3, 130.4, 130.6 (ArCH), 132.6, 135.5, 146.2 (ArC), 155.2 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{19}H_{24}N_2NaO_3S$ $[M+Na]^+$: 383.13998, found: 383.13895.

3.2 Preparation of (*E*)-3-benzylidene-1,1-diethylurea 1b:

Under argon atmosphere, dried dichloromethane (24 mL) was added over carefully dried caesium carbonate (4.5 mmol) and α-ureidosulfone 1,1-diethyl-3-(phenyl(tosyl)methyl)urea (1 mmol). After stirring the suspension for 3 hours, the solid material was filtered through a celite plug and the filtrate was evaporated under vacuum at room temperature to yield **1b** as a colourless liquid. (Note: it is important not to evaporate the filtrate at temperatures above 30ºC to avoid decomposition of the imine).

(*E*)-3-benzylidene-1,1-diethylurea (1b):

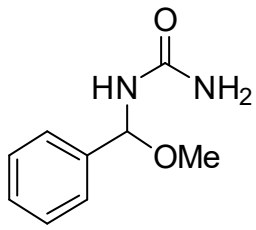


Colourless liquid; 92% yield; ^{1}H NMR (300 MHz, CD_3CN) δ: 1.08–1.22 (6H, m, CH_2CH_3), 3.37–3.48 (2H, q, *J* = 7.1, CH_2), 3.51–3.63 (2H, q, *J* = 7.2, CH_2), 7.34–48 (5H, m, 5×ArH), 7.44–7.67 (3H, m, 3×ArH), 7.92–8.03 (2H, m, 2×ArH), 8.93 (1H, s, CH); ^{13}C NMR (75.5 MHz, CD_3CN) δ: 13.6, 14.9 (CH_3), 41.9, 43.0 (CH_2), 129.9.0, 130.7, 133.9 (ArCH), 136.2 (ArC), 163.4 (N=CH), 167.9 (CO); HRMS (EI–TOF$^+$) Exact mass calcd. for $C_{12}H_{16}N_2O$ $[M]^+$: 204.1263, found: 204.1264.

3.3 General procedure for the synthesis of *N,O*-acetals 4 from imines 1 and alcohols 2 under SF-CF conditions:

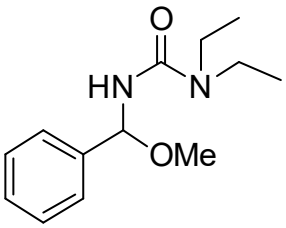
A liquid-liquid or solid-liquid mixture of the imine **1** (0.4 mmol) and the appropriate alcohol **2** (0.4 mmol) placed in a 5ml round bottom flask was stirred overnight. *N,O*-acetals **4** were thus obtained usually as white solids in pure form. Only in the case of *N,O*-acetal **4cb** the crude reaction material had to be washed with cold hexane to obtain the pure compound (slow evaporation of the mother liquids yielded a second crop of crystalline product). In some specific cases (**1a+2a**, **1f+2a** and **1g+2a**) an excess of alcohol **2** was required to achieve mutual solubilization. In these cases the crude reaction material was evaporated under vacuum prior to isolation of the pure *N,O*-acetals **4aa**, **4fa** and **4ga**. Physical, spectroscopic and analytical data, as well as literature references for known compounds, follow.

1-(Methoxy(phenyl)methyl)urea (4aa):



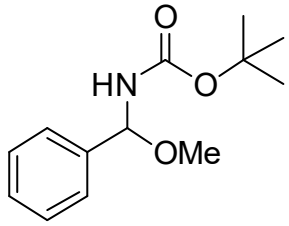
Resulting from the reaction of **1a** with **2a**. White solid, 99% yield; mp=119ºC; ^{1}H NMR (300 MHz, DMSO-D6) δ: 3.25 (3H, s, CH_3), 5.70 (2H, br s, NH_2), 5.77 (1H, d, *J* = 9.9, C*H*NH), 6.81 (1H, d, *J* = 9.9, CHN*H*), 7.26–7.48 (5H, m, 5×ArH); ^{13}C NMR (75.5 MHz, DMSO-D6) δ: 54.2 (OCH_3), 82.0 (CH), 126.0, 127.8, 128.2 (ArCH), 140.5 (ArC), 157.9 (CO); HRMS (EI-TOF^{+}) Exact mass calcd. for $C_9H_{12}N_2O_2$ [M]$^{+}$: 180.0899, found: 180.0903.

1,1-Diethyl-3-(methoxy(phenyl)methyl)urea (4ba):



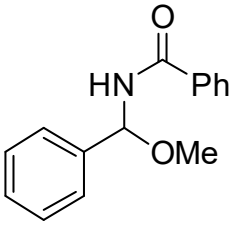
Resulting from the reaction of **1b** with **2a**. White solid, 99% yield; mp=58ºC; ^{1}H NMR (300 MHz, DMSO-D6) δ: 1.03 (6H, t, *J* = 7.0, 2×CCH_3), 3.22–3.41 (7H, m, 2×CH_2, OCH_3), 6.00 (1H, d, *J* = 9.3, CHN*H*), 6.88 (1H, d, *J* = 9.0, C*H*NH), 7.26–7.45 (5H, m, 5×ArH); ^{13}C NMR (75.5 MHz, DMSO-D6) δ: 13.9 (CH_2CH_3), 40.1 (CH_2), 54.5 (OCH_3), 83.0 (CH), 126.3, 127.5, 127.9 (ArCH), 140.9 (ArC), 156.3 (CO); HRMS (EI-TOF^{+}) Exact mass calcd. for $C_{13}H_{20}N_2O_2$ [M+Na]$^{+}$: 377.0936, found: 377.0931.

***tert*-Butyl (methoxy(phenyl)methyl)carbamate (4ca):**[5]



Resulting from the reaction of **1c** with **2a**. White solid, 99% yield; mp=70ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 1.48 (9H, s, 3×CCH_3), 3.45 (3H, s, OCH_3), 5.15 (1H, br s, CHN*H*), 5.82 (1H, d, *J* = 9.6, C*H*NH), 7.28–7.45 (5H, m, 5×ArH); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 28.4 (CCH_3), 55.6 (OCH_3), 80.2 (*C*CH_3), 83.6 (CH), 126.0, 128.5, 128.6 (ArCH), 139.5 (ArC), 155.4 (CO), 159.7 (ArC).

***N*-(Methoxy(phenyl)methyl)benzamide (4da):**[6]

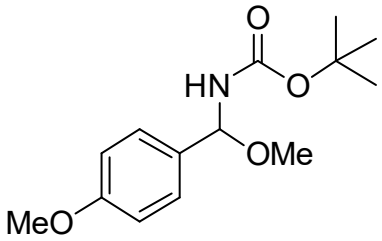


Resulting from the reaction of **1d** with **2a**. White solid, 99% yield; mp=101ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 3.52 (3H, s, CH_3), 6.36 (1H, d, *J* = 9.3, C*H*NH), 6.77 (1H, d, *J* = 9.9, CHN*H*), 7.30–7.54 (8H, m, 8×ArH), 7.78–7.82 (2H, m, 8×ArH); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 56.2 (CH_3), 81.9 (CH), 126.0, 127.2, 128.6, 128.7, 132.1 (ArCH), 133.8, 139.4 (ArC), 167.5 (CO).

[5] M. Terada, K. Machioka, K. Sorimachi, *Angew. Chem. Int. Ed.*, **2009**, *48*, 2553.

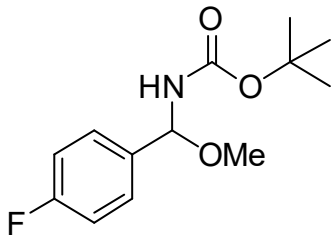
[6] Halli, K. Hofman, T. Beisel, G. Manolikakes, *Eur. J. Org. Chem.*, **2015**, 4624.

***tert*-Butyl (methoxy(4-methoxyphenyl)methyl)carbamate (4fa):**[5]



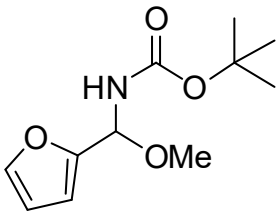
Resulting from the reaction of **1f** with **2a**. White solid, 99% yield; mp=78ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 1.49 (9H, s, 3×CCH_3), 3.44 (3H, s, CHOCH_3), 3.81 (3H, s, OCH_3), 5.19 (1H, br s, CHN*H*), 5.79 (1H, d, *J* = 9.6, C*H*NH), 6.89 (2H, d, *J* = 8.7, 2×ArH), 7.35 (2H, d, *J* = 8.7, 2×ArH); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 28.4 (CCH_3), 55.4, 55.5 (OCH_3), 80.1 (*C*CH_3), 83.3 (CH), 113.9, 127.2 (ArCH), 131.8 (ArC), 155.3 (CO), 159.7 (ArC).

***tert*-Butyl ((4-fluorophenyl)(methoxy)methyl)carbamate (4ga):**



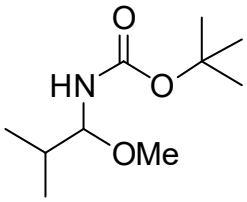
Resulting from the reaction of **1g** with **2a**. White solid, 99% yield; mp=58ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 1.49 (9H, s, 3×CCH_3), 3.44 (3H, s, CHOCH_3), 5.22 (1H, d, *J* = 8.7, CHN*H*), 5.82 (1H, d, *J* = 9.9, C*H*NH), 7.00–7.09 (2H, m, 2×ArH), 7.33–7.44 (2H, m, 2×ArH); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 28.4 (CCH_3), 55.6 (OCH_3), 80.3 (*C*CH_3), 83.0 (CH), 115.2, 115.4, 127.8, 127.9 (ArCH), 135.5, 135.5 (ArC), 155.4 (CO), 161.1, 164.31 (ArCF); HRMS (ESI$^+$) Exact mass calcd. for $C_{13}H_{18}FNNaO_3S$ $[M+Na]^+$: 278.1163, found: 278.1163.

***tert*-Butyl (furan-2-yl(methoxy)methyl)carbamate (4ha):**



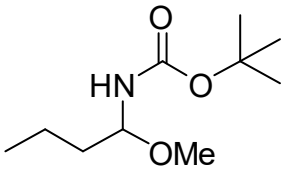
Resulting from the reaction of **1h** with **2a**. Colourless oil, 99% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 1.44 (9H, s, 3×CCH_3), 3.37 (3H, s, OCH_3), 5.53 (1H, d, *J* = 9.0, CHN*H*), 5.83 (1H, d, *J* = 10.2, C*H*NH), 6.29–6.31 (2H, m, 2×CHFur), 7.33–7.35 (1H, m, CHFur); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 28.3 (CCH_3), 55.2 (OCH_3), 78.1 (*C*CH_3), 80.4 (CH), 107.3, 110.2, 142.6 (CHFur), 151.2 (CFur), 155.0 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{11}H_{17}O_4Na$ $[M+Na]^+$: 250.1050, found: 250.1041.

***tert*-Butyl (1-methoxy-2-methylpropyl)carbamate (4ia):**[5]



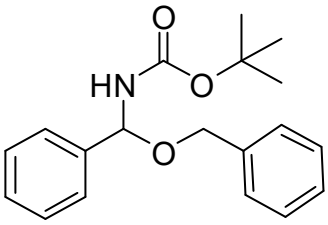
Resulting from the reaction of **1i** with **2a**. Colourless oil, 99% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 0.87 (6H, t, *J* = 7.0, CH(CH_3)$_2$), 1.41 (9H, s, 3×CCH_3), 3.28 (3H, s, OCH_3), 4.47–4.55 (1H, m, CH), 4.80 (1H d, *J* = 9.6, CHN*H*); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 17.3, 17.9 (CHCH_3), 28.4 (CCH_3), 55.6 (OCH_3), 79.6 (*C*CH_3), 87.3 (CH), 155.9 (CO).

***tert*-Butyl (1-methoxybutyl)carbamate (4ja)**:[7]



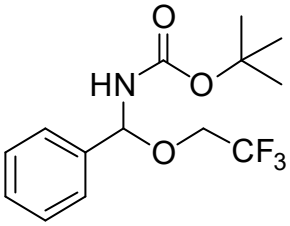
Resulting from the reaction of **1j** with **2a**. Colourless oil, 99% yield; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 0.89 (3H, t, *J* = 7.2, CH_2CH_3), 1.30–1.68 (13H, m, 3×CCH_3, 2×CH_2), 3.30 (3H, s, OCH_3), 4.72–4.84 (1H, m, CH), 4.93 (1H d, *J* = 9.9, CHN*H*); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 13.8 (CH_2CH_3), 18.3 (CH_2), 28.3 (CCH_3), 37.7 (CH_2), 55.3 (OCH_3), 79.6 (CCH_3), 82.8 (CH), 155.6 (CO).

***tert*-Butyl ((benzyloxy)(phenyl)methyl)carbamate (4cb):[8]**



Resulting from the reaction of **1c** with **2b**. White solid, 80% yield; mp=53ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 1.57 (9H, s, 3×CCH_3), 4.71 (1H, d, *J* = 11.7, CH*H*), 4.84 (1H, d, *J* = 11.7, C*H*H), 5.39 (1H, d, *J* = 9.9, CHN*H*), 6.15 (1H d, *J* = 9.9, C*H*NH), 7.32–7.58 (10H, m, 10×ArH); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 28.4 (CCH_3), 70.0 (CH_2), 80.1 (CCH_3), 81.9 (CH), 126.1, 127.6, 127.8, 128.4, 128.5 (ArCH), 138.2, 139.7 (ArC), 155.4 (CO).

***tert*-Butyl (phenyl(2,2,2-trifluoroethoxy)methyl)carbamate (4cc)**:



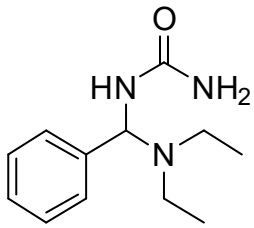
Resulting from the reaction of **1c** with **2c**. White solid, 99% yield; mp=72ºC; ^{1}H NMR (300 MHz, $CDCl_3$) δ: 1.51 (9H, s, 3×CCH_3), 4.05–4.21 (2H, m, CH_2), 5.32 (1H, d, *J* = 8.7, CHN*H*), 6.10 (1H d, *J* = 9.9, C*H*NH), 7.34–7.52 (5H, m, 5×ArH); ^{13}C NMR (75.5 MHz, $CDCl_3$) δ: 28.3 (CCH_3), 66.8 (m, CH_2), 81.2 (CCH_3), 83.3 (CH), 125.9–122.2 (q, *J* = 278, CF_3), 126.0, 128.8, 128.9 (ArCH), 138.2 (ArC), 155.5 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{14}H_{18}F_3NNaO_3$ $[M+Na]^+$: 328.1136, found: 328.1131.

[7] H. Nemoto, H. N. Jimenez, Y. Yamamoto, *J. Chem. Soc., Chem. Commun.*, **1990**, 1304.
[8] D. E. Carrera, *Chem. Commun.*, **2017**, *53*, 11185.

3.4 General procedure for the synthesis of *N,N*-acetals 5 by addition of amines 3 to imines 1 under SF-CF conditions:

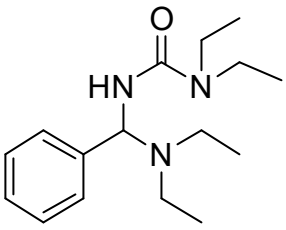
A liquid-liquid or solid-liquid mixture of the imine **1** (0.4 mmol) and the appropriate amine **3** (0.4 mmol) were quickly combined in a 5ml round bottom flask to ensure a homogeneous mixture (in some cases the solid product began to precipitate immediately after mixing) which was then gently stirred. In most cases the mixture thickened ostensibly till the point that the whole mass completely solidified. These solids were eventually identified as the pure *N,N*-acetals **5**. Products **5aa** and **5bb** in solution revert to their imine and amine components as shown by NMR in $CDCl_3$ (fast reversion) and DMSO-d6 (slow reversion). Physical, spectroscopic and analytical data, follow.

1-((Diethylamino)(phenyl)methyl)urea (5aa):



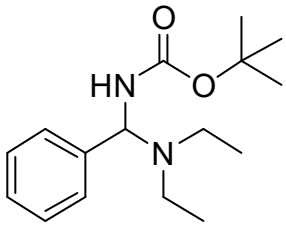
Resulting from the reaction of **1a** with **3a**. White solid, 99% yield; mp=106ºC; ^{1}H NMR (300 MHz, DMSO-d6) δ: 0.98 (6H, t, *J* = 6.9, 2×CH_3), 2.23–2.55 (4H, m, 2×CH_2), 5.63 (2H, br s, NH_2), 5.71 (1H, d, *J* = 9.6, C*H*NH), 6.59 (1H, d, *J* = 9.6, CHN*H*), 7.16–7.48 (5H, m, 5×ArH); ^{13}C NMR (75.5 MHz, DMSO-D6) δ: 13.7 (CH_3), 42.3 (CH_2), 67.0 (CH), 126.8, 126.8, 127.9 (ArCH), 142.6 (ArC), 158.9 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{12}H_{20}ON_3$ $[M+H]^+$: 222.1601, found: 222.1603.

3-((Diethylamino)(phenyl)methyl)-1,1-diethylurea (5ba):



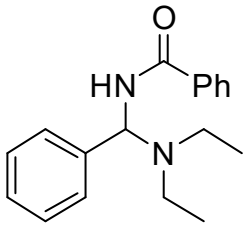
Resulting from the reaction of **1b** with **3a**. White solid, 99% yield; mp=66ºC; ^{1}H NMR (300 MHz, DMSO-d6) δ: 0.92–1.18 (12H, m, 4×CH_3), 2.23–2.38 (2H, m, 2×CH_2), 2.43–2.61 (2H, m, 2×CH_2), 3.11–3.49 (4H, m, 4×CH_2), 5.96 (1H, d, *J* = 9.3, C*H*NH), 6.26 (1H, d, *J* = 9.3, CHN*H*), 7.18–7.48 (5H, m, 5×ArH); ^{13}C NMR (75.5 MHz, DMSO-D6) δ: 13.6, 13.9 (CH_3), 40.3, 42.5 (CH_2), 67.9 (CH), 126.6, 127.0, 127.8 (ArCH), 142.5 (ArC), 156.9 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{16}H_{28}ON_3$ $[M+H]^+$: 278.2227, found: 278.2230.

***tert*-Butyl ((diethylamino)(phenyl)methyl)carbamate (5ca):**



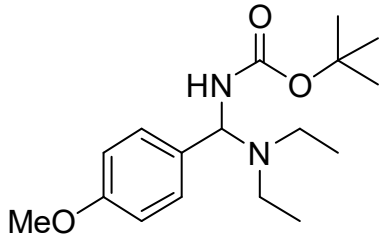
Resulting from the reaction of **1c** with **3a**. White solid, 99% yield; mp=59ºC; ^{1}H NMR (300 MHz, DMSO-d6) δ: 0.97 (6H, t, *J* = 6.9, 2×$CH_2C\mathit{H}_3$), 1.43 (9H, s, 3×CCH_3), 2.25–2.40 (2H, m, CH_2), 2.41–2.52 (2H, m, CH_2), 5.65 (1H, d, *J* = 9.9, C*H*NH), 7.19–7.50 (6H, m, 5×ArH, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 13.6 ($CH_2\mathit{C}H_3$), 28.2 ($CC\mathit{H}_3$), 42.4 (CH_2), 68.5 (CH), 77.8 ($\mathit{C}CH_3$), 126.8, 127.0, 127.9 (ArCH), 141.5 (ArC), 156.2 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{16}H_{27}O_2N_2$ $[M+H]^+$**:** 279.2067, found: 279.2067.

N-((Diethylamino)(phenyl)methyl)benzamide (5da):



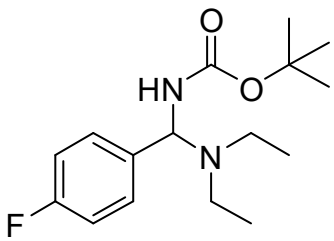
Resulting from the reaction of **1d** with **3a**. White solid, 99% yield; mp=101ºC; ^{1}H NMR (300 MHz, DMSO-d6) δ: 1.01 (6H, t, *J* = 7.0, 2×CH_3), 2.30–2.43 (2H, m, CH_2), 2.52–2.67 (2H, m, CH_2), 6.22 (1H, d, *J* = 9.3, C*H*NH), 7.13–7.61 (8H, m, 8×ArH), 7.91–7.96 (2H, m, 2×ArH), 8.69 (1H, d, *J* = 9.3, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 13.6 (CH_3), 42.7 (CH_2), 67.0 (CH), 127.1, 127.7, 128.0, 128.2, 131.3 (ArCH), 134.4, 141.0 (ArC), 167.5 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{18}H_{23}ON_2$ [M+H]$^+$: 283.1805, found: 283.1805.

***tert*-Butyl ((diethylamino)(4-methoxyphenyl)methyl)carbamate (5fa):**



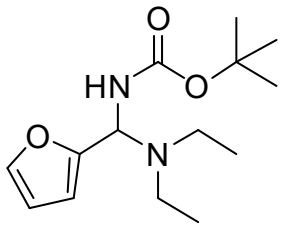
Resulting from the reaction of **1f** with **3a**. Colourless oil, 99% yield; ^{1}H NMR (300 MHz, DMSO-d6) δ: 0.96 (6H, t, *J* = 6.9, 2×CH_2CH_3), 1.42 (9H, s, 3×CCH_3), 2.23–2.41 (2H, m, CH_2), 2.42–2.60 (2H, m, CH_2), 3.73 (3H, s, OCH_3), 5.57 (1H, d, *J* = 9.9, C*H*NH), 6.88 (2H, d, *J* = 8.7, 2×ArH), 7.30 (2H, d, *J* = 8.7, 2×ArH), 7.38 (1H, d, *J* = 9.9, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 13.7 (CH_2CH_3), 28.2 (CCH_3), 42.3 (CH_2), 55.0 (OCH_3), 68.2 (CH), 77.8 (CCH_3), 113.2, 128.1 (ArCH), 133.3 (ArC), 156.1 (CO), 158.2 (ArC); HRMS (ESI$^+$) Exact mass calcd. for $C_{17}H_{29}O_3N_2$ [M+Na]$^+$: 309.2178, found: 309.2176.

***tert*-Butyl ((diethylamino)(4-fluorophenyl)methyl)carbamate (5ga):**



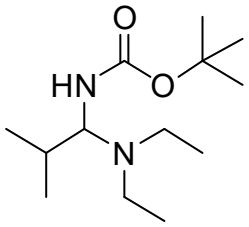
Resulting from the reaction of **1g** with **3a**. White solid, 99% yield; mp=65ºC; ^{1}H NMR (300 MHz, DMSO-d6) δ: 0.97 (6H, t, *J* = 6.9, 2×CH_2CH_3), 1.42 (9H, s, 3×CCH_3), 2.22–2.53 (4H, m, 2×CH_2), 5.63 (1H, d, *J* = 9.6, C*H*NH), 6.88 (2H, d, *J* = 8.7, 2×ArH), 7.09–7.19 (2H, m, 2×ArH), 7.38–7.52 (3H, m, 2×ArH, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 13.6 (CH_2CH_3), 28.2 (CCH_3), 42.4 (CH_2), 68.1 (CH), 77.9 (CCH_3), 114.4, 114.7, 128.8, 128.9 (ArCH), 137.6, 137.7 (ArC), 156.1 (CO), 159.6, 162.9 (ArCF); HRMS (ESI$^+$) Exact mass calcd. for $C_{16}H_{26}O_2N_2F$ [M+H]$^+$: 297.1973, found: 297.1974.

***tert*-Butyl ((diethylamino)(furan-2-yl)methyl)carbamate (5ha):**



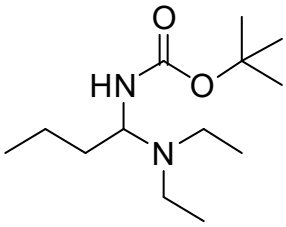
Resulting from the reaction of **1h** with **3a**. Yellow solid, 99% yield; mp=60ºC; ^{1}H NMR (300 MHz, DMSO-d6) δ: 0.92 (6H, t, *J* = 6.9, 2×CH_2CH_3), 1.37 (9H, s, 3×CCH_3), 2.22–2.39 (2H, m, CH_2), 2.40–2.55 (2H, m, CH_2), 5.57 (1H, d, *J* = 9.3, C*H*NH), 6.28 (1H, br s, CHFur), 6.34 (1H, br s, CHFur), 7.47–7.54 (2H, m, CHFur, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 13.7 (CH_2CH_3), 28.2 (CCH_3), 42.7 (CH_2), 64.6 (CH), 78.1 (CCH_3), 107.1, 110.2, 142.0 (CHFur), 153.8 (CFur), 155.8 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{14}H_{25}O_3N_2$ [M+H]$^+$: 269.1860, found: 269.1858.

***tert*-Butyl (1-(diethylamino)-2-methylpropyl)carbamate (5ia):**



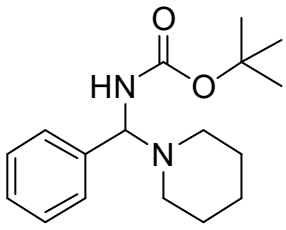
Resulting from the reaction of **1i** with **3a**. White solid, 99% yield; mp=61ºC**;** ^{1}H NMR (300 MHz, DMSO-d6) δ: 0.77 (3H, d, *J* = 6.3, CHC*H*$_3$), 0.83 (3H, d, *J* = 6.3, CHC*H*$_3$), 0.92 (6H, t, *J* = 7.0, 2×CH$_2$C*H*$_3$), 1.34 (9H, s, 3×CCH$_3$), 1.65–1.80 (1H, m, C*H*CH$_3$), 2.06–2.39 (2H, m, CH*H*), 2.35–2.52 (2H, m, C*H*H), 3.83–3.96 (1H, m, C*H*NH), 6.68 (1H, d, *J* = 9.3, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 13.9 (CH$_2$*C*H$_3$), 19.8, 20.2 (CHC*H*$_3$), 28.2 (C*C*H$_3$), 29.9 (C*H*CH$_3$), 42.4 (CH$_2$), 72.6 (CH), 77.1 (*C*CH$_3$), 156.4 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{13}H_{29}O_2N_2$ [M+H]$^+$: 245.2229, found: 245.2212.

***tert*-Butyl (1-(diethylamino)butyl)carbamate (5ja):**



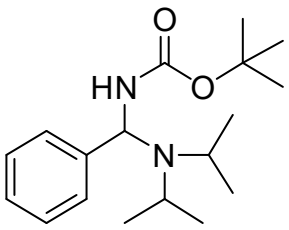
Resulting from the reaction of **1j** with **3a**. Colourless oil, 99% yield; ^{1}H NMR (300 MHz, DMSO-d6) δ: 0.84 (3H, t, *J* = 7.2, CH$_2$CH$_2$C*H*$_3$), 0.97 (3H, t, *J* = 7.2, 2×NCH$_2$C*H*$_3$), 1.13–1.54 (13H, m, 3×CCH$_3$, CH$_2$C*H*$_2$CH$_3$, C*H*$_2$CH$_2$CH$_3$), 2.14–2.30 (2H, m, CH*H*), 2.42–2.58 (2H, m, C*H*H), 4.33–4.45 (1H, m, C*H*NH), 6.74 (1H, d, *J* = 9.3, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 13.5, 14.2 (CH$_2$*C*H$_3$), 19.1 (CH$_2$*C*H$_2$CH$_3$), 28.2 (C*C*H$_3$), 29.9 (C*H*CH$_3$), 35.3 (*C*H$_2$CH$_2$CH$_3$), 42.4 (NCH$_2$), 66.2 (CH), 77.1 (*C*CH$_3$), 155.9 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{13}H_{29}O_2N_2$ [M+H]$^+$: 245.2229, found: 245.2224.

***tert*-Butyl (phenyl(piperidin-1-yl)methyl)carbamate (5cb):**



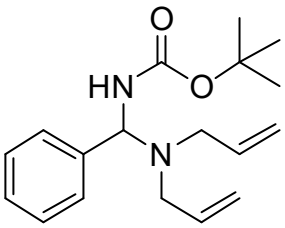
Resulting from the reaction of **1c** with **3b**. White solid, 99% yield; mp=82ºC; ^{1}H NMR (300 MHz, DMSO-d6) δ: 1.20–1.59 (15H, m, 3×CH$_2$, CCH$_3$), 2.37 (4H, br s, 2×CH$_2$), 5.40 (1H, d, *J* = 9.6, C*H*NH), 7.19–7.50 (5H, m, 5×ArH), 7.51 (1H, d, *J* = 9.3, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 24.2, 25.7 (CH$_2$), 28.2 (CH$_3$), 48.7 (CH$_2$), 73.0 (CH), 77.8 (*C*CH$_3$), 127.0, 127.1, 127.9 (ArCH), 140.2 (ArC), 155.8 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{17}H_{27}O_2N_2$ [M+H]$^+$: 291.2067, found: 291.2066.

***tert*-Butyl ((diisopropylamino)(phenyl)methyl)carbamate (5cc):**



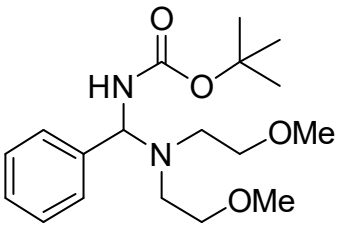
Resulting from the reaction of **1c** with **3c**. White solid, 99% yield; mp=58ºC; ^{1}H NMR (300 MHz, DMSO-d6) δ: 0.97 (6H, d, *J* = 6.6, 2×CHC*H*$_3$), 1.08 (6H, d, *J* = 6.3, 2×CHC*H*$_3$), 1.43 (9H, s, 3×CCH$_3$), 3.00–3.13 (2H, m, 2×C*H*CH$_3$), 5.69 (1H, d, *J* = 9.6, C*H*NH), 7.15–7.42 (5H, m, 5×ArH), 7.46 (1H, d, *J* = 9.3, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 21.8, 23.3 (CH*C*H$_3$), 28.2 (C*C*H$_3$), 44.6 (*C*HCH$_3$), 65.0 (CH), 77.7 (*C*CH$_3$), 126.5, 126.9, 127.7 (ArCH), 143.3 (ArC), 154.98 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{18}H_{31}O_2N_2$ [M+H]$^+$: 307.2386, found: 307.2385.

***tert*-Butyl ((diallylamino)(phenyl)methyl)carbamate (5cd):**



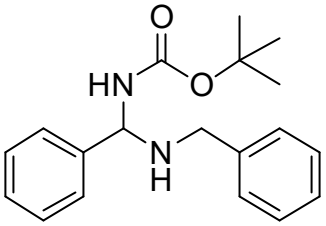
Resulting from the reaction of **1c** with **3d**. White solid, 99% yield; mp=98ºC; ^{1}H NMR (300 MHz, DMSO-d6) δ: 1.41 (9H, s, 3×CCH_3), 2.81–2.93 (2H, m, NCH_2), 2.97–3.07 (2H, m, NCH_2), 5.02–5.22 (4H, m, 2xCH=CH_2), 5.60 (1H, d, *J* = 9.6, C*H*NH), 5.68–5.83 (1H, m, 2xC*H*=CH_2), 7.18–7.44 (5H, m, 5×ArH), 7.51 (1H, d, *J* = 9.6, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 28.2 (CCH_3), 51.3 (NCH_2), 68.4 (CH), 77.9 (*C*CH_3), 116.7 (=CH_2), 126.9, 127.1, 128.0 (ArCH), 136.3 (=CH), 140.9 (ArC), 156.0 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{18}H_{27}O_2N_2$ $[M+H]^+$: 303.2067, found: 303.2065.

***tert*-Butyl ((bis(2-methoxyethyl)amino)(phenyl)methyl)carbamate (5ce):**



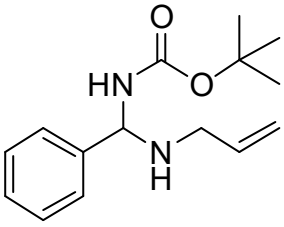
Resulting from the reaction of **1c** with **3e**. Colourless oil, 99% yield; ^{1}H NMR (300 MHz, DMSO-d6) δ: 1.43 (9H, s, 3×CCH_3), 2.55–2.68 (4H, m, 2×NCH_2), 3.19 (6H, s, 2×OCH_3), 3.22–3.43 (4H, m, OCH_2), 5.60 (1H, d, *J* = 9.6, C*H*NH), 7.18–7.44 (5H, m, 5×ArH), 7.57 (1H, d, *J* = 9.6, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 28.2 (CCH_3), 49.1 (NCH_2), 57.9 (OCH_3), 70.3 (CH), 71.1 (CH_2O), 78.0 (*C*CH_3), 127.0, 127.1, 127.9 (ArCH), 140.8 (ArC), 156.1 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{18}H_{30}O_4N_2Na$ $[M+Na]^+$: 361.2098, found: 361.2097.

***tert*-Butyl ((benzylamino)(phenyl)methyl)carbamate (5cf):**



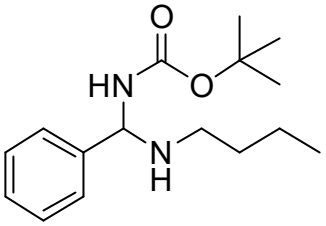
Resulting from the reaction of **1c** with **3f**. White solid, 99% yield; mp=83ºC; ^{1}H NMR (300 MHz, DMSO-D6) δ: 1.41 (9H, s, 3×CCH_3), 3.66–3.88 (2H, m, CH_2), 3.19 (6H, s, 2×OCH_3), 5.25 (1H, d, *J* = 7.8, CH), 7.16–7.46 (11H, m, 10×ArH, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 28.2 (CCH_3), 49.0 (CH_2), 67.0 (CH), 77.8 (*C*CH_3), 126.4, 126.6, 127.2, 128.0, 128.0, 128.1 (ArCH), 140.5, 142.4 (ArC), 155.2 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{19}H_{25}O_2N_2$ $[M+H]^+$: 313.1911, found: 313.1909.

***tert*-Butyl ((allylamino)(phenyl)methyl)carbamate (5cg):**



Resulting from the reaction of **1c** with **3g**. White solid, 99% yield; mp=61ºC; ^{1}H NMR (300 MHz, DMSO-d6) δ: 1.40 (9H, s, 3×CCH_3), 3.08–3.32(2H, m, NCH_2), 5.02–5.21 (2H, m, CH=CH_2), 5.27 (1H, d, *J* = 8.7, C*H*NH), 5.80–5.96 (1H, m, C*H*=CH_2), 7.14–7.48 (6H, m, 6×ArH, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 28.2 (CCH_3), 47.8 (NCH_2), 67.0 (CH), 77.7 (*C*CH_3), 115.3 (=CH_2), 126.4, 127.2, 128.0 (ArCH), 137.1 (=CH), 142.4 (ArC), 155.1 (CO); HRMS (ESI$^+$) Exact mass calcd. for $C_{15}H_{23}O_2N_2$ $[M+H]^+$: 263.1754, found: 263.1754.

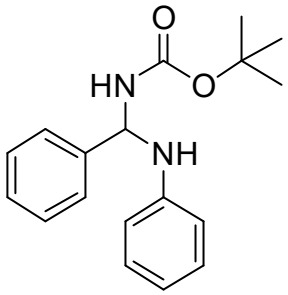
***tert*-Butyl ((butylamino)(phenyl)methyl)carbamate (5ch)**:



Resulting from the reaction of **1c** with **3h**. White solid, 99% yield; mp=46ºC; ^{1}H NMR (300 MHz, DMSO-d6) δ: 0.87 (3H, t, *J* = 7.0, CH_2CH_3), 1.23–1.50

(13H, m, 3×CCH_3, 2×CH_2), 2.42–2.53 (1H, m, NCH*H*), 2.56–2.69 (1H, m, NC*H*H), 5.26 (1H, d, *J* = 8.7, C*H*NH), 7.15 (1H, d, *J* = 8.4, CHN*H*), 7.18–7.44 (5H, m, 5×ArH); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 13.9 (CH_2CH_3), 20.0 (CH_2), 28.2 (CCH_3), 31.6 (CH_2), 44.9 (NCH_2), 67.7 (CH), 77.7 (CCH_3), 126.4, 127.1, 127.9 (ArCH), 142.6 (ArC), 155.2 (CO); HRMS (ESI^+) Exact mass calcd. for $C_{16}H_{27}O_2N_2$ $[M+H]^+$: 279.2067, found: 279.2067.

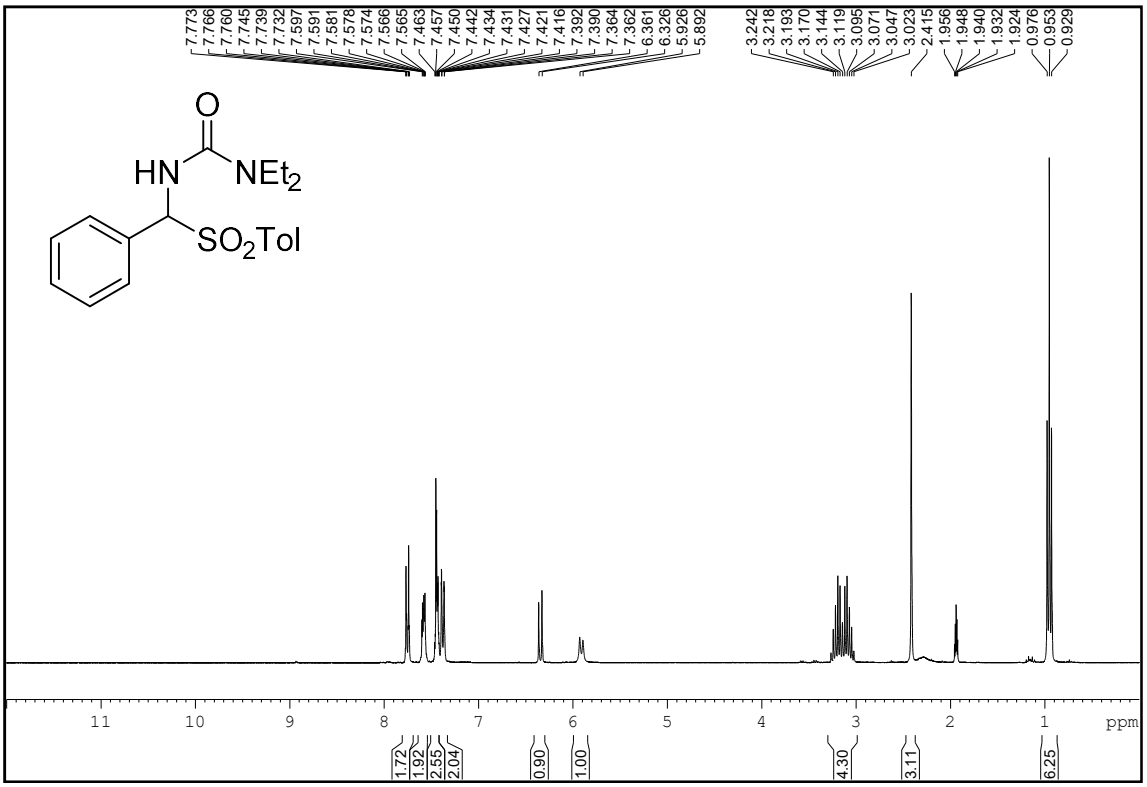
***tert*-Butyl (phenyl(phenylamino)methyl)carbamate (5ci):**

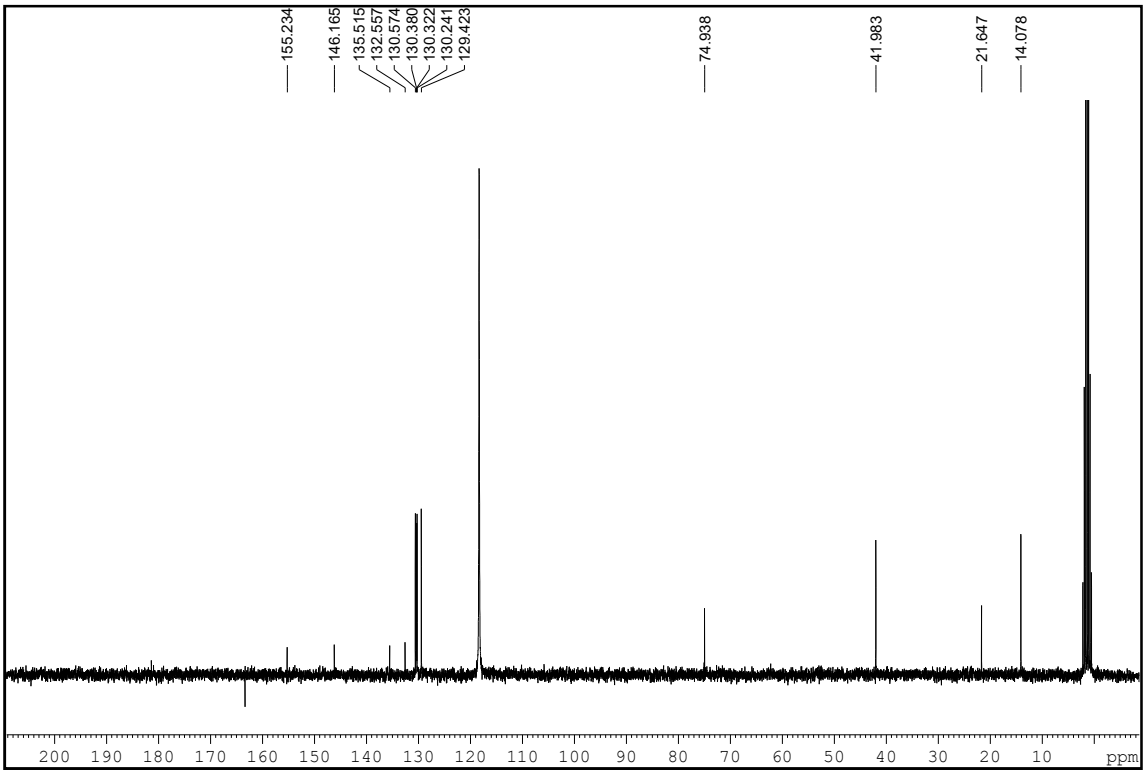


Resulting from the reaction of **1c** with **3i**. White solid, 99% yield; mp=104ºC ; ^{1}H NMR (300 MHz, DMSO-d6) δ: 1.37 (9H, s, 3×CCH_3), 5.92–6.13 (2H, m, CH, NHPh), 6.60 (1H, t, *J* = 7.2, ArH), 6.74 (2H, d, *J* = 7.8, 2×ArH), 7.03–7.12 (2H, m, 2×ArH), 7.25–7.40 (3H, m, 3×ArH), 7.46–7.52 (2H, m, 2×ArH), 7.58 (1H, d, *J* = 6.9, CHN*H*); ^{13}C NMR (75.5 MHz, DMSO-d6) δ: 28.2 (CCH_3), 63.0 (CH), 78.0 (CCH_3), 113.2, 116.8, 126.6, 127.6, 128.3, 128.7 (ArCH), 141.4, 146.7 (ArC), 155.1 (CO); HRMS (ESI^+) Exact mass calcd. for $C_{18}H_{23}O_2N_2$ $[M+H]^+$: 299.1760, found: 299.1761.

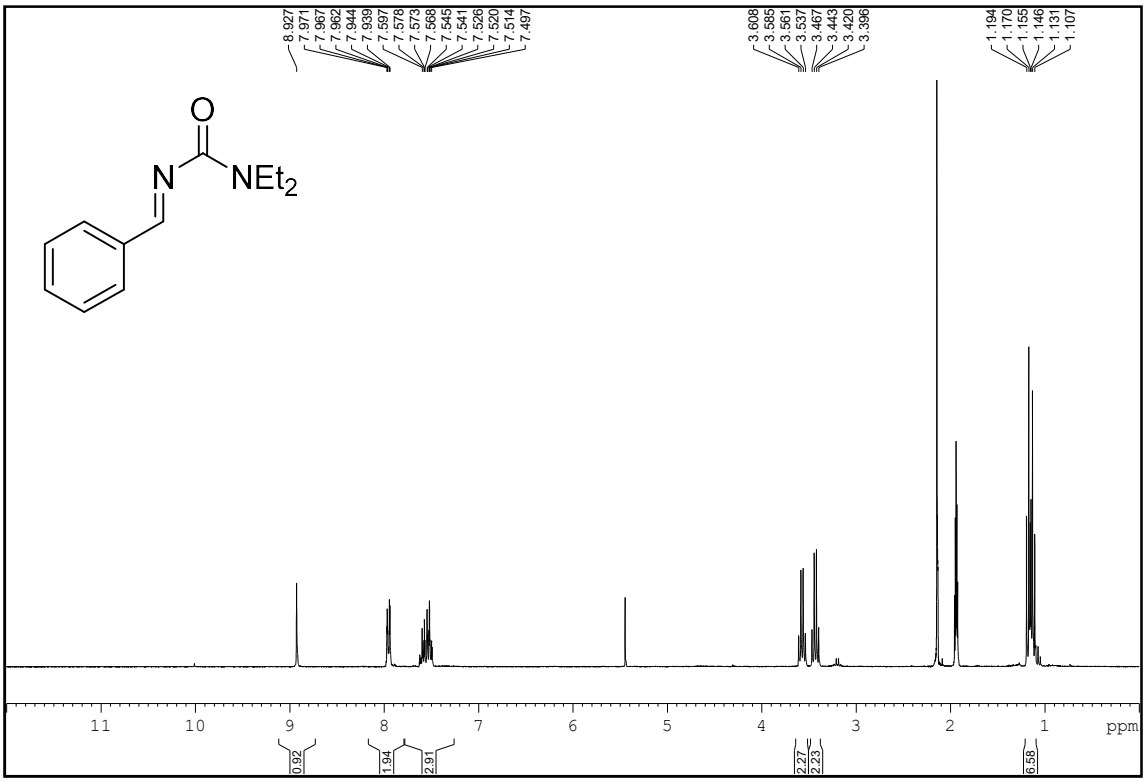
4. ^{1}H- and ^{13}C-NMR spectra

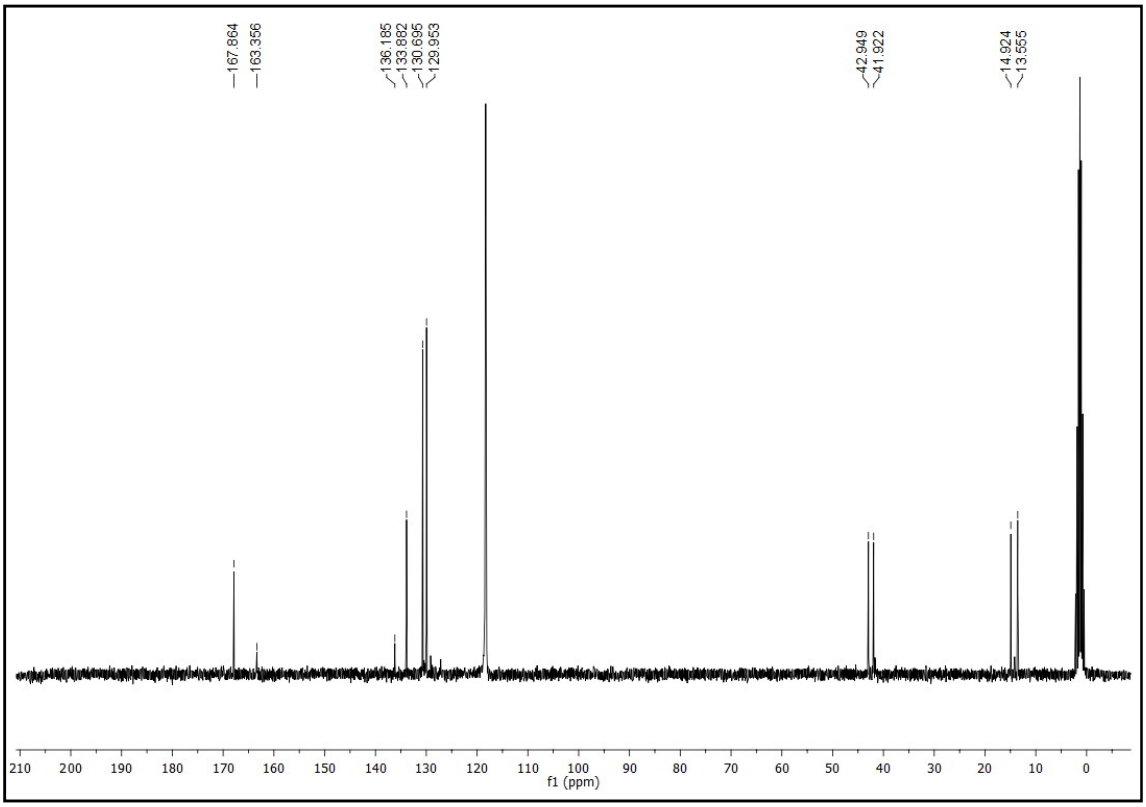
1,1-Diethyl-3-(phenyl(tosyl)methyl)urea:



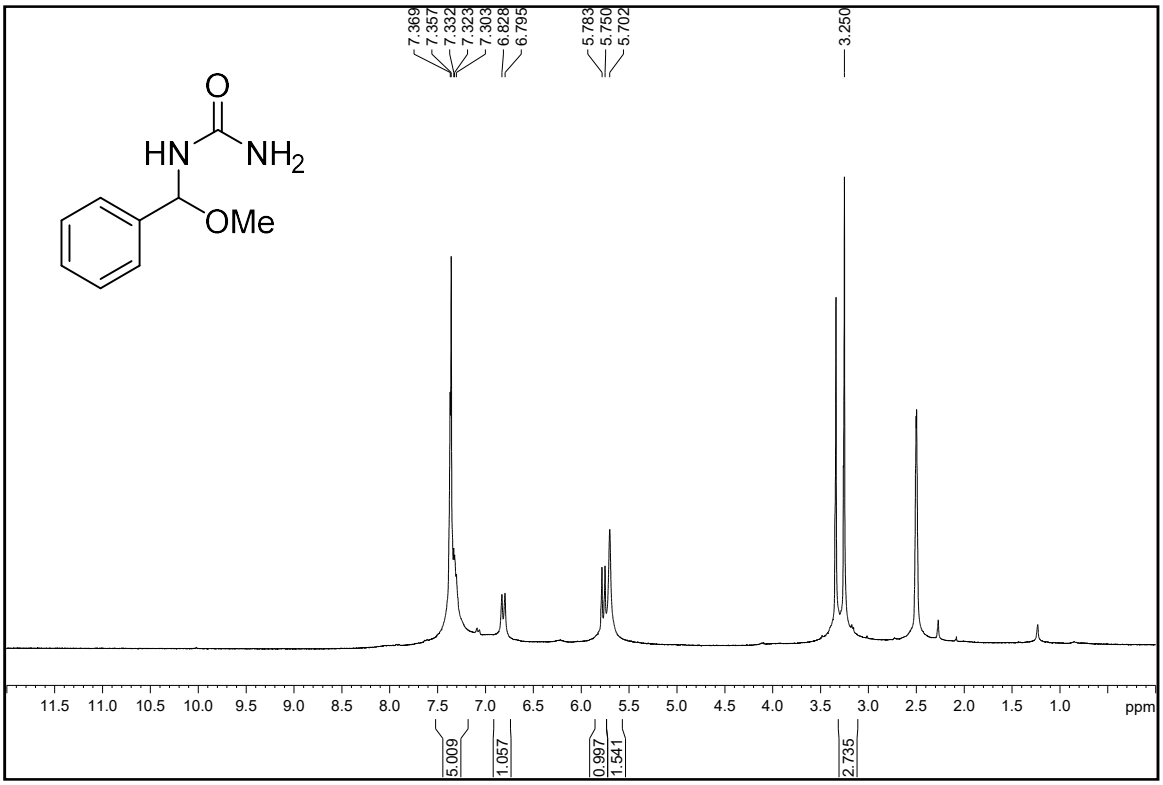


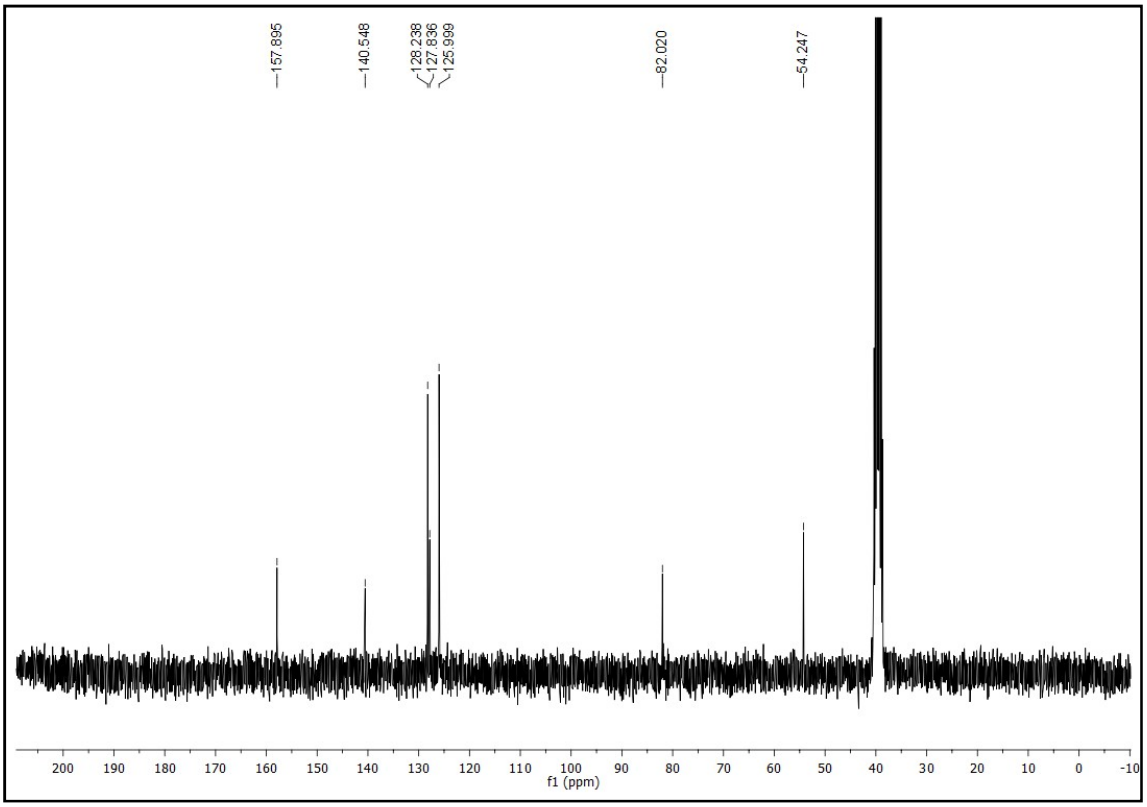
(*E*)-3-Benzylidene-1,1-diethylurea (1b):



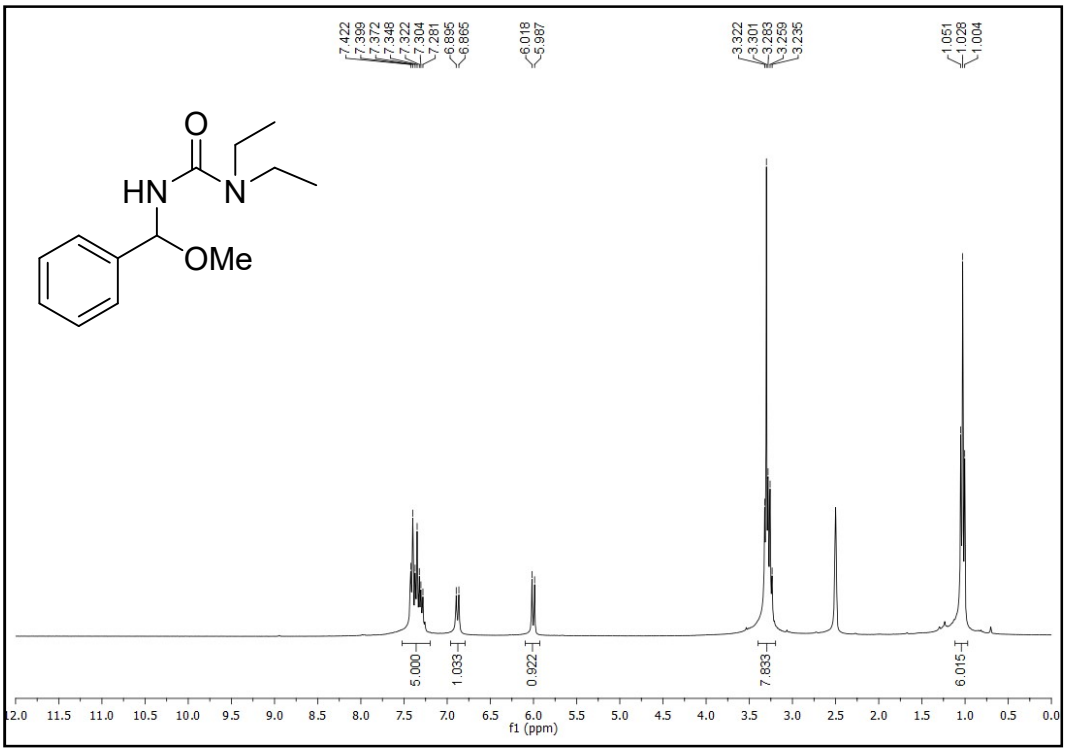


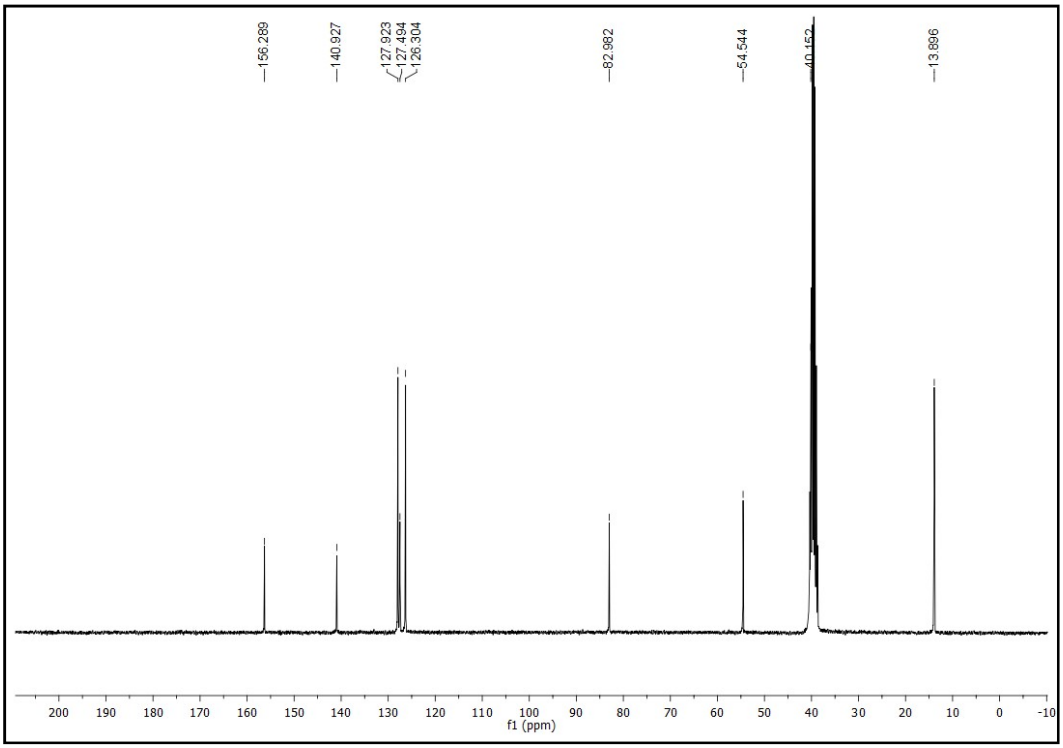
1-(Methoxy(phenyl)methyl)urea (4aa):



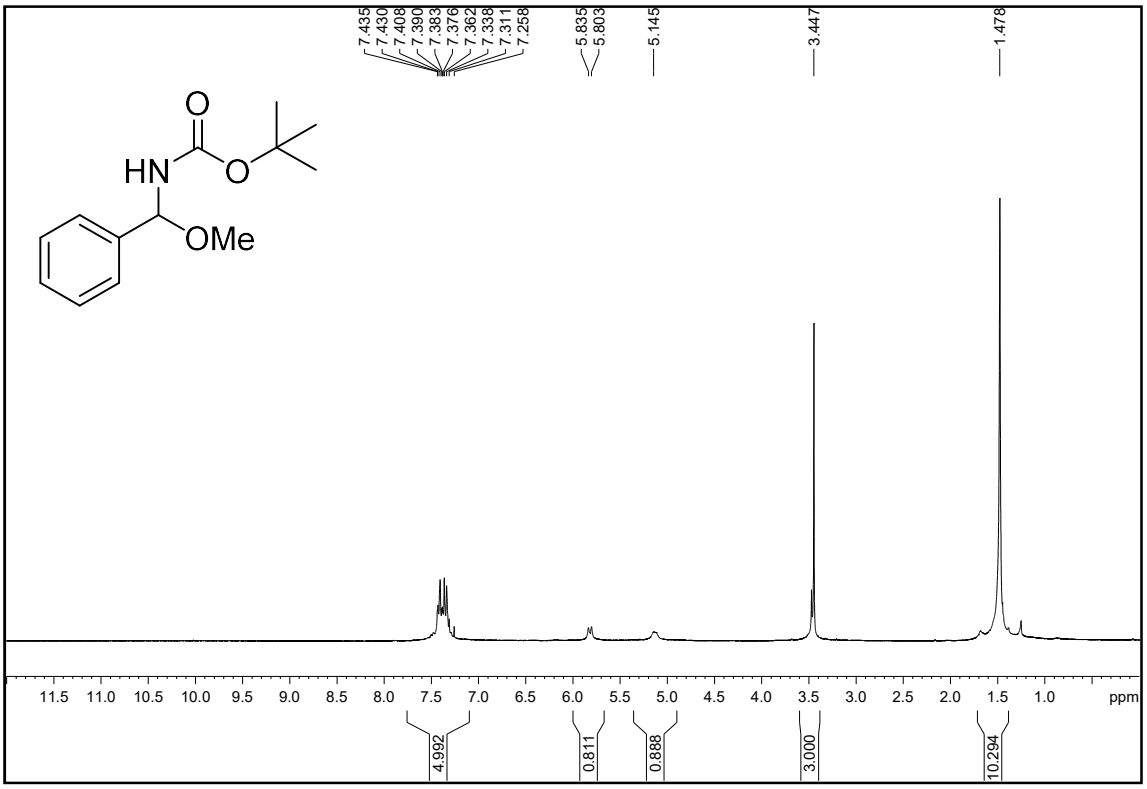


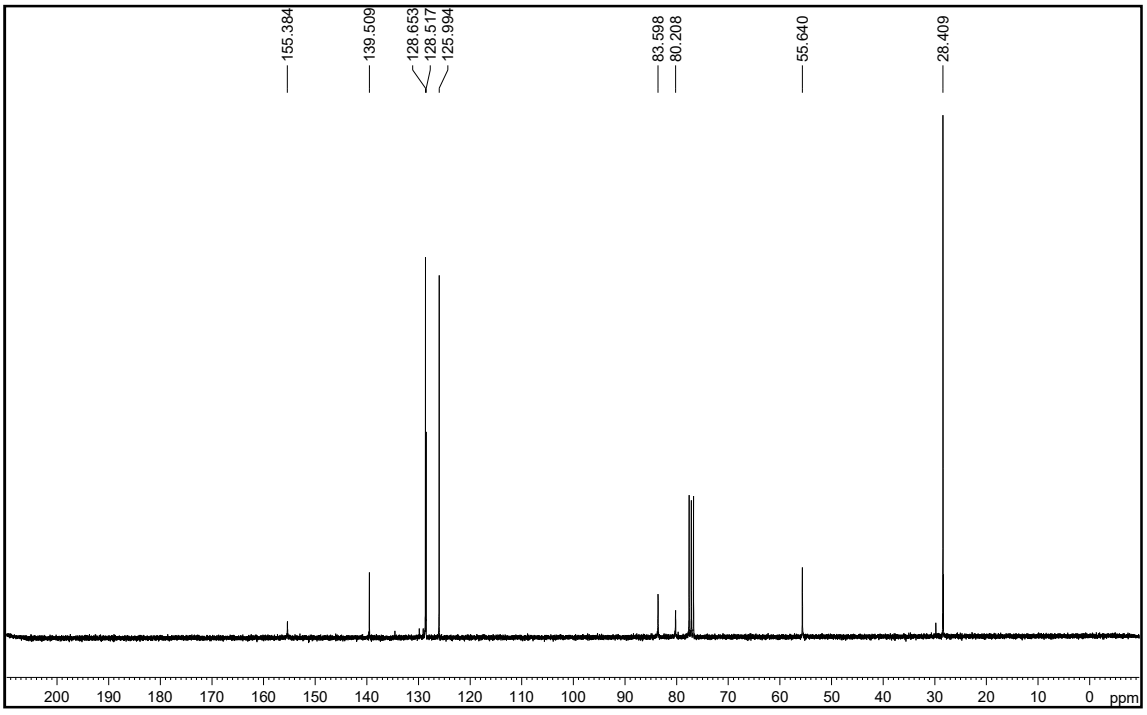
1,1-Diethyl-3-(methoxy(phenyl)methyl)urea (4ba):



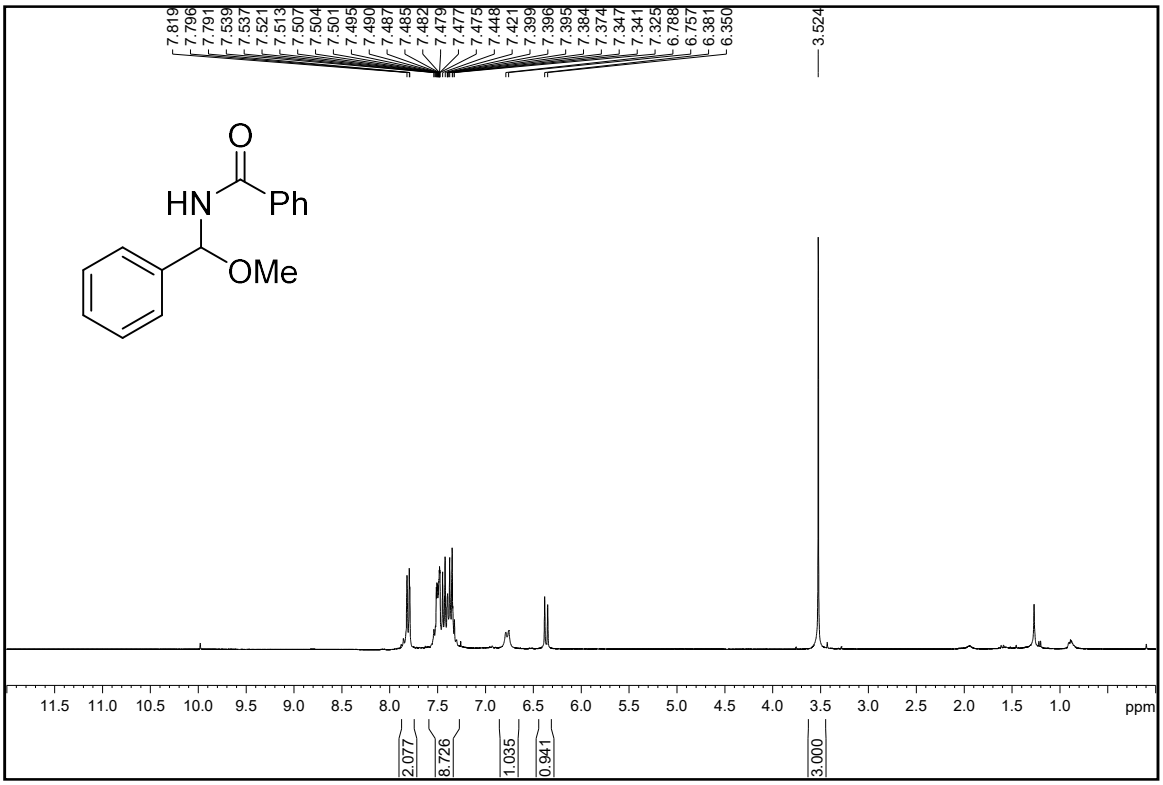


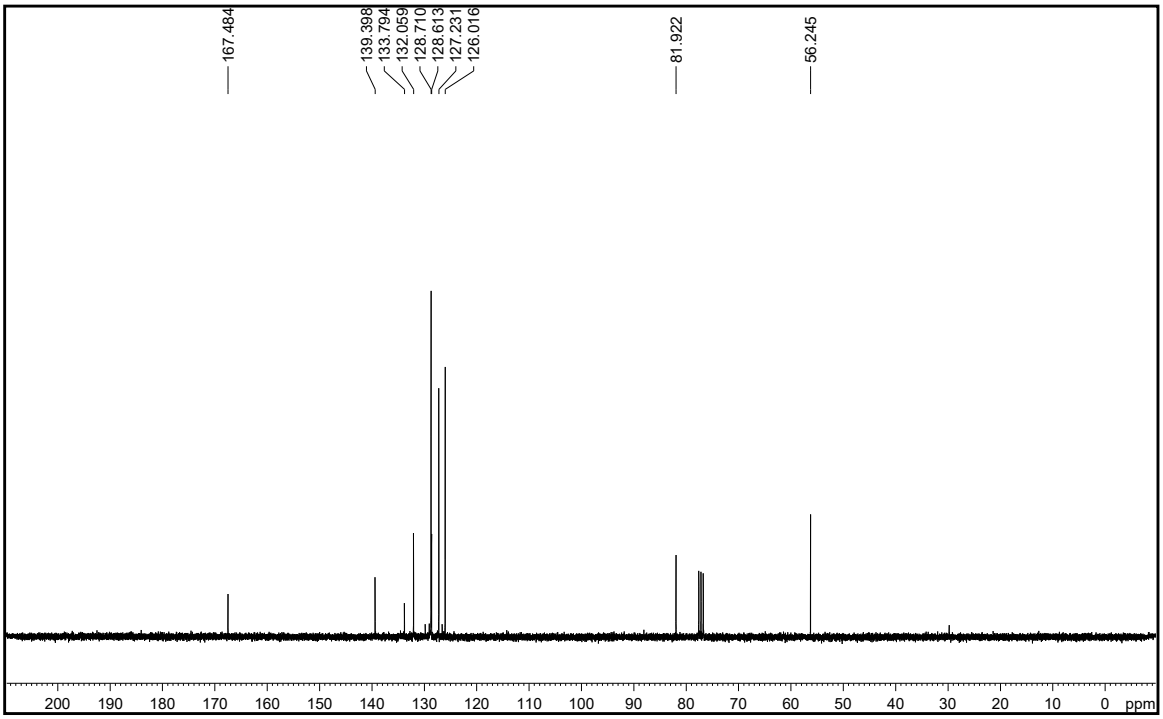
***tert*-Butyl (methoxy(phenyl)methyl)carbamate (4ca):**



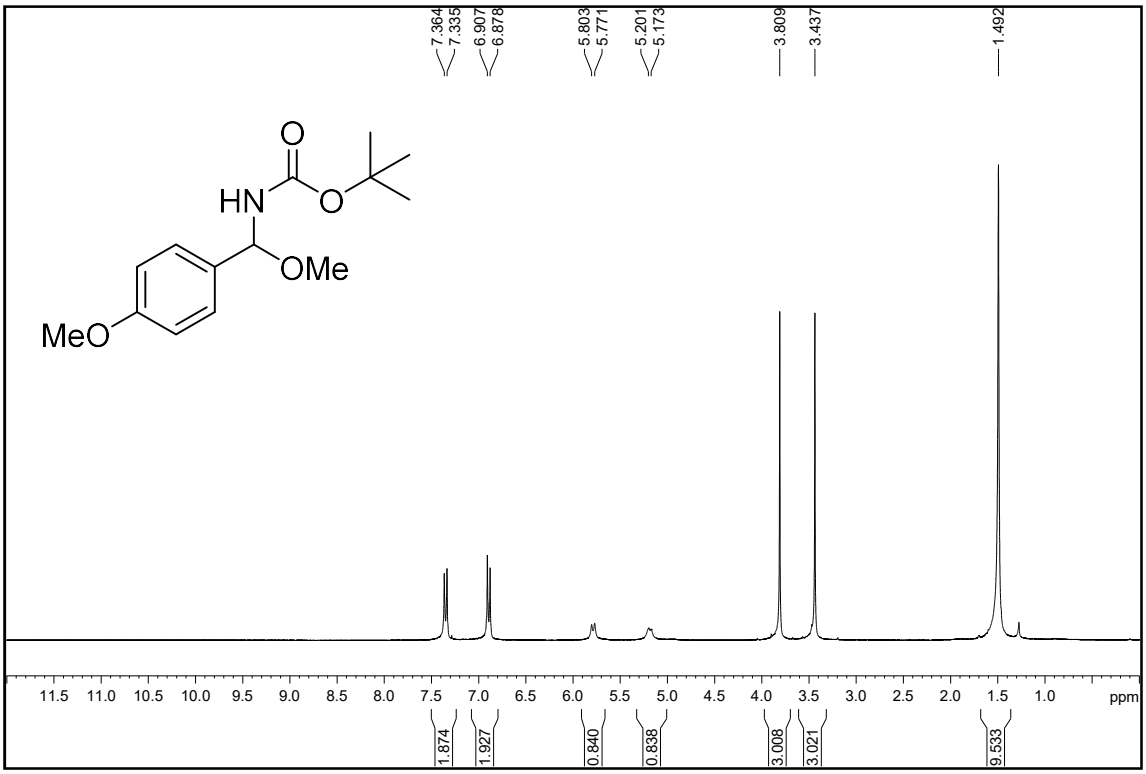


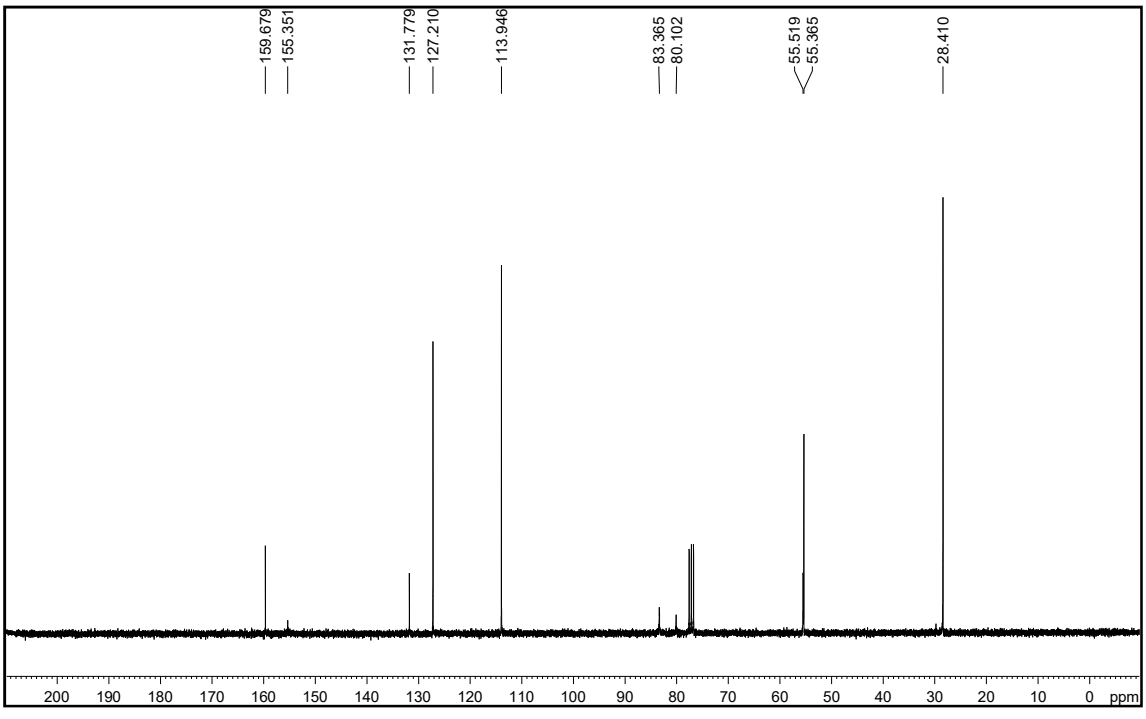
N-(Methoxy(phenyl)methyl)benzamide (4da):



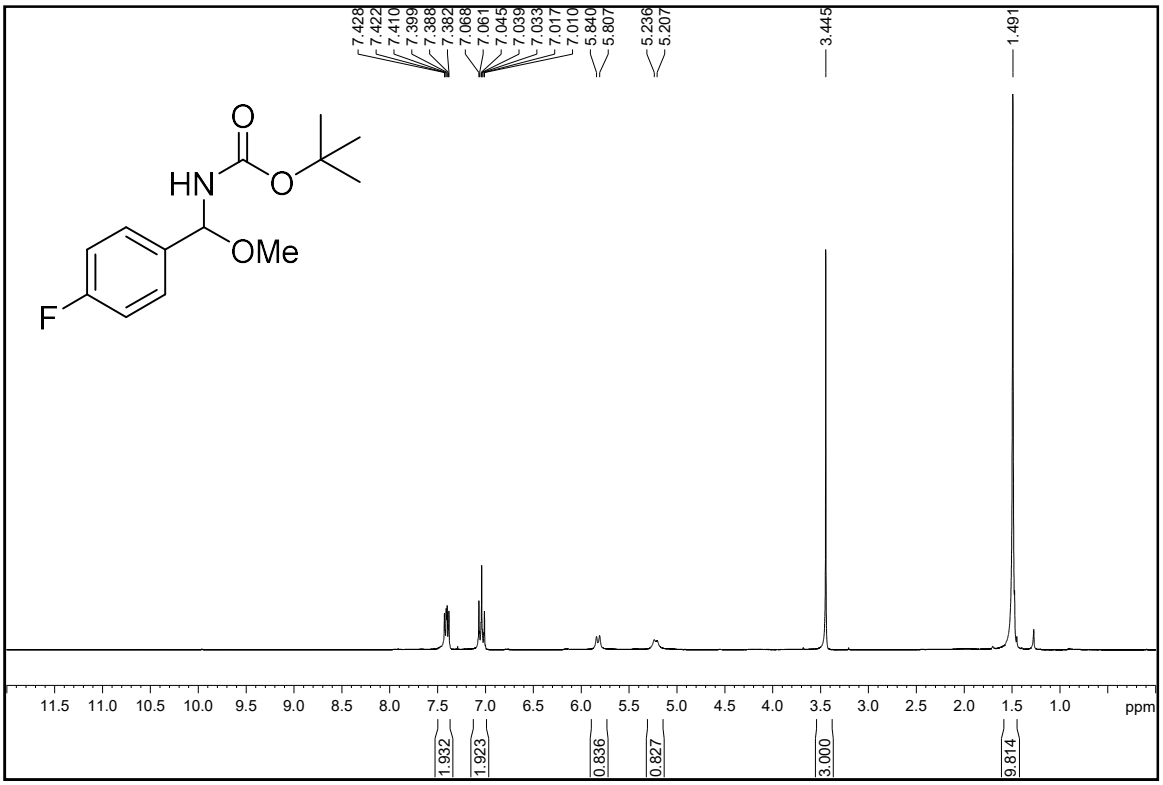


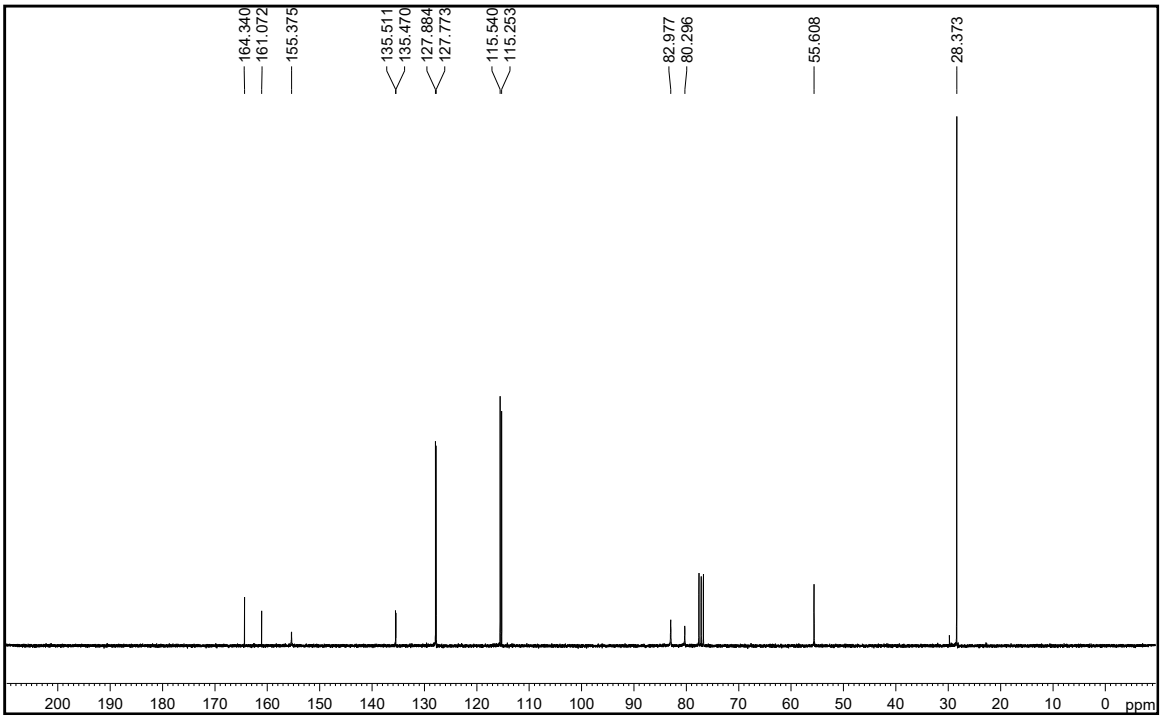
***tert*-Butyl (methoxy(4-methoxyphenyl)methyl)carbamate (4fa):**



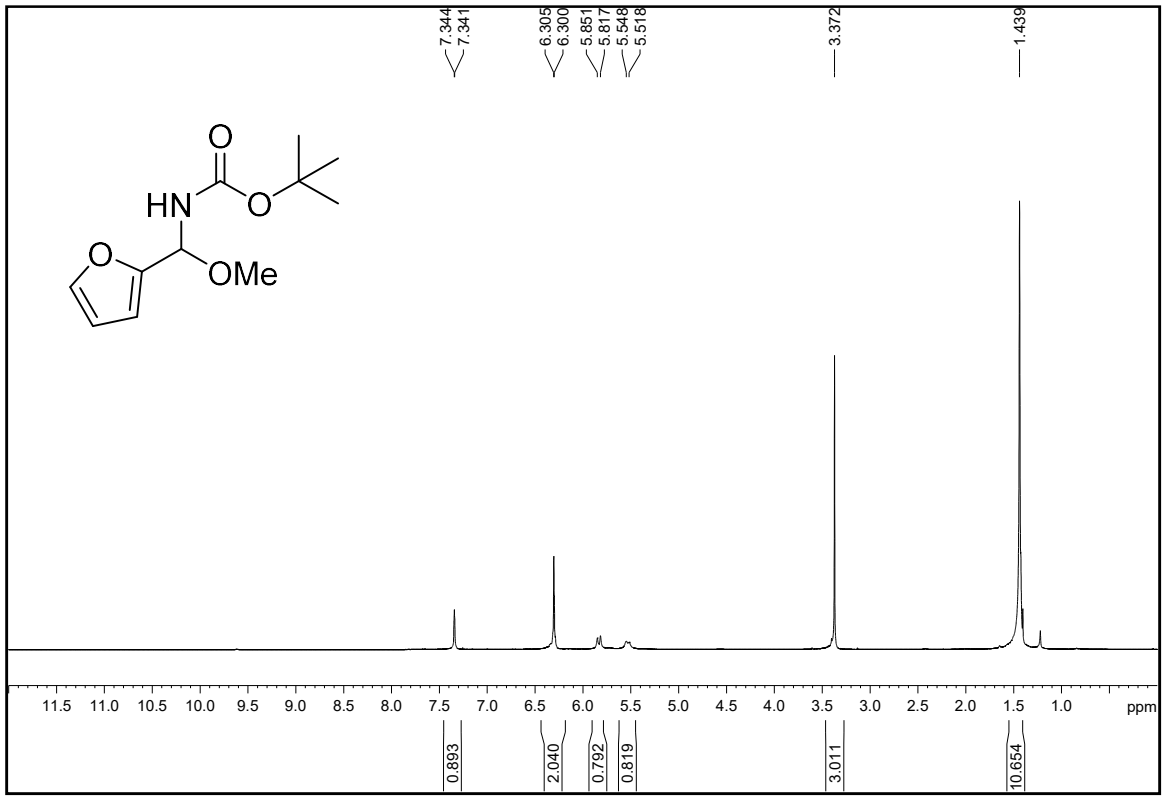


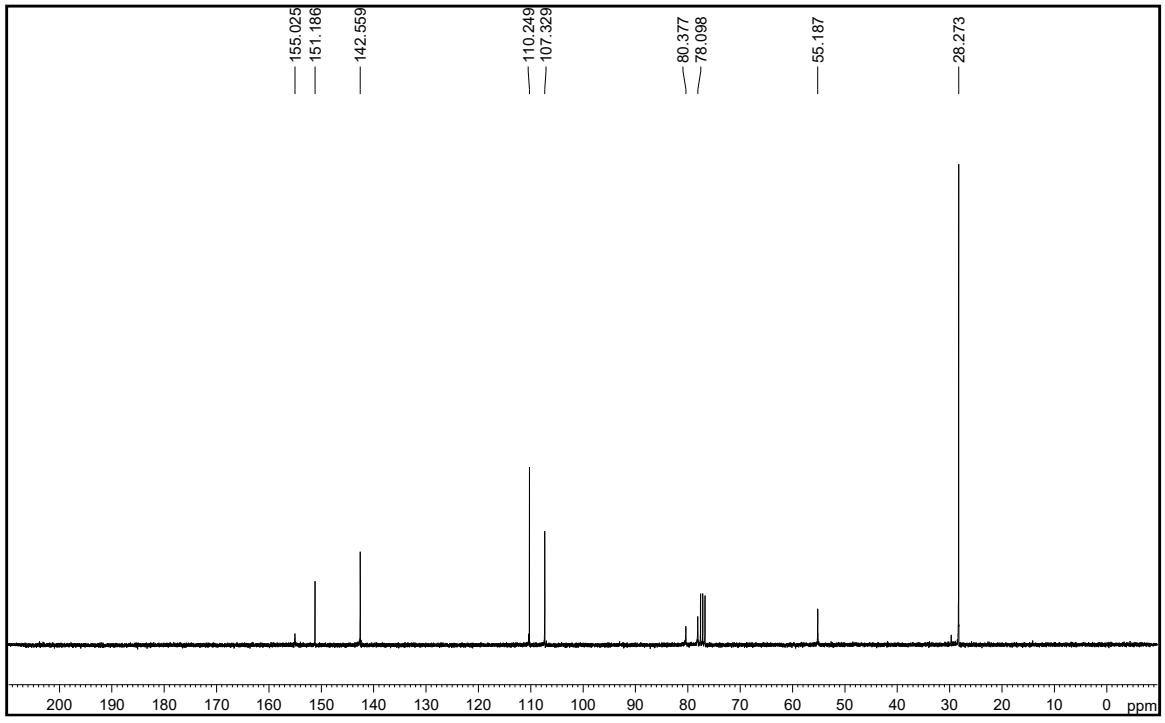
***tert*-Butyl ((4-fluorophenyl)(methoxy)methyl)carbamate (4ga):**



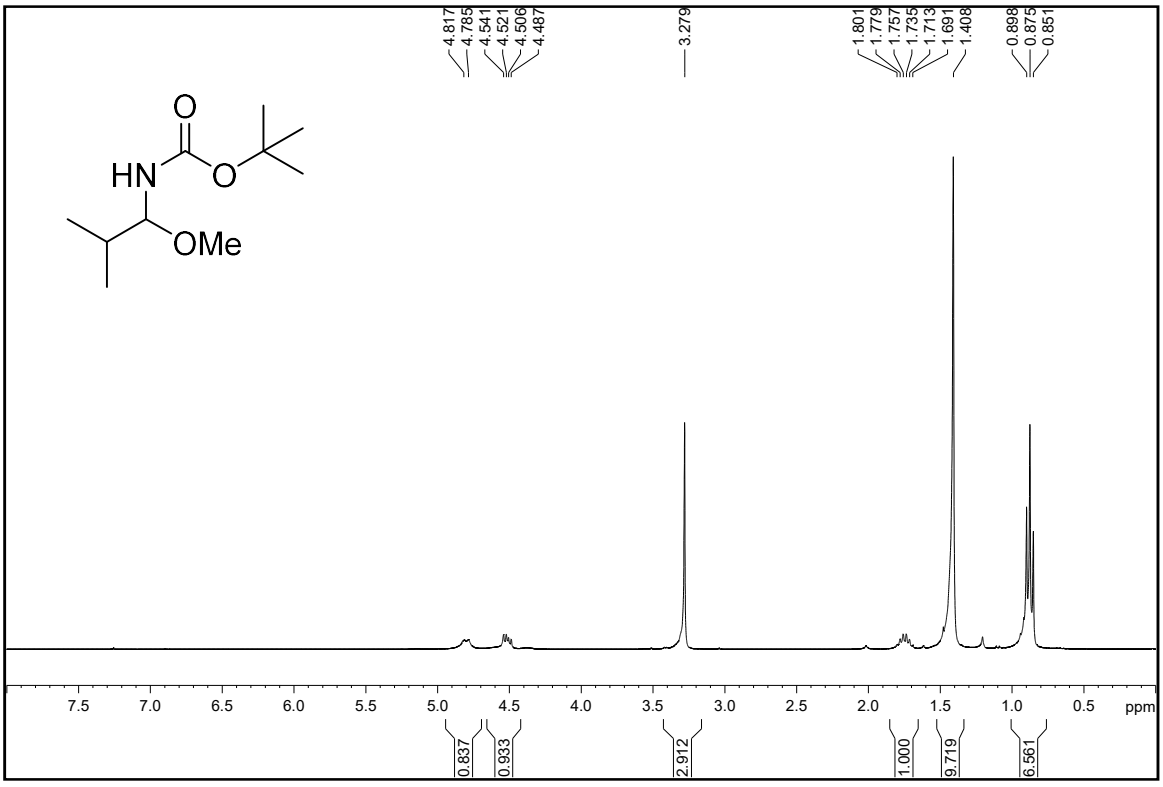


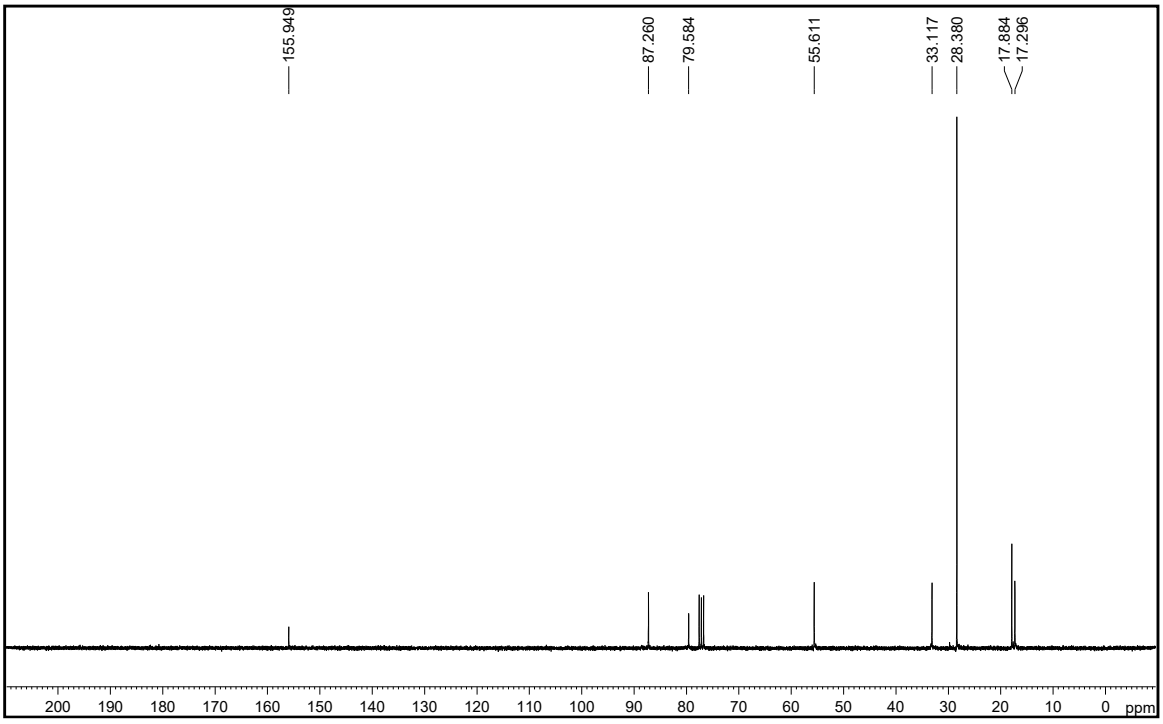
***tert*-Butyl (furan-2-yl(methoxy)methyl)carbamate (4ha):**



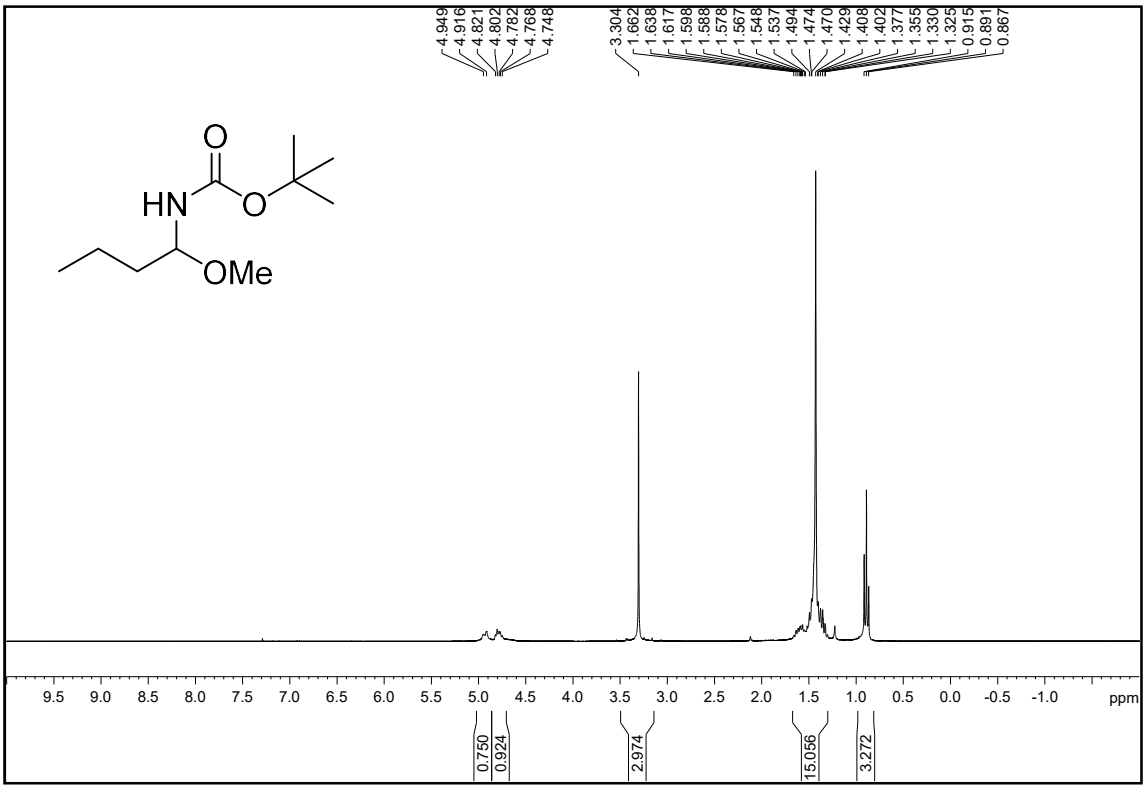


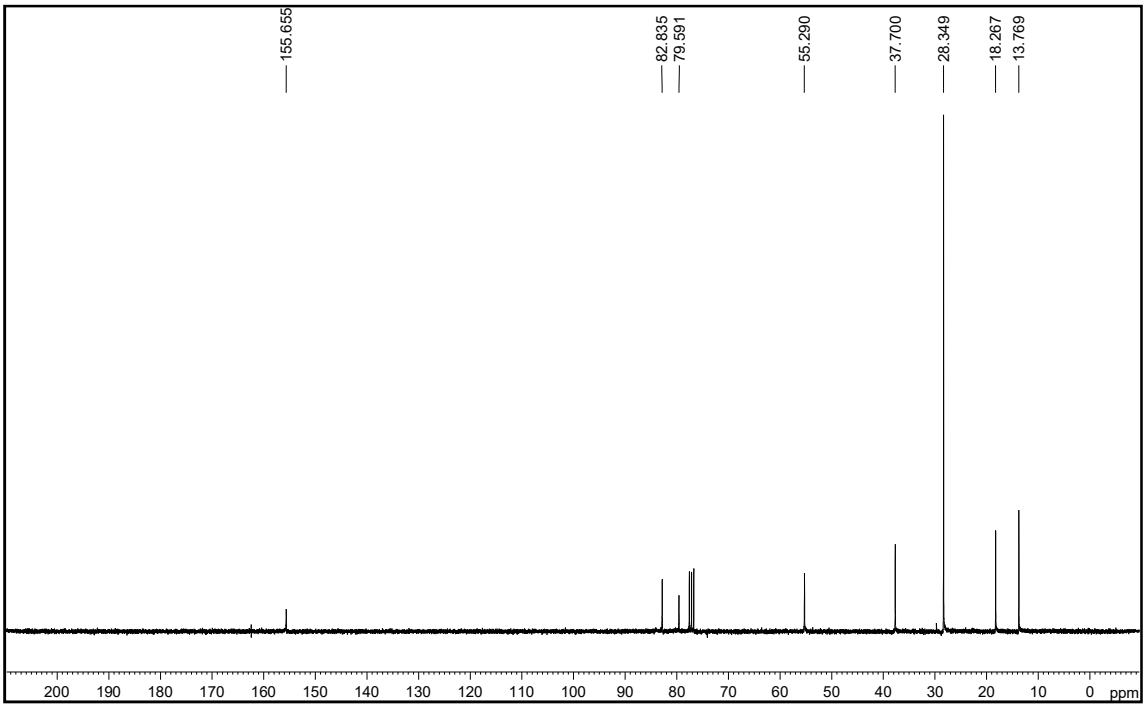
***tert*-Butyl (1-methoxy-2-methylpropyl)carbamate (4ia)**:



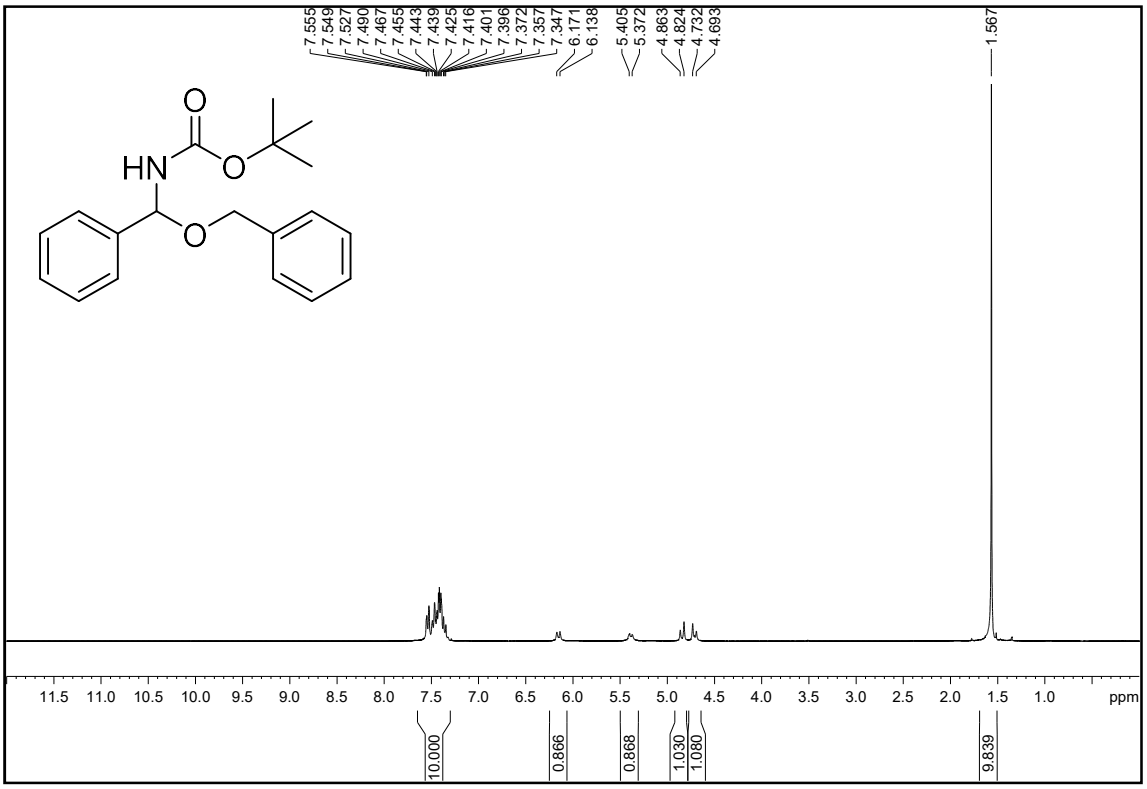


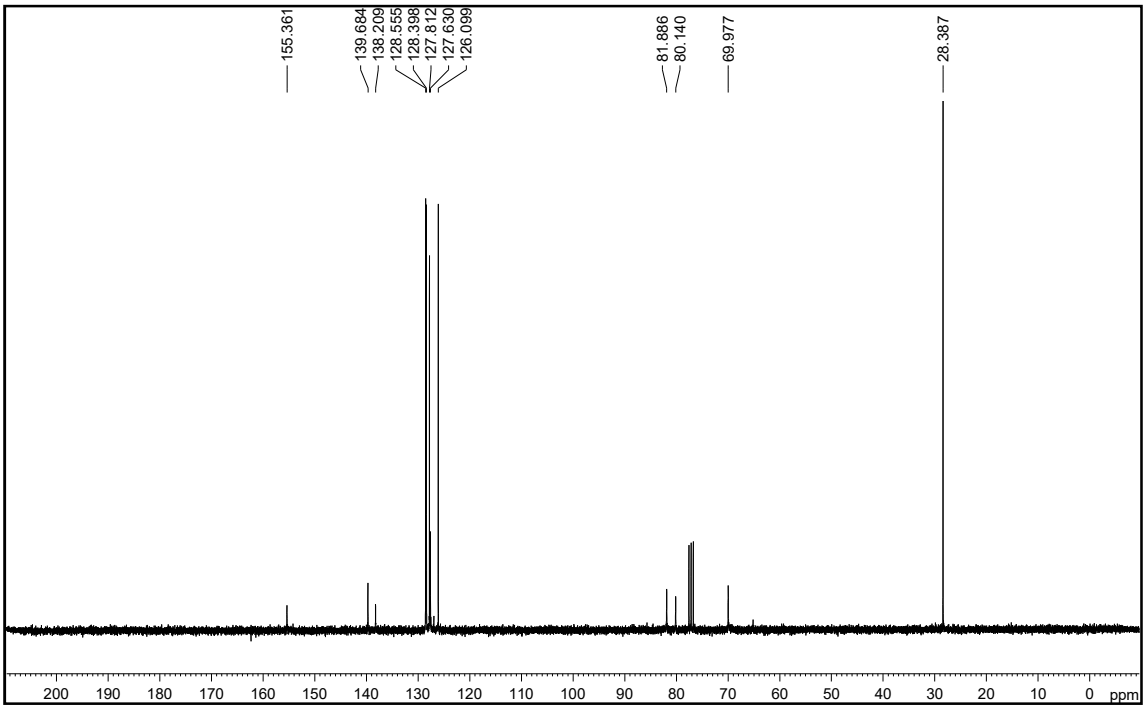
***tert*-Butyl (1-methoxybutyl)carbamate (4ja)**:



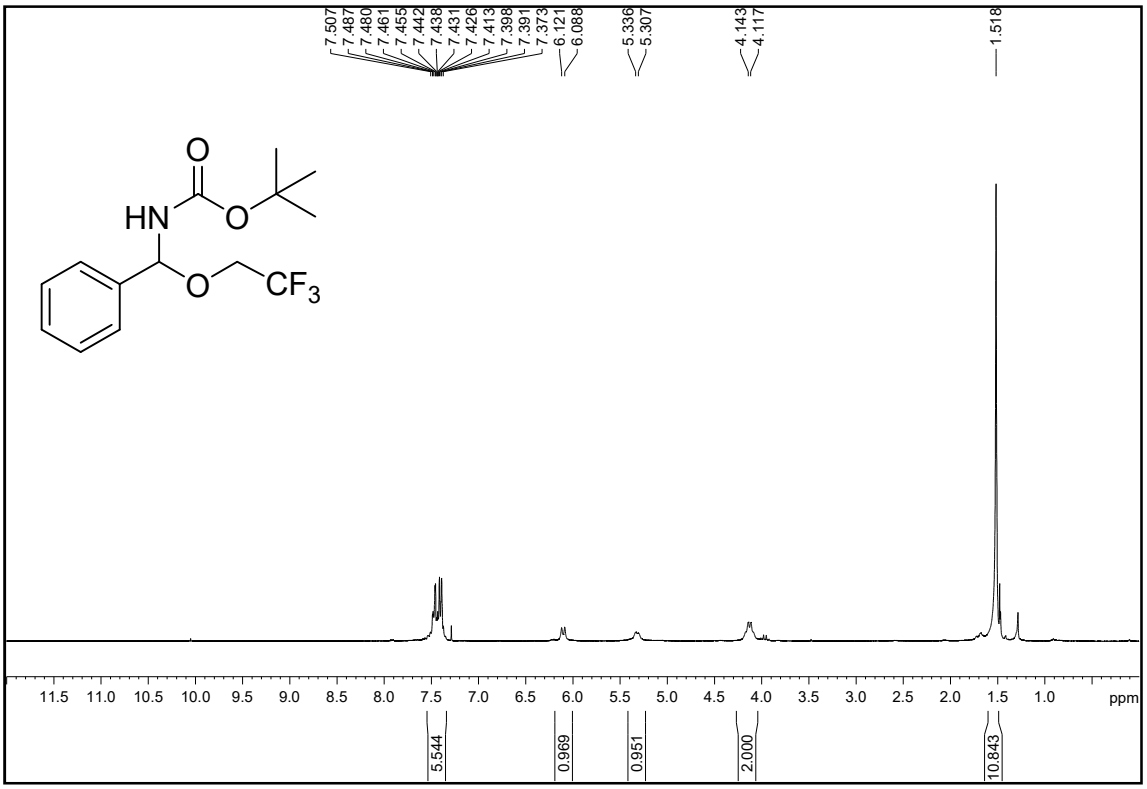


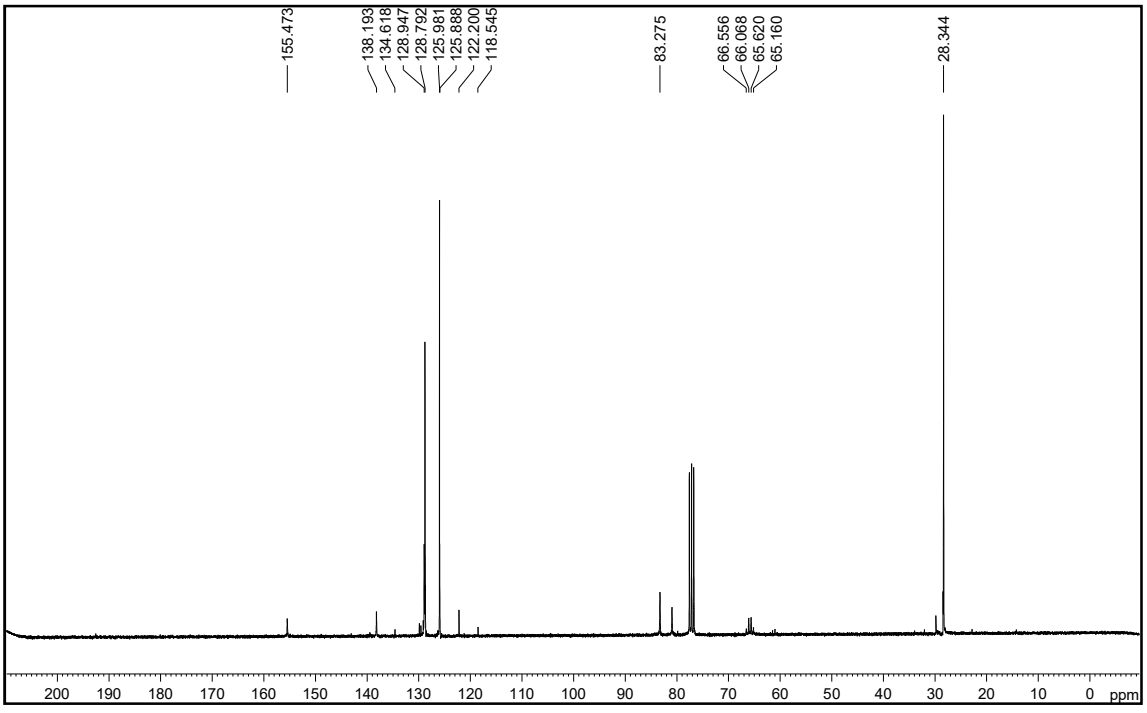
***tert*-Butyl ((benzyloxy)(phenyl)methyl)carbamate (4cb):**



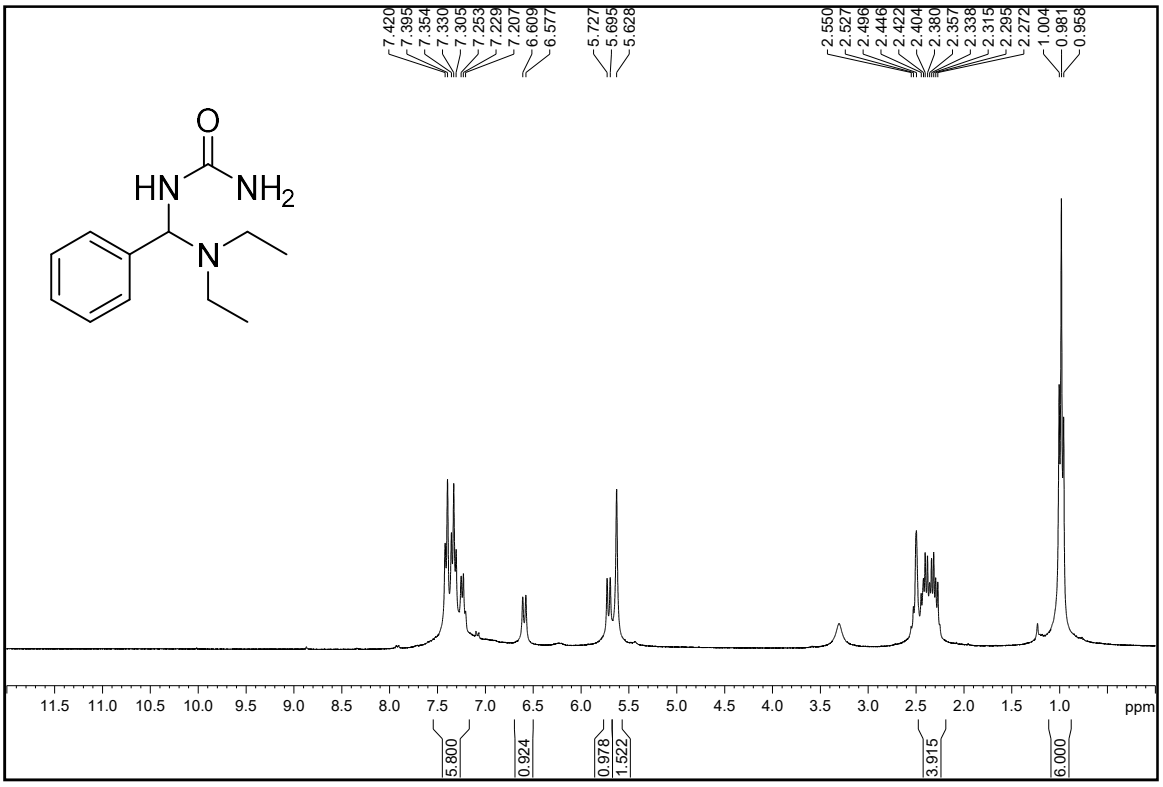


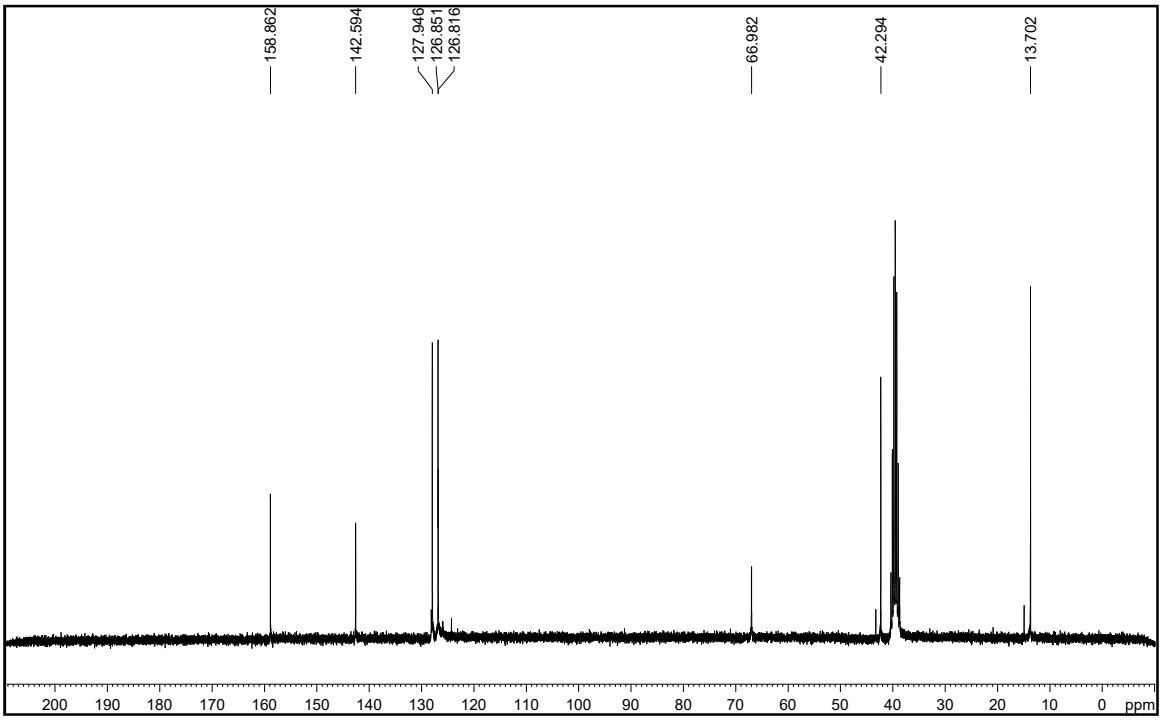
***tert*-Butyl (phenyl(2,2,2-trifluoroethoxy)methyl)carbamate (4cc)**:



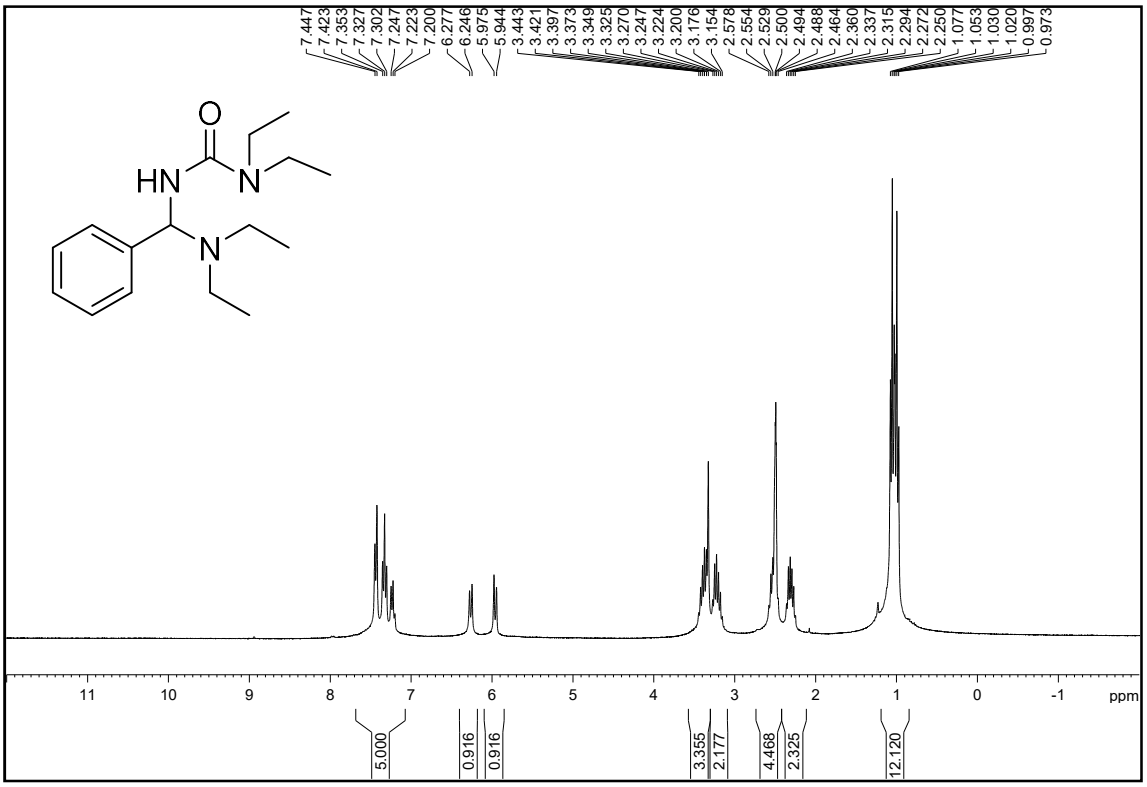


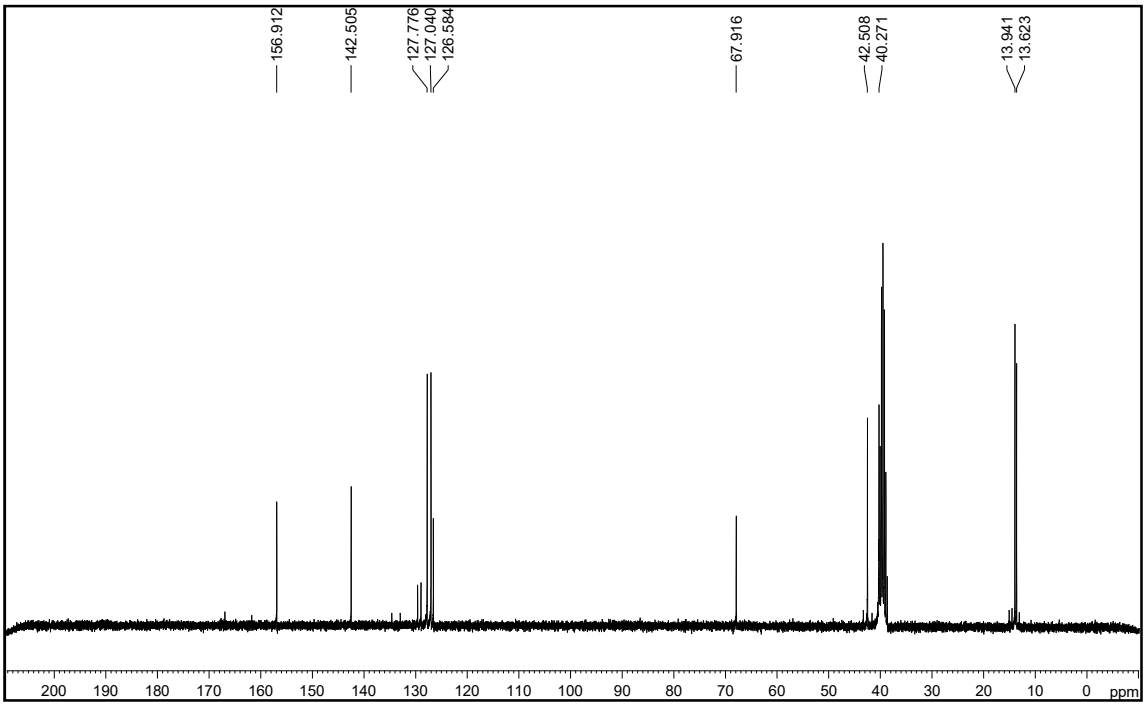
1-((Diethylamino)(phenyl)methyl)urea (5aa):



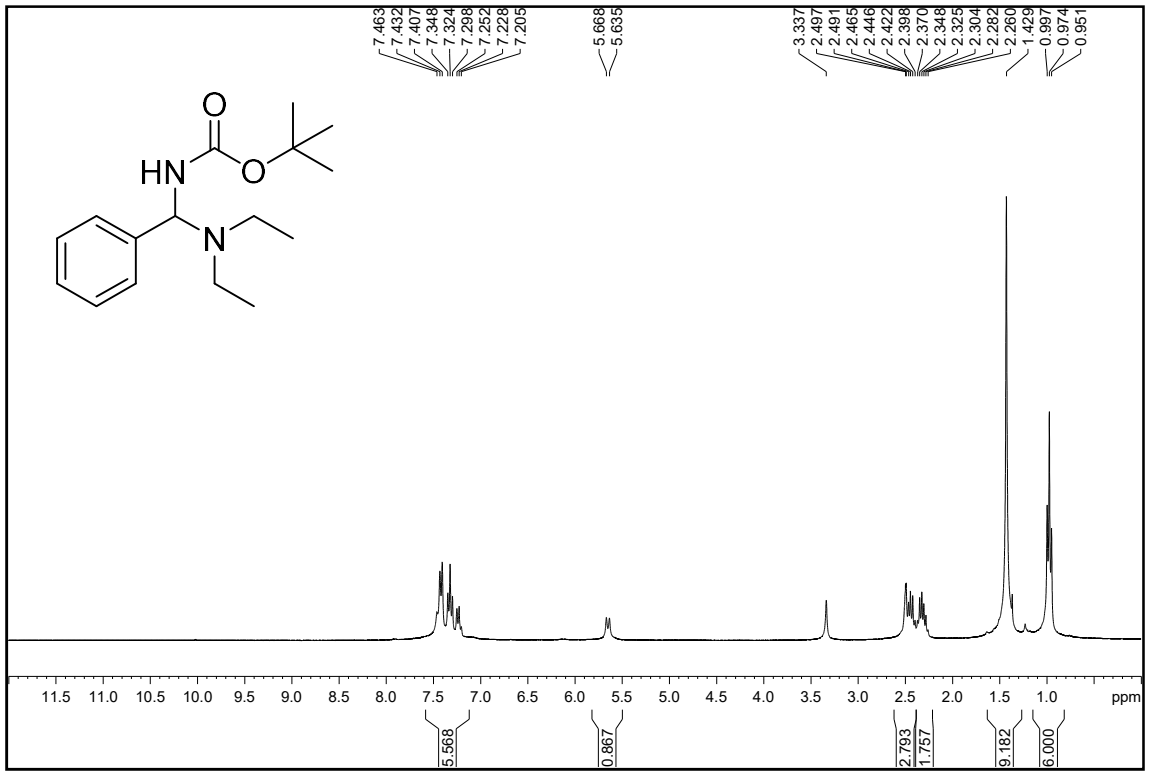


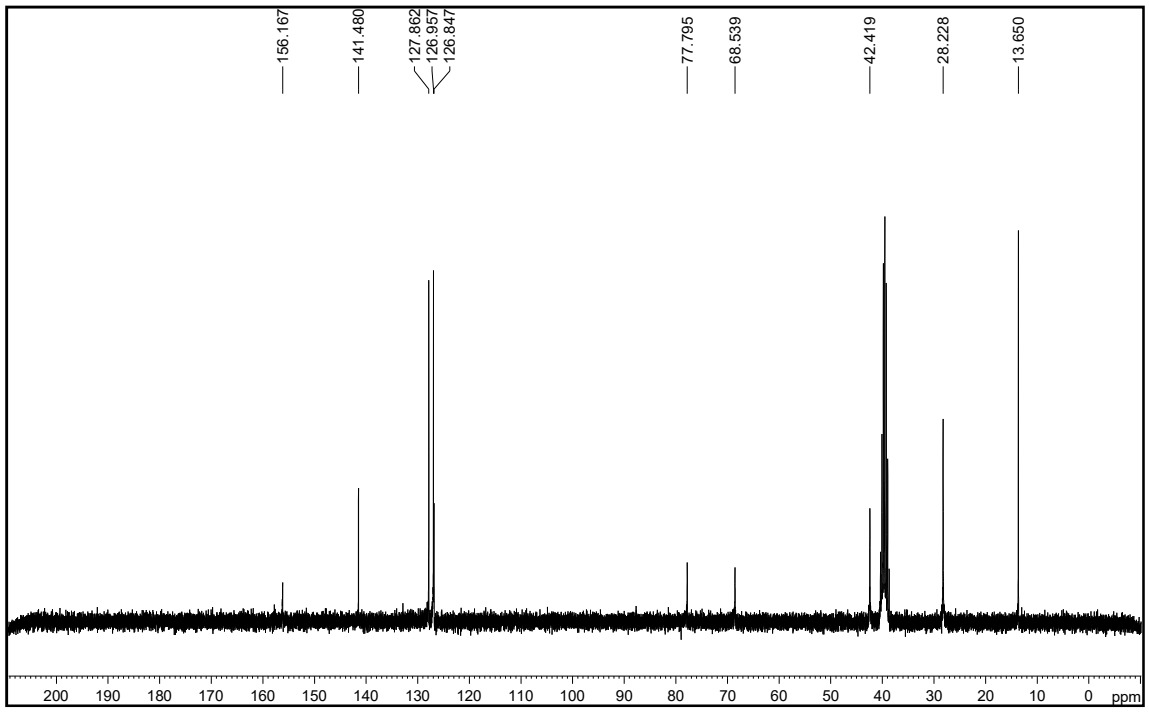
3-((Diethylamino)(phenyl)methyl)-1,1-diethylurea (5ba):



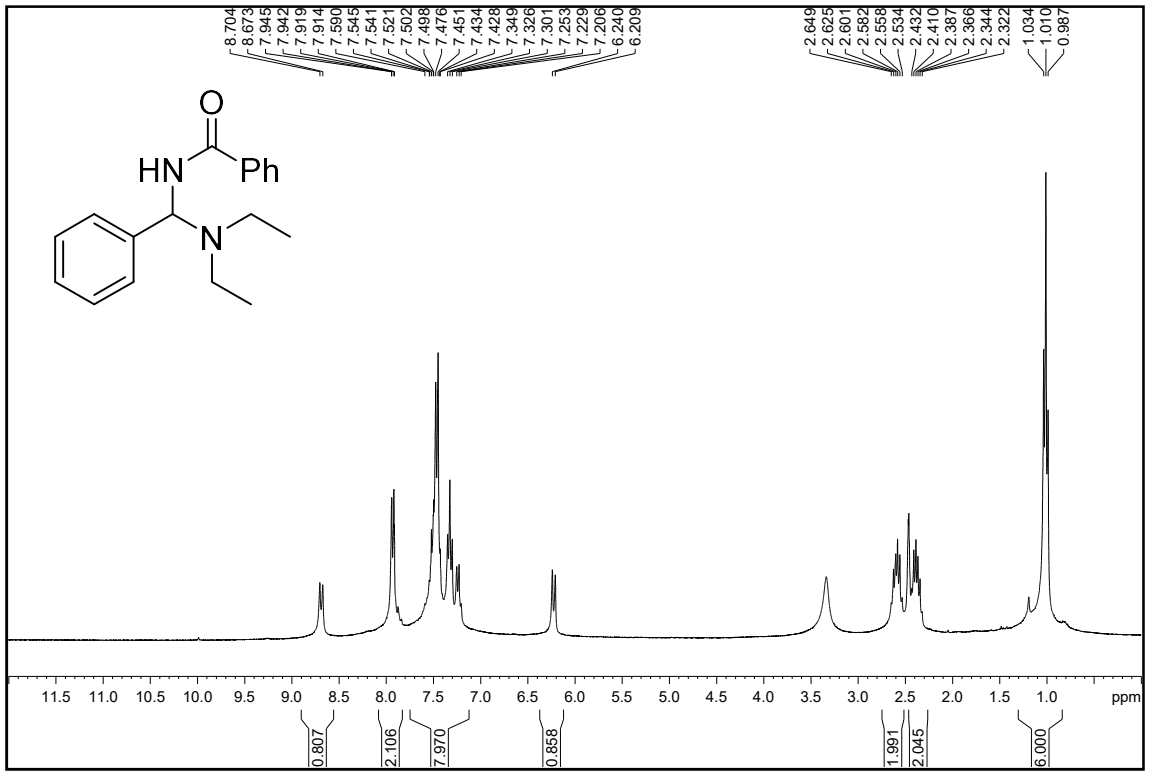


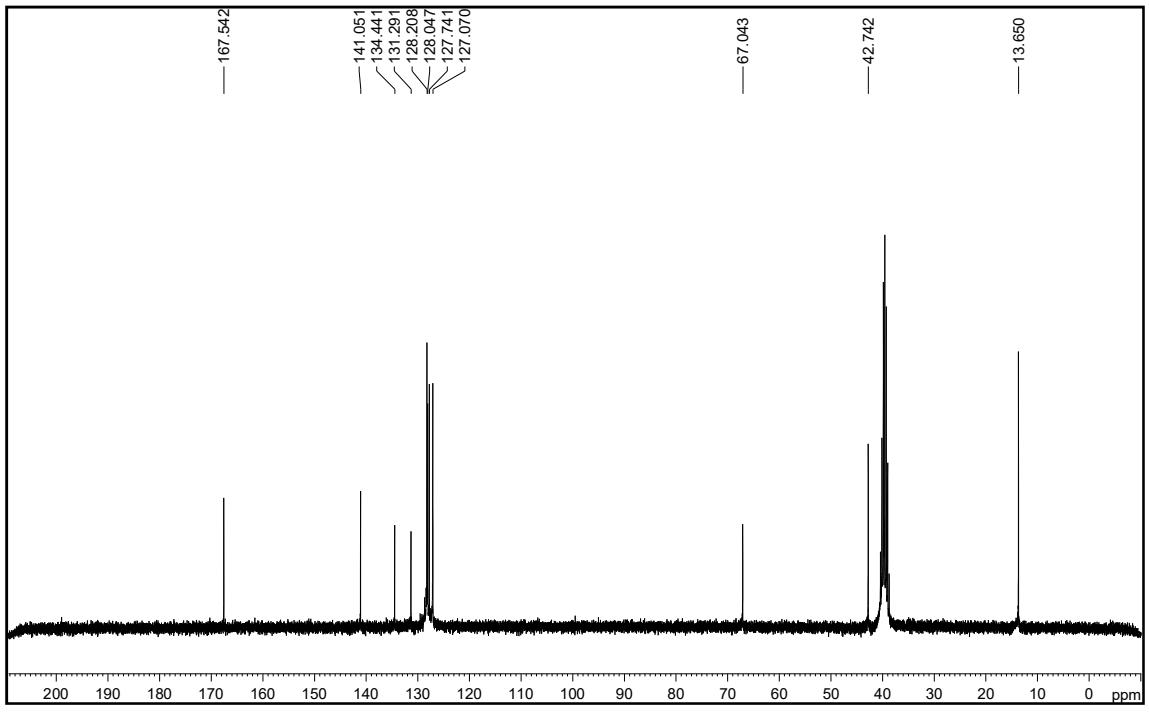
***tert*-Butyl((diethylamino)(phenyl)methyl)carbamate (5ca):**



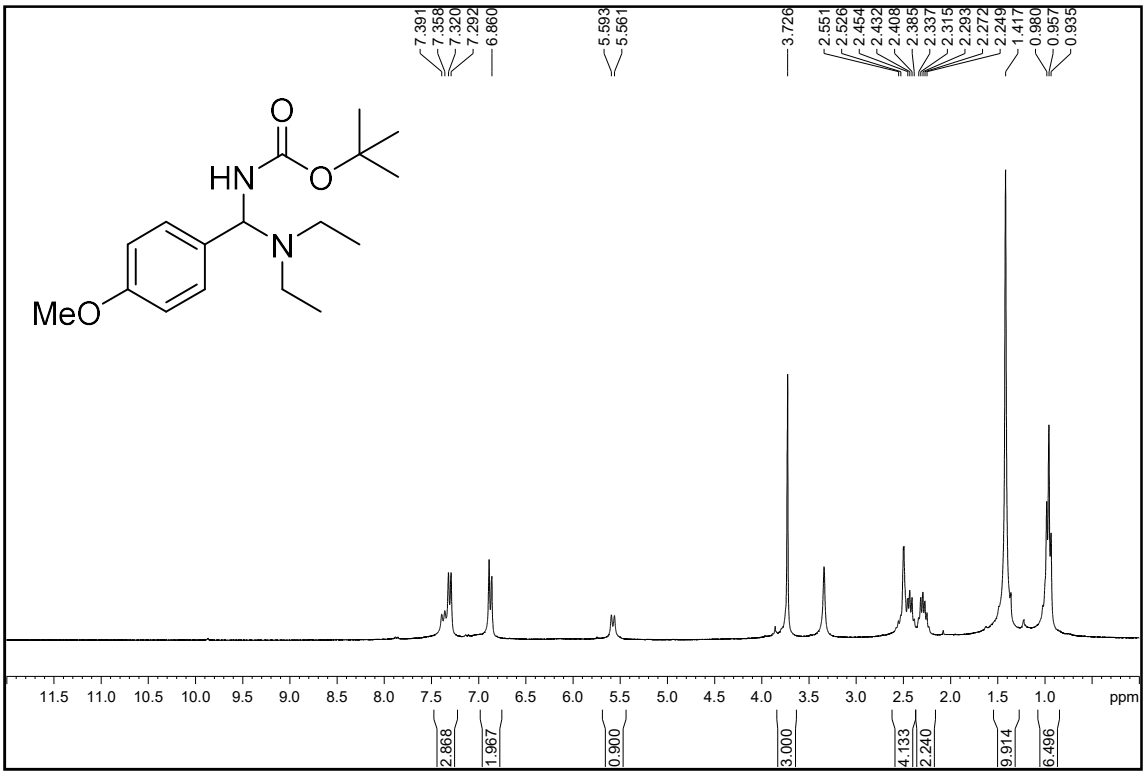


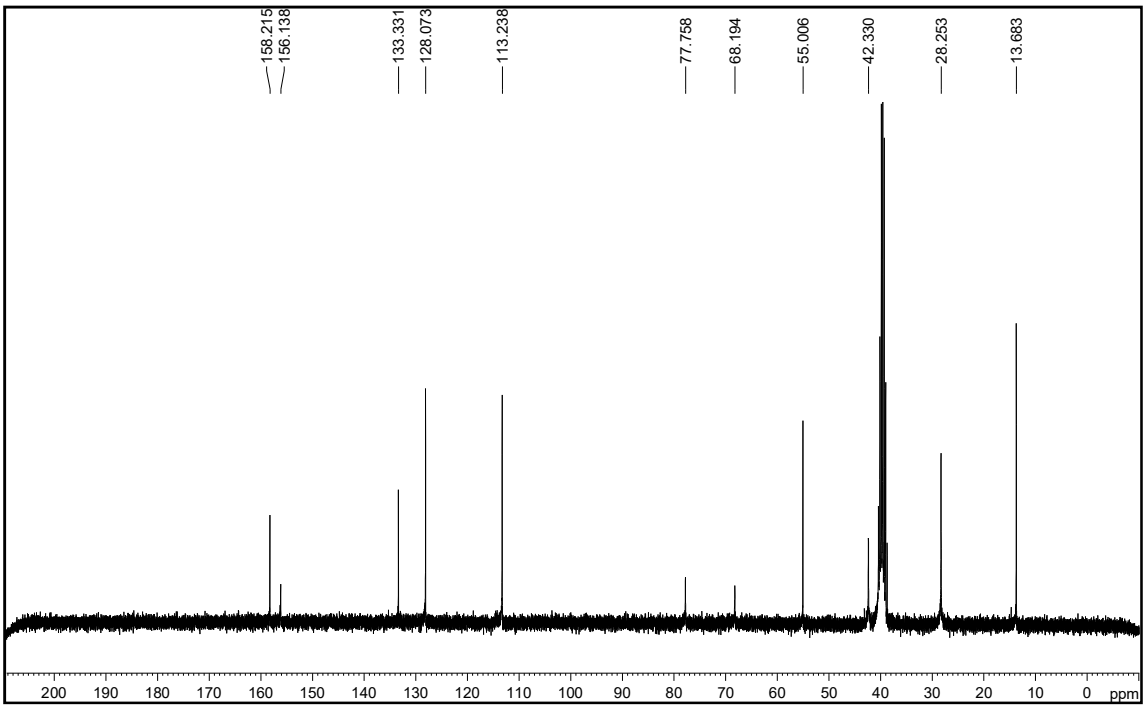
***N*-((Diethylamino)(phenyl)methyl)benzamide (5da):**



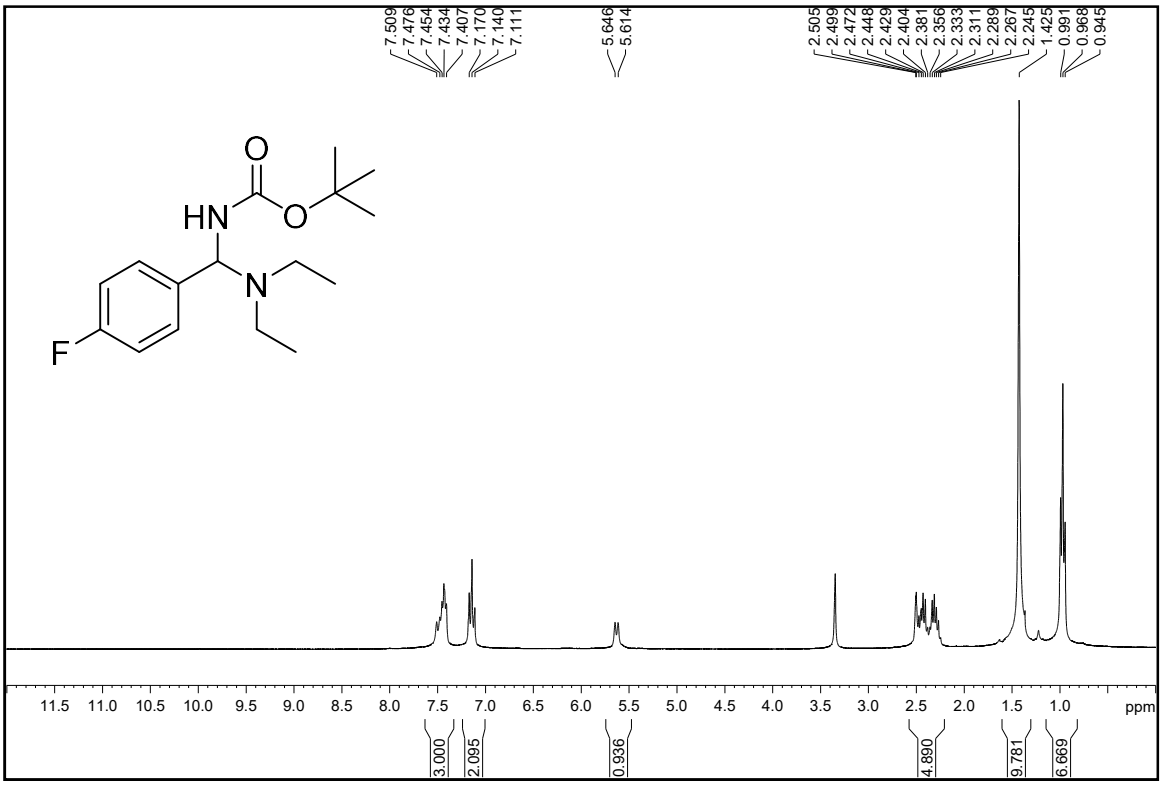


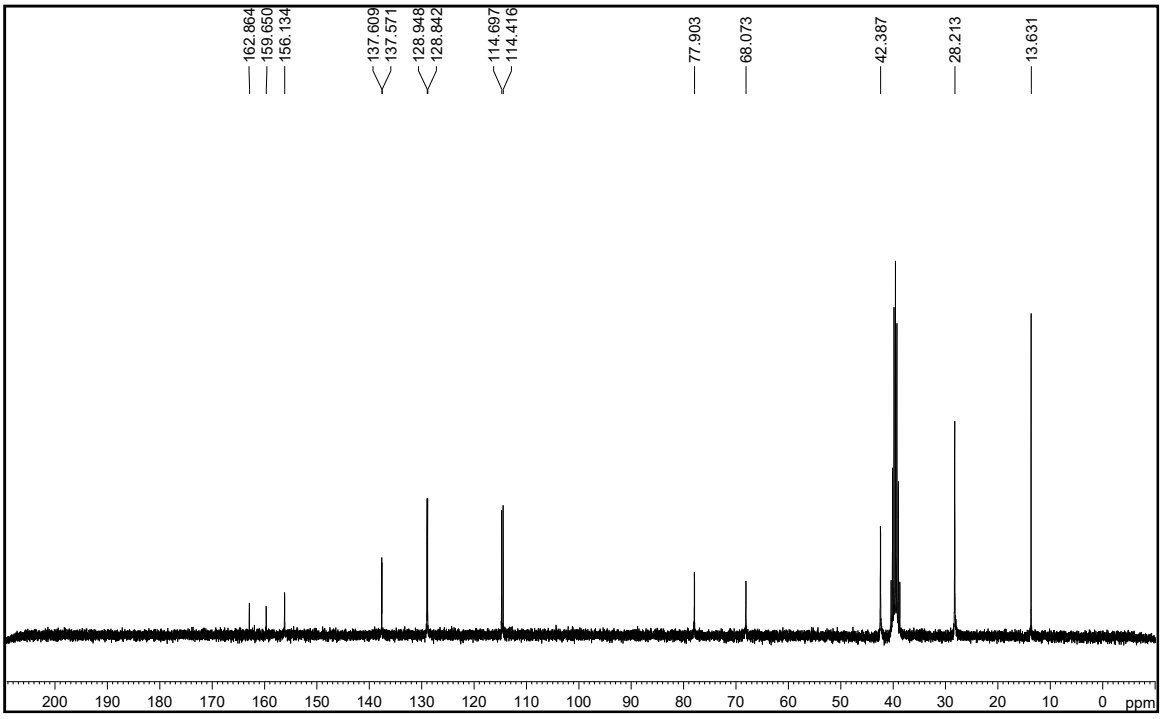
***tert*-Butyl((diethylamino)(4-methoxyphenyl)methyl)carbamate (5fa):**



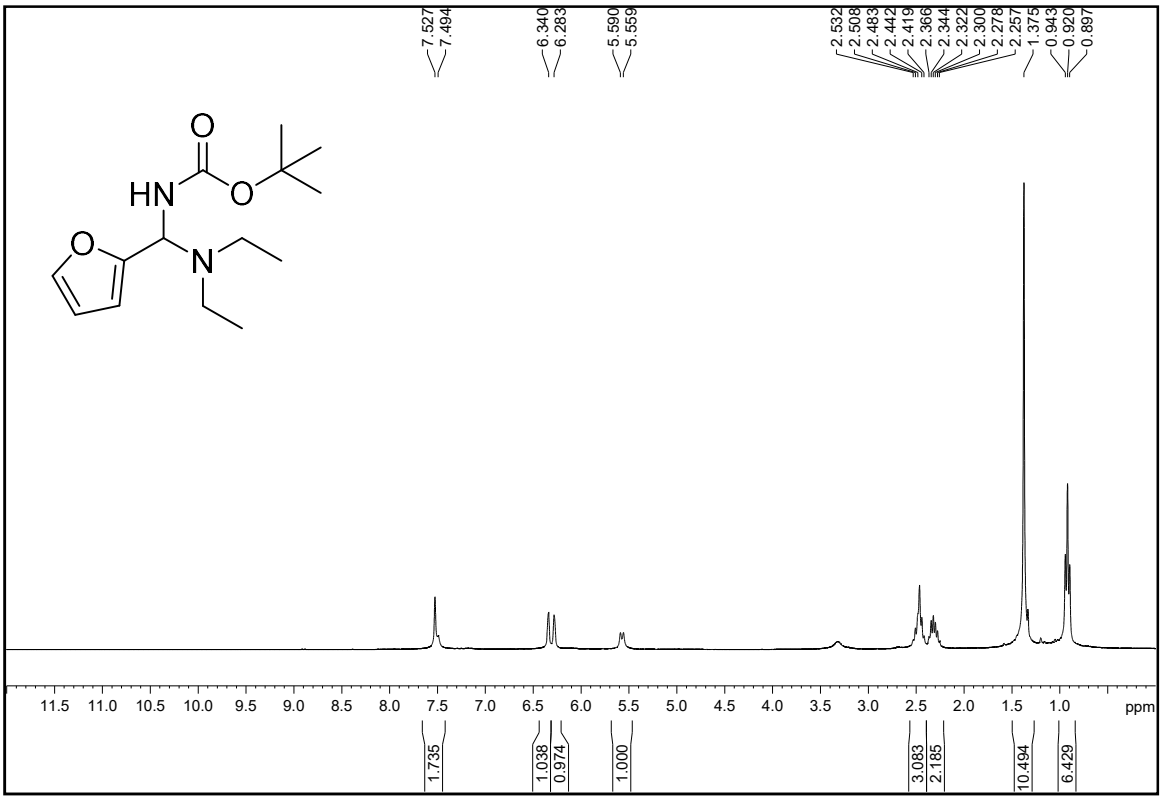


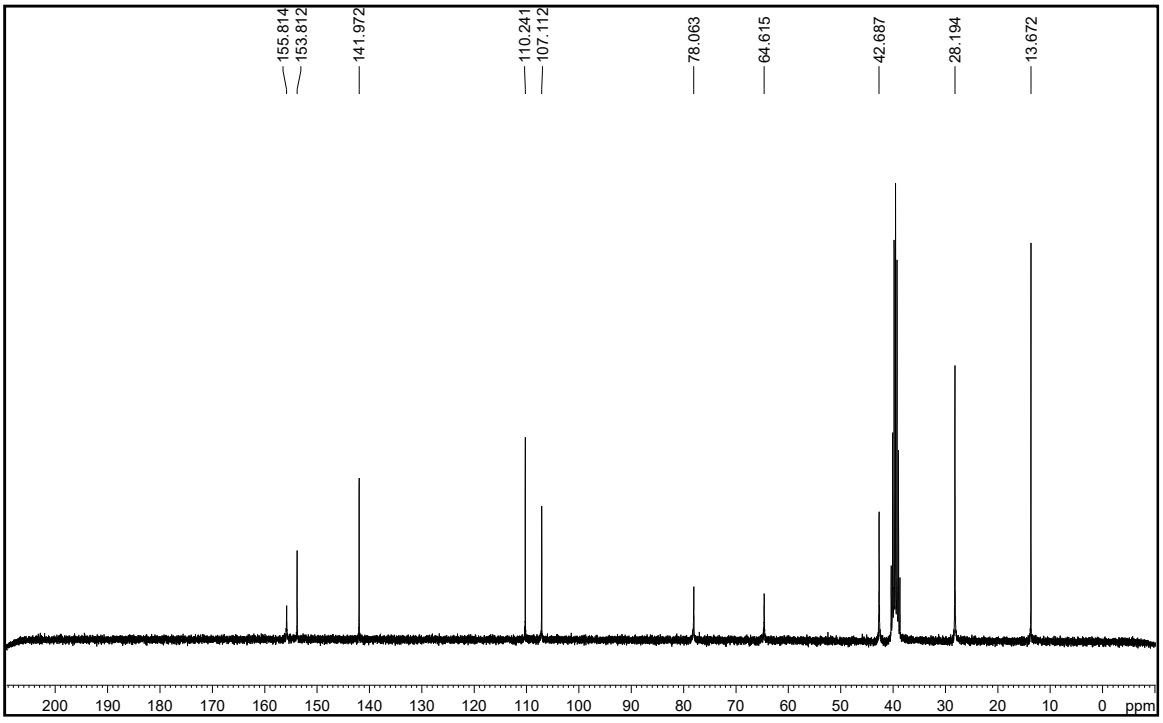
***tert*-Butyl ((diethylamino)(4-fluorophenyl)methyl)carbamate (5ga):**



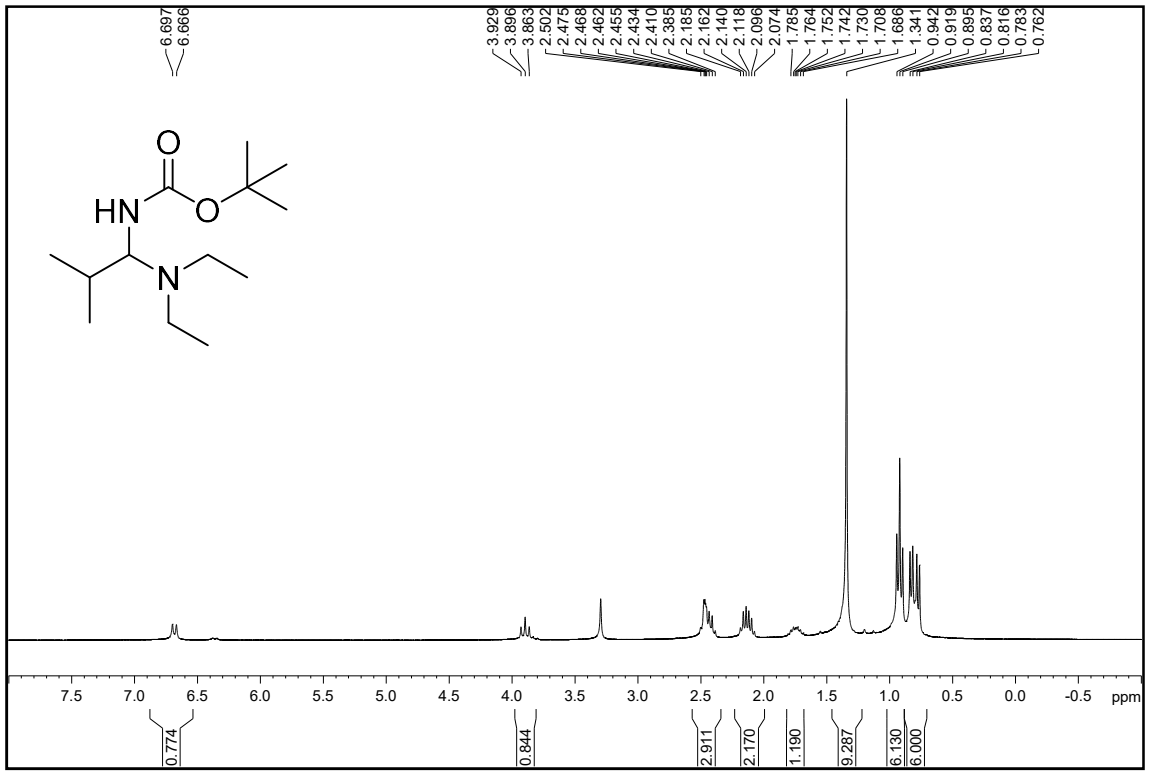


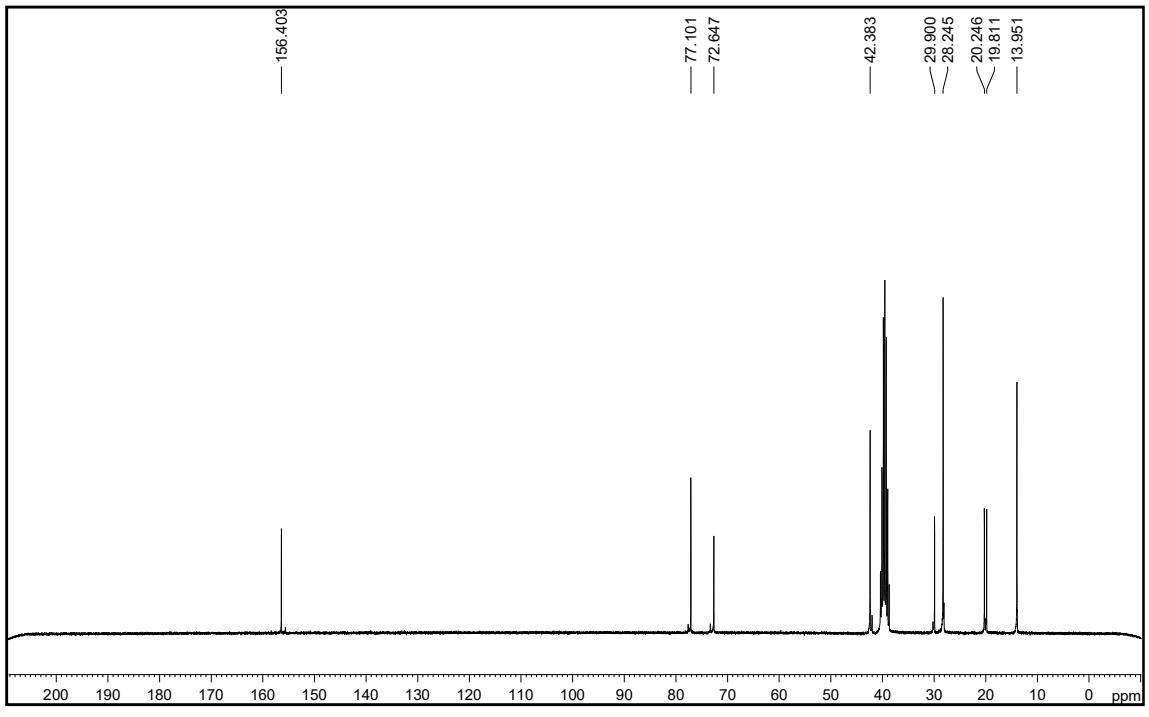
***tert*-Butyl ((diethylamino)(furan-2-yl)methyl)carbamate (5ha):**



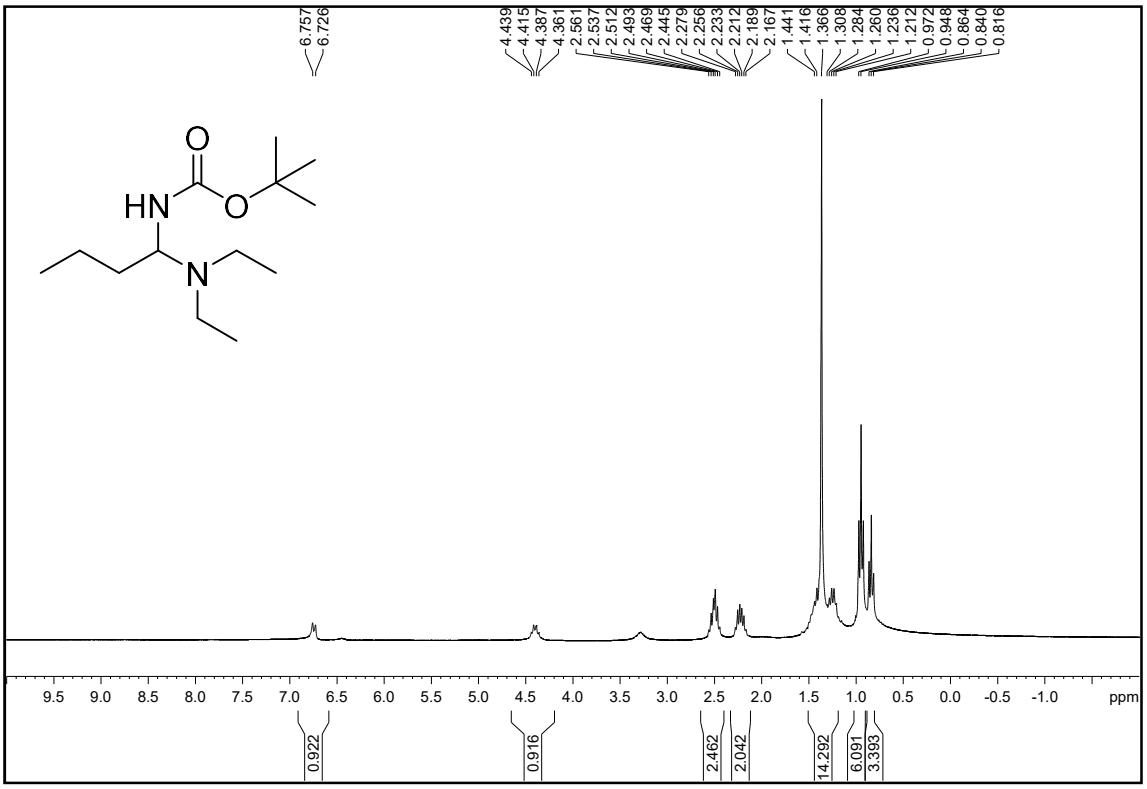


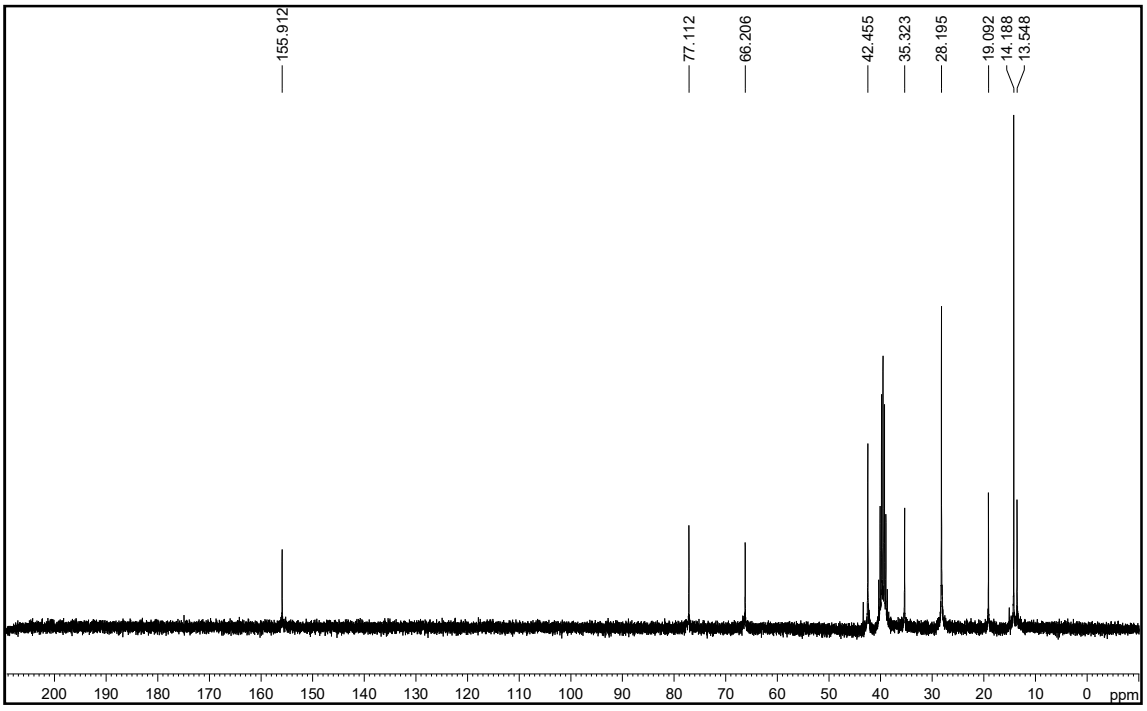
***tert*-Butyl (1-(diethylamino)-2-methylpropyl)carbamate (5ia):**



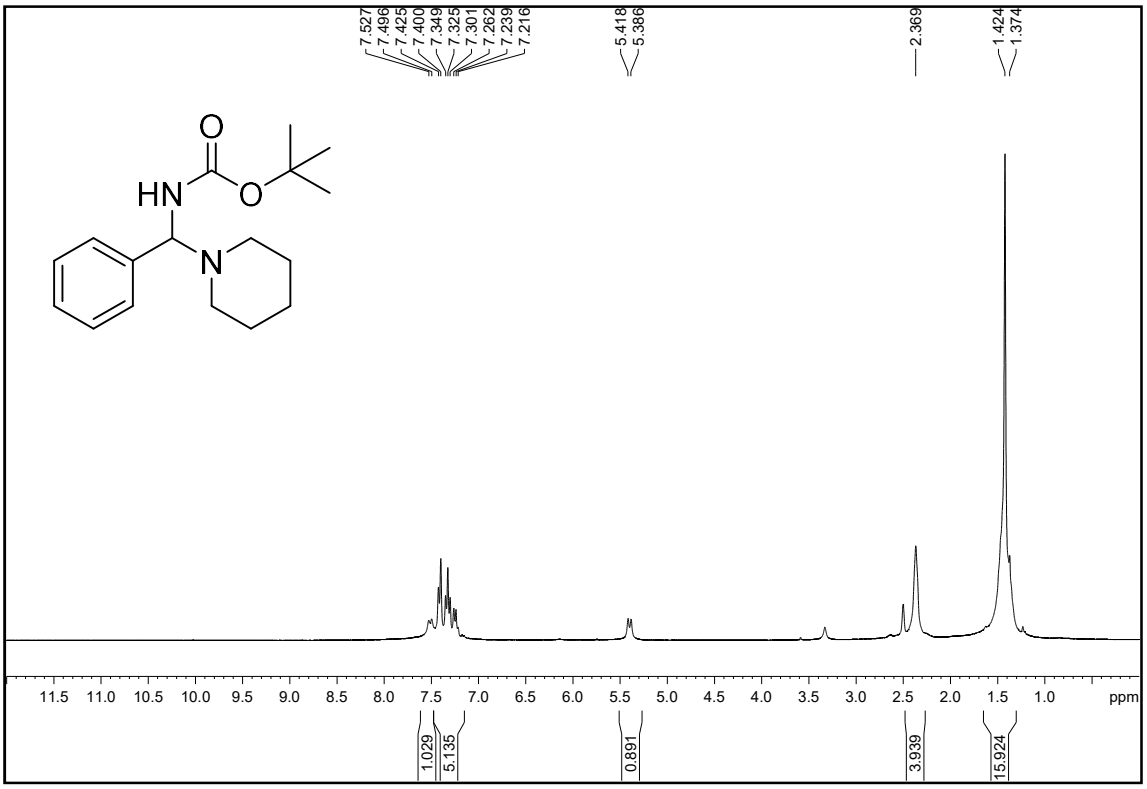


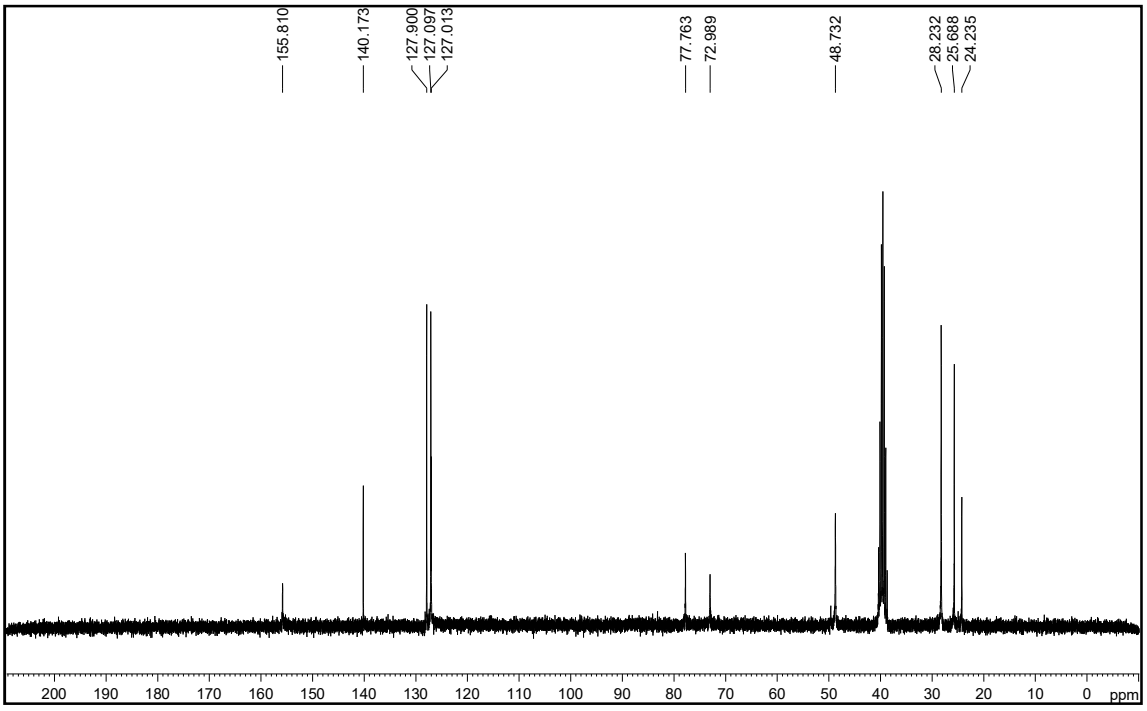
***tert*-Butyl (1-(diethylamino)butyl)carbamate (5ja):**



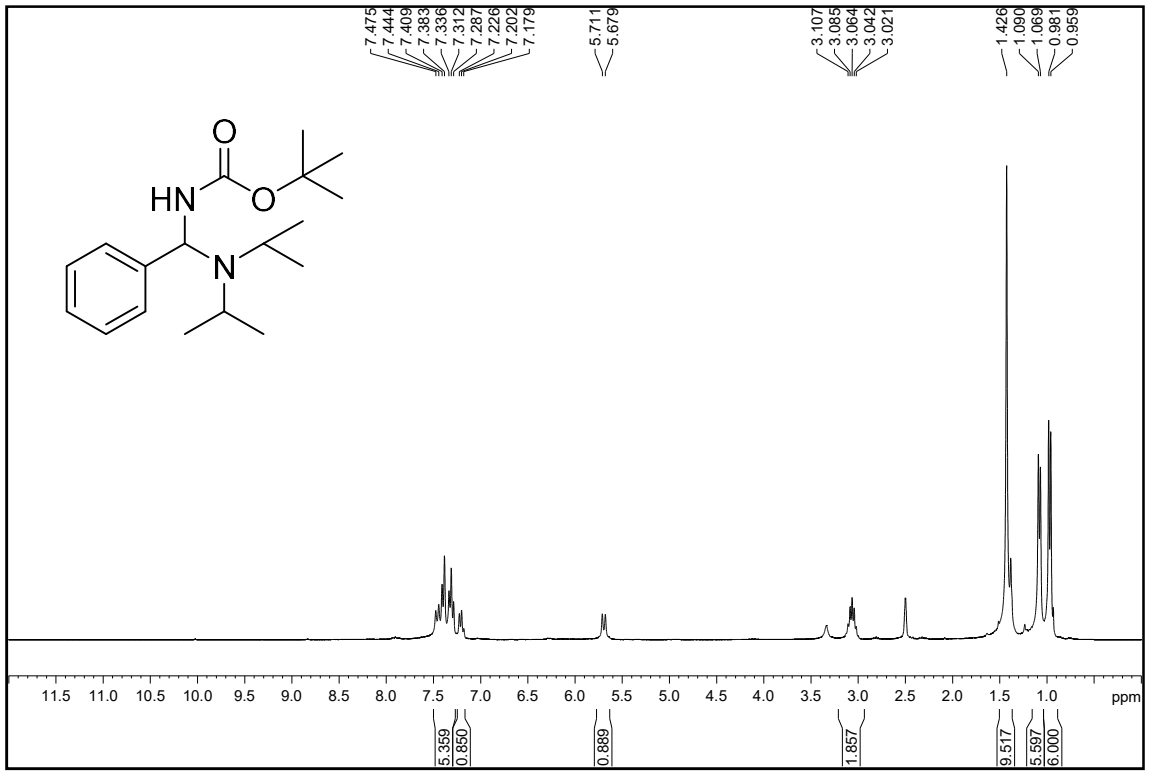


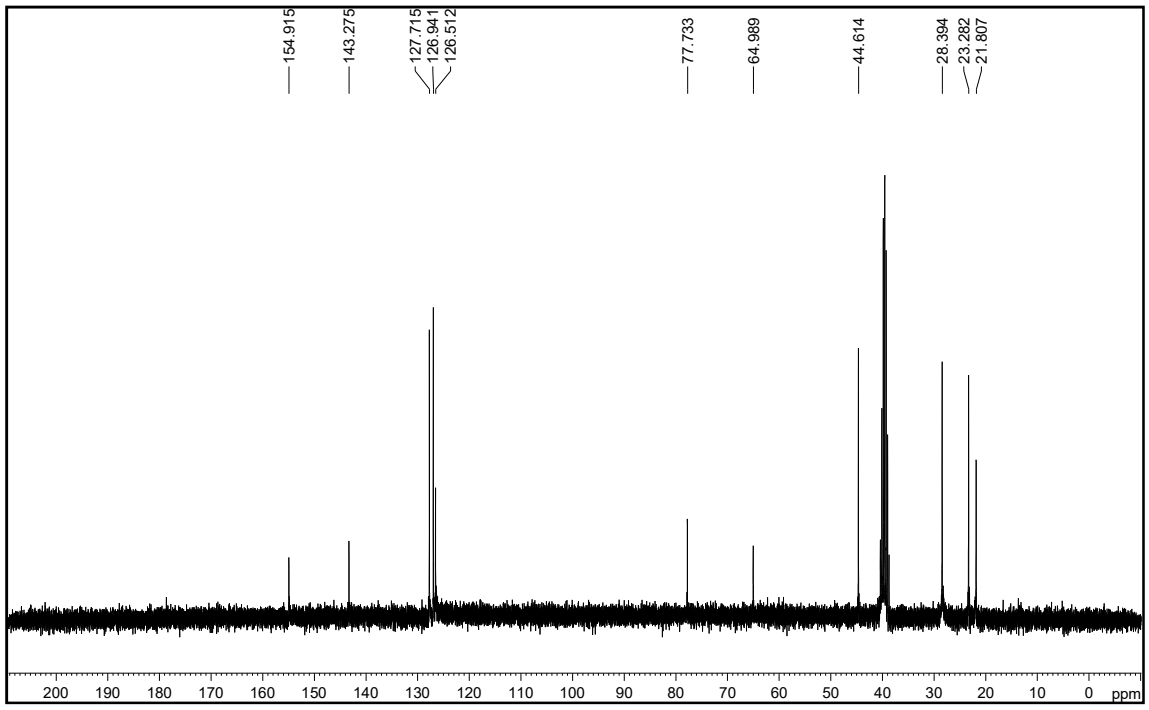
***tert*-Butyl (phenyl(piperidin-1-yl)methyl)carbamate (5cb):**



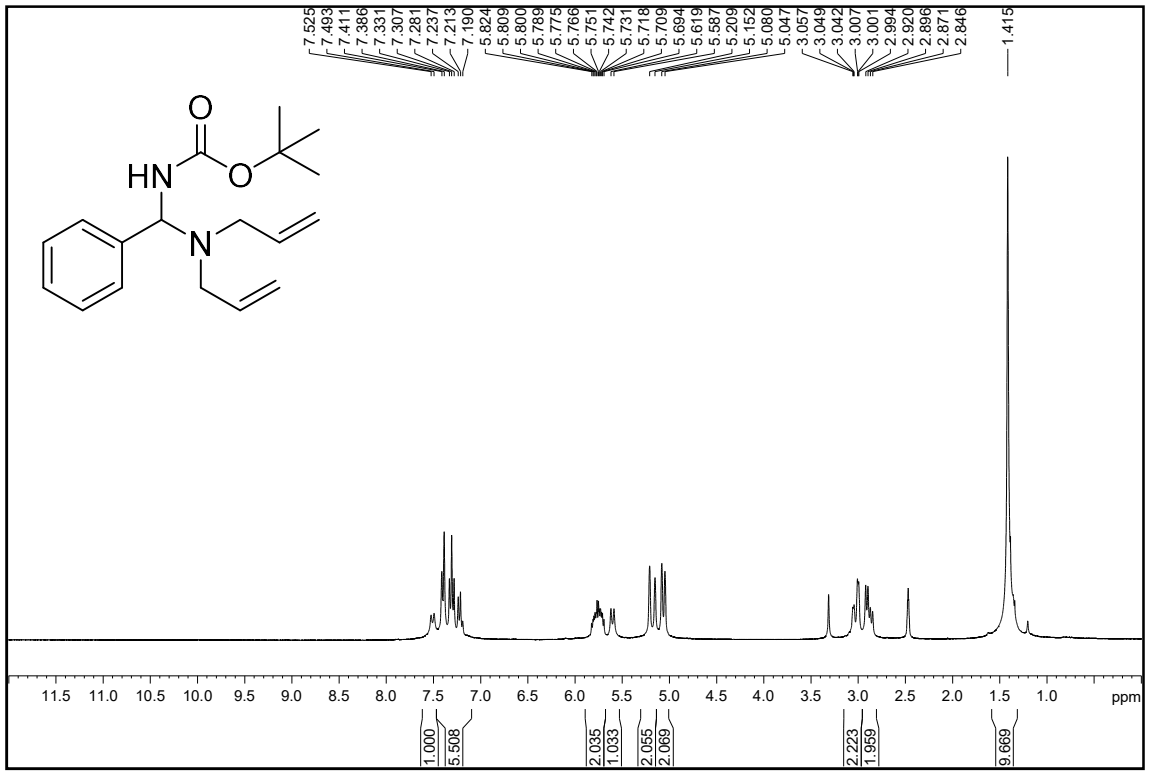


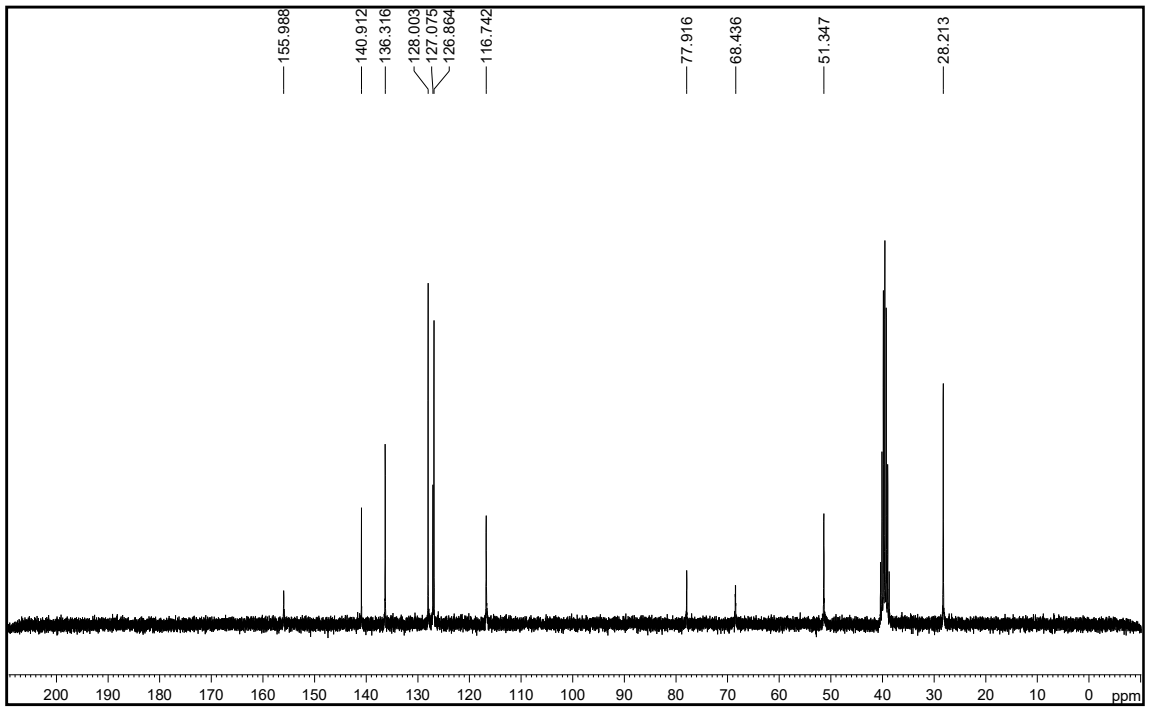
***tert*-Butyl ((diisopropylamino)(phenyl)methyl)carbamate (5cc):**



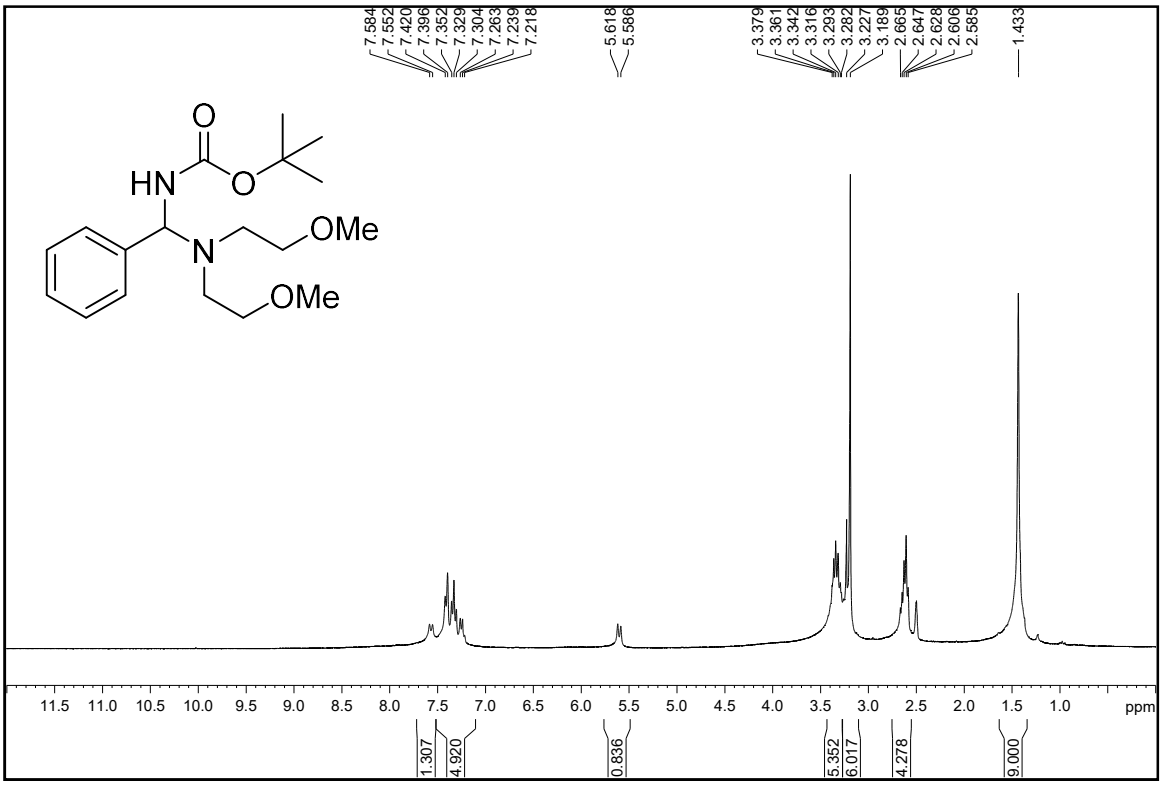


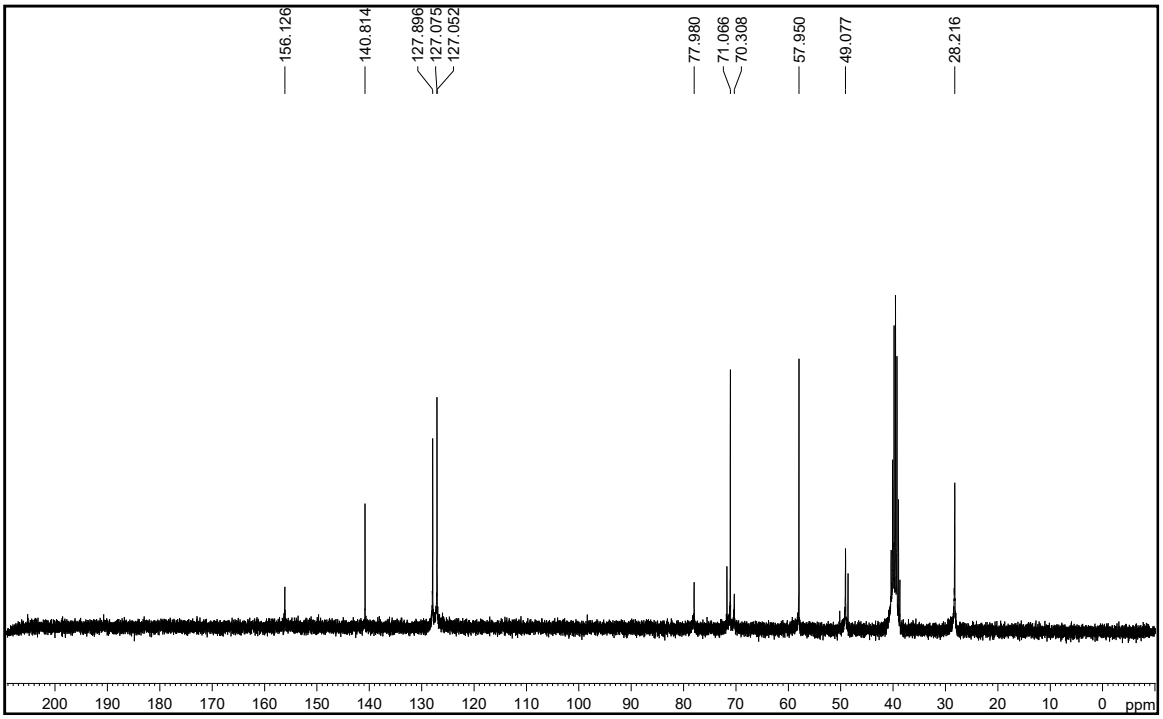
***tert*-Butyl ((diallylamino)(phenyl)methyl)carbamate (5cd):**



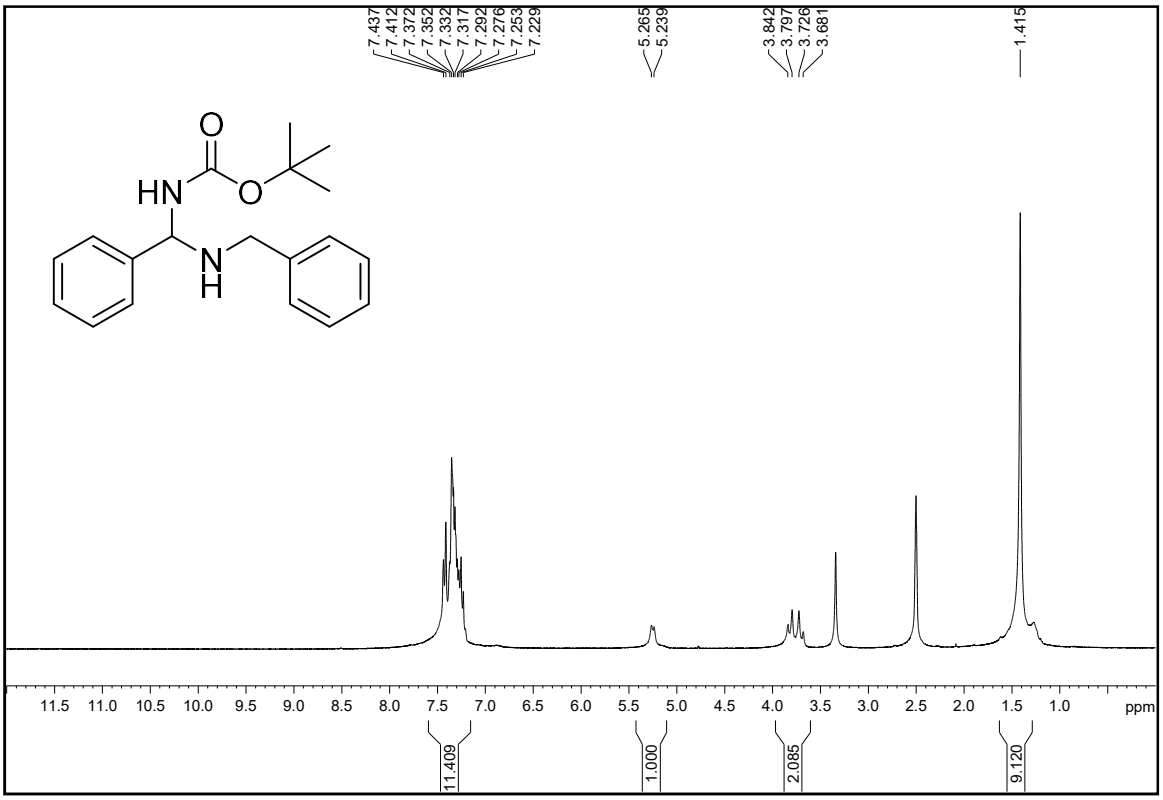


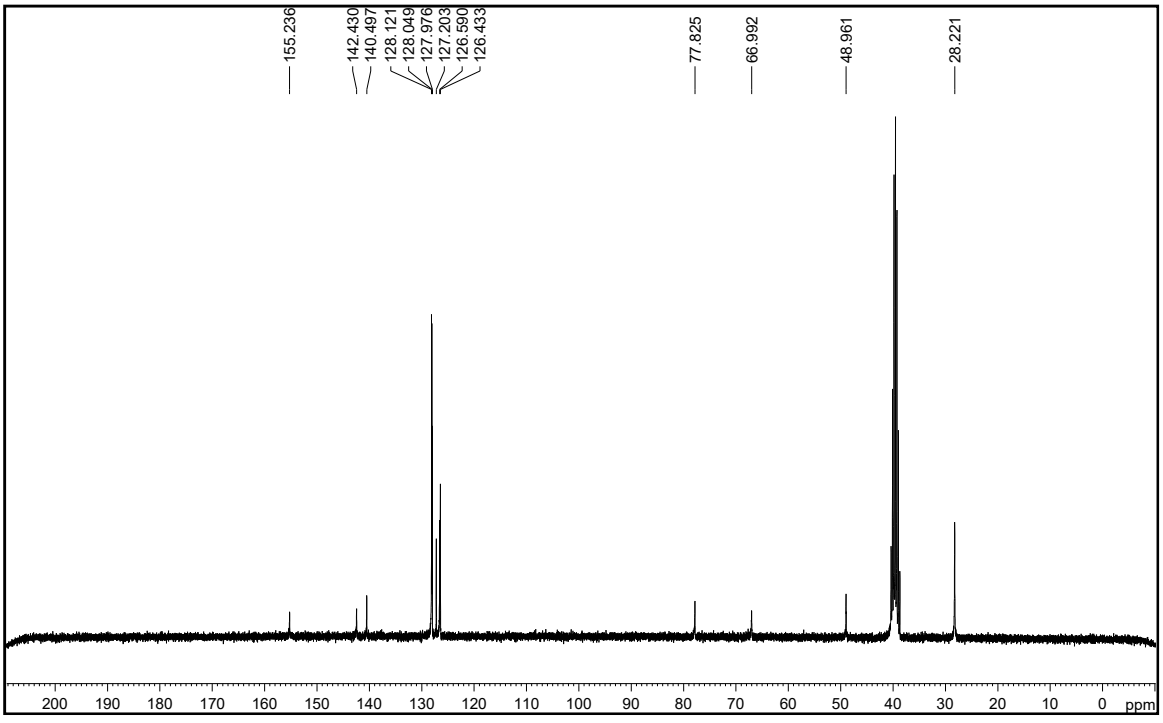
***tert*-Butyl ((bis(2-methoxyethyl)amino)(phenyl)methyl)carbamate (5ce):**



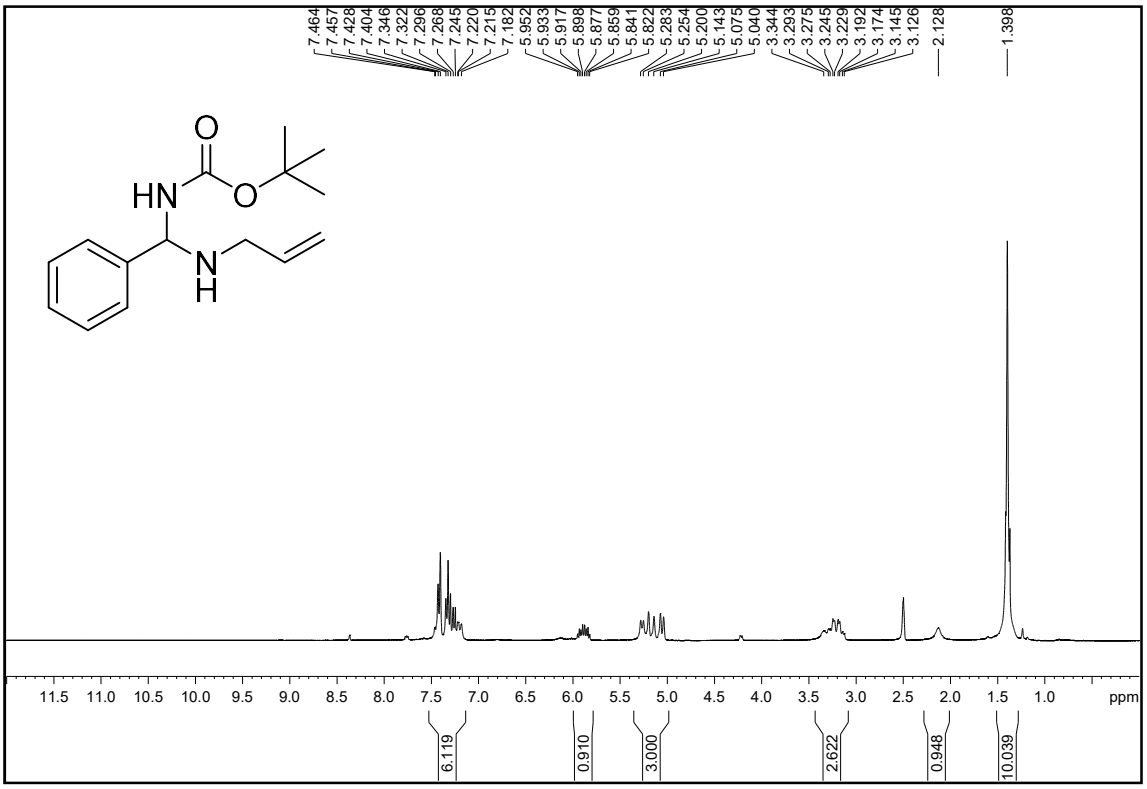


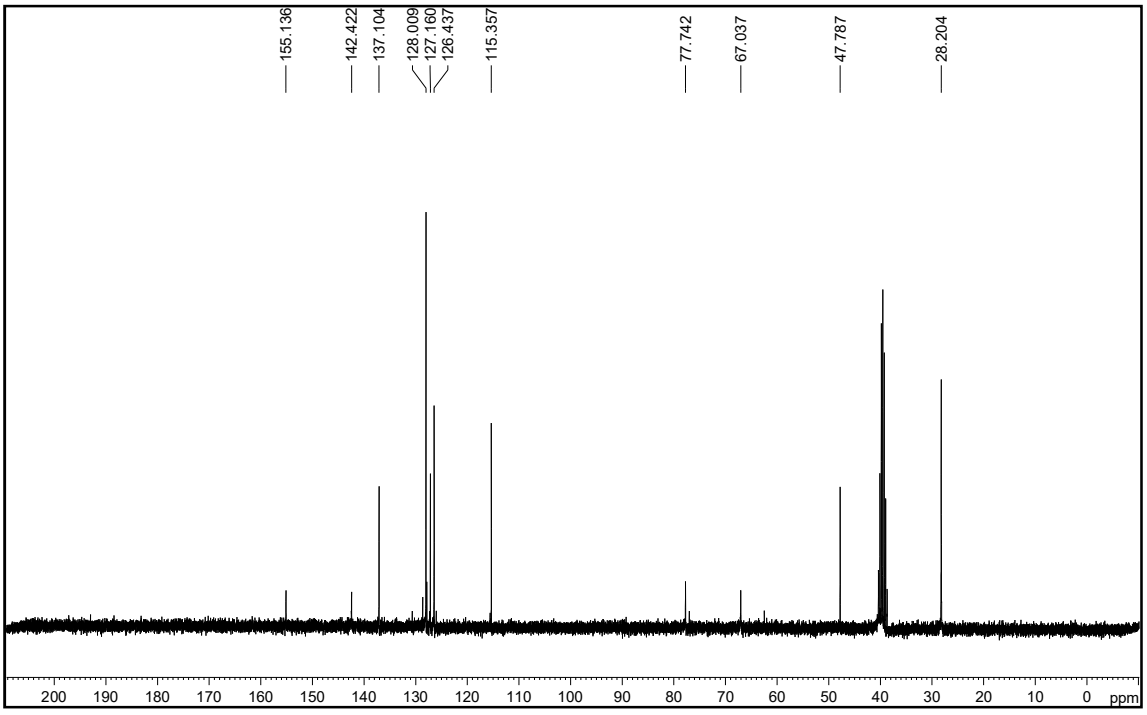
***tert*-Butyl ((benzylamino)(phenyl)methyl)carbamate (5cf):**



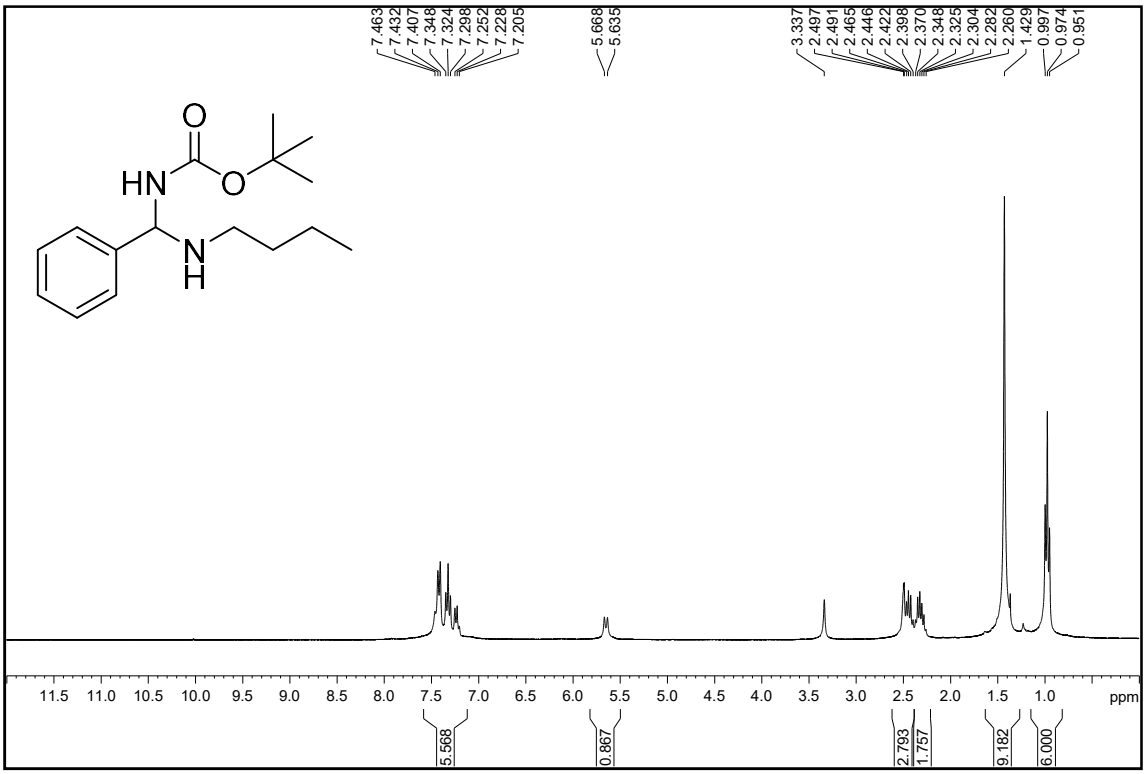


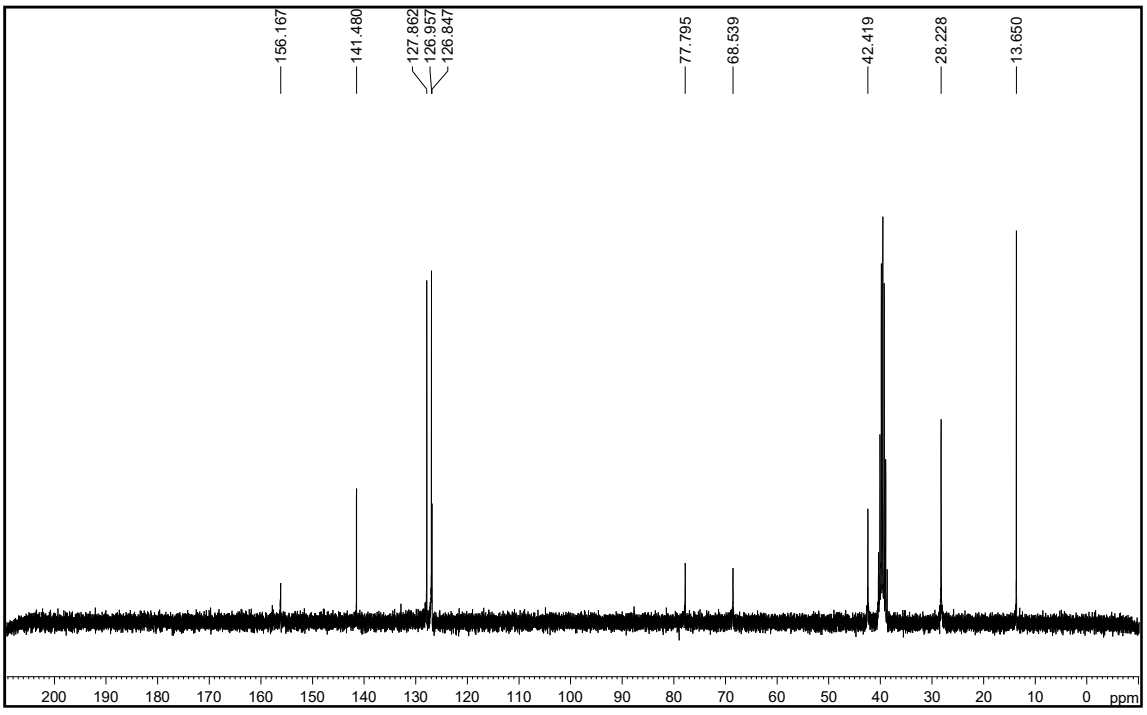
***tert*-Butyl ((allylamino)(phenyl)methyl)carbamate (5cg):**



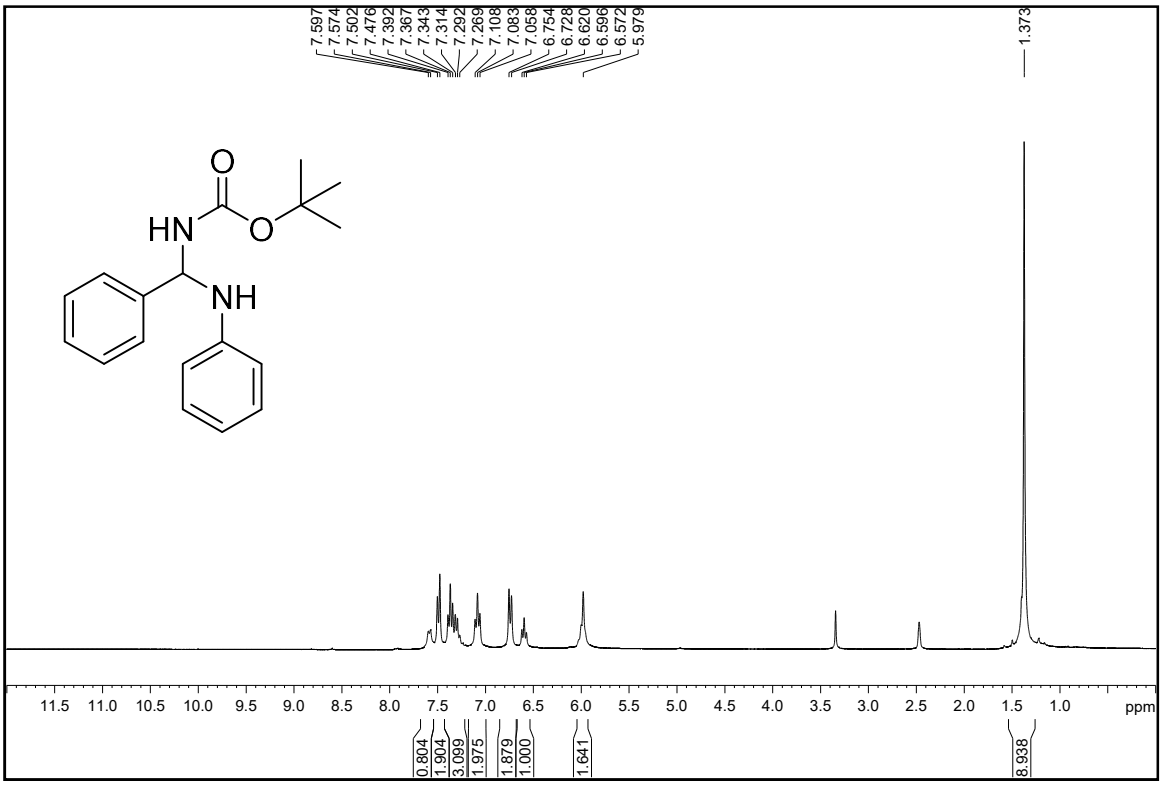


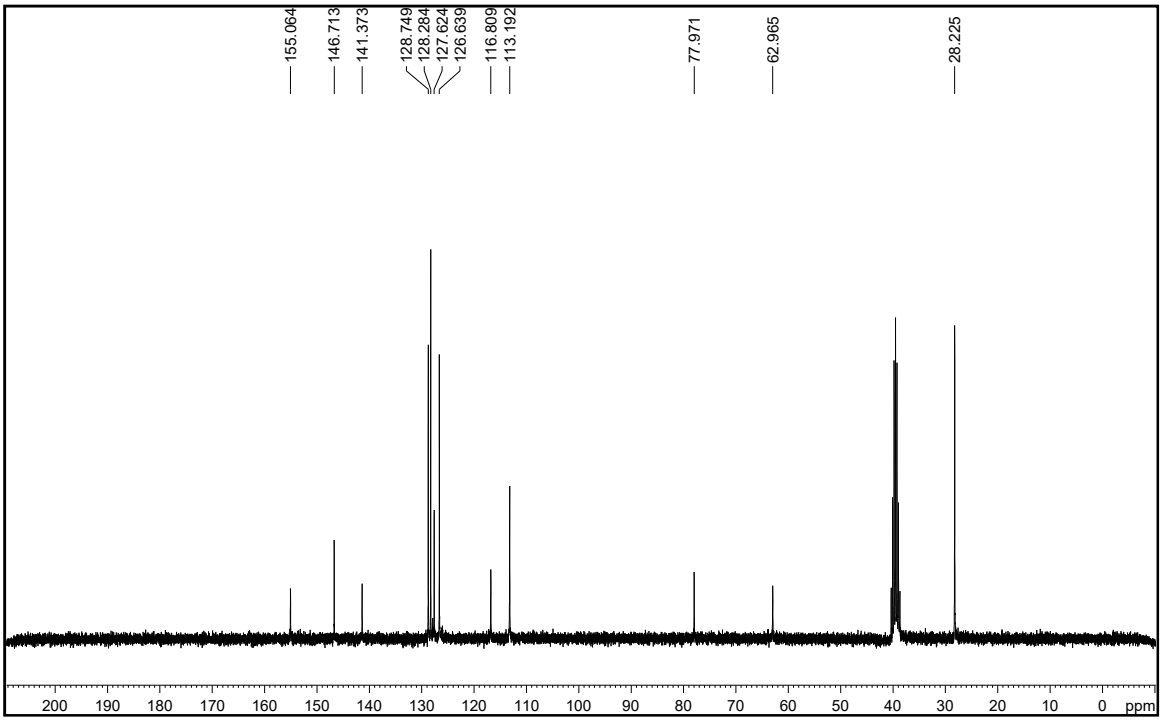
***tert*-Butyl ((butylamino)(phenyl)methyl)carbamate (5ch)**:





***tert*-Butyl (phenyl(phenylamino)methyl)carbamate (5ci):**





Supporting information 2 (SI2): Computational data on the addition of ROH to imine derivatives 1

Contents:

1.- Computational methods: general information

All calculations were performed within the density functional theory (DFT)[9] for which purpose we used the Gaussian 09 (Revision B.01) software package.[10] Computations were executed at the University of the Balearic Islands computational center. Truhlar's M06-2X functional has been employed throughout.[11] In some cases simplified models of imine derivatives **1** have been employed in computation, as follows. Authentic **1a** and **1e** were used for computational studies, as well as the *N,N*-dimethyl derivative (instead of the *N,N*-diethyl analog) of **1b**, and the methoxycarbonyl derivative (instead of the *tert*-butoxycarbonyl analog) of **1c**. Our model for **3a** (diethylamine) in computations was dimethylamine. The numbering system has not been changed though, to avoid confusion. Stationary points were optimized at the M06-2X/6-31+G(d,p) level of theory. The nature (local minimum or first-order saddle point) of these stationary points was determined by frequency analysis: local minima showed no imaginary frequencies, whereas saddle points showed the existence of a single imaginary frequency. Solvation effects were taken in consideration by means of full optimizations carried out at the M06-2X(PCM=solvent)/6-31+G(d,p) level of theory using the PCM(IEFPCM) method of Tomasi et al.[12] Gibbs energies of stationary points obtained with M06-2X/6-31+G(d,p) and M06-2X(PCM=solvent)/6-31+G(d,p) are provided, as well as their Cartesian coordinates. Absolute energies are given in Hartrees, whereas relative energies are reported in kcal/mol.

[9] R.G.Y. Parr, W. Yang, "*Density Functional Theory of Atoms and Molecules*", Oxford University Press, Oxford, **1989**.

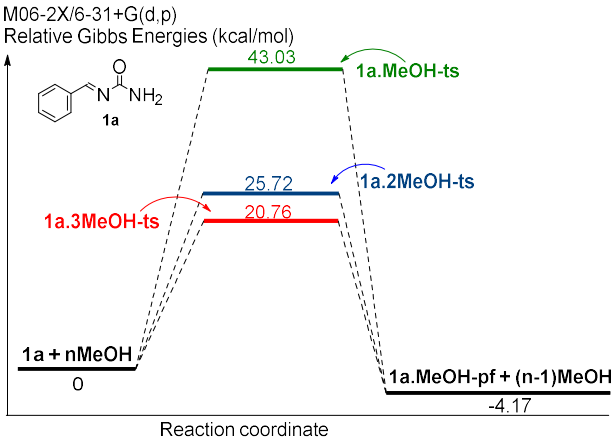
[10] M. J. Frisch, G. W. Trucks, H.B. Schlegel, G. E. Scuseria,M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Menucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, 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. Zakrezwski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J.Fox, Gaussian 09, Revision B.01, Gaussian, Inc., Wallingford CT, **2010**.

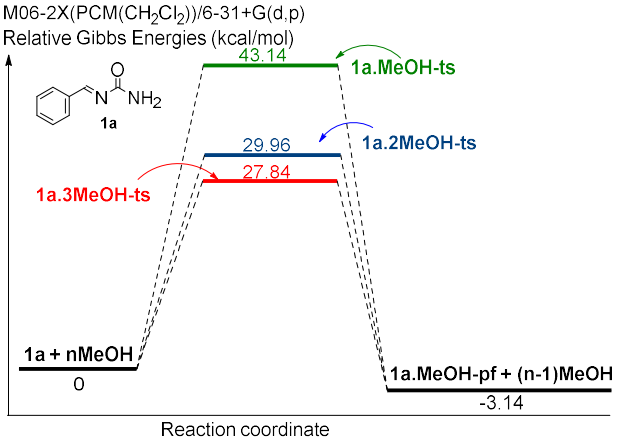
[11] Y. Zhao, D.G. Truhlar, *Theor. Chem. Account.* **2008**, *120*, 215-241.

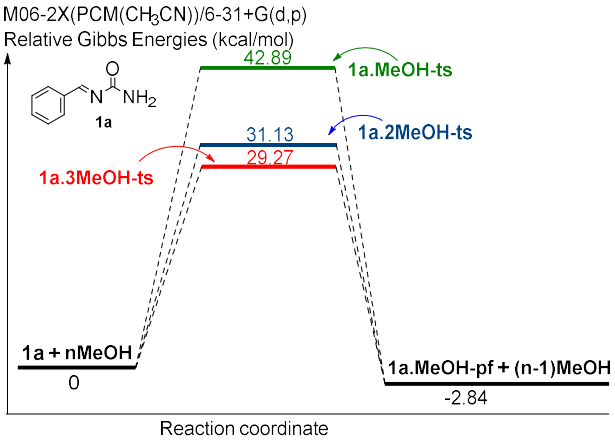
[12] a) E. Cancès, B. Mennucci, J. Tomasi, *J. Chem. Phys.* **1997**, *107*, 3032-3047; b) J. Tomasi, B. Mennucci, E. Cancès , *J. Mol. Struct. (Teochem)* **1999**, *464*, 211-226.

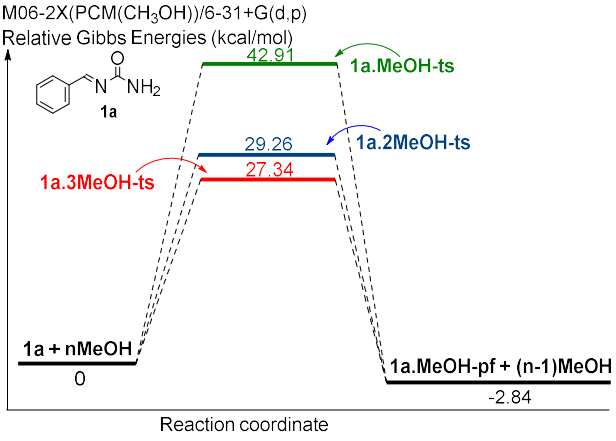
2.- Computational data on the addition of methanol (2a) to imine derivatives 1

2.1.-Energy profiles for the addition of n methanol (2a) molecules (n=1-3) to imine derivative 1a in gas phase, CH_2Cl_2, CH_3CN and CH_3OH.









2.2.-Computacional data for the addition of n methanol (2a) molecules (n=1-3) to imine derivative 1a

2.2.1 M06-2X/6-31+G(d,p) calculations

IMINE 1a

```
Zero-point correction=                           0.150878
(Hartree/Particle)
 Thermal correction to Energy=                    0.160513
 Thermal correction to Enthalpy=                  0.161457
 Thermal correction to Gibbs Free Energy=         0.114839
 Sum of electronic and zero-point Energies=           -494.076496
 Sum of electronic and thermal Energies=              -494.066861
 Sum of electronic and thermal Enthalpies=            -494.065917
 Sum of electronic and thermal Free Energies=         -494.112535
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.622748	-0.499022	-0.000089
2	7	0	1.509634	0.420514	-0.000204
3	6	0	-0.815418	-0.204058	-0.000026
4	6	0	2.860957	-0.063736	-0.000341
5	7	0	3.733509	0.971690	0.000127
6	8	0	3.194901	-1.234701	0.000083
7	1	0	4.721695	0.779076	0.000526
8	6	0	-3.559593	0.295537	0.000111
9	6	0	-1.724758	-1.266460	0.000053
10	6	0	-1.288143	1.115076	-0.000038
11	6	0	-2.654905	1.361056	0.000030
12	6	0	-3.095423	-1.018017	0.000123
13	1	0	-1.353280	-2.288175	0.000061
14	1	0	-0.567707	1.926727	-0.000097
15	1	0	-3.021848	2.382540	0.000023
16	1	0	-3.797574	-1.845407	0.000185
17	1	0	-4.627304	0.492368	0.000165
18	1	0	0.922139	-1.554672	-0.000087
19	1	0	3.389888	1.917466	0.000161

2a (MeOH)

```
 Zero-point correction=                           0.051816
(Hartree/Particle)
 Thermal correction to Energy=                    0.055178
 Thermal correction to Enthalpy=                  0.056122
 Thermal correction to Gibbs Free Energy=         0.029030
 Sum of electronic and zero-point Energies=           -115.619754
 Sum of electronic and thermal Energies=              -115.616391
 Sum of electronic and thermal Enthalpies=            -115.615447
```

Sum of electronic and thermal Free Energies= -115.642540

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.046265	-0.752857	0.000000
2	1	0	-0.861357	-1.070830	0.000000
3	6	0	0.046265	0.661884	0.000000
4	1	0	1.091273	0.974249	0.000000
5	1	0	-0.438813	1.074068	0.893412
6	1	0	-0.438813	1.074068	-0.893412

1a.MeOH-ts

Zero-point correction= 0.202338
(Hartree/Particle)
Thermal correction to Energy= 0.214728
Thermal correction to Enthalpy= 0.215673
Thermal correction to Gibbs Free Energy= 0.162732
Sum of electronic and zero-point Energies= -609.646887
Sum of electronic and thermal Energies= -609.634497
Sum of electronic and thermal Enthalpies= -609.633553
Sum of electronic and thermal Free Energies= -609.686494

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.542453	-0.202571	-0.423520
2	6	0	2.717605	-0.592665	0.200100
3	7	0	3.740894	-0.822864	-0.695476
4	8	0	2.883425	-0.717944	1.410028
5	6	0	-0.850132	-0.143136	0.239540
6	6	0	-3.508428	-0.900948	-0.141000
7	6	0	-1.818628	0.189990	1.189822
8	6	0	-1.213227	-0.872779	-0.894795
9	6	0	-2.540970	-1.246863	-1.084634
10	6	0	-3.146536	-0.185513	1.000232
11	1	0	-1.527980	0.738230	2.083428
12	1	0	-0.436973	-1.147476	-1.602381
13	1	0	-2.821448	-1.817688	-1.964332
14	1	0	-3.894940	0.070441	1.743660
15	1	0	-4.541922	-1.198997	-0.288627
16	6	0	0.566289	0.287878	0.444226
17	1	0	0.857468	0.387173	1.493192
18	8	0	0.724038	1.814206	-0.128699
19	6	0	-0.369814	2.528338	-0.716261
20	1	0	-0.830948	1.948748	-1.520191
21	1	0	0.033369	3.466760	-1.098197
22	1	0	-1.107181	2.729040	0.062281
23	1	0	1.402364	1.188637	-0.774476
24	1	0	3.482571	-1.007614	-1.652153
25	1	0	4.525535	-1.335122	-0.323236

1a.MeOH-pf

```
 Zero-point correction=                           0.208106
(Hartree/Particle)
 Thermal correction to Energy=                    0.220616
 Thermal correction to Enthalpy=                  0.221561
 Thermal correction to Gibbs Free Energy=         0.167619
 Sum of electronic and zero-point Energies=           -609.721232
 Sum of electronic and thermal Energies=              -609.708721
 Sum of electronic and thermal Enthalpies=            -609.707777
 Sum of electronic and thermal Free Energies=         -609.761719
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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.296521	-0.680633	-0.362778
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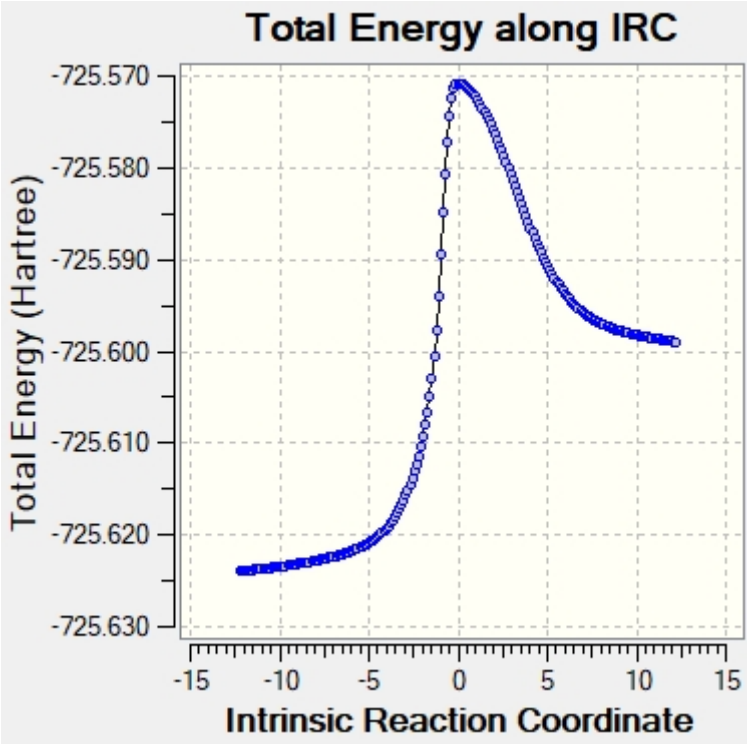
3	7	0	3.412156	-1.500580	-0.863289
4	8	0	3.114861	-0.068921	0.888062
5	6	0	-0.980880	-0.005666	0.113286
6	6	0	-3.678222	-0.713753	-0.088887
7	6	0	-1.479041	-1.097441	0.829914
8	6	0	-1.838243	0.728536	-0.703689
9	6	0	-3.184986	0.374031	-0.803802
10	6	0	-2.820647	-1.451079	0.730011
11	1	0	-0.806312	-1.671217	1.462931
12	1	0	-1.443312	1.574539	-1.257743
13	1	0	-3.847151	0.951864	-1.441351
14	1	0	-3.199831	-2.299352	1.291762
15	1	0	-4.726128	-0.986981	-0.164900
16	6	0	0.491814	0.354067	0.232437
17	1	0	0.785771	0.404073	1.289146
18	8	0	0.787130	1.584918	-0.389554
19	6	0	0.650298	2.691048	0.480966
20	1	0	0.889649	3.582788	-0.099410
21	1	0	1.351070	2.604654	1.321024
22	1	0	-0.375579	2.775832	0.865806
23	1	0	1.042112	-0.927777	-1.311345
24	1	0	2.974188	-2.276012	-1.337447
25	1	0	4.342009	-1.671805	-0.510148

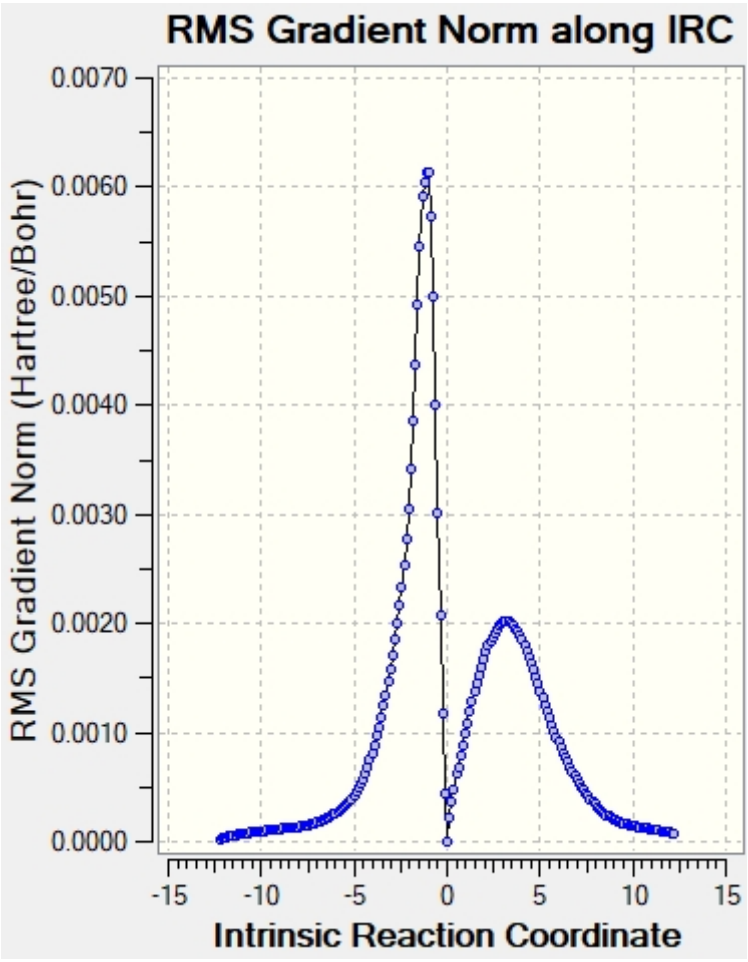
1a.2MeOH-ts

Zero-point correction=	0.257714
(Hartree/Particle)	
Thermal correction to Energy=	0.273261
Thermal correction to Enthalpy=	0.274206
Thermal correction to Gibbs Free Energy=	0.214152
Sum of electronic and zero-point Energies=	-725.313070
Sum of electronic and thermal Energies=	-725.297523
Sum of electronic and thermal Enthalpies=	-725.296579
Sum of electronic and thermal Free Energies=	-725.356632

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.458984	-1.054925	-0.127423
2	7	0	3.256267	-1.472526	0.920595
3	8	0	2.891735	-1.051814	-1.282557
4	6	0	-1.071332	-0.316859	-0.519804
5	6	0	-3.814887	-0.701182	-0.119221
6	6	0	-2.002861	0.462807	-1.213440
7	6	0	-1.523590	-1.297546	0.364729
8	6	0	-2.890684	-1.488700	0.563435
9	6	0	-3.367411	0.274323	-1.010689
10	1	0	-1.653905	1.226447	-1.901580
11	1	0	-0.789601	-1.898115	0.891438
12	1	0	-3.233135	-2.254134	1.253120
13	1	0	-4.082358	0.888413	-1.549542
14	1	0	-4.879041	-0.848458	0.037634
15	6	0	0.413974	-0.138617	-0.740228
16	8	0	0.555634	1.450981	-0.786805
17	6	0	1.845837	1.885574	-1.261150
18	1	0	1.815687	2.974510	-1.306875
19	1	0	2.009568	1.456097	-2.249255
20	1	0	2.633115	1.546103	-0.584189
21	7	0	1.212182	-0.635437	0.277250
22	1	0	0.496759	1.653227	0.319330
23	1	0	4.073275	-1.996684	0.647050
24	1	0	2.793096	-1.757887	1.769320
25	8	0	0.649088	1.418303	1.597793
26	6	0	-0.483778	1.486823	2.460570
27	1	0	-0.683189	2.538255	2.674243
28	1	0	-0.259324	0.970840	3.397410
29	1	0	-1.365735	1.031532	1.996225
30	1	0	0.947397	0.425581	1.362181
31	1	0	0.741083	-0.409935	-1.749534

1a.2MeOH-ts IRC



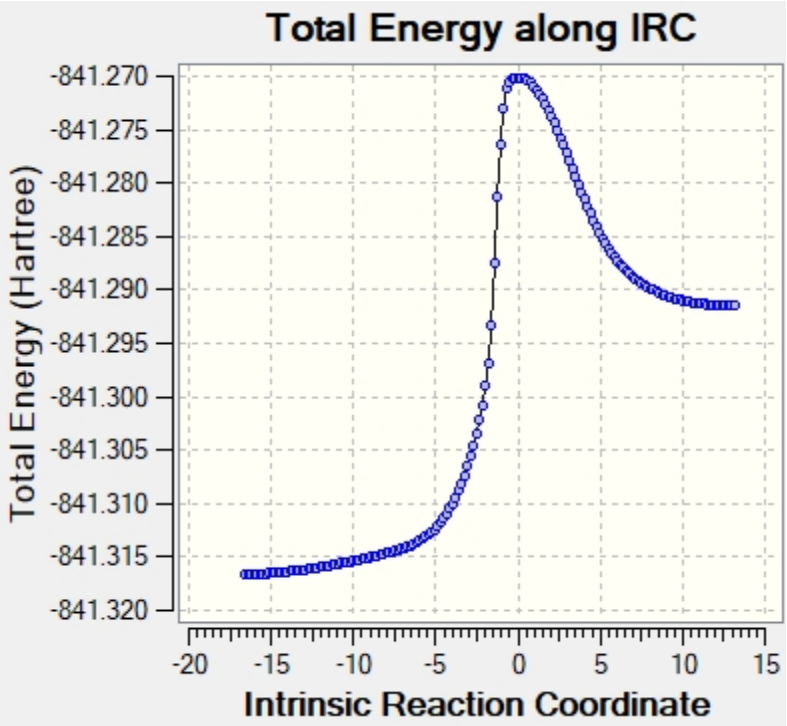


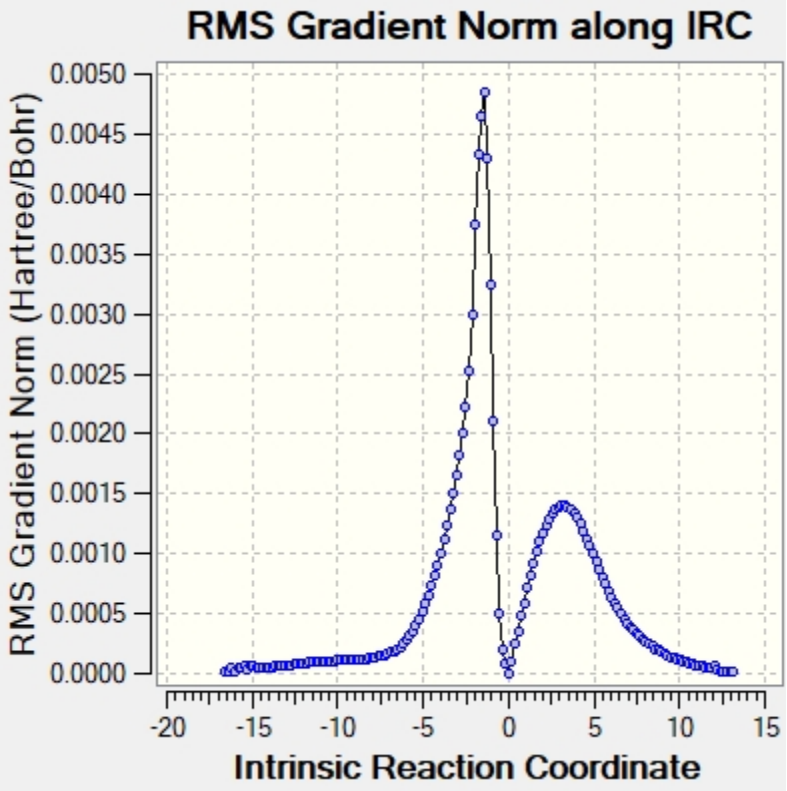
1a.3MeOH-ts

Zero-point correction= (Hartree/Particle)	0.312208
Thermal correction to Energy=	0.331877
Thermal correction to Enthalpy=	0.332821
Thermal correction to Gibbs Free Energy=	0.263097
Sum of electronic and zero-point Energies=	-840.957953
Sum of electronic and thermal Energies=	-840.938284
Sum of electronic and thermal Enthalpies=	-840.937339
Sum of electronic and thermal Free Energies=	-841.007064

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.265065	-1.532373	0.235219
2	7	0	3.101362	-1.351005	1.314058
3	8	0	2.589395	-2.259443	-0.704888
4	6	0	-1.251758	-0.796066	-0.370124
5	6	0	-3.971109	-0.577606	0.251381
6	6	0	-2.191095	-0.562908	-1.380759
7	6	0	-1.686937	-0.939515	0.947055
8	6	0	-3.041633	-0.826770	1.257623
9	6	0	-3.542779	-0.450499	-1.070334
10	1	0	-1.856126	-0.459632	-2.408397
11	1	0	-0.954872	-1.155342	1.718056
12	1	0	-3.369919	-0.939903	2.286474
13	1	0	-4.264072	-0.265525	-1.860263
14	1	0	-5.026173	-0.490202	0.491992
15	6	0	0.213140	-0.954904	-0.694629
16	1	0	0.427213	-1.784567	-1.376477
17	8	0	0.444690	0.279137	-1.751543
18	8	0	0.048909	2.274440	-0.397021
19	6	0	0.724951	3.463372	-0.784690
20	1	0	1.809578	3.361758	-0.663902
21	1	0	0.373549	4.305958	-0.183149
22	1	0	0.494230	3.662688	-1.833665
23	6	0	1.805253	0.362267	-2.203617
24	1	0	1.850079	1.147534	-2.960647
25	1	0	2.087521	-0.603807	-2.621981
26	1	0	2.466790	0.599433	-1.364588
27	7	0	1.073920	-0.847801	0.361251
28	1	0	0.220123	1.187131	-1.192526
29	1	0	4.048265	-1.674163	1.197910
30	1	0	2.935291	-0.572922	1.934206
31	8	0	0.890445	1.285177	1.726777
32	1	0	0.345746	1.977416	0.550582
33	6	0	0.122741	1.228288	2.914513
34	1	0	0.314003	0.290174	3.450187
35	1	0	-0.952233	1.295355	2.702845
36	1	0	0.409777	2.060787	3.562647
37	1	0	0.951713	0.335267	1.247108

1a.3MeOH-ts IRC





2.2.2 M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

IMINE 1a

```
 Zero-point correction=                           0.150659
(Hartree/Particle)
 Thermal correction to Energy=                    0.160286
 Thermal correction to Enthalpy=                  0.161230
 Thermal correction to Gibbs Free Energy=         0.114509
 Sum of electronic and zero-point Energies=           -494.087106
 Sum of electronic and thermal Energies=              -494.077479
 Sum of electronic and thermal Enthalpies=            -494.076535
 Sum of electronic and thermal Free Energies=         -494.123256
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.620447	-0.498752	-0.000020
2	7	0	1.512619	0.418478	-0.000050
3	6	0	-0.815812	-0.201705	-0.000006
4	6	0	2.863099	-0.057477	-0.000085
5	7	0	3.733897	0.969215	0.000035
6	8	0	3.198465	-1.236687	0.000026
7	1	0	4.725120	0.784910	0.000136
8	6	0	-3.561252	0.293292	0.000023
9	6	0	-1.723340	-1.267212	0.000018
10	6	0	-1.290918	1.117741	-0.000016
11	6	0	-2.658514	1.361635	-0.000002
12	6	0	-3.094794	-1.020312	0.000033
13	1	0	-1.351212	-2.288464	0.000025
14	1	0	-0.576754	1.934832	-0.000037
15	1	0	-3.027232	2.382294	-0.000010
16	1	0	-3.795513	-1.848726	0.000053
17	1	0	-4.629167	0.488375	0.000034
18	1	0	0.910663	-1.555925	-0.000022
19	1	0	3.397268	1.919079	0.000051

2a (MeOH)

```
 Zero-point correction=                           0.051726
(Hartree/Particle)
 Thermal correction to Energy=                    0.055103
 Thermal correction to Enthalpy=                  0.056047
 Thermal correction to Gibbs Free Energy=         0.028919
 Sum of electronic and zero-point Energies=           -115.625091
 Sum of electronic and thermal Energies=              -115.621715
 Sum of electronic and thermal Enthalpies=            -115.620771
 Sum of electronic and thermal Free Energies=         -115.647898
```

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	8	0	0.047053	-0.755604	0.000000
2	1	0	-0.864768	-1.066764	0.000000
3	6	0	0.047053	0.664968	0.000000
4	1	0	1.090796	0.981812	0.000000
5	1	0	-0.442385	1.069988	0.892601
6	1	0	-0.442385	1.069988	-0.892601

1a.2MeOH-ts

Zero-point correction= (Hartree/Particle)	0.202345
Thermal correction to Energy=	0.214689
Thermal correction to Enthalpy=	0.215633
Thermal correction to Gibbs Free Energy=	0.162524
Sum of electronic and zero-point Energies=	-609.662582
Sum of electronic and thermal Energies=	-609.650239
Sum of electronic and thermal Enthalpies=	-609.649294
Sum of electronic and thermal Free Energies=	-609.702403

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.582601	-0.061498	-0.426722
2	6	0	2.668330	-0.647491	0.158197
3	7	0	3.762089	-0.748126	-0.676452
4	8	0	2.728361	-1.056539	1.328487
5	6	0	-0.834528	-0.111946	0.212040
6	6	0	-3.457415	-0.967174	-0.212306
7	6	0	-1.806538	0.087287	1.196545
8	6	0	-1.176394	-0.751349	-0.981786
9	6	0	-2.486429	-1.175835	-1.193275
10	6	0	-3.116765	-0.337378	0.984972
11	1	0	-1.534203	0.571930	2.131408
12	1	0	-0.405587	-0.916769	-1.727844
13	1	0	-2.749968	-1.675257	-2.120288
14	1	0	-3.867478	-0.184195	1.753529
15	1	0	-4.476442	-1.303188	-0.377476
16	6	0	0.563749	0.371979	0.453604
17	1	0	0.827667	0.379788	1.513673
18	8	0	0.710447	1.869301	0.005286
19	6	0	-0.395663	2.626617	-0.525282
20	1	0	-0.852453	2.103706	-1.366971
21	1	0	0.017513	3.584222	-0.837877
22	1	0	-1.121832	2.769718	0.274405
23	1	0	1.436966	1.357453	-0.679956
24	1	0	3.593785	-0.666963	-1.668269
25	1	0	4.458661	-1.423432	-0.398564

1a.2MeOH-pf

```
 Zero-point correction=                           0.207637
(Hartree/Particle)
 Thermal correction to Energy=                    0.220250
 Thermal correction to Enthalpy=                  0.221195
 Thermal correction to Gibbs Free Energy=         0.167261
 Sum of electronic and zero-point Energies=           -609.735782
 Sum of electronic and thermal Energies=              -609.723168
 Sum of electronic and thermal Enthalpies=            -609.722224
 Sum of electronic and thermal Free Energies=         -609.776158

Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0        1.335651   -0.619077   -0.340392
      2          6           0        2.673324   -0.698143   -0.018537
      3          7           0        3.421336   -1.494714   -0.841205
      4          8           0        3.158278   -0.096893    0.936929
      5          6           0       -0.946096    0.006218    0.139019
      6          6           0       -3.610380   -0.796632   -0.121758
      7          6           0       -1.536508   -0.796684    1.116567
      8          6           0       -1.695207    0.412570   -0.966288
      9          6           0       -3.024673    0.010461   -1.096668
     10          6           0       -2.864381   -1.199036    0.987108
     11          1           0       -0.953298   -1.107119    1.980231
     12          1           0       -1.234977    1.052596   -1.714144
     13          1           0       -3.603610    0.330082   -1.957691
     14          1           0       -3.318443   -1.821133    1.752188
     15          1           0       -4.645919   -1.106649   -0.221708
     16          6           0        0.517227    0.395486    0.262913
     17          1           0        0.805239    0.459847    1.320390
     18          8           0        0.794976    1.631361   -0.368278
     19          6           0        0.326712    2.743456    0.374941
     20          1           0        0.626517    3.638957   -0.169630
     21          1           0        0.778798    2.757630    1.375182
     22          1           0       -0.765988    2.729224    0.474541
     23          1           0        1.029270   -0.973485   -1.237624
     24          1           0        2.977803   -2.170593   -1.445281
     25          1           0        4.339551   -1.734735   -0.498254
 ---------------------------------------------------------------------
```

1a.2MeOH-ts

```
 Zero-point correction=                           0.257363
(Hartree/Particle)
 Thermal correction to Energy=                    0.273170
 Thermal correction to Enthalpy=                  0.274114
 Thermal correction to Gibbs Free Energy=         0.212965
 Sum of electronic and zero-point Energies=           -725.326905
 Sum of electronic and thermal Energies=              -725.311098
 Sum of electronic and thermal Enthalpies=            -725.310154
 Sum of electronic and thermal Free Energies=         -725.371303

Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -2.429710   -1.072665   -0.306887
```

2	7	0	-3.271824	-0.974500	-1.397985
3	8	0	-2.810738	-1.668921	0.716675
4	6	0	1.077998	-0.490386	0.328134
5	6	0	3.815378	-0.700804	-0.215207
6	6	0	2.020259	-0.162074	1.309384
7	6	0	1.514985	-0.934335	-0.920586
8	6	0	2.880271	-1.038409	-1.191267
9	6	0	3.382103	-0.263881	1.038571
10	1	0	1.682428	0.183843	2.281953
11	1	0	0.775688	-1.192456	-1.671638
12	1	0	3.211706	-1.383429	-2.165784
13	1	0	4.105997	-0.003712	1.804698
14	1	0	4.877366	-0.780271	-0.426173
15	6	0	-0.401806	-0.401847	0.630583
16	8	0	-0.528572	1.014942	1.299705
17	6	0	-1.775106	1.200709	2.002938
18	1	0	-1.787105	2.229078	2.361459
19	1	0	-1.796428	0.501896	2.838992
20	1	0	-2.616024	1.013677	1.331378
21	7	0	-1.230693	-0.450036	-0.487251
22	1	0	-0.526866	1.664391	0.387264
23	1	0	-4.033268	-1.636567	-1.417820
24	1	0	-2.848298	-0.759534	-2.288717
25	8	0	-0.730981	2.004682	-0.870023
26	6	0	0.378457	2.463438	-1.648982
27	1	0	1.275987	1.873885	-1.436360
28	1	0	0.555926	3.508108	-1.392597
29	1	0	0.132738	2.388740	-2.710097
30	1	0	-1.002312	1.022081	-1.080862
31	1	0	-0.704567	-1.062082	1.450009

1a.3MeOH-ts

Zero-point correction= 0.312142
(Hartree/Particle)
Thermal correction to Energy= 0.332317
Thermal correction to Enthalpy= 0.333261
Thermal correction to Gibbs Free Energy= 0.262089
Sum of electronic and zero-point Energies= -840.972537
Sum of electronic and thermal Energies= -840.952362
Sum of electronic and thermal Enthalpies= -840.951417
Sum of electronic and thermal Free Energies= -841.022590

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.351128	-1.464578	0.324399
2	7	0	3.231150	-1.120727	1.319104
3	8	0	2.657002	-2.317418	-0.521568
4	6	0	-1.205670	-0.908460	-0.226821
5	6	0	-3.919462	-0.683588	0.414011
6	6	0	-2.174018	-0.933766	-1.237151
7	6	0	-1.606625	-0.789636	1.104223
8	6	0	-2.959670	-0.673595	1.423822
9	6	0	-3.523824	-0.818630	-0.918487
10	1	0	-1.863418	-1.034756	-2.273060

11	1	0	-0.853658	-0.808244	1.885244
12	1	0	-3.261885	-0.581391	2.462576
13	1	0	-4.268296	-0.836480	-1.708408
14	1	0	-4.972717	-0.594551	0.661662
15	6	0	0.251166	-1.059777	-0.569093
16	1	0	0.473741	-1.917740	-1.210109
17	8	0	0.388627	0.116597	-1.787512
18	8	0	-0.198339	2.228045	-0.633704
19	6	0	0.301752	3.430500	-1.218710
20	1	0	1.393960	3.473852	-1.157098
21	1	0	-0.126505	4.299107	-0.712557
22	1	0	-0.001585	3.444903	-2.266803
23	6	0	1.738497	0.274543	-2.248275
24	1	0	1.738744	1.045170	-3.020777
25	1	0	2.068219	-0.679364	-2.658966
26	1	0	2.389523	0.569045	-1.419232
27	7	0	1.143572	-0.809735	0.421167
28	1	0	0.086841	1.027688	-1.337950
29	1	0	4.187494	-1.419459	1.206874
30	1	0	3.062635	-0.283484	1.856928
31	8	0	0.953807	1.539903	1.537909
32	1	0	0.202289	2.090625	0.285939
33	6	0	0.297644	1.590269	2.796254
34	1	0	0.586864	0.735314	3.417915
35	1	0	-0.792857	1.586553	2.677676
36	1	0	0.594836	2.508562	3.307876
37	1	0	1.018429	0.571169	1.194345

2.2.3 M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

IMINE 1a

Zero-point correction=	0.150588
(Hartree/Particle)	
Thermal correction to Energy=	0.160225
Thermal correction to Enthalpy=	0.161170
Thermal correction to Gibbs Free Energy=	0.114397
Sum of electronic and zero-point Energies=	-494.088775
Sum of electronic and thermal Energies=	-494.079137
Sum of electronic and thermal Enthalpies=	-494.078193
Sum of electronic and thermal Free Energies=	-494.124965

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.620170	-0.499736	-0.000002
2	7	0	-1.512791	0.417525	-0.000001
3	6	0	0.815792	-0.202022	0.000001
4	6	0	-2.863103	-0.056507	-0.000002
5	7	0	-3.733390	0.969394	-0.000003
6	8	0	-3.199034	-1.236732	-0.000006
7	1	0	-4.725014	0.786176	-0.000008
8	6	0	3.561198	0.293783	0.000005

9	6	0	1.723662	-1.267530	0.000000
10	6	0	1.290581	1.117788	0.000003
11	6	0	2.658189	1.362063	0.000005
12	6	0	3.095088	-1.020135	0.000003
13	1	0	1.351988	-2.288899	-0.000001
14	1	0	0.576971	1.935404	0.000003
15	1	0	3.026579	2.382808	0.000007
16	1	0	3.796005	-1.848341	0.000002
17	1	0	4.629017	0.489198	0.000006
18	1	0	-0.909473	-1.557067	-0.000002
19	1	0	-3.397955	1.919915	-0.000003

2a (MeOH)

Zero-point correction= 0.051716
(Hartree/Particle)
Thermal correction to Energy= 0.055090
Thermal correction to Enthalpy= 0.056034
Thermal correction to Gibbs Free Energy= 0.028911
Sum of electronic and zero-point Energies= -115.625915
Sum of electronic and thermal Energies= -115.622541
Sum of electronic and thermal Enthalpies= -115.621596
Sum of electronic and thermal Free Energies= -115.648720

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.047226	-0.755832	0.000000
2	1	0	-0.865422	-1.065796	0.000000
3	6	0	0.047226	0.665026	0.000000
4	1	0	1.090620	0.983565	0.000000
5	1	0	-0.443182	1.069365	0.892097
6	1	0	-0.443182	1.069365	-0.892097

1a.MeOH-ts

Zero-point correction= 0.202233
(Hartree/Particle)
Thermal correction to Energy= 0.214616
Thermal correction to Enthalpy= 0.215560
Thermal correction to Gibbs Free Energy= 0.162265
Sum of electronic and zero-point Energies= -609.665368
Sum of electronic and thermal Energies= -609.652985
Sum of electronic and thermal Enthalpies= -609.652041
Sum of electronic and thermal Free Energies= -609.705336

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.591854	-0.028070	-0.421292
2	6	0	2.655964	-0.660982	0.145547

3	7	0	3.765382	-0.733218	-0.671027
4	8	0	2.687990	-1.137857	1.293724
5	6	0	-0.829928	-0.105684	0.208729
6	6	0	-3.444298	-0.978196	-0.233740
7	6	0	-1.800209	0.049802	1.202816
8	6	0	-1.169353	-0.708877	-1.004720
9	6	0	-2.475100	-1.142038	-1.225264
10	6	0	-3.106208	-0.383806	0.982219
11	1	0	-1.530699	0.508732	2.151296
12	1	0	-0.401428	-0.838660	-1.760755
13	1	0	-2.736866	-1.611853	-2.168145
14	1	0	-3.855808	-0.262747	1.757522
15	1	0	-4.460111	-1.320088	-0.406361
16	6	0	0.563766	0.387522	0.462106
17	1	0	0.821744	0.375128	1.523755
18	8	0	0.707522	1.882686	0.041891
19	6	0	-0.401018	2.647592	-0.476028
20	1	0	-0.849001	2.143328	-1.333353
21	1	0	0.010498	3.613983	-0.761910
22	1	0	-1.131154	2.766702	0.323809
23	1	0	1.445053	1.391785	-0.649964
24	1	0	3.620801	-0.585754	-1.659203
25	1	0	4.440529	-1.442175	-0.425372

1a.MeOH-pf

Zero-point correction= 0.207710
(Hartree/Particle)
Thermal correction to Energy= 0.220312
Thermal correction to Enthalpy= 0.221257
Thermal correction to Gibbs Free Energy= 0.167670
Sum of electronic and zero-point Energies= -609.738169
Sum of electronic and thermal Energies= -609.725567
Sum of electronic and thermal Enthalpies= -609.724622
Sum of electronic and thermal Free Energies= -609.778209

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.343714	-0.623081	-0.317061
2	6	0	2.679429	-0.696018	0.007287
3	7	0	3.426202	-1.520071	-0.786207
4	8	0	3.166374	-0.061635	0.942703
5	6	0	-0.942067	0.007090	0.139932
6	6	0	-3.605382	-0.801449	-0.110827
7	6	0	-1.568230	-0.678400	1.181983
8	6	0	-1.655019	0.294500	-1.025857
9	6	0	-2.983363	-0.110670	-1.151504
10	6	0	-2.896630	-1.083563	1.057438
11	1	0	-1.014434	-0.896144	2.092010
12	1	0	-1.168290	0.844996	-1.826306
13	1	0	-3.533825	0.117082	-2.059023
14	1	0	-3.379473	-1.613543	1.872489
15	1	0	-4.640627	-1.113556	-0.207175
16	6	0	0.519404	0.402434	0.258385
17	1	0	0.802367	0.497924	1.314882

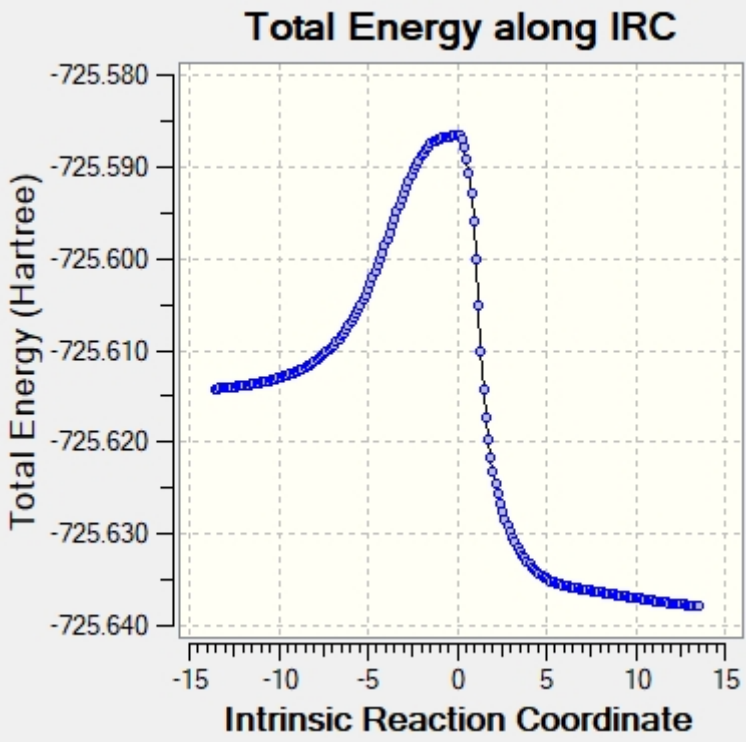
18	8	0	0.794939	1.623090	-0.406134
19	6	0	0.286810	2.750100	0.287848
20	1	0	0.585694	3.633300	-0.276801
21	1	0	0.709481	2.804645	1.299529
22	1	0	-0.807591	2.718318	0.357367
23	1	0	1.030736	-1.024707	-1.191938
24	1	0	2.982872	-2.208297	-1.376658
25	1	0	4.343457	-1.753736	-0.436158

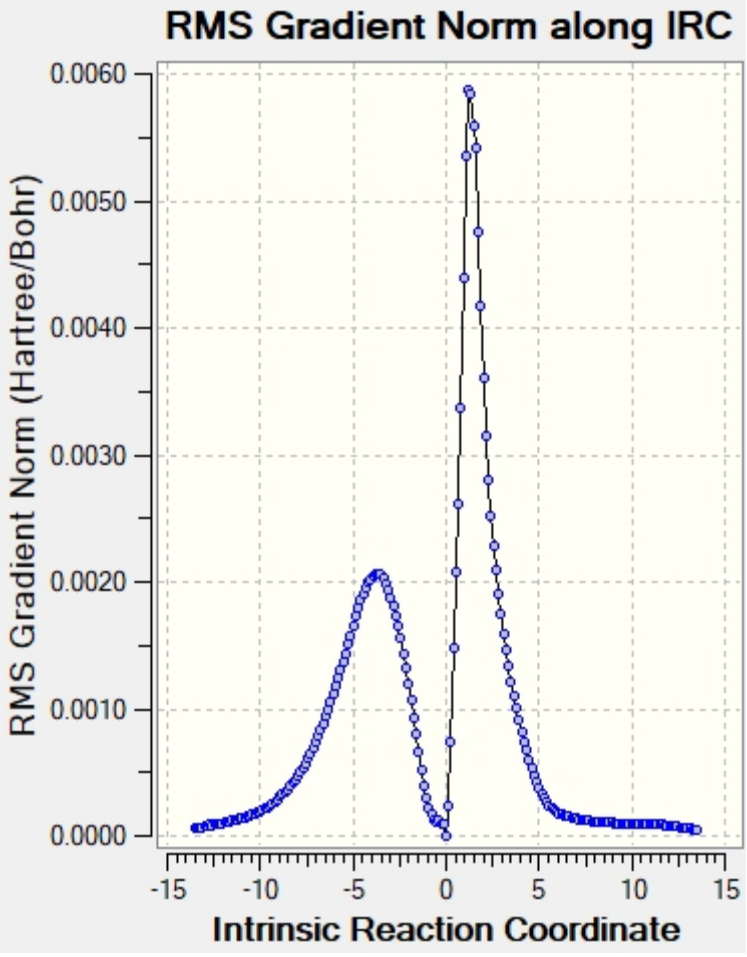
1a.2MeOH-ts

Zero-point correction= 0.256986
(Hartree/Particle)
Thermal correction to Energy= 0.271994
Thermal correction to Enthalpy= 0.272938
Thermal correction to Gibbs Free Energy= 0.213811
Sum of electronic and zero-point Energies= -725.329615
Sum of electronic and thermal Energies= -725.314607
Sum of electronic and thermal Enthalpies= -725.313663
Sum of electronic and thermal Free Energies= -725.372790

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.425992	-1.034002	-0.441853
2	7	0	-3.276176	-0.795617	-1.505226
3	8	0	-2.799732	-1.769260	0.492929
4	6	0	1.078438	-0.527728	0.257041
5	6	0	3.815951	-0.667368	-0.307780
6	6	0	2.020073	-0.370983	1.280918
7	6	0	1.515914	-0.766132	-1.046190
8	6	0	2.881569	-0.834025	-1.327980
9	6	0	3.381981	-0.437671	0.999947
10	1	0	1.681471	-0.187410	2.296752
11	1	0	0.777675	-0.893209	-1.830824
12	1	0	3.213234	-1.016917	-2.345457
13	1	0	4.105762	-0.311136	1.798951
14	1	0	4.877983	-0.718750	-0.526979
15	6	0	-0.400490	-0.476130	0.573200
16	8	0	-0.524726	0.839523	1.414042
17	6	0	-1.761918	0.929048	2.152033
18	1	0	-1.777408	1.908593	2.627785
19	1	0	-1.762020	0.138195	2.902007
20	1	0	-2.611011	0.812858	1.474740
21	7	0	-1.234929	-0.384143	-0.540077
22	1	0	-0.532167	1.604124	0.594811
23	1	0	-4.026148	-1.461771	-1.618416
24	1	0	-2.858564	-0.454292	-2.358880
25	8	0	-0.742771	2.109796	-0.602200
26	6	0	0.364156	2.679081	-1.310792
27	1	0	0.570973	3.654727	-0.871014
28	1	0	0.095996	2.804012	-2.361437
29	1	0	1.249498	2.040770	-1.228671
30	1	0	-1.009308	1.170529	-0.947805
31	1	0	-0.698498	-1.237016	1.302132

1a.2MeOH-ts IRC



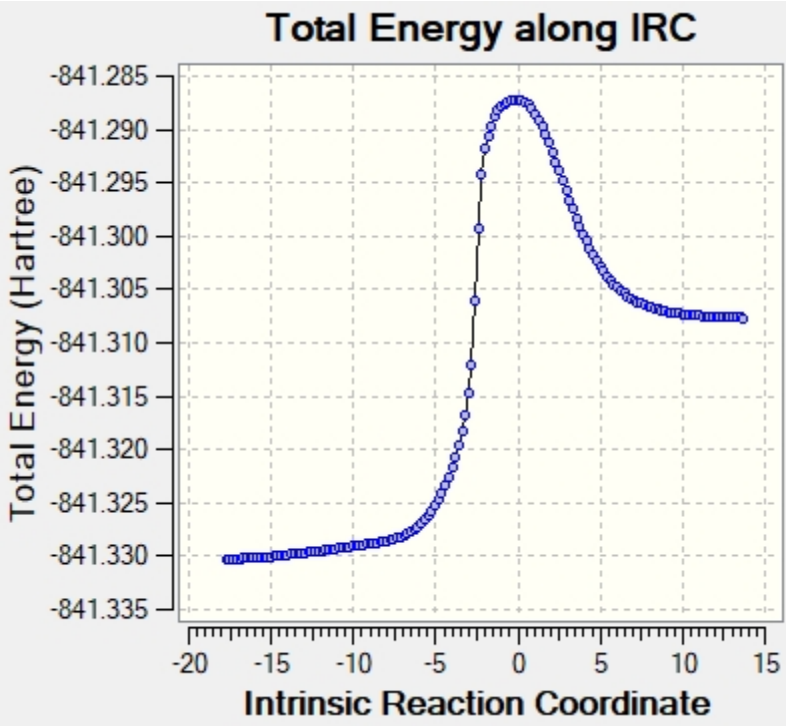


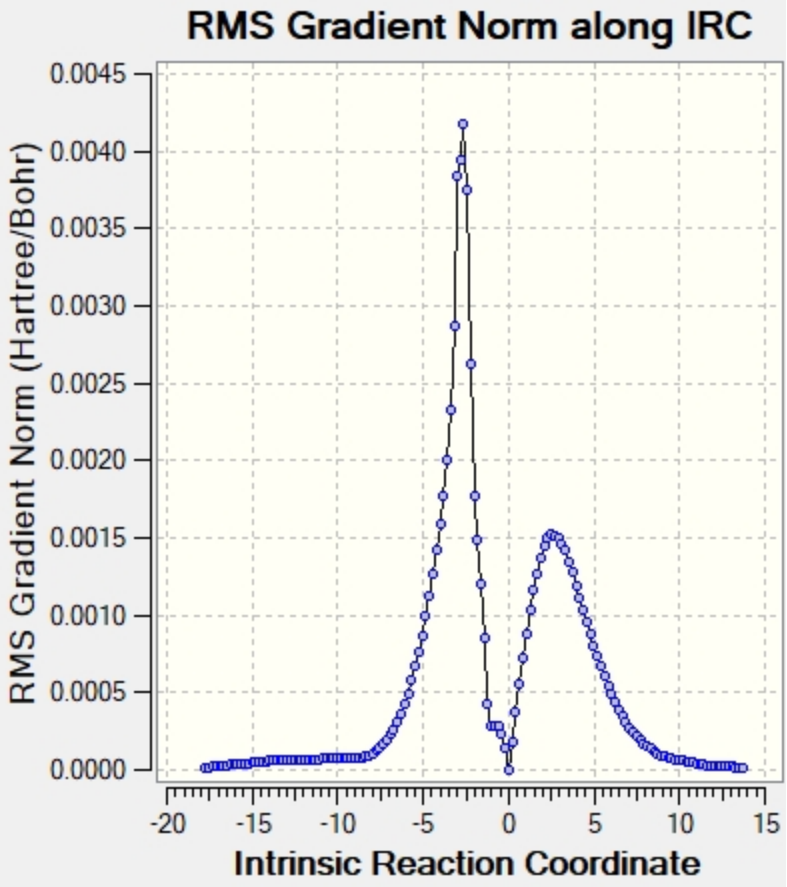
1a.3MeOH-ts

Zero-point correction=	0.312767
(Hartree/Particle)	
Thermal correction to Energy=	0.332881
Thermal correction to Enthalpy=	0.333825
Thermal correction to Gibbs Free Energy=	0.262693
Sum of electronic and zero-point Energies=	-840.974406
Sum of electronic and thermal Energies=	-840.954293
Sum of electronic and thermal Enthalpies=	-840.953348
Sum of electronic and thermal Free Energies=	-841.024480

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.376978	-1.417640	0.405696
2	7	0	3.281476	-0.963150	1.331261
3	8	0	2.670775	-2.350242	-0.357889
4	6	0	-1.199069	-0.949723	-0.117631
5	6	0	-3.906635	-0.658842	0.524109
6	6	0	-2.180720	-1.129003	-1.099556
7	6	0	-1.583513	-0.646057	1.188992
8	6	0	-2.933372	-0.496373	1.508410
9	6	0	-3.527460	-0.981769	-0.780958
10	1	0	-1.883155	-1.373896	-2.115255
11	1	0	-0.822076	-0.545113	1.954914
12	1	0	-3.221945	-0.257490	2.527417
13	1	0	-4.282271	-1.119489	-1.548651
14	1	0	-4.957244	-0.542984	0.771765
15	6	0	0.252539	-1.117736	-0.469900
16	1	0	0.472316	-2.020648	-1.046705
17	8	0	0.349352	-0.039447	-1.787275
18	8	0	-0.265075	2.151216	-0.796449
19	6	0	0.135860	3.317564	-1.517397
20	1	0	1.226590	3.399242	-1.558610
21	1	0	-0.279602	4.210729	-1.044643
22	1	0	-0.258732	3.234471	-2.531114
23	6	0	1.685607	0.103751	-2.290503
24	1	0	1.657199	0.819244	-3.113748
25	1	0	2.017627	-0.871923	-2.644292
26	1	0	2.352639	0.464043	-1.500973
27	7	0	1.161867	-0.774565	0.475152
28	1	0	0.038009	0.896781	-1.409677
29	1	0	4.239747	-1.254907	1.214317
30	1	0	3.120101	-0.071383	1.776457
31	8	0	1.016871	1.676993	1.370447
32	1	0	0.193587	2.115821	0.102460
33	6	0	0.420169	1.843627	2.649016
34	1	0	0.702152	1.022436	3.317732
35	1	0	-0.673711	1.879456	2.576362
36	1	0	0.776175	2.781702	3.080531
37	1	0	1.061507	0.682957	1.114485

1a.3MeOH-ts IRC





2.2.4 M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

IMINE 1a

```
 Zero-point correction=                           0.150591
(Hartree/Particle)
 Thermal correction to Energy=                    0.160227
 Thermal correction to Enthalpy=                  0.161172
 Thermal correction to Gibbs Free Energy=         0.114406
 Sum of electronic and zero-point Energies=           -494.088719
 Sum of electronic and thermal Energies=              -494.079082
 Sum of electronic and thermal Enthalpies=            -494.078138
 Sum of electronic and thermal Free Energies=         -494.124904

Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0       -0.620170   -0.499736   -0.000002
      2          7           0       -1.512791    0.417525   -0.000001
      3          6           0        0.815792   -0.202022    0.000001
      4          6           0       -2.863103   -0.056507   -0.000002
      5          7           0       -3.733390    0.969394   -0.000003
      6          8           0       -3.199034   -1.236732   -0.000006
      7          1           0       -4.725014    0.786176   -0.000008
      8          6           0        3.561198    0.293783    0.000005
      9          6           0        1.723662   -1.267530    0.000000
     10          6           0        1.290581    1.117788    0.000003
     11          6           0        2.658189    1.362063    0.000005
     12          6           0        3.095088   -1.020135    0.000003
     13          1           0        1.351988   -2.288899   -0.000001
     14          1           0        0.576971    1.935404    0.000003
     15          1           0        3.026579    2.382808    0.000007
     16          1           0        3.796005   -1.848341    0.000002
     17          1           0        4.629017    0.489198    0.000006
     18          1           0       -0.909473   -1.557067   -0.000002
     19          1           0       -3.397955    1.919915   -0.000003
 ---------------------------------------------------------------------
```

2a (MeOH)

```
 Zero-point correction=                           0.051717
(Hartree/Particle)
 Thermal correction to Energy=                    0.055091
 Thermal correction to Enthalpy=                  0.056035
 Thermal correction to Gibbs Free Energy=         0.028912
 Sum of electronic and zero-point Energies=           -115.625887
 Sum of electronic and thermal Energies=              -115.622513
 Sum of electronic and thermal Enthalpies=            -115.621569
 Sum of electronic and thermal Free Energies=         -115.648692

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

1	8	0	0.047226	-0.755832	0.000000
2	1	0	-0.865422	-1.065796	0.000000
3	6	0	0.047226	0.665026	0.000000
4	1	0	1.090620	0.983565	0.000000
5	1	0	-0.443182	1.069365	0.892097
6	1	0	-0.443182	1.069365	-0.892097

1a.MeOH-ts

Zero-point correction= 0.202243
(Hartree/Particle)
Thermal correction to Energy= 0.214622
Thermal correction to Enthalpy= 0.215566
Thermal correction to Gibbs Free Energy= 0.162294
Sum of electronic and zero-point Energies= -609.665268
Sum of electronic and thermal Energies= -609.652889
Sum of electronic and thermal Enthalpies= -609.651945
Sum of electronic and thermal Free Energies= -609.705216

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.591570	-0.029143	-0.421477
2	6	0	2.656375	-0.660495	0.146075
3	7	0	3.765314	-0.733678	-0.671089
4	8	0	2.689315	-1.135101	1.295075
5	6	0	-0.830075	-0.105862	0.208824
6	6	0	-3.444703	-0.977961	-0.232912
7	6	0	-1.800511	0.051485	1.202471
8	6	0	-1.169470	-0.710745	-1.003779
9	6	0	-2.475347	-1.143701	-1.223960
10	6	0	-3.106636	-0.381891	0.982232
11	1	0	-1.530987	0.511642	2.150355
12	1	0	-0.401378	-0.842024	-1.759378
13	1	0	-2.737079	-1.614888	-2.166166
14	1	0	-3.856345	-0.259432	1.757209
15	1	0	-4.460611	-1.319726	-0.405233
16	6	0	0.563757	0.387117	0.461761
17	1	0	0.821906	0.375528	1.523373
18	8	0	0.707569	1.882302	0.040452
19	6	0	-0.400909	2.646864	-0.477996
20	1	0	-0.849432	2.141637	-1.334483
21	1	0	0.010728	3.612792	-0.765290
22	1	0	-1.130725	2.767221	0.321950
23	1	0	1.444767	1.390701	-0.651122
24	1	0	3.619914	-0.588544	-1.659482
25	1	0	4.441099	-1.441620	-0.424273

1a.MeOH-pf

```
 Zero-point correction=                           0.207711
(Hartree/Particle)
 Thermal correction to Energy=                    0.220313
 Thermal correction to Enthalpy=                  0.221257
 Thermal correction to Gibbs Free Energy=         0.167675
 Sum of electronic and zero-point Energies=           -609.738084
 Sum of electronic and thermal Energies=              -609.725482
 Sum of electronic and thermal Enthalpies=            -609.724538
 Sum of electronic and thermal Free Energies=         -609.778121

Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0        1.343714   -0.623081   -0.317061
      2          6           0        2.679429   -0.696018    0.007287
      3          7           0        3.426202   -1.520071   -0.786207
      4          8           0        3.166374   -0.061635    0.942703
      5          6           0       -0.942067    0.007090    0.139932
      6          6           0       -3.605382   -0.801449   -0.110827
      7          6           0       -1.568230   -0.678400    1.181983
      8          6           0       -1.655019    0.294500   -1.025857
      9          6           0       -2.983363   -0.110670   -1.151504
     10          6           0       -2.896630   -1.083563    1.057438
     11          1           0       -1.014434   -0.896144    2.092010
     12          1           0       -1.168290    0.844996   -1.826306
     13          1           0       -3.533825    0.117082   -2.059023
     14          1           0       -3.379473   -1.613543    1.872489
     15          1           0       -4.640627   -1.113556   -0.207175
     16          6           0        0.519404    0.402434    0.258385
     17          1           0        0.802367    0.497924    1.314882
     18          8           0        0.794939    1.623090   -0.406134
     19          6           0        0.286810    2.750100    0.287848
     20          1           0        0.585694    3.633300   -0.276801
     21          1           0        0.709481    2.804645    1.299529
     22          1           0       -0.807591    2.718318    0.357367
     23          1           0        1.030736   -1.024707   -1.191938
     24          1           0        2.982872   -2.208297   -1.376658
     25          1           0        4.343457   -1.753736   -0.436158
 ---------------------------------------------------------------------
```

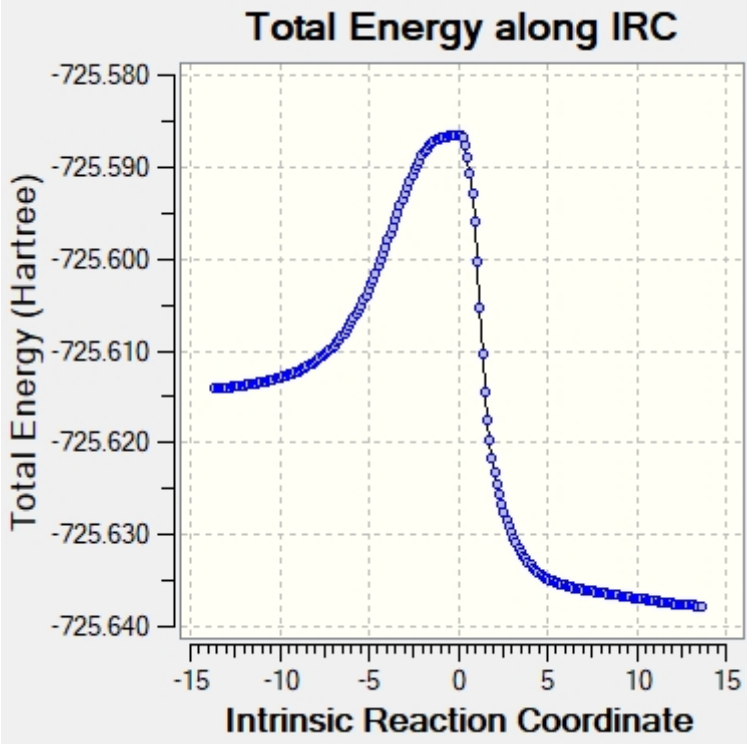
1a.2MeOH-ts

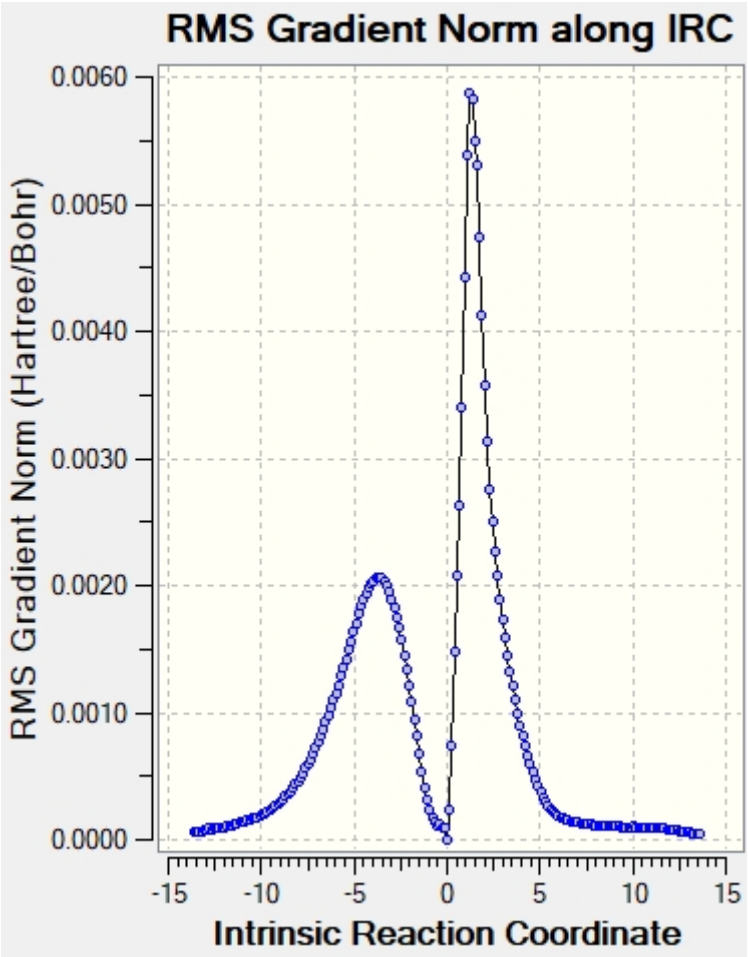
```
 Zero-point correction=                           0.257031
(Hartree/Particle)
 Thermal correction to Energy=                    0.272961
 Thermal correction to Enthalpy=                  0.273905
 Thermal correction to Gibbs Free Energy=         0.210864
 Sum of electronic and zero-point Energies=           -725.329491
 Sum of electronic and thermal Energies=              -725.313561
 Sum of electronic and thermal Enthalpies=            -725.312617
 Sum of electronic and thermal Free Energies=         -725.375659

Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	6	0	-2.425831	-1.036452	-0.436539
2	7	0	-3.275950	-0.803813	-1.501208
3	8	0	-2.799344	-1.766833	0.502038
4	6	0	1.078497	-0.526054	0.259780
5	6	0	3.816008	-0.669175	-0.304244
6	6	0	2.020166	-0.362559	1.282563
7	6	0	1.515956	-0.772834	-1.041904
8	6	0	2.881591	-0.842485	-1.323302
9	6	0	3.382061	-0.430968	1.001958
10	1	0	1.681668	-0.172419	2.297215
11	1	0	0.777621	-0.904935	-1.825628
12	1	0	3.213199	-1.032003	-2.339582
13	1	0	4.105864	-0.299255	1.800107
14	1	0	4.878037	-0.721973	-0.523127
15	6	0	-0.400454	-0.473126	0.575479
16	8	0	-0.524877	0.847038	1.409987
17	6	0	-1.762240	0.940139	2.147249
18	1	0	-1.777910	1.921992	2.618210
19	1	0	-1.762470	0.152954	2.901075
20	1	0	-2.611178	0.820578	1.470353
21	7	0	-1.234805	-0.386809	-0.538137
22	1	0	-0.532225	1.607169	0.587191
23	1	0	-4.026031	-1.470444	-1.610754
24	1	0	-2.858421	-0.466861	-2.356628
25	8	0	-0.743014	2.106978	-0.612996
26	6	0	0.363828	2.672036	-1.324982
27	1	0	0.571082	3.650037	-0.890652
28	1	0	0.095493	2.791284	-2.376254
29	1	0	1.249047	2.033960	-1.239596
30	1	0	-1.009662	1.165889	-0.953468
31	1	0	-0.698448	-1.230212	1.308362

1a.2MeOH-ts IRC



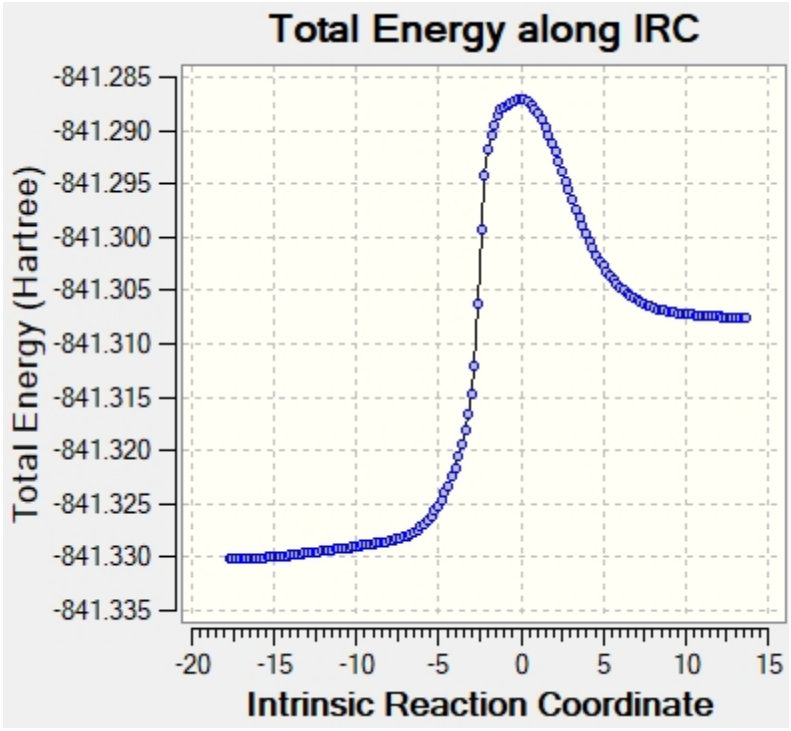


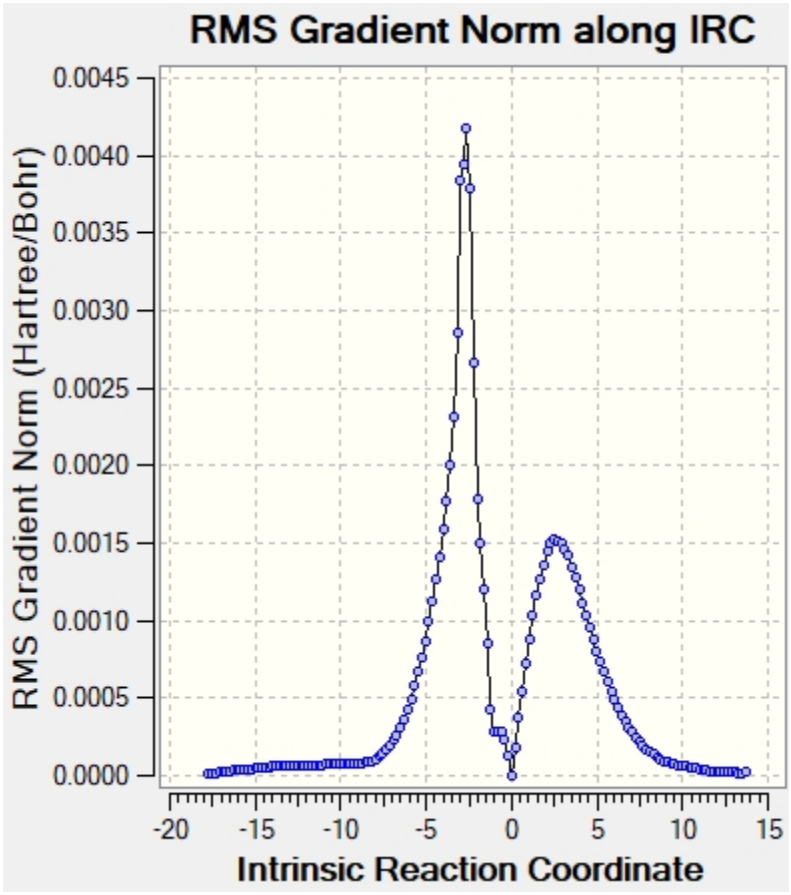
1a.3MeOH-ts

Zero-point correction=	0.312755
(Hartree/Particle)	
Thermal correction to Energy=	0.332869
Thermal correction to Enthalpy=	0.333813
Thermal correction to Gibbs Free Energy=	0.262671
Sum of electronic and zero-point Energies=	-840.974333
Sum of electronic and thermal Energies=	-840.954218
Sum of electronic and thermal Enthalpies=	-840.953274
Sum of electronic and thermal Free Energies=	-841.024416

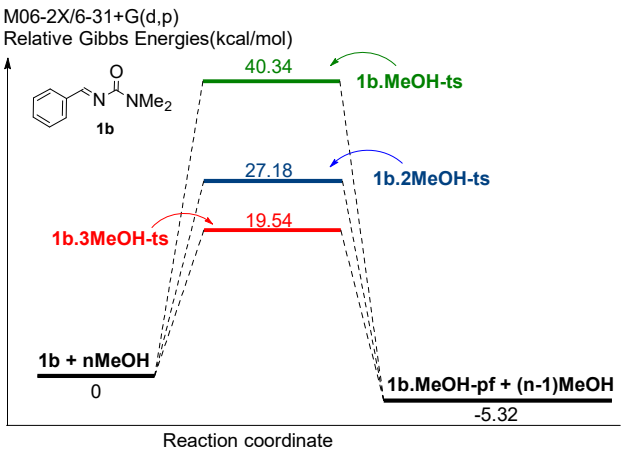
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.375913	-1.418494	0.406128
2	7	0	3.280303	-0.964715	1.332198
3	8	0	2.669537	-2.350947	-0.357640
4	6	0	-1.199763	-0.948851	-0.118086
5	6	0	-3.907329	-0.657277	0.523315
6	6	0	-2.181312	-1.127395	-1.100238
7	6	0	-1.584321	-0.645552	1.188579
8	6	0	-2.934178	-0.495527	1.507829
9	6	0	-3.528048	-0.979817	-0.781809
10	1	0	-1.883665	-1.372030	-2.115975
11	1	0	-0.822943	-0.545211	1.954643
12	1	0	-3.222843	-0.256954	2.526884
13	1	0	-4.282780	-1.117012	-1.549675
14	1	0	-4.957941	-0.541169	0.770845
15	6	0	0.251865	-1.117464	-0.470089
16	1	0	0.471357	-2.020651	-1.046586
17	8	0	0.349602	-0.039537	-1.787232
18	8	0	-0.263127	2.151528	-0.796720
19	6	0	0.140659	3.317295	-1.516953
20	1	0	1.231579	3.397386	-1.556472
21	1	0	-0.274189	4.211053	-1.044775
22	1	0	-0.252509	3.234916	-2.531291
23	6	0	1.686062	0.102578	-2.290247
24	1	0	1.658228	0.817589	-3.113935
25	1	0	2.017637	-0.873512	-2.643303
26	1	0	2.353109	0.462944	-1.500766
27	7	0	1.161136	-0.774747	0.475267
28	1	0	0.038910	0.897069	-1.409663
29	1	0	4.238430	-1.257036	1.215548
30	1	0	3.119221	-0.073004	1.777594
31	8	0	1.016727	1.676328	1.370889
32	1	0	0.194410	2.115384	0.102813
33	6	0	0.419939	1.842858	2.649401
34	1	0	0.701296	1.021222	3.317842
35	1	0	-0.673909	1.879395	2.576595
36	1	0	0.776453	2.780539	3.081373
37	1	0	1.061239	0.682203	1.114692

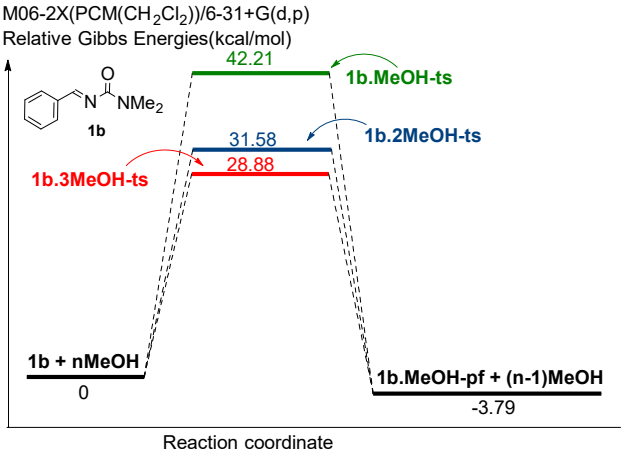
1a.3MeOH-ts IRC

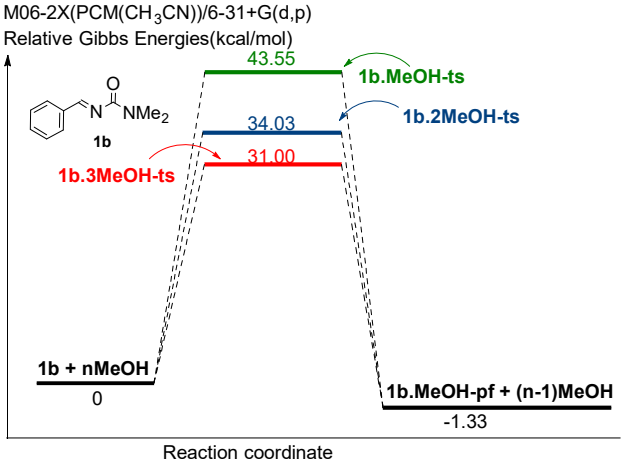


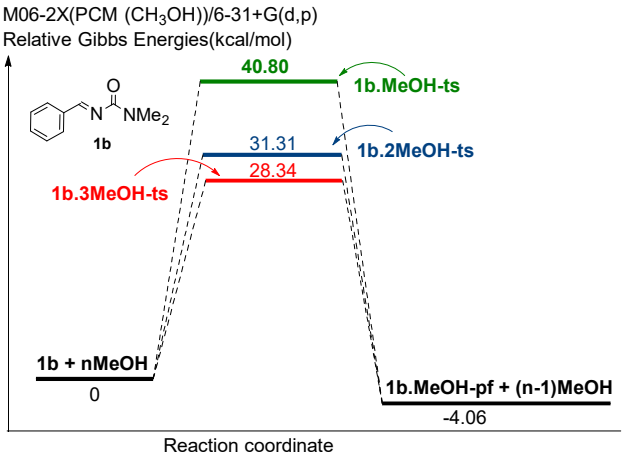


2.3.-Energy profiles for the addition of n methanol (2a) molecules (n=1-3) to imine derivative 1b in gas phase, CH_2Cl_2, CH_3CN and CH_3OH.









2.4.-Computacional data for the addition of n methanol (2a) molecules (n=1-3) to imine derivative 1b

2.4.1 M06-2X/6-31+G(d,p) calculations

IMINE 1b

```
 Zero-point correction=                           0.207154
(Hartree/Particle)
 Thermal correction to Energy=                    0.218337
 Thermal correction to Enthalpy=                  0.219281
 Thermal correction to Gibbs Free Energy=         0.168649
 Sum of electronic and zero-point Energies=           -572.593307
 Sum of electronic and thermal Energies=              -572.582124
 Sum of electronic and thermal Enthalpies=            -572.581180
 Sum of electronic and thermal Free Energies=         -572.631812
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.731564	-0.278656	0.000000
2	6	0	2.140380	-0.015507	0.000000
3	6	0	0.000000	0.768172	0.000000
4	7	0	2.880985	-1.149944	0.000000
5	8	0	2.643261	1.101516	0.000000
6	1	0	0.458174	1.765469	0.000000
7	6	0	-1.467375	0.696799	0.000000
8	6	0	-4.255852	0.619877	0.000000
9	6	0	-2.205047	1.884880	0.000000
10	6	0	-2.135242	-0.534995	0.000000
11	6	0	-3.523360	-0.570877	0.000000
12	6	0	-3.597578	1.847556	0.000000
13	1	0	-1.682232	2.838113	0.000000
14	1	0	-1.544916	-1.445804	0.000000
15	1	0	-4.041596	-1.524681	0.000000
16	1	0	-4.166449	2.771699	0.000000
17	1	0	-5.341076	0.587477	0.000000
18	6	0	4.325660	-0.972197	0.000000
19	1	0	4.805254	-1.950680	0.000000
20	1	0	4.642822	-0.410063	0.883187
21	1	0	4.642822	-0.410063	-0.883187
22	6	0	2.282128	-2.480950	0.000000
23	1	0	3.087675	-3.215777	0.000000
24	1	0	1.661651	-2.637087	-0.885588
25	1	0	1.661651	-2.637087	0.885588

-

1b.MeOH-ts

```
 Zero-point correction=                           0.258599
(Hartree/Particle)
 Thermal correction to Energy=                    0.274158
 Thermal correction to Enthalpy=                  0.275102
 Thermal correction to Gibbs Free Energy=         0.214366
 Sum of electronic and zero-point Energies=           -688.164833
 Sum of electronic and thermal Energies=              -688.149274
 Sum of electronic and thermal Enthalpies=            -688.148329
 Sum of electronic and thermal Free Energies=         -688.209066
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.928964	-0.002934	-0.187495
2	6	0	2.080059	-0.160421	0.578600
3	7	0	3.190187	-0.523655	-0.147354
4	8	0	2.124799	-0.025839	1.803840
5	6	0	-1.503156	-0.095340	0.298205
6	6	0	-4.036581	-1.192465	-0.106889
7	6	0	-2.575117	0.294022	1.105956
8	6	0	-1.699700	-1.048570	-0.703511
9	6	0	-2.965506	-1.592616	-0.906547
10	6	0	-3.840865	-0.251000	0.903337
11	1	0	-2.412826	1.020424	1.899332
12	1	0	-0.843824	-1.358401	-1.295179
13	1	0	-3.116003	-2.337910	-1.681252
14	1	0	-4.669909	0.049649	1.536100
15	1	0	-5.020823	-1.623715	-0.261906
16	6	0	-0.155635	0.511215	0.518760
17	1	0	0.036047	0.821008	1.548940
18	8	0	-0.101602	1.939555	-0.309002
19	6	0	4.478699	-0.565325	0.511156
20	1	0	4.322137	-0.552055	1.588159
21	1	0	5.096615	0.298065	0.226615
22	1	0	5.012219	-1.479413	0.228003
23	6	0	3.202752	-0.577225	-1.593020
24	1	0	2.210413	-0.828113	-1.963743
25	1	0	3.910011	-1.349346	-1.913191
26	1	0	3.519728	0.379003	-2.036505
27	6	0	-1.204780	2.414507	-1.087398
28	1	0	-1.544724	1.653178	-1.794477
29	1	0	-0.862599	3.305439	-1.615647
30	1	0	-2.018697	2.675633	-0.409040
31	1	0	0.681591	1.282254	-0.782863

1b.MeOH-pf

```
 Zero-point correction=                           0.265365
(Hartree/Particle)
 Thermal correction to Energy=                    0.280799
 Thermal correction to Enthalpy=                  0.281743
 Thermal correction to Gibbs Free Energy=         0.221328
 Sum of electronic and zero-point Energies=           -688.238792
 Sum of electronic and thermal Energies=              -688.223358
 Sum of electronic and thermal Enthalpies=            -688.222414
 Sum of electronic and thermal Free Energies=         -688.282828

Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -0.766174   -0.333725   -0.005845
      2          6           0       -2.078349    0.014083   -0.316378
      3          7           0       -3.039629   -0.839539    0.157082
      4          8           0       -2.331434    0.993807   -1.008960
      5          6           0        1.622021    0.040101   -0.146677
      6          6           0        4.163946   -1.114021    0.040397
      7          6           0        1.945165   -1.085480   -0.912223
      8          6           0        2.577833    0.583842    0.709523
      9          6           0        3.845442    0.006397    0.802583
     10          6           0        3.209392   -1.659294   -0.820363
     11          1           0        1.197416   -1.508427   -1.578312
     12          1           0        2.317112    1.453758    1.302704
     13          1           0        4.583012    0.433774    1.475051
     14          1           0        3.452433   -2.531765   -1.419153
     15          1           0        5.150039   -1.562112    0.114533
     16          6           0        0.241450    0.664952   -0.274959
     17          1           0        0.076090    1.004828   -1.304642
     18          8           0        0.093604    1.758421    0.603548
     19          6           0       -4.436964   -0.474554    0.012901
     20          1           0       -4.893763   -0.296721    0.994042
     21          1           0       -4.987092   -1.275580   -0.492317
     22          1           0       -4.496327    0.434170   -0.583257
     23          6           0       -2.730567   -2.013848    0.948956
     24          1           0       -2.501194   -1.769201    1.995935
     25          1           0       -1.893898   -2.567415    0.514300
     26          1           0       -3.601331   -2.672575    0.941848
     27          6           0        0.068498    3.016320   -0.047548
     28          1           0       -0.075160    3.769291    0.728712
     29          1           0       -0.762133    3.057662   -0.761231
     30          1           0        1.018127    3.214583   -0.564180
     31          1           0       -0.607259   -0.860240    0.843337
 ---------------------------------------------------------------------
```

1b.2MeOH-ts

Zero-point correction= (Hartree/Particle)	0.311641
Thermal correction to Energy=	0.330627
Thermal correction to Enthalpy=	0.331572
Thermal correction to Gibbs Free Energy=	0.263003
Sum of electronic and zero-point Energies=	-803.824736
Sum of electronic and thermal Energies=	-803.805750
Sum of electronic and thermal Enthalpies=	-803.804805
Sum of electronic and thermal Free Energies=	-803.873374

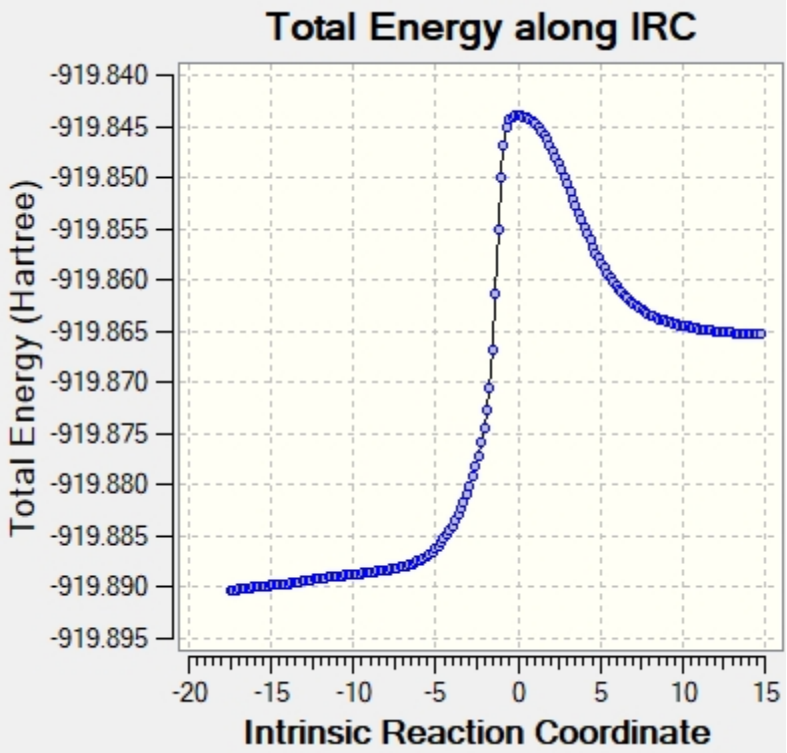
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.878857	-0.198582	-0.314067
2	6	0	2.073242	-0.916566	-0.246331
3	7	0	3.157139	-0.231682	-0.739796
4	8	0	2.172146	-2.066914	0.182540
5	6	0	-1.541638	-0.522822	-0.324340
6	6	0	-4.089748	0.068229	-1.320417
7	6	0	-2.596133	-1.423458	-0.153538
8	6	0	-1.766838	0.664075	-1.026655
9	6	0	-3.036256	0.962754	-1.513698
10	6	0	-3.865753	-1.131586	-0.648199
11	1	0	-2.417539	-2.365030	0.360558
12	1	0	-0.931842	1.331664	-1.214696
13	1	0	-3.202448	1.887140	-2.058394
14	1	0	-4.674953	-1.842651	-0.515175
15	1	0	-5.077313	0.298646	-1.707981
16	6	0	-0.190877	-0.847625	0.239847
17	1	0	-0.033959	-1.908094	0.451056
18	8	0	-0.243375	-0.276456	1.820709
19	1	0	0.105736	0.778001	1.700462
20	1	0	0.893273	1.068646	0.277361
21	8	0	0.729663	1.779040	1.130115
22	6	0	4.482362	-0.793978	-0.582769
23	1	0	4.387177	-1.803133	-0.186384
24	1	0	5.083070	-0.187219	0.107912
25	1	0	4.996855	-0.828930	-1.550211
26	6	0	3.082624	1.134032	-1.218406
27	1	0	3.200769	1.865156	-0.405749
28	1	0	2.128390	1.306463	-1.717423
29	1	0	3.885709	1.292024	-1.944344
30	6	0	0.080307	2.998573	0.822126
31	1	0	-1.007594	2.871759	0.744803
32	1	0	0.454331	3.392783	-0.129394
33	1	0	0.298415	3.726927	1.607753
34	6	0	-1.394238	-0.480298	2.630569
35	1	0	-1.165036	-0.111119	3.632548
36	1	0	-1.595879	-1.552897	2.682919
37	1	0	-2.268929	0.038376	2.225374

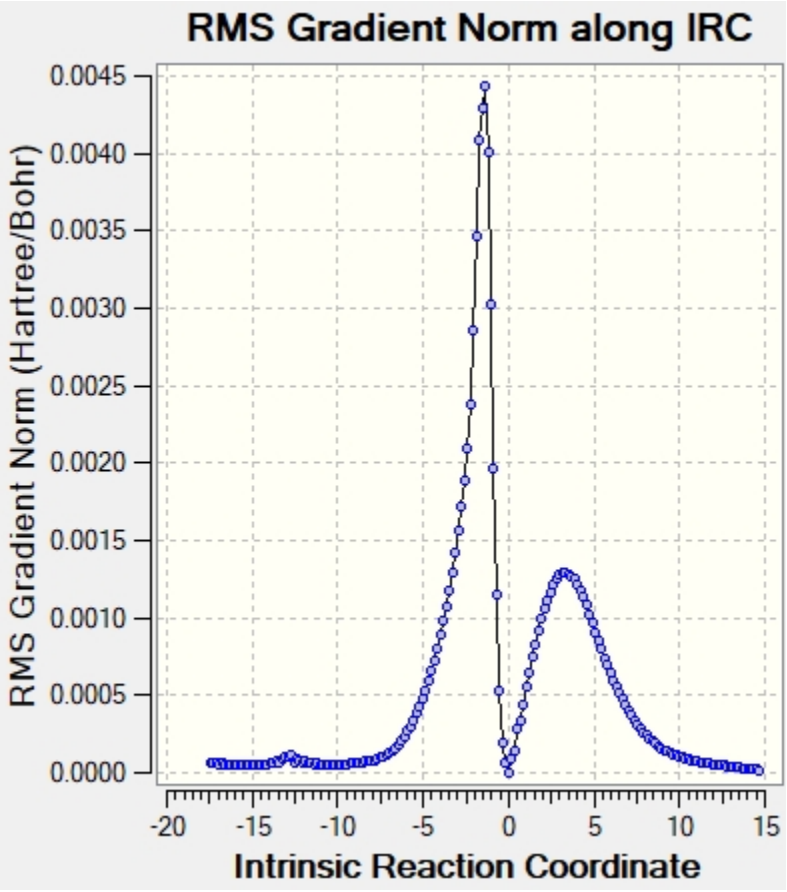
1b.3MeOH-ts

Zero-point correction=	0.368665
(Hartree/Particle)	
Thermal correction to Energy=	0.391158
Thermal correction to Enthalpy=	0.392103
Thermal correction to Gibbs Free Energy=	0.315655
Sum of electronic and zero-point Energies=	-919.475275
Sum of electronic and thermal Energies=	-919.452782
Sum of electronic and thermal Enthalpies=	-919.451838
Sum of electronic and thermal Free Energies=	-919.528286

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.153499	-0.471536	-0.842716
2	7	0	3.131286	-0.911218	0.017210
3	8	0	2.419471	-0.187573	-2.019564
4	6	0	-1.477749	-0.636924	-0.802827
5	6	0	-3.986708	-1.721087	-0.190075
6	6	0	-2.633045	-0.142420	-1.418680
7	6	0	-1.589822	-1.689367	0.106184
8	6	0	-2.839006	-2.227396	0.414021
9	6	0	-3.879481	-0.678252	-1.110669
10	1	0	-2.551349	0.669459	-2.134581
11	1	0	-0.685834	-2.086106	0.557357
12	1	0	-2.912777	-3.046296	1.123449
13	1	0	-4.769462	-0.282955	-1.590524
14	1	0	-4.959726	-2.139871	0.047909
15	6	0	-0.111858	-0.100266	-1.166081
16	1	0	0.151616	-0.270383	-2.214986
17	8	0	-0.402568	1.494015	-1.254888
18	8	0	-1.125429	2.154092	0.972460
19	6	0	-0.835558	3.485494	1.377992
20	1	0	0.245372	3.656759	1.438107
21	1	0	-1.285594	3.682046	2.354794
22	1	0	-1.271187	4.171308	0.647797
23	6	0	0.768291	2.269273	-1.559780
24	1	0	0.452365	3.312124	-1.630327
25	1	0	1.179435	1.913168	-2.502978
26	1	0	1.517366	2.142831	-0.772663
27	7	0	0.893603	-0.386400	-0.276694
28	1	0	-0.782025	1.815689	-0.276908
29	8	0	0.297232	0.456409	2.067424
30	1	0	-0.590011	1.468413	1.548144
31	6	0	-0.238530	-0.463438	2.999447
32	1	0	0.354762	-1.385421	3.016068
33	1	0	-1.278599	-0.719283	2.762065
34	1	0	-0.200744	-0.014017	3.995686
35	1	0	0.590995	0.001691	1.154823
36	6	0	4.515582	-0.910631	-0.407299
37	1	0	5.123938	-0.291577	0.264135
38	1	0	4.568855	-0.510445	-1.418159
39	1	0	4.923679	-1.929042	-0.403695
40	6	0	2.846986	-1.365506	1.363967
41	1	0	3.678937	-1.990828	1.698712
42	1	0	1.937240	-1.971128	1.375420
43	1	0	2.723279	-0.536000	2.072389

1b.3MeOH-ts IRC





2.4.2 M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

IMINE 1b

```
 Zero-point correction=                           0.206733
(Hartree/Particle)
 Thermal correction to Energy=                    0.218020
 Thermal correction to Enthalpy=                  0.218964
 Thermal correction to Gibbs Free Energy=         0.167209
 Sum of electronic and zero-point Energies=           -572.602520
 Sum of electronic and thermal Energies=              -572.591233
 Sum of electronic and thermal Enthalpies=            -572.590289
 Sum of electronic and thermal Free Energies=         -572.642044
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.734568	-0.277717	0.000000
2	6	0	2.141882	-0.026226	0.000000
3	6	0	0.000000	0.769199	0.000000
4	7	0	2.876522	-1.156713	0.000000
5	8	0	2.651705	1.096527	0.000000
6	1	0	0.451202	1.768782	0.000000
7	6	0	-1.466207	0.699895	0.000000
8	6	0	-4.255695	0.638249	0.000000
9	6	0	-2.197319	1.893353	0.000000
10	6	0	-2.141118	-0.529390	0.000000
11	6	0	-3.529938	-0.557637	0.000000
12	6	0	-3.590533	1.863108	0.000000
13	1	0	-1.670438	2.844091	0.000000
14	1	0	-1.561899	-1.447299	0.000000
15	1	0	-4.053321	-1.508418	0.000000
16	1	0	-4.154228	2.790245	0.000000
17	1	0	-5.340959	0.611711	0.000000
18	6	0	4.325149	-0.996547	0.000000
19	1	0	4.791440	-1.980321	0.000000
20	1	0	4.650299	-0.443246	0.885520
21	1	0	4.650299	-0.443246	-0.885520
22	6	0	2.273520	-2.489584	0.000000
23	1	0	3.077281	-3.224730	0.000000
24	1	0	1.655305	-2.642641	-0.886857
25	1	0	1.655305	-2.642641	0.886857

1b.MeOH-ts

```
 Zero-point correction=                           0.258486
(Hartree/Particle)
 Thermal correction to Energy=                    0.273982
 Thermal correction to Enthalpy=                  0.274926
 Thermal correction to Gibbs Free Energy=         0.214099
 Sum of electronic and zero-point Energies=           -688.178286
 Sum of electronic and thermal Energies=              -688.162790
 Sum of electronic and thermal Enthalpies=            -688.161846
 Sum of electronic and thermal Free Energies=         -688.222674
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.951541	0.125349	0.187737
2	6	0	-2.038620	-0.368775	-0.486159
3	7	0	-3.174382	-0.506668	0.280920
4	8	0	-2.028742	-0.719219	-1.681948
5	6	0	1.492654	-0.132067	-0.249689
6	6	0	3.993084	-1.185178	0.408827
7	6	0	2.553295	-0.042575	-1.155325
8	6	0	1.684467	-0.760810	0.983142
9	6	0	2.933170	-1.283149	1.312022
10	6	0	3.802240	-0.566969	-0.827201
11	1	0	2.398573	0.433958	-2.120615
12	1	0	0.844216	-0.840261	1.665794
13	1	0	3.079519	-1.771665	2.270255
14	1	0	4.621670	-0.498653	-1.535613
15	1	0	4.964367	-1.597317	0.664711
16	6	0	0.162474	0.457405	-0.612197
17	1	0	-0.011956	0.477385	-1.690388
18	8	0	0.111856	1.976961	-0.185667
19	6	0	-4.433647	-0.791864	-0.380532
20	1	0	-4.240062	-1.334074	-1.303752
21	1	0	-4.982191	0.130708	-0.619045
22	1	0	-5.057532	-1.404318	0.276448
23	6	0	-3.267906	0.081700	1.604248
24	1	0	-2.331852	-0.059033	2.142669
25	1	0	-4.072376	-0.417010	2.150652
26	1	0	-3.493577	1.157413	1.562157
27	6	0	1.235807	2.647701	0.418395
28	1	0	1.591385	2.095221	1.289566
29	1	0	0.881651	3.637725	0.701500
30	1	0	2.023172	2.727503	-0.330899
31	1	0	-0.700560	1.537201	0.443704

1b.MeOH-pf

```
 Zero-point correction=                           0.264319
(Hartree/Particle)
 Thermal correction to Energy=                    0.279977
 Thermal correction to Enthalpy=                  0.280921
 Thermal correction to Gibbs Free Energy=         0.219457
 Sum of electronic and zero-point Energies=           -688.251117
 Sum of electronic and thermal Energies=              -688.235459
 Sum of electronic and thermal Enthalpies=            -688.234515
 Sum of electronic and thermal Free Energies=         -688.295979
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.825894	-0.221990	-0.019657
2	6	0	2.129762	0.076731	0.346975
3	7	0	3.080380	-0.787826	-0.107061
4	8	0	2.381853	1.039295	1.077222
5	6	0	-1.563142	0.061143	0.168254
6	6	0	-4.012458	-1.277734	0.014995
7	6	0	-2.087621	-0.576132	1.294355
8	6	0	-2.272051	0.032169	-1.033715
9	6	0	-3.493746	-0.637391	-1.109884
10	6	0	-3.307831	-1.244766	1.219580
11	1	0	-1.535886	-0.549119	2.231085
12	1	0	-1.867179	0.544953	-1.901766
13	1	0	-4.042100	-0.655184	-2.046768
14	1	0	-3.711089	-1.735458	2.100000
15	1	0	-4.964910	-1.795311	-0.044372
16	6	0	-0.205860	0.740658	0.248802
17	1	0	-0.036155	1.130055	1.260508
18	8	0	-0.092110	1.802609	-0.680671
19	6	0	4.485473	-0.491732	0.120124
20	1	0	4.995795	-0.310470	-0.832330
21	1	0	4.970417	-1.332697	0.625334
22	1	0	4.561632	0.395755	0.744435
23	6	0	2.768703	-1.931558	-0.949697
24	1	0	2.529162	-1.636790	-1.979324
25	1	0	1.941021	-2.512521	-0.533938
26	1	0	3.644413	-2.580767	-0.979293
27	6	0	-0.772001	2.971537	-0.258497
28	1	0	-0.612413	3.729312	-1.025781
29	1	0	-0.366226	3.330235	0.696327
30	1	0	-1.849231	2.792301	-0.147190
31	1	0	0.665516	-0.818365	-0.820056

1b.2MeOH-ts

Zero-point correction=	0.312444
(Hartree/Particle)	
Thermal correction to Energy=	0.331313
Thermal correction to Enthalpy=	0.332257
Thermal correction to Gibbs Free Energy=	0.263924
Sum of electronic and zero-point Energies=	-803.838991
Sum of electronic and thermal Energies=	-803.820123
Sum of electronic and thermal Enthalpies=	-803.819179
Sum of electronic and thermal Free Energies=	-803.887512

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.885526	-0.212793	-0.257808
2	6	0	2.054908	-0.930205	-0.166875
3	7	0	3.132239	-0.340579	-0.791477
4	8	0	2.174381	-2.040337	0.385328
5	6	0	-1.539209	-0.538766	-0.247391
6	6	0	-4.058392	-0.101365	-1.390315
7	6	0	-2.590214	-1.429159	-0.009818
8	6	0	-1.753387	0.559597	-1.085025
9	6	0	-3.008426	0.781850	-1.647603
10	6	0	-3.845492	-1.212964	-0.576601
11	1	0	-2.423564	-2.302818	0.616015
12	1	0	-0.924063	1.219863	-1.319220
13	1	0	-3.164691	1.636401	-2.298801
14	1	0	-4.651742	-1.914830	-0.388524
15	1	0	-5.033896	0.068468	-1.835315
16	6	0	-0.198508	-0.786208	0.392537
17	1	0	-0.059582	-1.830059	0.686086
18	8	0	-0.235616	-0.082274	1.831040
19	1	0	0.105482	0.968440	1.635234
20	1	0	0.913531	1.211961	0.240646
21	8	0	0.731754	1.929136	1.013228
22	6	0	4.460532	-0.880045	-0.571245
23	1	0	4.377928	-1.921418	-0.267648
24	1	0	4.994963	-0.321579	0.210244
25	1	0	5.039709	-0.816515	-1.497360
26	6	0	3.076172	1.011030	-1.318692
27	1	0	3.231895	1.767668	-0.536180
28	1	0	2.113699	1.189948	-1.797806
29	1	0	3.865062	1.125320	-2.066569
30	6	0	0.030532	3.099644	0.597772
31	1	0	-1.040734	2.900248	0.486348
32	1	0	0.432801	3.451233	-0.356011
33	1	0	0.176979	3.873239	1.353000
34	6	0	-1.378235	-0.243283	2.680279
35	1	0	-1.130896	0.218155	3.636476
36	1	0	-1.551798	-1.311231	2.822588
37	1	0	-2.261268	0.228171	2.242891

1b.3MeOH-ts

Zero-point correction= (Hartree/Particle)	0.369517
Thermal correction to Energy=	0.392271
Thermal correction to Enthalpy=	0.393215
Thermal correction to Gibbs Free Energy=	0.316408
Sum of electronic and zero-point Energies=	-919.486606
Sum of electronic and thermal Energies=	-919.463851
Sum of electronic and thermal Enthalpies=	-919.462907
Sum of electronic and thermal Free Energies=	-919.539714

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.195634	-0.546098	-0.801870
2	7	0	3.185983	-0.814104	0.107430
3	8	0	2.459733	-0.437772	-2.016090
4	6	0	-1.428545	-0.799333	-0.734301
5	6	0	-3.929965	-1.806818	0.020719
6	6	0	-2.570389	-0.495130	-1.485367
7	6	0	-1.547035	-1.627646	0.382012
8	6	0	-2.793858	-2.126263	0.761478
9	6	0	-3.814277	-0.992729	-1.107981
10	1	0	-2.481535	0.141266	-2.361080
11	1	0	-0.652775	-1.886507	0.939832
12	1	0	-2.873736	-2.768005	1.633832
13	1	0	-4.694116	-0.746424	-1.694152
14	1	0	-4.900148	-2.194535	0.315741
15	6	0	-0.075337	-0.284540	-1.160009
16	1	0	0.180132	-0.537273	-2.193089
17	8	0	-0.429650	1.312369	-1.427267
18	8	0	-1.338128	2.159526	0.692611
19	6	0	-1.229114	3.564958	0.920806
20	1	0	-0.180763	3.879934	0.944677
21	1	0	-1.708822	3.825950	1.867194
22	1	0	-1.743375	4.079254	0.107422
23	6	0	0.723557	2.112572	-1.735063
24	1	0	0.379720	3.138765	-1.873491
25	1	0	1.168796	1.723817	-2.649224
26	1	0	1.448078	2.057345	-0.917459
27	7	0	0.935139	-0.427563	-0.253171
28	1	0	-0.880558	1.699226	-0.534325
29	8	0	0.311792	0.770706	2.002988
30	1	0	-0.741771	1.646484	1.341969
31	6	0	-0.111895	-0.017283	3.104635
32	1	0	0.613972	-0.809650	3.318148
33	1	0	-1.092181	-0.472507	2.920325
34	1	0	-0.182908	0.631573	3.980435
35	1	0	0.604671	0.199601	1.197454
36	6	0	4.576891	-0.816818	-0.301278
37	1	0	5.153399	-0.117440	0.315500
38	1	0	4.641171	-0.515171	-1.344396
39	1	0	5.014836	-1.816019	-0.189555
40	6	0	2.917884	-1.072713	1.510496
41	1	0	3.751025	-1.649733	1.919523
42	1	0	2.004748	-1.661369	1.618105
43	1	0	2.813016	-0.148480	2.093195

2.4.3 M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

IMINE 1b

```
 Zero-point correction=                           0.207191
(Hartree/Particle)
 Thermal correction to Energy=                    0.219957
 Thermal correction to Enthalpy=                  0.220901
 Thermal correction to Gibbs Free Energy=         0.165315
 Sum of electronic and zero-point Energies=           -572.605294
 Sum of electronic and thermal Energies=              -572.592528
 Sum of electronic and thermal Enthalpies=            -572.591584
 Sum of electronic and thermal Free Energies=         -572.647170
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.773180	0.073012	-0.194711
2	6	0	2.066104	-0.528790	-0.177628
3	6	0	-0.198338	-0.724808	0.037306
4	7	0	3.071620	0.354268	0.014994
5	8	0	2.251058	-1.734472	-0.362546
6	1	0	-0.014336	-1.783295	0.256501
7	6	0	-1.598854	-0.284574	0.020385
8	6	0	-4.281766	0.483689	0.001050
9	6	0	-2.602426	-1.223638	0.284557
10	6	0	-1.946258	1.046538	-0.253208
11	6	0	-3.282567	1.426584	-0.262763
12	6	0	-3.942291	-0.840624	0.274231
13	1	0	-2.330724	-2.254287	0.497685
14	1	0	-1.159137	1.766640	-0.453666
15	1	0	-3.551217	2.456466	-0.475106
16	1	0	-4.717537	-1.572033	0.477702
17	1	0	-5.324749	0.784803	-0.007069
18	6	0	4.441333	-0.128442	0.078643
19	1	0	5.086609	0.554530	-0.480452
20	1	0	4.497910	-1.124099	-0.355398
21	1	0	4.788145	-0.165018	1.117962
22	6	0	2.887221	1.755262	0.366498
23	1	0	3.151954	1.917629	1.417512
24	1	0	1.853626	2.047876	0.204877
25	1	0	3.544444	2.368424	-0.256575

1b.MeOH-ts

Zero-point correction=	0.258091
(Hartree/Particle)	
Thermal correction to Energy=	0.273804
Thermal correction to Enthalpy=	0.274748
Thermal correction to Gibbs Free Energy=	0.212786
Sum of electronic and zero-point Energies=	-688.181187
Sum of electronic and thermal Energies=	-688.165475
Sum of electronic and thermal Enthalpies=	-688.164530
Sum of electronic and thermal Free Energies=	-688.226492

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.954800	0.145708	0.181520
2	6	0	-2.029591	-0.398186	-0.466713
3	7	0	-3.170102	-0.502139	0.298692
4	8	0	-2.006579	-0.822083	-1.640834
5	6	0	1.491804	-0.131082	-0.242135
6	6	0	3.984185	-1.182517	0.450115
7	6	0	2.549024	-0.091777	-1.155294
8	6	0	1.683472	-0.707225	1.016464
9	6	0	2.927979	-1.229082	1.361845
10	6	0	3.793996	-0.615463	-0.810395
11	1	0	2.395925	0.347280	-2.138414
12	1	0	0.847503	-0.746226	1.707837
13	1	0	3.073895	-1.676895	2.339820
14	1	0	4.611167	-0.585324	-1.524039
15	1	0	4.952205	-1.593678	0.719478
16	6	0	0.164449	0.453272	-0.625952
17	1	0	-0.005959	0.432908	-1.704841
18	8	0	0.109528	1.976171	-0.253798
19	6	0	-4.424172	-0.827199	-0.355320
20	1	0	-4.223166	-1.421620	-1.244149
21	1	0	-4.971847	0.079231	-0.650439
22	1	0	-5.052688	-1.401668	0.330717
23	6	0	-3.277093	0.172300	1.580449
24	1	0	-2.353583	0.052893	2.145375
25	1	0	-4.099048	-0.278442	2.141897
26	1	0	-3.483337	1.246126	1.464484
27	6	0	1.233145	2.672518	0.324100
28	1	0	1.567102	2.174382	1.235435
29	1	0	0.885125	3.682080	0.535686
30	1	0	2.032522	2.694187	-0.416288
31	1	0	-0.708283	1.563731	0.390021

1b.MeOH-pf

```
 Zero-point correction=                           0.264244
(Hartree/Particle)
 Thermal correction to Energy=                    0.279921
 Thermal correction to Enthalpy=                  0.280865
 Thermal correction to Gibbs Free Energy=         0.219555
 Sum of electronic and zero-point Energies=           -688.253321
 Sum of electronic and thermal Energies=              -688.237644
 Sum of electronic and thermal Enthalpies=            -688.236700
 Sum of electronic and thermal Free Energies=         -688.298010
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.831303	-0.207555	-0.024675
2	6	0	2.134212	0.086819	0.343863
3	7	0	3.081836	-0.784536	-0.099011
4	8	0	2.388494	1.056107	1.067655
5	6	0	-1.558385	0.062132	0.167969
6	6	0	-4.000079	-1.292018	0.024868
7	6	0	-2.096480	-0.539091	1.307266
8	6	0	-2.250071	-0.010038	-1.042548
9	6	0	-3.467852	-0.686875	-1.113611
10	6	0	-3.312970	-1.215788	1.237450
11	1	0	-1.559908	-0.477561	2.251169
12	1	0	-1.835498	0.474260	-1.922311
13	1	0	-4.002329	-0.738381	-2.057246
14	1	0	-3.726728	-1.678386	2.128098
15	1	0	-4.949383	-1.815695	-0.030736
16	6	0	-0.205127	0.749693	0.243765
17	1	0	-0.037517	1.143955	1.254026
18	8	0	-0.098195	1.810348	-0.689443
19	6	0	4.488512	-0.495053	0.129502
20	1	0	5.002049	-0.327974	-0.823604
21	1	0	4.966130	-1.334141	0.644352
22	1	0	4.570097	0.398338	0.744538
23	6	0	2.766702	-1.936767	-0.930086
24	1	0	2.525070	-1.651052	-1.961400
25	1	0	1.939282	-2.512366	-0.506646
26	1	0	3.641809	-2.586650	-0.955364
27	6	0	-0.818203	2.963703	-0.289279
28	1	0	-0.653092	3.724669	-1.052156
29	1	0	-0.451242	3.332340	0.677377
30	1	0	-1.893434	2.759055	-0.210734
31	1	0	0.668776	-0.817724	-0.814227

1b.2MeOH-ts

Zero-point correction=	0.312557
(Hartree/Particle)	
Thermal correction to Energy=	0.331439
Thermal correction to Enthalpy=	0.332384
Thermal correction to Gibbs Free Energy=	0.264014
Sum of electronic and zero-point Energies=	-803.841828
Sum of electronic and thermal Energies=	-803.822946
Sum of electronic and thermal Enthalpies=	-803.822002
Sum of electronic and thermal Free Energies=	-803.890372

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.884780	-0.223312	-0.251593
2	6	0	2.051891	-0.934788	-0.141029
3	7	0	3.126094	-0.373716	-0.798856
4	8	0	2.178671	-2.023859	0.455793
5	6	0	-1.539993	-0.546269	-0.228122
6	6	0	-4.055460	-0.147853	-1.393953
7	6	0	-2.586475	-1.438710	0.021143
8	6	0	-1.756932	0.535038	-1.087344
9	6	0	-3.010101	0.737998	-1.661447
10	6	0	-3.839911	-1.242060	-0.557520
11	1	0	-2.418900	-2.297783	0.666608
12	1	0	-0.932473	1.198875	-1.328558
13	1	0	-3.168432	1.580066	-2.328122
14	1	0	-4.642974	-1.944881	-0.359660
15	1	0	-5.029715	0.007474	-1.846871
16	6	0	-0.200525	-0.771644	0.424968
17	1	0	-0.065954	-1.807547	0.748120
18	8	0	-0.232247	-0.025608	1.828189
19	1	0	0.110079	1.022843	1.603130
20	1	0	0.915664	1.243805	0.206141
21	8	0	0.734753	1.964344	0.962306
22	6	0	4.456607	-0.898988	-0.555126
23	1	0	4.382001	-1.938432	-0.243033
24	1	0	4.976970	-0.328526	0.227399
25	1	0	5.046197	-0.838285	-1.474431
26	6	0	3.069634	0.964840	-1.360487
27	1	0	3.228330	1.740427	-0.597349
28	1	0	2.105963	1.133410	-1.840678
29	1	0	3.856924	1.059885	-2.112442
30	6	0	0.029916	3.129792	0.531172
31	1	0	-1.038503	2.922038	0.413298
32	1	0	0.440425	3.475177	-0.420739
33	1	0	0.166755	3.906853	1.284028
34	6	0	-1.373940	-0.164939	2.685405
35	1	0	-1.124783	0.327350	3.625237
36	1	0	-1.543563	-1.228558	2.859980
37	1	0	-2.257808	0.291479	2.234813

1b.3MeOH-ts

Zero-point correction=	0.368843
(Hartree/Particle)	
Thermal correction to Energy=	0.391929
Thermal correction to Enthalpy=	0.392873
Thermal correction to Gibbs Free Energy=	0.314530
Sum of electronic and zero-point Energies=	-919.489567
Sum of electronic and thermal Energies=	-919.466481
Sum of electronic and thermal Enthalpies=	-919.465537
Sum of electronic and thermal Free Energies=	-919.543880

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.191817	-0.599570	-0.781476
2	7	0	3.185928	-0.812929	0.137591
3	8	0	2.453968	-0.557925	-2.001607
4	6	0	-1.433432	-0.851215	-0.686688
5	6	0	-3.938587	-1.789234	0.140787
6	6	0	-2.569958	-0.618605	-1.470236
7	6	0	-1.558255	-1.575206	0.499586
8	6	0	-2.807372	-2.038357	0.915146
9	6	0	-3.816217	-1.082404	-1.057794
10	1	0	-2.474770	-0.065011	-2.400027
11	1	0	-0.667984	-1.784896	1.083684
12	1	0	-2.892707	-2.597733	1.841919
13	1	0	-4.692211	-0.892910	-1.670323
14	1	0	-4.910241	-2.150161	0.463408
15	6	0	-0.081304	-0.364643	-1.146282
16	1	0	0.167295	-0.670198	-2.166674
17	8	0	-0.439152	1.218663	-1.497807
18	8	0	-1.352252	2.180381	0.574321
19	6	0	-1.256525	3.599606	0.712305
20	1	0	-0.211510	3.925556	0.701513
21	1	0	-1.726527	3.914386	1.647037
22	1	0	-1.786480	4.055663	-0.125210
23	6	0	0.710813	2.008104	-1.844083
24	1	0	0.363913	3.026662	-2.024085
25	1	0	1.152342	1.582322	-2.743442
26	1	0	1.438348	1.989792	-1.027425
27	7	0	0.932657	-0.457715	-0.238049
28	1	0	-0.893123	1.649808	-0.629980
29	8	0	0.340912	0.897863	1.948325
30	1	0	-0.741671	1.719237	1.245924
31	6	0	-0.044878	0.201786	3.124355
32	1	0	0.713077	-0.537073	3.406420
33	1	0	-1.007525	-0.306215	2.993535
34	1	0	-0.138305	0.929616	3.933122
35	1	0	0.617443	0.268078	1.187153
36	6	0	4.577690	-0.810360	-0.269611
37	1	0	5.140679	-0.077388	0.319892
38	1	0	4.640785	-0.549368	-1.323703
39	1	0	5.031649	-1.796720	-0.116398
40	6	0	2.928116	-0.994474	1.554780
41	1	0	3.747531	-1.577964	1.982320
42	1	0	1.998018	-1.545914	1.701819
43	1	0	2.862632	-0.039479	2.092144

2.4.4 M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

IMINE 1b

```
 Zero-point correction=                           0.206703
(Hartree/Particle)
 Thermal correction to Energy=                    0.217962
 Thermal correction to Enthalpy=                  0.218906
 Thermal correction to Gibbs Free Energy=         0.167899
 Sum of electronic and zero-point Energies=           -572.603974
 Sum of electronic and thermal Energies=              -572.592716
 Sum of electronic and thermal Enthalpies=            -572.591771
 Sum of electronic and thermal Free Energies=         -572.642778
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.735049	-0.277539	0.000000
2	6	0	2.141831	-0.027420	0.000000
3	6	0	0.000000	0.769427	0.000000
4	7	0	2.876163	-1.157009	0.000000
5	8	0	2.651742	1.096766	0.000000
6	1	0	0.450387	1.769296	0.000000
7	6	0	-1.466057	0.700120	0.000000
8	6	0	-4.255714	0.639543	0.000000
9	6	0	-2.196736	1.894164	0.000000
10	6	0	-2.141573	-0.529110	0.000000
11	6	0	-3.530498	-0.556834	0.000000
12	6	0	-3.590004	1.864347	0.000000
13	1	0	-1.669738	2.844816	0.000000
14	1	0	-1.563663	-1.447843	0.000000
15	1	0	-4.054177	-1.507432	0.000000
16	1	0	-4.153326	2.791684	0.000000
17	1	0	-5.340960	0.613392	0.000000
18	6	0	4.325261	-0.998625	0.000000
19	1	0	4.789921	-1.982946	0.000000
20	1	0	4.651041	-0.446147	0.885792
21	1	0	4.651041	-0.446147	-0.885792
22	6	0	2.273271	-2.490488	0.000000
23	1	0	3.077387	-3.224946	0.000000
24	1	0	1.655490	-2.643382	-0.887078
25	1	0	1.655490	-2.643382	0.887078

1b.MeOH-ts

Zero-point correction=	0.258088
(Hartree/Particle)	
Thermal correction to Energy=	0.273806
Thermal correction to Enthalpy=	0.274750
Thermal correction to Gibbs Free Energy=	0.212750
Sum of electronic and zero-point Energies=	-688.181104
Sum of electronic and thermal Energies=	-688.165387
Sum of electronic and thermal Enthalpies=	-688.164442
Sum of electronic and thermal Free Energies=	-688.226442

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.954678	0.144860	0.181761
2	6	0	-2.029994	-0.396791	-0.467712
3	7	0	-3.170263	-0.502389	0.297820
4	8	0	-2.007607	-0.817277	-1.642984
5	6	0	1.491817	-0.131062	-0.242520
6	6	0	3.984460	-1.182889	0.448159
7	6	0	2.549298	-0.089241	-1.155264
8	6	0	1.683340	-0.709971	1.014821
9	6	0	2.927983	-1.232003	1.359436
10	6	0	3.794397	-0.613118	-0.811146
11	1	0	2.396268	0.351845	-2.137488
12	1	0	0.847110	-0.750964	1.705761
13	1	0	3.073797	-1.681937	2.336453
14	1	0	4.611761	-0.581043	-1.524485
15	1	0	4.952589	-1.594205	0.716896
16	6	0	0.164380	0.453728	-0.625308
17	1	0	-0.006168	0.435383	-1.704207
18	8	0	0.109673	1.976288	-0.250367
19	6	0	-4.424613	-0.825497	-0.356581
20	1	0	-4.223983	-1.417433	-1.247152
21	1	0	-4.972343	0.081788	-0.648959
22	1	0	-5.052892	-1.401856	0.328093
23	6	0	-3.276533	0.168009	1.581712
24	1	0	-2.352616	0.046960	2.145620
25	1	0	-4.098039	-0.284622	2.142304
26	1	0	-3.483060	1.242168	1.469273
27	6	0	1.233428	2.671407	0.328639
28	1	0	1.569218	2.169956	1.237484
29	1	0	0.884812	3.679818	0.544726
30	1	0	2.031715	2.696773	-0.412817
31	1	0	-0.707900	1.562547	0.392832

1b.MeOH-pf

Zero-point correction=	0.264245
(Hartree/Particle)	
Thermal correction to Energy=	0.279922
Thermal correction to Enthalpy=	0.280866
Thermal correction to Gibbs Free Energy=	0.219556
Sum of electronic and zero-point Energies=	-688.253249
Sum of electronic and thermal Energies=	-688.237571
Sum of electronic and thermal Enthalpies=	-688.236627
Sum of electronic and thermal Free Energies=	-688.297937

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.831303	-0.207555	-0.024675
2	6	0	2.134212	0.086819	0.343863
3	7	0	3.081836	-0.784536	-0.099011
4	8	0	2.388494	1.056107	1.067655
5	6	0	-1.558385	0.062132	0.167969
6	6	0	-4.000079	-1.292018	0.024868
7	6	0	-2.096480	-0.539091	1.307266
8	6	0	-2.250071	-0.010038	-1.042548
9	6	0	-3.467852	-0.686875	-1.113611
10	6	0	-3.312970	-1.215788	1.237450
11	1	0	-1.559908	-0.477561	2.251169
12	1	0	-1.835498	0.474260	-1.922311
13	1	0	-4.002329	-0.738381	-2.057246
14	1	0	-3.726728	-1.678386	2.128098
15	1	0	-4.949383	-1.815695	-0.030736
16	6	0	-0.205127	0.749693	0.243765
17	1	0	-0.037517	1.143955	1.254026
18	8	0	-0.098195	1.810348	-0.689443
19	6	0	4.488512	-0.495053	0.129502
20	1	0	5.002049	-0.327974	-0.823604
21	1	0	4.966130	-1.334141	0.644352
22	1	0	4.570097	0.398338	0.744538
23	6	0	2.766702	-1.936767	-0.930086
24	1	0	2.525070	-1.651052	-1.961400
25	1	0	1.939282	-2.512366	-0.506646
26	1	0	3.641809	-2.586650	-0.955364
27	6	0	-0.818203	2.963703	-0.289279
28	1	0	-0.653092	3.724669	-1.052156
29	1	0	-0.451242	3.332340	0.677377
30	1	0	-1.893434	2.759055	-0.210734
31	1	0	0.668776	-0.817724	-0.814227

1b.2MeOH-ts

Zero-point correction=	0.312557
(Hartree/Particle)	
Thermal correction to Energy=	0.331438
Thermal correction to Enthalpy=	0.332383
Thermal correction to Gibbs Free Energy=	0.264022
Sum of electronic and zero-point Energies=	-803.841726
Sum of electronic and thermal Energies=	-803.822845
Sum of electronic and thermal Enthalpies=	-803.821901
Sum of electronic and thermal Free Energies=	-803.890261

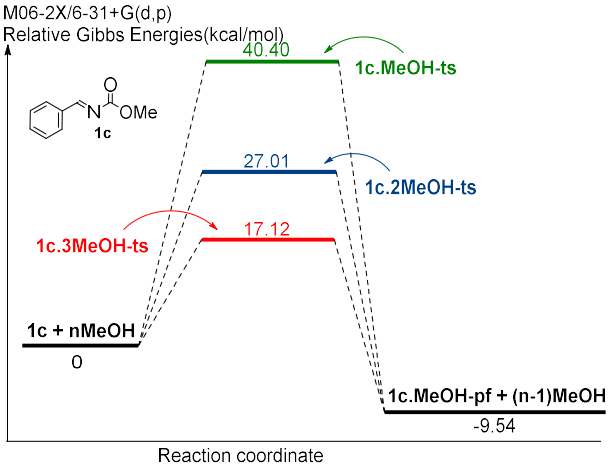
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.884840	-0.223071	-0.251435
2	6	0	2.051947	-0.934830	-0.141223
3	7	0	3.126289	-0.373224	-0.798290
4	8	0	2.178384	-2.024355	0.454656
5	6	0	-1.539928	-0.546228	-0.228309
6	6	0	-4.055437	-0.147497	-1.393924
7	6	0	-2.586487	-1.438564	0.020999
8	6	0	-1.756804	0.535098	-1.087514
9	6	0	-3.009994	0.738219	-1.661504
10	6	0	-3.839944	-1.241754	-0.557546
11	1	0	-2.418922	-2.297715	0.666362
12	1	0	-0.932223	1.198746	-1.328822
13	1	0	-3.168270	1.580273	-2.328211
14	1	0	-4.643060	-1.944515	-0.359682
15	1	0	-5.029703	0.007932	-1.846786
16	6	0	-0.200451	-0.771756	0.424627
17	1	0	-0.065711	-1.807669	0.747641
18	8	0	-0.232491	-0.025943	1.828436
19	1	0	0.109904	1.022332	1.603589
20	1	0	0.915694	1.243003	0.206584
21	8	0	0.734739	1.964036	0.962690
22	6	0	4.456680	-0.899031	-0.555191
23	1	0	4.381662	-1.938304	-0.242631
24	1	0	4.977732	-0.328508	0.226826
25	1	0	5.045800	-0.838993	-1.474855
26	6	0	3.069954	0.965455	-1.359556
27	1	0	3.228754	1.740848	-0.596243
28	1	0	2.106291	1.134206	-1.839708
29	1	0	3.857224	1.060600	-2.111532
30	6	0	0.029996	3.129278	0.531123
31	1	0	-1.038472	2.921611	0.413347
32	1	0	0.440423	3.474290	-0.420981
33	1	0	0.166889	3.906738	1.283579
34	6	0	-1.374393	-0.165128	2.685308
35	1	0	-1.125412	0.326939	3.625315
36	1	0	-1.544302	-1.228733	2.859712
37	1	0	-2.258092	0.291505	2.234573

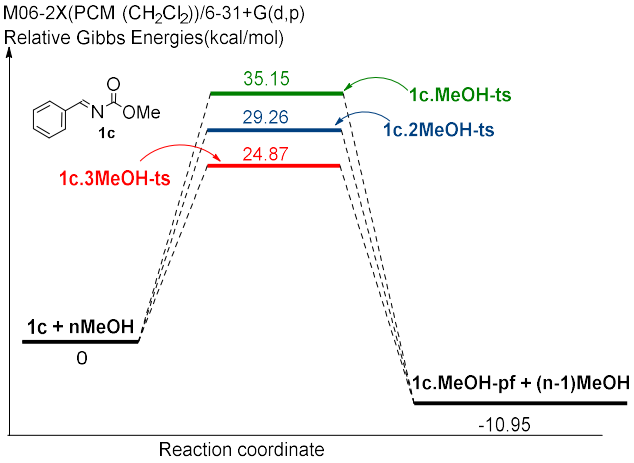
1b.3MeOH-ts

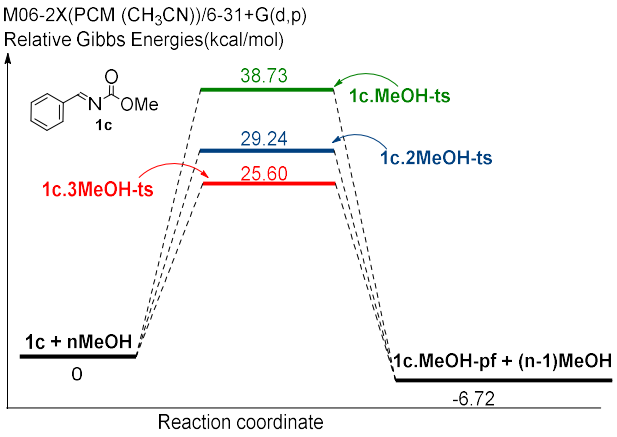
Zero-point correction=	0.368870
(Hartree/Particle)	
Thermal correction to Energy=	0.391940
Thermal correction to Enthalpy=	0.392884
Thermal correction to Gibbs Free Energy=	0.314644
Sum of electronic and zero-point Energies=	-919.489461
Sum of electronic and thermal Energies=	-919.466391
Sum of electronic and thermal Enthalpies=	-919.465447
Sum of electronic and thermal Free Energies=	-919.543687

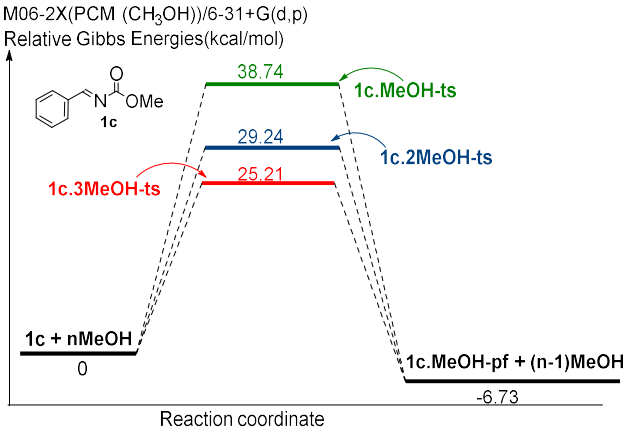
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.191859	-0.597971	-0.782162
2	7	0	3.185884	-0.812971	0.136639
3	8	0	2.454038	-0.554377	-2.002182
4	6	0	-1.433322	-0.849738	-0.688160
5	6	0	-3.938408	-1.789673	0.137366
6	6	0	-2.569926	-0.615358	-1.471072
7	6	0	-1.558039	-1.576454	0.496444
8	6	0	-2.807115	-2.040571	0.911041
9	6	0	-3.816134	-1.080117	-1.059599
10	1	0	-2.474855	-0.059591	-2.399578
11	1	0	-0.667696	-1.787400	1.079978
12	1	0	-2.892344	-2.602084	1.836536
13	1	0	-4.692184	-0.889189	-1.671600
14	1	0	-4.910039	-2.151310	0.459268
15	6	0	-0.081195	-0.362153	-1.146772
16	1	0	0.167660	-0.666240	-2.167537
17	8	0	-0.438970	1.221372	-1.495651
18	8	0	-1.351822	2.180028	0.577782
19	6	0	-1.254986	3.598880	0.718458
20	1	0	-0.209650	3.923877	0.710047
21	1	0	-1.726301	3.912419	1.652950
22	1	0	-1.783116	4.056974	-0.119104
23	6	0	0.711041	2.011332	-1.840627
24	1	0	0.364068	3.030054	-2.019561
25	1	0	1.152923	1.586649	-2.740323
26	1	0	1.438319	1.992121	-1.023770
27	7	0	0.932712	-0.456712	-0.238506
28	1	0	-0.893002	1.651131	-0.626982
29	8	0	0.340018	0.894294	1.949964
30	1	0	-0.741931	1.716995	1.248824
31	6	0	-0.046655	0.195199	3.123882
32	1	0	0.710243	-0.545693	3.403497
33	1	0	-1.010060	-0.310979	2.991609
34	1	0	-0.138845	0.920630	3.934968
35	1	0	0.617214	0.266271	1.187348
36	6	0	4.577596	-0.810809	-0.270682
37	1	0	5.141206	-0.079045	0.319738
38	1	0	4.640702	-0.548455	-1.324437
39	1	0	5.030886	-1.797691	-0.118879
40	6	0	2.927639	-0.997272	1.553390
41	1	0	3.747916	-1.579918	1.980409
42	1	0	1.998490	-1.550747	1.699017
43	1	0	2.859988	-0.043314	2.092306

2.5.-Energy profiles for the addition of n methanol (2a) molecules (n=1-3) to imine derivative 1c in gas phase, CH_2Cl_2, CH_3CN and CH_3OH.









2.6.-Computacional data for the addition of n methanol (2a) molecules (n=1-3) to imine derivative 1c

2.6.1 M06-2X/6-31+G(d,p) calculations

IMINE 1c

```
 Zero-point correction=                           0.167279
(Hartree/Particle)
 Thermal correction to Energy=                    0.178016
 Thermal correction to Enthalpy=                  0.178961
 Thermal correction to Gibbs Free Energy=         0.129302
 Sum of electronic and zero-point Energies=           -553.201074
 Sum of electronic and thermal Energies=              -553.190337
 Sum of electronic and thermal Enthalpies=            -553.189393
 Sum of electronic and thermal Free Energies=         -553.239051
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.029746	-0.333860	-0.077834
2	6	0	-2.349802	0.172967	-0.090134
3	6	0	-0.119713	0.559754	0.017399
4	8	0	-3.206725	-0.820688	0.148877
5	8	0	-2.686240	1.317989	-0.297995
6	1	0	-0.381680	1.622577	0.100612
7	6	0	1.306219	0.218063	0.015034
8	6	0	4.027224	-0.382611	0.013366
9	6	0	2.252414	1.242934	0.118886
10	6	0	1.728334	-1.114347	-0.089095
11	6	0	3.084943	-1.410070	-0.090555
12	6	0	3.612592	0.943417	0.118265
13	1	0	1.918209	2.274391	0.199303
14	1	0	0.977107	-1.893836	-0.167054
15	1	0	3.415108	-2.440782	-0.171263
16	1	0	4.345142	1.739799	0.199803
17	1	0	5.086917	-0.618988	0.012865
18	6	0	-4.582496	-0.439457	0.163147
19	1	0	-5.136016	-1.350702	0.381679
20	1	0	-4.872290	-0.033204	-0.808405
21	1	0	-4.758842	0.315461	0.932370

1c.MeOH-ts

Zero-point correction=	0.218939
(Hartree/Particle)	
Thermal correction to Energy=	0.232409
Thermal correction to Enthalpy=	0.233353
Thermal correction to Gibbs Free Energy=	0.177761
Sum of electronic and zero-point Energies=	-668.776028
Sum of electronic and thermal Energies=	-668.762559
Sum of electronic and thermal Enthalpies=	-668.761615
Sum of electronic and thermal Free Energies=	-668.817207

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.168746	0.057859	-0.408897
2	6	0	2.335412	-0.312390	0.198099
3	8	0	2.503999	-0.588566	1.377362
4	6	0	-1.222194	-0.142732	0.233401
5	6	0	-3.786704	-1.152101	-0.191355
6	6	0	-2.224617	0.063834	1.184847
7	6	0	-1.501206	-0.870756	-0.925353
8	6	0	-2.783682	-1.371206	-1.136429
9	6	0	-3.506594	-0.437461	0.972998
10	1	0	-1.995007	0.610936	2.096746
11	1	0	-0.697287	-1.043388	-1.634574
12	1	0	-3.000834	-1.940764	-2.034619
13	1	0	-4.281224	-0.280771	1.716823
14	1	0	-4.783418	-1.549705	-0.356181
15	6	0	0.142157	0.421643	0.465281
16	1	0	0.406818	0.518224	1.521940
17	8	0	0.156775	1.965790	-0.064058
18	6	0	-0.996727	2.587801	-0.647516
19	1	0	-1.396939	1.981027	-1.463340
20	1	0	-0.675180	3.563872	-1.011595
21	1	0	-1.751431	2.708886	0.130428
22	1	0	0.895184	1.451732	-0.723903
23	8	0	3.343018	-0.362261	-0.703621
24	6	0	4.597470	-0.773219	-0.171676
25	1	0	5.284330	-0.787730	-1.017312
26	1	0	4.519380	-1.766729	0.276152
27	1	0	4.944156	-0.070791	0.590456

1c.MeOH-pf

```
 Zero-point correction=                           0.224740
(Hartree/Particle)
 Thermal correction to Energy=                    0.238459
 Thermal correction to Enthalpy=                  0.239403
 Thermal correction to Gibbs Free Energy=         0.182708
 Sum of electronic and zero-point Energies=           -668.854771
 Sum of electronic and thermal Energies=              -668.841052
 Sum of electronic and thermal Enthalpies=            -668.840108
 Sum of electronic and thermal Free Energies=         -668.896803
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.009604	-0.398415	-0.261611
2	6	0	2.327198	-0.310403	0.097453
3	8	0	3.090103	-1.055327	-0.726656
4	8	0	2.753056	0.315573	1.043839
5	6	0	-1.340826	-0.012252	0.136802
6	6	0	-3.897925	-1.094210	-0.171035
7	6	0	-1.815031	-0.963560	1.042123
8	6	0	-2.151073	0.397714	-0.921292
9	6	0	-3.427870	-0.143674	-1.074427
10	6	0	-3.089047	-1.503618	0.889819
11	1	0	-1.179490	-1.282398	1.864956
12	1	0	-1.776052	1.144713	-1.615072
13	1	0	-4.055256	0.179007	-1.899604
14	1	0	-3.453176	-2.240858	1.598585
15	1	0	-4.892201	-1.513527	-0.289359
16	6	0	0.068603	0.535872	0.288295
17	1	0	0.320377	0.653613	1.351697
18	8	0	0.230360	1.776028	-0.366233
19	6	0	-0.271398	2.863629	0.384759
20	1	0	-0.069148	3.766455	-0.192290
21	1	0	0.240194	2.931812	1.353980
22	1	0	-1.353508	2.775258	0.551911
23	1	0	0.799642	-0.821035	-1.155889
24	6	0	4.479768	-1.074808	-0.399071
25	1	0	4.947159	-1.707842	-1.151486
26	1	0	4.629145	-1.489970	0.599697
27	1	0	4.892540	-0.064654	-0.434010

1c.2MeOH-ts

Zero-point correction= (Hartree/Particle)	0.273315
Thermal correction to Energy=	0.290129
Thermal correction to Enthalpy=	0.291074
Thermal correction to Gibbs Free Energy=	0.227778
Sum of electronic and zero-point Energies=	-784.435542
Sum of electronic and thermal Energies=	-784.418728
Sum of electronic and thermal Enthalpies=	-784.417784
Sum of electronic and thermal Free Energies=	-784.481080

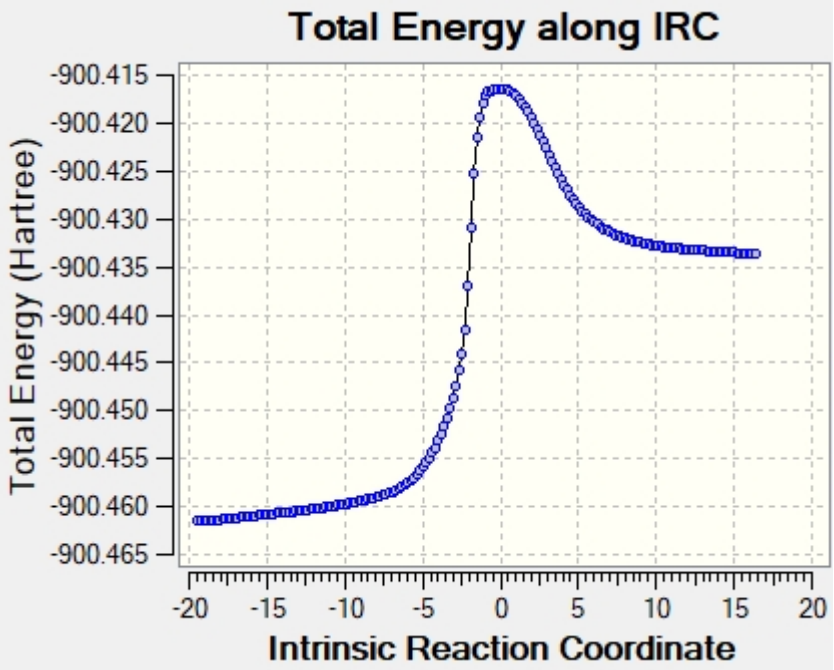
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.086899	-0.181120	-0.348437
2	6	0	2.288162	-0.805167	-0.153520
3	8	0	3.247078	-0.204458	-0.897860
4	8	0	2.529425	-1.774620	0.550344
5	6	0	-1.303352	-0.604670	-0.085821
6	6	0	-3.905904	-0.602304	-1.113287
7	6	0	-2.292595	-1.406064	0.489380
8	6	0	-1.619664	0.174821	-1.201769
9	6	0	-2.917153	0.183179	-1.706714
10	6	0	-3.589571	-1.406665	-0.020028
11	1	0	-2.041871	-2.043487	1.334290
12	1	0	-0.830402	0.738306	-1.689297
13	1	0	-3.154912	0.788110	-2.576316
14	1	0	-4.348293	-2.039231	0.429900
15	1	0	-4.914823	-0.601499	-1.513979
16	6	0	0.083767	-0.602943	0.489416
17	1	0	0.311804	-1.491449	1.085151
18	8	0	0.057439	0.533790	1.690790
19	1	0	0.334902	1.476906	1.148769
20	1	0	1.080581	1.315820	-0.309123
21	8	0	0.865044	2.223808	0.223442
22	6	0	0.097265	3.176574	-0.497349
23	1	0	-0.971401	2.929338	-0.476559
24	1	0	0.433705	3.212757	-1.537208
25	1	0	0.249029	4.158632	-0.044316
26	6	0	-1.045179	0.611161	2.588955
27	1	0	-0.800963	1.360044	3.344947
28	1	0	-1.166654	-0.360814	3.072495
29	1	0	-1.967966	0.880867	2.066706
30	6	0	4.536986	-0.797011	-0.801554
31	1	0	5.182411	-0.203539	-1.448348
32	1	0	4.509550	-1.836483	-1.137269
33	1	0	4.898551	-0.770062	0.229216

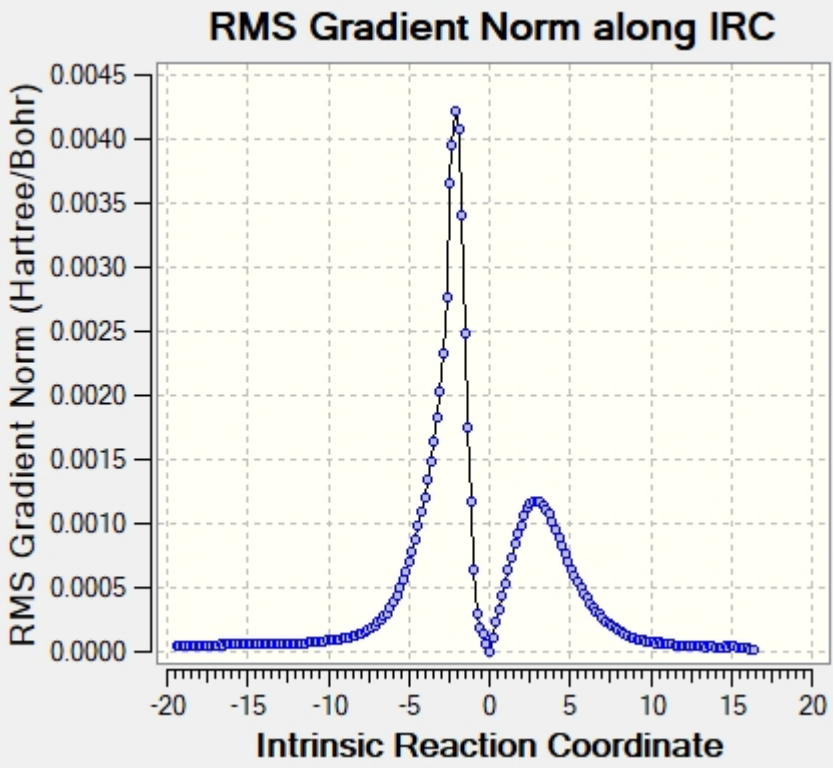
1c.3MeOH-ts

Zero-point correction=	0.329081
(Hartree/Particle)	
Thermal correction to Energy=	0.350257
Thermal correction to Enthalpy=	0.351201
Thermal correction to Gibbs Free Energy=	0.277018
Sum of electronic and zero-point Energies=	-900.087323
Sum of electronic and thermal Energies=	-900.066147
Sum of electronic and thermal Enthalpies=	-900.065203
Sum of electronic and thermal Free Energies=	-900.139386

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.287579	-0.942595	-0.258932
2	8	0	3.124632	-0.766958	0.791500
3	8	0	2.685355	-1.376717	-1.333073
4	6	0	-1.332402	-0.955605	-0.410186
5	6	0	-3.949686	-1.415524	0.455964
6	6	0	-2.393039	-0.921192	-1.321176
7	6	0	-1.588054	-1.239188	0.931385
8	6	0	-2.894397	-1.464253	1.363363
9	6	0	-3.696004	-1.147457	-0.889894
10	1	0	-2.191862	-0.704543	-2.366486
11	1	0	-0.752833	-1.297695	1.621440
12	1	0	-3.085853	-1.684652	2.409227
13	1	0	-4.514427	-1.115571	-1.602345
14	1	0	-4.966543	-1.592575	0.792762
15	6	0	0.079396	-0.731850	-0.881488
16	1	0	0.371731	-1.357699	-1.730783
17	8	0	-0.118889	0.693907	-1.746434
18	8	0	-0.964911	2.275458	-0.069451
19	6	0	-0.709443	3.654496	-0.301896
20	1	0	0.363984	3.872187	-0.260703
21	1	0	-1.228418	4.262573	0.444191
22	1	0	-1.094769	3.911355	-1.291351
23	6	0	1.128173	1.227527	-2.210941
24	1	0	0.907132	2.125625	-2.791268
25	1	0	1.611447	0.473511	-2.832576
26	1	0	1.774661	1.471926	-1.361802
27	7	0	1.020619	-0.572973	0.088119
28	1	0	-0.547608	1.395886	-1.052258
29	8	0	0.488450	1.355509	1.743246
30	1	0	-0.474131	1.964544	0.777844
31	6	0	0.168883	0.970094	3.066618
32	1	0	0.773711	0.106803	3.365068
33	1	0	-0.893628	0.710605	3.162067
34	1	0	0.392241	1.800944	3.741007
35	1	0	0.770515	0.535927	1.184036
36	6	0	4.477072	-1.139409	0.552875
37	1	0	5.005405	-0.941901	1.485067
38	1	0	4.904199	-0.548389	-0.261251
39	1	0	4.545144	-2.197907	0.290827

1c.3MeOH-ts IRC





2.6.2 M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

IMINE 1c

```
 Zero-point correction=                           0.167056
(Hartree/Particle)
 Thermal correction to Energy=                    0.177803
 Thermal correction to Enthalpy=                  0.178747
 Thermal correction to Gibbs Free Energy=         0.129144
 Sum of electronic and zero-point Energies=           -553.209863
 Sum of electronic and thermal Energies=              -553.199116
 Sum of electronic and thermal Enthalpies=            -553.198171
 Sum of electronic and thermal Free Energies=         -553.247775
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.034929	-0.337351	-0.096520
2	6	0	-2.350947	0.168704	-0.113438
3	6	0	-0.118189	0.550946	0.018827
4	8	0	-3.205208	-0.807236	0.189254
5	8	0	-2.689360	1.303506	-0.382556
6	1	0	-0.374506	1.612152	0.123534
7	6	0	1.305894	0.211021	0.017343
8	6	0	4.030987	-0.372108	0.019265
9	6	0	2.244835	1.240999	0.150452
10	6	0	1.737719	-1.116881	-0.114520
11	6	0	3.096374	-1.404431	-0.113893
12	6	0	3.607075	0.949413	0.151250
13	1	0	1.903695	2.267969	0.252517
14	1	0	0.997520	-1.903969	-0.215399
15	1	0	3.434040	-2.430669	-0.215500
16	1	0	4.334054	1.748031	0.254862
17	1	0	5.092022	-0.601710	0.020301
18	6	0	-4.588036	-0.433612	0.209513
19	1	0	-5.131227	-1.338548	0.472222
20	1	0	-4.893462	-0.072290	-0.773974
21	1	0	-4.755368	0.346024	0.954693

1c.MeOH-ts

Zero-point correction=	0.218204
(Hartree/Particle)	
Thermal correction to Energy=	0.231995
Thermal correction to Enthalpy=	0.232939
Thermal correction to Gibbs Free Energy=	0.175615
Sum of electronic and zero-point Energies=	-668.791066
Sum of electronic and thermal Energies=	-668.777276
Sum of electronic and thermal Enthalpies=	-668.776331
Sum of electronic and thermal Free Energies=	-668.833656

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.203500	0.251495	-0.392789
2	6	0	2.296841	-0.293746	0.181033
3	8	0	2.390308	-0.780565	1.308036
4	6	0	-1.199310	-0.101190	0.214681
5	6	0	-3.684265	-1.284524	-0.243904
6	6	0	-2.193292	-0.048502	1.195589
7	6	0	-1.447681	-0.757960	-0.992910
8	6	0	-2.689682	-1.346427	-1.221344
9	6	0	-3.435420	-0.637296	0.966546
10	1	0	-1.991947	0.449792	2.141066
11	1	0	-0.657942	-0.808849	-1.736018
12	1	0	-2.880470	-1.858434	-2.159172
13	1	0	-4.203868	-0.596200	1.731890
14	1	0	-4.649938	-1.747479	-0.421838
15	6	0	0.122993	0.555563	0.475918
16	1	0	0.366067	0.590942	1.541052
17	8	0	0.100901	2.049427	0.030664
18	6	0	-1.078111	2.663001	-0.533037
19	1	0	-1.430350	2.095317	-1.395355
20	1	0	-0.781574	3.669967	-0.820926
21	1	0	-1.843002	2.698153	0.242192
22	1	0	0.903991	1.643184	-0.638970
23	8	0	3.351627	-0.275870	-0.672988
24	6	0	4.547966	-0.877014	-0.182452
25	1	0	5.278659	-0.775606	-0.983629
26	1	0	4.383339	-1.932141	0.047211
27	1	0	4.899614	-0.364477	0.715593

1c.MeOH-pf

```
 Zero-point correction=                           0.224018
(Hartree/Particle)
 Thermal correction to Energy=                    0.237835
 Thermal correction to Enthalpy=                  0.238779
 Thermal correction to Gibbs Free Energy=         0.181790
 Sum of electronic and zero-point Energies=           -668.864900
 Sum of electronic and thermal Energies=              -668.851084
 Sum of electronic and thermal Enthalpies=            -668.850140
 Sum of electronic and thermal Free Energies=         -668.907129
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.029779	-0.369511	-0.235055
2	6	0	2.344785	-0.281522	0.112249
3	8	0	3.093825	-1.088158	-0.658491
4	8	0	2.786120	0.406627	1.014431
5	6	0	-1.326405	-0.009723	0.144932
6	6	0	-3.864974	-1.134838	-0.159135
7	6	0	-1.877598	-0.782459	1.167903
8	6	0	-2.050611	0.204242	-1.028778
9	6	0	-3.317795	-0.358224	-1.180401
10	6	0	-3.143993	-1.345882	1.016421
11	1	0	-1.314690	-0.943662	2.084257
12	1	0	-1.622597	0.821502	-1.813809
13	1	0	-3.878388	-0.186450	-2.094042
14	1	0	-3.569095	-1.944093	1.816327
15	1	0	-4.852516	-1.570064	-0.276244
16	6	0	0.072518	0.562794	0.292854
17	1	0	0.309330	0.715122	1.354909
18	8	0	0.226375	1.788546	-0.395562
19	6	0	-0.433399	2.867319	0.245758
20	1	0	-0.200833	3.765288	-0.326552
21	1	0	-0.068928	2.987358	1.274154
22	1	0	-1.520274	2.719452	0.263428
23	1	0	0.798273	-0.880708	-1.076909
24	6	0	4.490776	-1.114746	-0.345432
25	1	0	4.935270	-1.800757	-1.063378
26	1	0	4.643767	-1.476407	0.672889
27	1	0	4.921847	-0.117887	-0.450899

1c.2MeOH-ts

Zero-point correction=	0.273789
(Hartree/Particle)	
Thermal correction to Energy=	0.290707
Thermal correction to Enthalpy=	0.291652
Thermal correction to Gibbs Free Energy=	0.227806
Sum of electronic and zero-point Energies=	-784.450958
Sum of electronic and thermal Energies=	-784.434040
Sum of electronic and thermal Enthalpies=	-784.433096
Sum of electronic and thermal Free Energies=	-784.496941

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.085388	-0.195854	-0.343588
2	6	0	2.269731	-0.806187	-0.118091
3	8	0	3.222690	-0.310432	-0.953549
4	8	0	2.539013	-1.700591	0.685968
5	6	0	-1.310353	-0.596624	-0.049248
6	6	0	-3.900155	-0.691400	-1.106244
7	6	0	-2.278038	-1.426313	0.522985
8	6	0	-1.642647	0.169101	-1.170912
9	6	0	-2.933714	0.128213	-1.691889
10	6	0	-3.568610	-1.475795	-0.002395
11	1	0	-2.019233	-2.044060	1.379613
12	1	0	-0.877043	0.769627	-1.652044
13	1	0	-3.183273	0.724379	-2.564025
14	1	0	-4.310341	-2.129385	0.445542
15	1	0	-4.903720	-0.729055	-1.518370
16	6	0	0.071802	-0.544770	0.547416
17	1	0	0.285152	-1.419203	1.169329
18	8	0	0.075883	0.603631	1.632692
19	1	0	0.346374	1.533774	1.079862
20	1	0	1.082396	1.417898	-0.388994
21	8	0	0.881284	2.284819	0.142123
22	6	0	0.083644	3.241611	-0.560205
23	1	0	0.218196	4.209532	-0.076709
24	1	0	-0.974977	2.964050	-0.534007
25	1	0	0.417909	3.307448	-1.597422
26	6	0	-1.003534	0.694487	2.574091
27	1	0	-0.734857	1.473568	3.286980
28	1	0	-1.086398	-0.264323	3.088060
29	1	0	-1.940300	0.937155	2.068114
30	6	0	4.512877	-0.903956	-0.840147
31	1	0	5.137089	-0.394750	-1.573543
32	1	0	4.468806	-1.972943	-1.061062
33	1	0	4.919531	-0.762359	0.163756

1c.3MeOH-ts

Zero-point correction=	0.329306
(Hartree/Particle)	
Thermal correction to Energy=	0.350790
Thermal correction to Enthalpy=	0.351734
Thermal correction to Gibbs Free Energy=	0.276793
Sum of electronic and zero-point Energies=	-900.099320
Sum of electronic and thermal Energies=	-900.077836
Sum of electronic and thermal Enthalpies=	-900.076891
Sum of electronic and thermal Free Energies=	-900.151832

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.313698	-0.995305	-0.112458
2	8	0	3.171720	-0.554836	0.835405
3	8	0	2.699441	-1.654262	-1.073151
4	6	0	-1.313280	-1.059087	-0.231529
5	6	0	-3.949453	-1.332084	0.655790
6	6	0	-2.352711	-1.230468	-1.152450
7	6	0	-1.598359	-1.046093	1.134684
8	6	0	-2.914542	-1.178268	1.576595
9	6	0	-3.665617	-1.363661	-0.711364
10	1	0	-2.127750	-1.246481	-2.215167
11	1	0	-0.782848	-0.950976	1.843783
12	1	0	-3.129232	-1.166740	2.640775
13	1	0	-4.467023	-1.492843	-1.431782
14	1	0	-4.973471	-1.435318	1.001083
15	6	0	0.098537	-0.926600	-0.718303
16	1	0	0.382014	-1.641488	-1.495984
17	8	0	-0.122967	0.404682	-1.830696
18	8	0	-1.045116	2.215861	-0.392362
19	6	0	-0.917488	3.550141	-0.882317
20	1	0	0.133824	3.851169	-0.936173
21	1	0	-1.461255	4.242203	-0.234167
22	1	0	-1.353589	3.583459	-1.882282
23	6	0	1.116707	0.904441	-2.345650
24	1	0	0.896029	1.752551	-2.996286
25	1	0	1.593185	0.104734	-2.912571
26	1	0	1.769309	1.222902	-1.526125
27	7	0	1.040943	-0.605796	0.193610
28	1	0	-0.571775	1.166505	-1.265591
29	8	0	0.567862	1.645103	1.517180
30	1	0	-0.496040	2.099259	0.445373
31	6	0	0.201445	1.508117	2.881949
32	1	0	0.828949	0.758718	3.375799
33	1	0	-0.850941	1.216090	2.985508
34	1	0	0.349801	2.470030	3.377407
35	1	0	0.803199	0.742286	1.120618
36	6	0	4.539918	-0.914352	0.647897
37	1	0	5.078971	-0.460932	1.478193
38	1	0	4.913021	-0.527683	-0.302787
39	1	0	4.658374	-1.999946	0.667027

2.6.3 M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

IMINE 1c

```
 Zero-point correction=                           0.167019
(Hartree/Particle)
 Thermal correction to Energy=                    0.177768
 Thermal correction to Enthalpy=                  0.178713
 Thermal correction to Gibbs Free Energy=         0.129112
 Sum of electronic and zero-point Energies=           -553.211305
 Sum of electronic and thermal Energies=              -553.200556
 Sum of electronic and thermal Enthalpies=            -553.199611
 Sum of electronic and thermal Free Energies=         -553.249212
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.035586	-0.336972	-0.099808
2	6	0	-2.351191	0.168686	-0.115889
3	6	0	-0.117908	0.550273	0.021212
4	8	0	-3.204945	-0.806039	0.190955
5	8	0	-2.689985	1.302807	-0.389117
6	1	0	-0.373505	1.610842	0.132317
7	6	0	1.305805	0.210149	0.018927
8	6	0	4.031561	-0.371085	0.018424
9	6	0	2.244216	1.240798	0.152955
10	6	0	1.738709	-1.117446	-0.114755
11	6	0	3.097584	-1.404143	-0.115285
12	6	0	3.606728	0.950052	0.152339
13	1	0	1.902614	2.267357	0.256809
14	1	0	1.000175	-1.906076	-0.215813
15	1	0	3.435911	-2.430016	-0.218077
16	1	0	4.333168	1.749045	0.256526
17	1	0	5.092723	-0.599983	0.018569
18	6	0	-4.588918	-0.433746	0.213302
19	1	0	-5.130320	-1.338465	0.480052
20	1	0	-4.896796	-0.076649	-0.770855
21	1	0	-4.754945	0.347371	0.957044

1c.MeOH-ts

Zero-point correction=	0.218104
(Hartree/Particle)	
Thermal correction to Energy=	0.231901
Thermal correction to Enthalpy=	0.232845
Thermal correction to Gibbs Free Energy=	0.175440
Sum of electronic and zero-point Energies=	-668.793548
Sum of electronic and thermal Energies=	-668.779752
Sum of electronic and thermal Enthalpies=	-668.778808
Sum of electronic and thermal Free Energies=	-668.836213

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.207821	0.273656	-0.388888
2	6	0	2.291064	-0.294404	0.177258
3	8	0	2.371905	-0.811169	1.293221
4	6	0	-1.196219	-0.096341	0.212544
5	6	0	-3.670996	-1.299147	-0.253053
6	6	0	-2.185610	-0.070372	1.199143
7	6	0	-1.444582	-0.735158	-1.004921
8	6	0	-2.681236	-1.333479	-1.236852
9	6	0	-3.422495	-0.669242	0.966628
10	1	0	-1.985753	0.415950	2.151059
11	1	0	-0.660560	-0.763334	-1.755304
12	1	0	-2.871816	-1.830224	-2.182885
13	1	0	-4.187480	-0.648558	1.736278
14	1	0	-4.632849	-1.768837	-0.433867
15	6	0	0.120325	0.571393	0.478544
16	1	0	0.360854	0.599446	1.544419
17	8	0	0.096465	2.057824	0.040838
18	6	0	-1.087844	2.676511	-0.508011
19	1	0	-1.444601	2.118261	-1.374382
20	1	0	-0.793115	3.686464	-0.786329
21	1	0	-1.846574	2.702217	0.273541
22	1	0	0.906534	1.657668	-0.632124
23	8	0	3.352670	-0.266121	-0.668080
24	6	0	4.542679	-0.885968	-0.183852
25	1	0	5.278094	-0.773510	-0.979026
26	1	0	4.369782	-1.944460	0.022829
27	1	0	4.893902	-0.393705	0.725597

1c.MeOH-pf

```
 Zero-point correction=                           0.224154
(Hartree/Particle)
 Thermal correction to Energy=                    0.237952
 Thermal correction to Enthalpy=                  0.238896
 Thermal correction to Gibbs Free Energy=         0.181850
 Sum of electronic and zero-point Energies=           -668.866339
 Sum of electronic and thermal Energies=              -668.852541
 Sum of electronic and thermal Enthalpies=            -668.851597
 Sum of electronic and thermal Free Energies=         -668.908643
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.036959	-0.380143	-0.215095
2	6	0	2.351514	-0.275370	0.126193
3	8	0	3.103316	-1.103726	-0.616832
4	8	0	2.791353	0.447221	1.003216
5	6	0	-1.322959	-0.013001	0.145761
6	6	0	-3.867547	-1.127927	-0.143590
7	6	0	-1.923760	-0.673810	1.217615
8	6	0	-2.000611	0.095265	-1.070366
9	6	0	-3.270166	-0.462418	-1.215019
10	6	0	-3.193840	-1.232488	1.073301
11	1	0	-1.398519	-0.749945	2.166608
12	1	0	-1.535016	0.628661	-1.894808
13	1	0	-3.794323	-0.373989	-2.161528
14	1	0	-3.658540	-1.742872	1.911049
15	1	0	-4.857501	-1.559052	-0.255255
16	6	0	0.074921	0.561572	0.287370
17	1	0	0.305205	0.740929	1.346457
18	8	0	0.231915	1.771091	-0.431001
19	6	0	-0.471418	2.854821	0.154594
20	1	0	-0.224131	3.743303	-0.426192
21	1	0	-0.158620	3.002508	1.196410
22	1	0	-1.555544	2.691459	0.124480
23	1	0	0.805521	-0.922027	-1.037813
24	6	0	4.501622	-1.114844	-0.306133
25	1	0	4.947625	-1.818916	-1.005190
26	1	0	4.658007	-1.446901	0.721672
27	1	0	4.927917	-0.119641	-0.441657

1c.2MeOH-ts

Zero-point correction=	0.273693
(Hartree/Particle)	
Thermal correction to Energy=	0.290635
Thermal correction to Enthalpy=	0.291580
Thermal correction to Gibbs Free Energy=	0.227612
Sum of electronic and zero-point Energies=	-784.453968
Sum of electronic and thermal Energies=	-784.437026
Sum of electronic and thermal Enthalpies=	-784.436082
Sum of electronic and thermal Free Energies=	-784.500049

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.083026	-0.204566	-0.344904
2	6	0	2.264966	-0.810016	-0.108523
3	8	0	3.216376	-0.341544	-0.962873
4	8	0	2.539098	-1.682335	0.720420
5	6	0	-1.313768	-0.594689	-0.039797
6	6	0	-3.902288	-0.712433	-1.098229
7	6	0	-2.275237	-1.430458	0.534108
8	6	0	-1.652033	0.167272	-1.162473
9	6	0	-2.942392	0.114767	-1.684362
10	6	0	-3.565124	-1.491588	0.007689
11	1	0	-2.012953	-2.042725	1.393545
12	1	0	-0.893735	0.777020	-1.643799
13	1	0	-3.196642	0.709165	-2.556290
14	1	0	-4.302136	-2.149276	0.457366
15	1	0	-4.905386	-0.758676	-1.510565
16	6	0	0.067782	-0.531053	0.558953
17	1	0	0.278007	-1.398914	1.191299
18	8	0	0.079767	0.626982	1.615744
19	1	0	0.358914	1.553875	1.051651
20	1	0	1.086328	1.426752	-0.417102
21	8	0	0.894999	2.290507	0.114073
22	6	0	0.094197	3.253392	-0.580504
23	1	0	0.233548	4.217274	-0.091124
24	1	0	-0.963891	2.976294	-0.548614
25	1	0	0.424221	3.322909	-1.618464
26	6	0	-0.998899	0.733230	2.559029
27	1	0	-0.725539	1.522129	3.258789
28	1	0	-1.082988	-0.218261	3.085951
29	1	0	-1.934653	0.972537	2.050268
30	6	0	4.506999	-0.933357	-0.839749
31	1	0	5.127156	-0.447666	-1.592154
32	1	0	4.460474	-2.008332	-1.028610
33	1	0	4.920953	-0.761423	0.156430

1c.3MeOH-ts

Zero-point correction=	0.329005
(Hartree/Particle)	
Thermal correction to Energy=	0.350582
Thermal correction to Enthalpy=	0.351526
Thermal correction to Gibbs Free Energy=	0.276277
Sum of electronic and zero-point Energies=	-900.101847
Sum of electronic and thermal Energies=	-900.080271
Sum of electronic and thermal Enthalpies=	-900.079327
Sum of electronic and thermal Free Energies=	-900.154576

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.317487	-0.999124	-0.038620
2	8	0	3.178198	-0.486176	0.868713
3	8	0	2.700774	-1.731366	-0.946155
4	6	0	-1.311551	-1.078350	-0.139760
5	6	0	-3.953765	-1.262722	0.751792
6	6	0	-2.338543	-1.387423	-1.038555
7	6	0	-1.611714	-0.882631	1.209294
8	6	0	-2.931060	-0.970149	1.652871
9	6	0	-3.654701	-1.476854	-0.595759
10	1	0	-2.102110	-1.547631	-2.086863
11	1	0	-0.806295	-0.679749	1.907090
12	1	0	-3.157299	-0.814797	2.703236
13	1	0	-4.447136	-1.713523	-1.298673
14	1	0	-4.980261	-1.331567	1.098240
15	6	0	0.099253	-0.987712	-0.634856
16	1	0	0.380143	-1.761552	-1.354659
17	8	0	-0.130134	0.251953	-1.858559
18	8	0	-1.065382	2.163835	-0.552226
19	6	0	-0.948078	3.457533	-1.146131
20	1	0	0.102293	3.730130	-1.291638
21	1	0	-1.434491	4.206224	-0.515887
22	1	0	-1.449518	3.425769	-2.114597
23	6	0	1.106703	0.712323	-2.416355
24	1	0	0.881761	1.492646	-3.145616
25	1	0	1.590736	-0.134080	-2.903456
26	1	0	1.755214	1.112658	-1.630067
27	7	0	1.045086	-0.588703	0.240923
28	1	0	-0.580000	1.051329	-1.355799
29	8	0	0.585983	1.766367	1.384754
30	1	0	-0.508030	2.118378	0.283920
31	6	0	0.235894	1.730211	2.761075
32	1	0	0.821480	0.969700	3.288604
33	1	0	-0.830875	1.512821	2.895034
34	1	0	0.453204	2.705948	3.201039
35	1	0	0.814547	0.836676	1.054645
36	6	0	4.548403	-0.851129	0.700502
37	1	0	5.085837	-0.353550	1.505869
38	1	0	4.919952	-0.511997	-0.268750
39	1	0	4.669781	-1.933645	0.776655

2.6.4 M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

IMINE 1c

```
 Zero-point correction=                           0.167020
(Hartree/Particle)
 Thermal correction to Energy=                    0.177769
 Thermal correction to Enthalpy=                  0.178713
 Thermal correction to Gibbs Free Energy=         0.129114
 Sum of electronic and zero-point Energies=           -553.211257
 Sum of electronic and thermal Energies=              -553.200508
 Sum of electronic and thermal Enthalpies=            -553.199564
 Sum of electronic and thermal Free Energies=         -553.249163
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.035586	-0.336972	-0.099808
2	6	0	-2.351191	0.168686	-0.115889
3	6	0	-0.117908	0.550273	0.021212
4	8	0	-3.204945	-0.806039	0.190955
5	8	0	-2.689985	1.302807	-0.389117
6	1	0	-0.373505	1.610842	0.132317
7	6	0	1.305805	0.210149	0.018927
8	6	0	4.031561	-0.371085	0.018424
9	6	0	2.244216	1.240798	0.152955
10	6	0	1.738709	-1.117446	-0.114755
11	6	0	3.097584	-1.404143	-0.115285
12	6	0	3.606728	0.950052	0.152339
13	1	0	1.902614	2.267357	0.256809
14	1	0	1.000175	-1.906076	-0.215813
15	1	0	3.435911	-2.430016	-0.218077
16	1	0	4.333168	1.749045	0.256526
17	1	0	5.092723	-0.599983	0.018569
18	6	0	-4.588918	-0.433746	0.213302
19	1	0	-5.130320	-1.338465	0.480052
20	1	0	-4.896796	-0.076649	-0.770855
21	1	0	-4.754945	0.347371	0.957044

1c.MeOH-ts

Zero-point correction=	0.218109
(Hartree/Particle)	
Thermal correction to Energy=	0.231903
Thermal correction to Enthalpy=	0.232847
Thermal correction to Gibbs Free Energy=	0.175461
Sum of electronic and zero-point Energies=	-668.793464
Sum of electronic and thermal Energies=	-668.779670
Sum of electronic and thermal Enthalpies=	-668.778725
Sum of electronic and thermal Free Energies=	-668.836111

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.207616	0.272300	-0.389206
2	6	0	2.291400	-0.294335	0.177507
3	8	0	2.372897	-0.809388	1.294163
4	6	0	-1.196399	-0.096594	0.212592
5	6	0	-3.671718	-1.298491	-0.252361
6	6	0	-2.186128	-0.068783	1.198805
7	6	0	-1.444676	-0.736833	-1.004131
8	6	0	-2.681611	-1.334703	-1.235738
9	6	0	-3.423291	-0.667182	0.966608
10	1	0	-1.986276	0.418565	2.150201
11	1	0	-0.660316	-0.766512	-1.754098
12	1	0	-2.872138	-1.832610	-2.181171
13	1	0	-4.188538	-0.645060	1.735956
14	1	0	-4.633778	-1.767859	-0.432920
15	6	0	0.120422	0.570714	0.478189
16	1	0	0.361044	0.599401	1.544027
17	8	0	0.096744	2.057194	0.039595
18	6	0	-1.087483	2.675946	-0.509273
19	1	0	-1.445505	2.116556	-1.374393
20	1	0	-0.792160	3.685188	-0.789563
21	1	0	-1.845529	2.703631	0.272874
22	1	0	0.906312	1.656430	-0.633342
23	8	0	3.352726	-0.266586	-0.668201
24	6	0	4.543065	-0.885436	-0.183561
25	1	0	5.278394	-0.773195	-0.978852
26	1	0	4.370707	-1.943862	0.023927
27	1	0	4.894047	-0.392345	0.725528

1c.MeOH-pf

Zero-point correction=	0.224155
(Hartree/Particle)	
Thermal correction to Energy=	0.237953
Thermal correction to Enthalpy=	0.238897
Thermal correction to Gibbs Free Energy=	0.181855
Sum of electronic and zero-point Energies=	-668.866284
Sum of electronic and thermal Energies=	-668.852486
Sum of electronic and thermal Enthalpies=	-668.851541
Sum of electronic and thermal Free Energies=	-668.908583

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.036959	-0.380143	-0.215095
2	6	0	2.351514	-0.275370	0.126193
3	8	0	3.103316	-1.103726	-0.616832
4	8	0	2.791353	0.447221	1.003216
5	6	0	-1.322959	-0.013001	0.145761
6	6	0	-3.867547	-1.127927	-0.143590
7	6	0	-1.923760	-0.673810	1.217615
8	6	0	-2.000611	0.095265	-1.070366
9	6	0	-3.270166	-0.462418	-1.215019
10	6	0	-3.193840	-1.232488	1.073301
11	1	0	-1.398519	-0.749945	2.166608
12	1	0	-1.535016	0.628661	-1.894808
13	1	0	-3.794323	-0.373989	-2.161528
14	1	0	-3.658540	-1.742872	1.911049
15	1	0	-4.857501	-1.559052	-0.255255
16	6	0	0.074921	0.561572	0.287370
17	1	0	0.305205	0.740929	1.346457
18	8	0	0.231915	1.771091	-0.431001
19	6	0	-0.471418	2.854821	0.154594
20	1	0	-0.224131	3.743303	-0.426192
21	1	0	-0.158620	3.002508	1.196410
22	1	0	-1.555544	2.691459	0.124480
23	1	0	0.805521	-0.922027	-1.037813
24	6	0	4.501622	-1.114844	-0.306133
25	1	0	4.947625	-1.818916	-1.005190
26	1	0	4.658007	-1.446901	0.721672
27	1	0	4.927917	-0.119641	-0.441657

1c.2MeOH-ts

Zero-point correction= (Hartree/Particle)	0.273696
Thermal correction to Energy=	0.290638
Thermal correction to Enthalpy=	0.291583
Thermal correction to Gibbs Free Energy=	0.227615
Sum of electronic and zero-point Energies=	-784.453865
Sum of electronic and thermal Energies=	-784.436923
Sum of electronic and thermal Enthalpies=	-784.435979
Sum of electronic and thermal Free Energies=	-784.499946

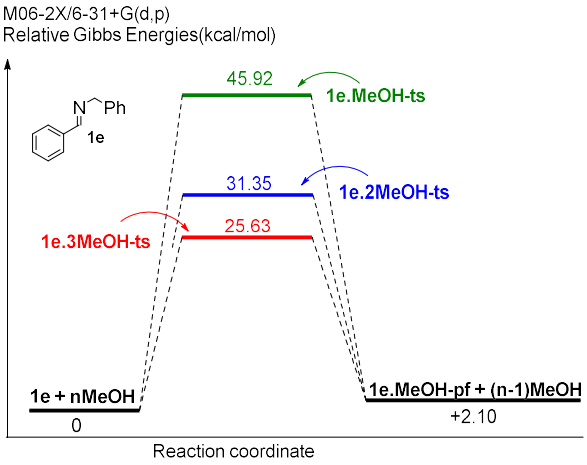
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.083203	-0.204097	-0.344942
2	6	0	2.265278	-0.809650	-0.109045
3	8	0	3.216729	-0.339958	-0.962623
4	8	0	2.539304	-1.682888	0.718882
5	6	0	-1.313534	-0.594813	-0.040250
6	6	0	-3.902118	-0.711637	-1.098591
7	6	0	-2.275268	-1.430270	0.533660
8	6	0	-1.651543	0.167224	-1.162947
9	6	0	-2.941942	0.115183	-1.684780
10	6	0	-3.565194	-1.490929	0.007306
11	1	0	-2.013122	-2.042722	1.393008
12	1	0	-0.892932	0.776521	-1.644343
13	1	0	-3.196000	0.709610	-2.556746
14	1	0	-4.302415	-2.148397	0.456968
15	1	0	-4.905241	-0.757539	-1.510903
16	6	0	0.068052	-0.531646	0.558413
17	1	0	0.278435	-1.399853	1.190224
18	8	0	0.079730	0.625800	1.616466
19	1	0	0.358231	1.552947	1.052945
20	1	0	1.085926	1.426711	-0.415939
21	8	0	0.893951	2.290427	0.115322
22	6	0	0.092779	3.252817	-0.579366
23	1	0	0.231743	4.216894	-0.090236
24	1	0	-0.965226	2.975335	-0.547419
25	1	0	0.422668	3.322302	-1.617384
26	6	0	-0.998758	0.731042	2.559985
27	1	0	-0.725491	1.519403	3.260402
28	1	0	-1.082518	-0.220901	3.086154
29	1	0	-1.934708	0.970501	2.051639
30	6	0	4.507382	-0.931755	-0.839907
31	1	0	5.127668	-0.445049	-1.591552
32	1	0	4.461023	-2.006509	-1.030071
33	1	0	4.921032	-0.761024	0.156609

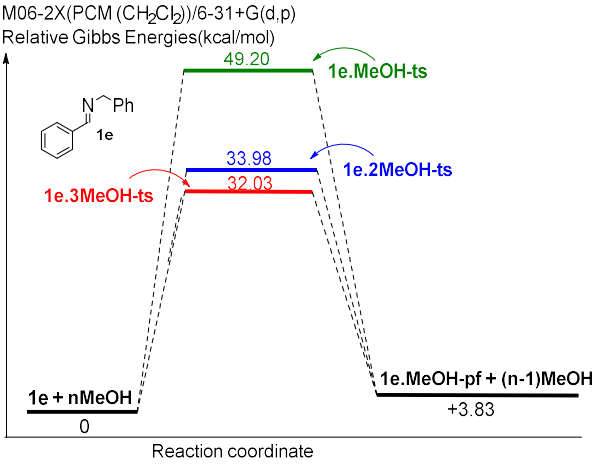
1c.3MeOH-ts

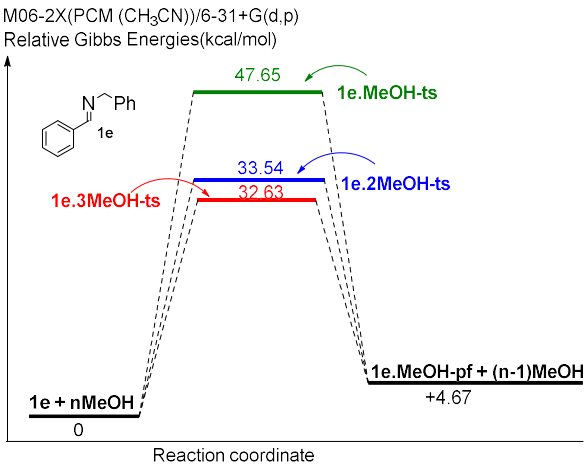
Zero-point correction=	0.329021
(Hartree/Particle)	
Thermal correction to Energy=	0.350586
Thermal correction to Enthalpy=	0.351530
Thermal correction to Gibbs Free Energy=	0.276357
Sum of electronic and zero-point Energies=	-900.101756
Sum of electronic and thermal Energies=	-900.080191
Sum of electronic and thermal Enthalpies=	-900.079247
Sum of electronic and thermal Free Energies=	-900.154421

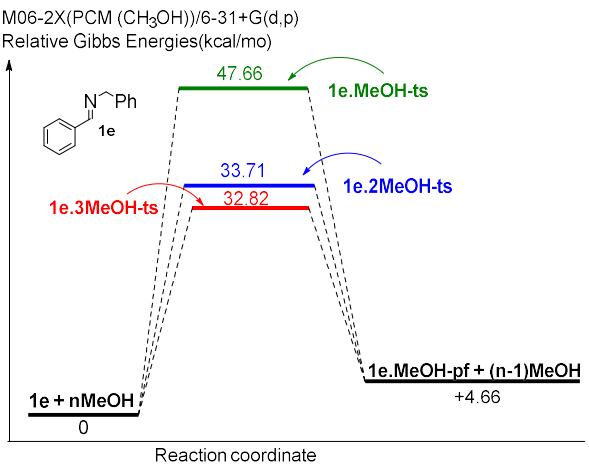
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.317198	-0.999223	-0.039040
2	8	0	3.177854	-0.487063	0.868813
3	8	0	2.700486	-1.730955	-0.946970
4	6	0	-1.311815	-1.077967	-0.140392
5	6	0	-3.953918	-1.262936	0.751359
6	6	0	-2.338962	-1.386117	-1.039321
7	6	0	-1.611776	-0.883448	1.208869
8	6	0	-2.931067	-0.971264	1.652549
9	6	0	-3.655059	-1.475848	-0.596425
10	1	0	-2.102689	-1.545381	-2.087807
11	1	0	-0.806211	-0.681290	1.906710
12	1	0	-3.157149	-0.816865	2.703090
13	1	0	-4.447612	-1.711803	-1.299447
14	1	0	-4.980370	-1.332029	1.097891
15	6	0	0.098997	-0.987161	-0.635517
16	1	0	0.379878	-1.760881	-1.355464
17	8	0	-0.130219	0.252770	-1.858580
18	8	0	-1.064127	2.164443	-0.551352
19	6	0	-0.946772	3.458484	-1.144390
20	1	0	0.103524	3.729719	-1.293010
21	1	0	-1.430032	4.207299	-0.511866
22	1	0	-1.451398	3.428438	-2.111250
23	6	0	1.106696	0.712825	-2.416460
24	1	0	0.881859	1.493109	-3.145801
25	1	0	1.590554	-0.133723	-2.903481
26	1	0	1.755319	1.113098	-1.630234
27	7	0	1.044861	-0.588616	0.240490
28	1	0	-0.579686	1.052247	-1.355392
29	8	0	0.586242	1.765603	1.385630
30	1	0	-0.506671	2.118313	0.284807
31	6	0	0.235680	1.728941	2.761785
32	1	0	0.821467	0.968581	3.289311
33	1	0	-0.831038	1.511019	2.895329
34	1	0	0.452369	2.704677	3.202065
35	1	0	0.814719	0.835964	1.055108
36	6	0	4.547966	-0.852250	0.700592
37	1	0	5.085401	-0.355289	1.506345
38	1	0	4.919765	-0.512648	-0.268405
39	1	0	4.669078	-1.934846	0.776083

2.7.-Energy profiles of the addition of n methanol (2a) molecules (n=1-3) to benzylimine 1e in gas phase, CH_2Cl_2, CH_3CN and CH_3OH.









2.8.-Computacional data of the addition of n methanol (2a) molecules (n=1-3) to imine derivative 1e

2.8.1 M06-2X/6-31+G(d,p) calculations

IMINE 1e

```
 Zero-point correction=                           0.233399
(Hartree/Particle)
 Thermal correction to Energy=                    0.245686
 Thermal correction to Enthalpy=                  0.246630
 Thermal correction to Gibbs Free Energy=         0.192346
 Sum of electronic and zero-point Energies=           -595.592068
 Sum of electronic and thermal Energies=              -595.579780
 Sum of electronic and thermal Enthalpies=            -595.578836
 Sum of electronic and thermal Free Energies=         -595.633120
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.018509	-0.623350	0.644354
2	6	0	0.988931	-1.026904	-0.065886
3	1	0	0.886850	-1.891558	-0.743099
4	6	0	2.317417	-0.383432	-0.046407
5	6	0	4.848334	0.796686	-0.048418
6	6	0	3.326071	-0.878084	-0.876874
7	6	0	2.582908	0.709119	0.788382
8	6	0	3.842860	1.294662	0.784814
9	6	0	4.589438	-0.290412	-0.879677
10	1	0	3.118099	-1.727368	-1.523634
11	1	0	1.789484	1.077897	1.430966
12	1	0	4.047790	2.141233	1.432836
13	1	0	5.367766	-0.680030	-1.528080
14	1	0	5.831678	1.256947	-0.046811
15	6	0	-1.230110	-1.349718	0.553022
16	1	0	-1.421404	-1.799419	1.535769
17	1	0	-1.171689	-2.174644	-0.177807
18	6	0	-2.404448	-0.456899	0.202021
19	6	0	-4.625208	1.116230	-0.473754
20	6	0	-3.695650	-0.992843	0.242327
21	6	0	-2.236211	0.874103	-0.177942
22	6	0	-3.342922	1.656258	-0.513319
23	6	0	-4.799225	-0.215210	-0.093640
24	1	0	-3.836260	-2.029812	0.540921
25	1	0	-1.236945	1.296991	-0.201722
26	1	0	-3.198240	2.691963	-0.805912
27	1	0	-5.795347	-0.645782	-0.056209
28	1	0	-5.484456	1.725695	-0.735597

1e.MeOH-ts

Zero-point correction=	0.282668
(Hartree/Particle)	
Thermal correction to Energy=	0.298526
Thermal correction to Enthalpy=	0.299470
Thermal correction to Gibbs Free Energy=	0.236683
Sum of electronic and zero-point Energies=	-711.149520
Sum of electronic and thermal Energies=	-711.133663
Sum of electronic and thermal Enthalpies=	-711.132719
Sum of electronic and thermal Free Energies=	-711.195505

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.164923	-0.633887	-0.456787
2	6	0	2.268323	-0.377386	-0.377308
3	6	0	4.750553	-0.585489	0.876813
4	6	0	3.416256	0.119130	-1.003295
5	6	0	2.367820	-0.984276	0.879204
6	6	0	3.607256	-1.083154	1.503671
7	6	0	4.655345	0.014874	-0.378641
8	1	0	3.329971	0.597657	-1.975900
9	1	0	1.469131	-1.379325	1.342386
10	1	0	3.685631	-1.554972	2.478073
11	1	0	5.544120	0.401635	-0.866867
12	1	0	5.716645	-0.669707	1.364932
13	6	0	0.964234	-0.221806	-1.037223
14	1	0	0.988272	-0.018720	-2.112967
15	8	0	0.463647	1.540692	-0.230438
16	6	0	1.244939	2.472619	0.460272
17	1	0	2.195657	2.027054	0.800181
18	1	0	0.710519	2.830062	1.350716
19	1	0	1.471754	3.341403	-0.172018
20	1	0	-0.143783	0.409989	0.156871
21	6	0	-1.347835	-0.698585	-1.327454
22	1	0	-1.415399	-1.702395	-1.761082
23	1	0	-1.254346	0.021610	-2.155131
24	6	0	-2.607600	-0.401892	-0.549956
25	6	0	-4.919987	0.172927	0.921996
26	6	0	-3.495115	-1.419467	-0.200751
27	6	0	-2.886038	0.910456	-0.153366
28	6	0	-4.035354	1.196102	0.578635
29	6	0	-4.648150	-1.135881	0.531430
30	1	0	-3.281441	-2.442000	-0.502229
31	1	0	-2.186778	1.701847	-0.416135
32	1	0	-4.243984	2.218427	0.879358
33	1	0	-5.331372	-1.937183	0.795999
34	1	0	-5.817189	0.397259	1.490661

1e.MeOH-pf

Zero-point correction=	0.290659
(Hartree/Particle)	
Thermal correction to Energy=	0.305948
Thermal correction to Enthalpy=	0.306892
Thermal correction to Gibbs Free Energy=	0.245577
Sum of electronic and zero-point Energies=	-711.227226
Sum of electronic and thermal Energies=	-711.211937
Sum of electronic and thermal Enthalpies=	-711.210992
Sum of electronic and thermal Free Energies=	-711.272307

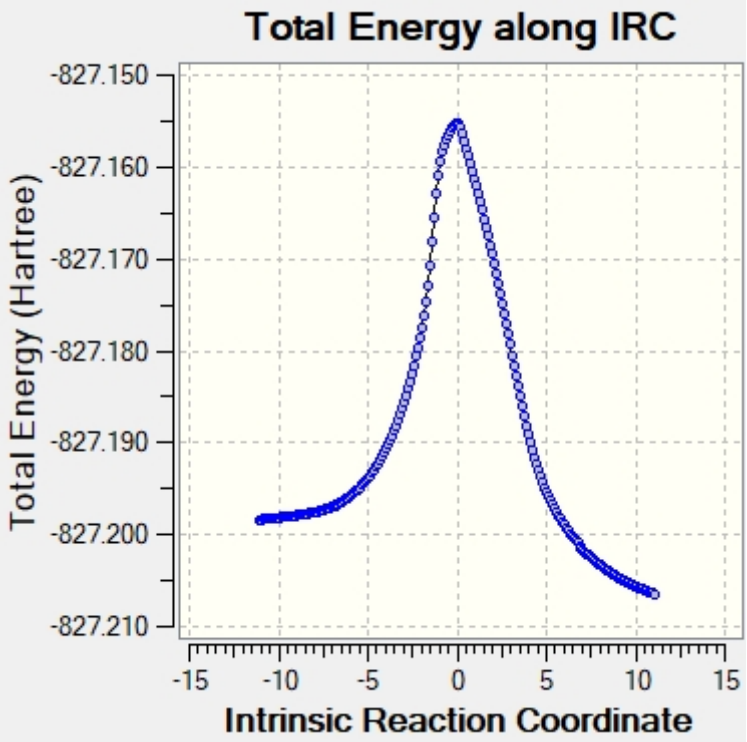
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.240593	1.019111	0.014961
2	6	0	2.034531	0.013278	-0.141586
3	6	0	3.579588	-2.267957	0.349302
4	6	0	2.424676	-0.813758	-1.192911
5	6	0	2.428518	-0.305431	1.161468
6	6	0	3.197751	-1.438634	1.406412
7	6	0	3.192968	-1.954063	-0.950762
8	1	0	2.125320	-0.565704	-2.209494
9	1	0	2.138291	0.352174	1.977898
10	1	0	3.503783	-1.676707	2.420653
11	1	0	3.490095	-2.592445	-1.777169
12	1	0	4.178834	-3.152480	0.541704
13	6	0	1.135646	1.221089	-0.386742
14	1	0	1.133562	1.442317	-1.469579
15	8	0	1.577333	2.342558	0.337591
16	1	0	-0.275435	0.887933	1.025060
17	6	0	2.834594	2.827151	-0.083750
18	1	0	3.033770	3.730049	0.494425
19	1	0	2.816507	3.080854	-1.153146
20	1	0	3.634151	2.096848	0.094715
21	6	0	-0.900995	-0.086366	-0.665718
22	1	0	-0.417892	-1.060830	-0.485908
23	1	0	-0.822695	0.105116	-1.746068
24	6	0	-2.360647	-0.180701	-0.280308
25	6	0	-5.081301	-0.381177	0.368013
26	6	0	-2.975363	-1.429794	-0.171354
27	6	0	-3.120616	0.970542	-0.053603
28	6	0	-4.472295	0.869518	0.269245
29	6	0	-4.328689	-1.532546	0.146404
30	1	0	-2.388142	-2.330696	-0.333698
31	1	0	-2.637308	1.940182	-0.127160
32	1	0	-5.051816	1.770815	0.445919
33	1	0	-4.791562	-2.511206	0.230051
34	1	0	-6.134175	-0.457364	0.621683

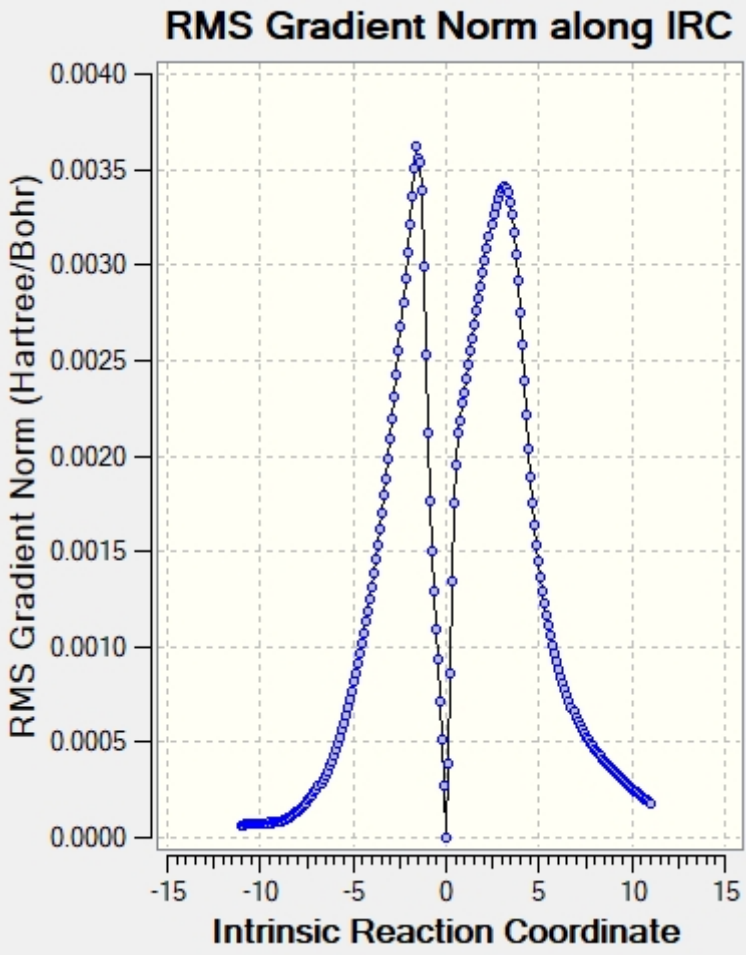
1e.2MeOH-ts

Zero-point correction= (Hartree/Particle)	0.337489
Thermal correction to Energy=	0.357011
Thermal correction to Enthalpy=	0.357956
Thermal correction to Gibbs Free Energy=	0.287027
Sum of electronic and zero-point Energies=	-826.817775
Sum of electronic and thermal Energies=	-826.798253
Sum of electronic and thermal Enthalpies=	-826.797308
Sum of electronic and thermal Free Energies=	-826.868237

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.354281	-0.650032	0.279925
2	6	0	-2.037744	-0.885677	-0.127166
3	6	0	-4.416496	-0.629539	-1.560755
4	6	0	-3.214948	-1.471840	0.349026
5	6	0	-2.053933	-0.174494	-1.333556
6	6	0	-3.242912	-0.046025	-2.041994
7	6	0	-4.402191	-1.346429	-0.365956
8	1	0	-3.199355	-2.015169	1.290453
9	1	0	-1.147248	0.290420	-1.706349
10	1	0	-3.255196	0.512761	-2.972133
11	1	0	-5.312945	-1.800519	0.010446
12	1	0	-5.341785	-0.525850	-2.118952
13	6	0	-0.827048	-1.015250	0.689195
14	1	0	-0.881266	-1.664183	1.561670
15	8	0	-1.211930	0.760631	1.904582
16	1	0	-0.707981	1.377281	1.085794
17	1	0	0.335955	0.264139	-0.268032
18	8	0	-0.049459	1.801566	0.069946
19	6	0	-0.536553	2.907371	-0.625200
20	1	0	-1.496812	2.699767	-1.132974
21	1	0	0.177136	3.231582	-1.398154
22	1	0	-0.702725	3.767620	0.042375
23	6	0	-2.521377	1.214525	2.108509
24	1	0	-2.525567	2.159214	2.670943
25	1	0	-3.091862	0.477795	2.689606
26	1	0	-3.055899	1.382338	1.158301
27	6	0	1.504994	-0.737484	1.188166
28	1	0	1.497006	-1.721561	1.666845
29	1	0	1.368453	0.029304	1.960759
30	6	0	2.795200	-0.513120	0.439604
31	6	0	5.171334	-0.060144	-0.961366
32	6	0	3.722151	-1.542152	0.274223
33	6	0	3.061770	0.750032	-0.101006
34	6	0	4.244357	0.970943	-0.801785
35	6	0	4.909953	-1.316989	-0.421345
36	1	0	3.517463	-2.524816	0.692588
37	1	0	2.325757	1.543227	0.026286
38	1	0	4.445756	1.952044	-1.221071
39	1	0	5.627860	-2.122342	-0.542063
40	1	0	6.095055	0.117215	-1.503597

1e.2MeOH-ts IRC





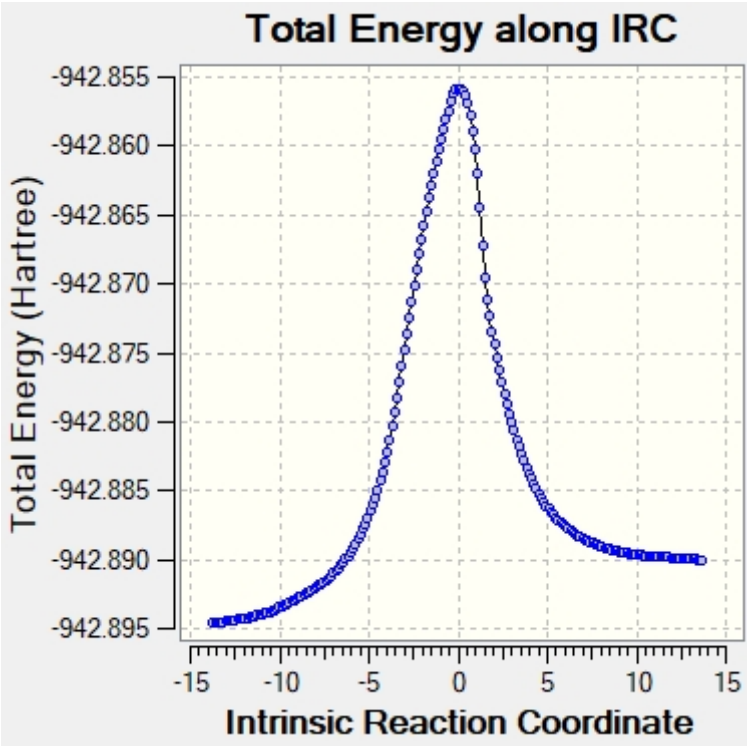
1e.3MeOH-ts

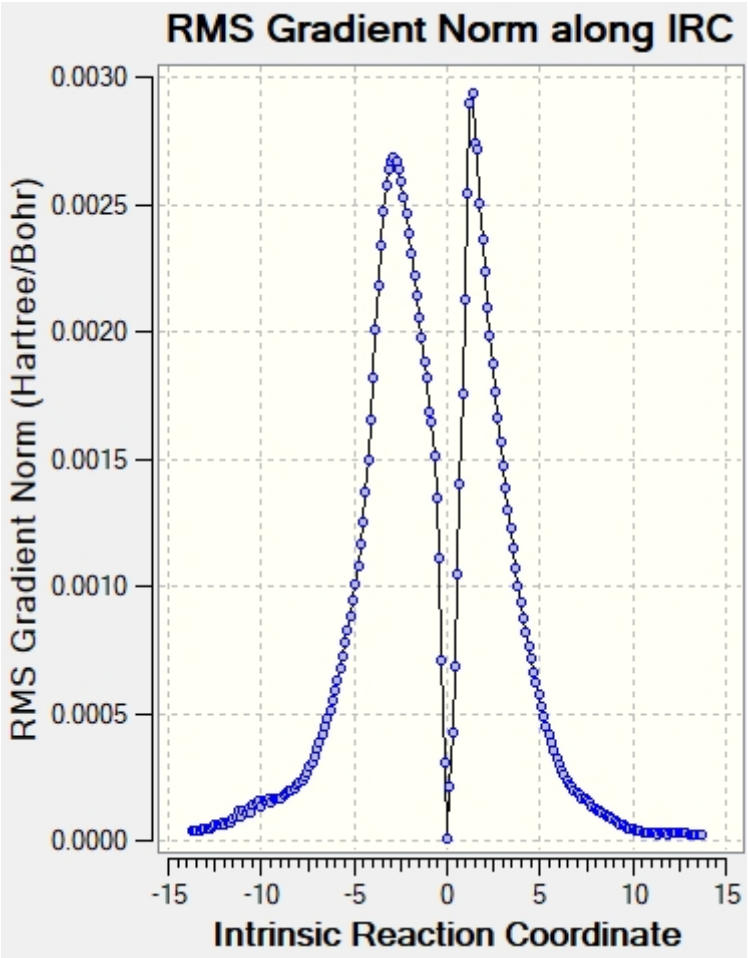
Zero-point correction=	0.390893
(Hartree/Particle)	
Thermal correction to Energy=	0.413983
Thermal correction to Enthalpy=	0.414927
Thermal correction to Gibbs Free Energy=	0.335942
Sum of electronic and zero-point Energies=	-942.464923
Sum of electronic and thermal Energies=	-942.441833
Sum of electronic and thermal Enthalpies=	-942.440888
Sum of electronic and thermal Free Energies=	-942.519874

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.597277	-0.946049	-0.879802
2	6	0	-3.529290	-2.780984	-0.063658
3	6	0	-2.850703	-0.964672	-1.500660
4	6	0	-1.308691	-1.861458	0.135962
5	6	0	-2.276860	-2.773750	0.545721
6	6	0	-3.812623	-1.879406	-1.090600
7	1	0	-3.069118	-0.225281	-2.264054
8	1	0	-0.324178	-1.871057	0.594549
9	1	0	-2.049999	-3.480783	1.337492
10	1	0	-4.789480	-1.882703	-1.563343
11	1	0	-4.284573	-3.491215	0.258696
12	6	0	-0.568694	0.013354	-1.331649
13	1	0	-0.491286	0.233185	-2.394945
14	8	0	-1.916148	1.695091	-1.304409
15	8	0	-2.158480	1.449549	1.076866
16	6	0	-2.731202	2.571144	1.694506
17	1	0	-2.004489	3.093054	2.336398
18	1	0	-3.590453	2.286518	2.317238
19	1	0	-3.090564	3.292750	0.944932
20	6	0	-1.176459	2.872693	-1.474384
21	1	0	-1.833224	3.723013	-1.702743
22	1	0	-0.470088	2.768431	-2.312935
23	1	0	-0.600734	3.122939	-0.568417
24	7	0	0.446464	0.299263	-0.573381
25	1	0	-2.102755	1.574025	-0.195453
26	8	0	-0.061734	0.605266	1.930269
27	1	0	-1.034002	1.020178	1.624596
28	6	0	-0.216028	-0.328166	2.972777
29	1	0	0.583248	-1.079939	2.921150
30	1	0	-1.182669	-0.846505	2.903370
31	1	0	-0.155103	0.162817	3.952522
32	1	0	0.318230	0.229744	0.497092
33	6	0	1.623581	1.044412	-1.011280
34	1	0	1.574173	2.049681	-0.577515
35	1	0	1.600884	1.140591	-2.101263
36	6	0	2.883475	0.345982	-0.552151
37	6	0	5.192665	-0.956818	0.334892
38	6	0	3.798804	-0.166735	-1.470441
39	6	0	3.127694	0.202339	0.818309
40	6	0	4.276528	-0.449174	1.257788
41	6	0	4.953307	-0.813822	-1.029287
42	1	0	3.611176	-0.059573	-2.536049
43	1	0	2.408553	0.598751	1.533908
44	1	0	4.460973	-0.557588	2.322192
45	1	0	5.661819	-1.207224	-1.751532

46	1	0	6.089949	-1.461238	0.679704

1e.3MeOH-ts IRC





2.8.2 M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

IMINE 1e

```
 Zero-point correction=                           0.233837
(Hartree/Particle)
 Thermal correction to Energy=                    0.246091
 Thermal correction to Enthalpy=                  0.247036
 Thermal correction to Gibbs Free Energy=         0.192549
 Sum of electronic and zero-point Energies=           -595.598345
 Sum of electronic and thermal Energies=              -595.586091
 Sum of electronic and thermal Enthalpies=            -595.585147
 Sum of electronic and thermal Free Energies=         -595.639634
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.005239	-0.105589	-1.018947
2	6	0	0.958178	-0.832502	-0.621483
3	1	0	0.872068	-1.929608	-0.582060
4	6	0	2.256924	-0.277070	-0.188850
5	6	0	4.738203	0.712792	0.634458
6	6	0	3.270925	-1.154123	0.207772
7	6	0	2.492594	1.103974	-0.170227
8	6	0	3.727323	1.594304	0.239461
9	6	0	4.509350	-0.661865	0.618234
10	1	0	3.088004	-2.225828	0.193939
11	1	0	1.698638	1.776465	-0.479165
12	1	0	3.906491	2.664875	0.253087
13	1	0	5.291434	-1.349067	0.925124
14	1	0	5.700602	1.099368	0.955260
15	6	0	-1.236002	-0.781932	-1.413551
16	1	0	-1.131978	-1.876242	-1.360814
17	1	0	-1.446418	-0.508354	-2.453064
18	6	0	-2.383927	-0.332026	-0.536401
19	6	0	-4.461848	0.530009	1.135688
20	6	0	-2.652980	-0.999136	0.661557
21	6	0	-3.163824	0.772564	-0.887889
22	6	0	-4.197604	1.203447	-0.056999
23	6	0	-3.686848	-0.573506	1.494362
24	1	0	-2.049101	-1.859420	0.941725
25	1	0	-2.959722	1.296539	-1.818397
26	1	0	-4.798034	2.062030	-0.341727
27	1	0	-3.889224	-1.102997	2.420363
28	1	0	-5.268864	0.861781	1.781567

1e.MeOH-ts

Zero-point correction=	0.286578
(Hartree/Particle)	
Thermal correction to Energy=	0.302456
Thermal correction to Enthalpy=	0.303400
Thermal correction to Gibbs Free Energy=	0.241834
Sum of electronic and zero-point Energies=	-711.164376
Sum of electronic and thermal Energies=	-711.148498
Sum of electronic and thermal Enthalpies=	-711.147553
Sum of electronic and thermal Free Energies=	-711.209120

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.137539	-1.052555	-1.093203
2	6	0	-1.796715	-0.574131	0.306739
3	6	0	-4.488250	-0.166045	0.920067
4	6	0	-2.172003	-0.150623	1.587294
5	6	0	-2.781074	-0.799350	-0.667769
6	6	0	-4.118715	-0.597540	-0.358212
7	6	0	-3.514989	0.061933	1.890435
8	1	0	-1.408438	0.019306	2.341290
9	1	0	-2.507891	-1.140912	-1.661312
10	1	0	-4.878491	-0.776026	-1.111817
11	1	0	-3.799099	0.397512	2.882148
12	1	0	-5.536179	-0.009080	1.155114
13	6	0	-0.382320	-0.792350	0.058412
14	1	0	0.287222	-0.829706	0.917517
15	8	0	-0.643268	1.385877	-1.265322
16	6	0	-1.650463	2.311606	-1.190876
17	1	0	-2.453349	2.011885	-0.472388
18	1	0	-2.179834	2.480770	-2.155280
19	1	0	-1.315581	3.320144	-0.859626
20	1	0	-0.421070	-0.755302	-1.893112
21	6	0	1.556185	-1.353631	-1.337313
22	1	0	1.735749	-1.111093	-2.387116
23	1	0	1.708628	-2.429899	-1.214578
24	6	0	2.498753	-0.574788	-0.447524
25	6	0	4.310231	0.876135	1.105161
26	6	0	3.586448	-1.217395	0.144523
27	6	0	2.307139	0.799344	-0.255896
28	6	0	3.213537	1.516069	0.522554
29	6	0	4.495718	-0.491866	0.916403
30	1	0	3.727059	-2.286120	0.002631
31	1	0	1.426791	1.279871	-0.691738
32	1	0	3.063792	2.580658	0.676024
33	1	0	5.340238	-0.997431	1.374197
34	1	0	5.012924	1.442085	1.709064

1e.MeOH-pf

```
 Zero-point correction=                           0.290664
(Hartree/Particle)
 Thermal correction to Energy=                    0.306008
 Thermal correction to Enthalpy=                  0.306952
 Thermal correction to Gibbs Free Energy=         0.244635
 Sum of electronic and zero-point Energies=           -711.235403
 Sum of electronic and thermal Energies=              -711.220058
 Sum of electronic and thermal Enthalpies=            -711.219114
 Sum of electronic and thermal Free Energies=         -711.281431
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.241607	1.013963	0.040899
2	6	0	2.033438	0.012291	-0.130301
3	6	0	3.590905	-2.266105	0.338892
4	6	0	2.449491	-0.788019	-1.193271
5	6	0	2.406373	-0.331645	1.173334
6	6	0	3.182137	-1.463466	1.407619
7	6	0	3.224050	-1.927201	-0.961548
8	1	0	2.166518	-0.521021	-2.209462
9	1	0	2.095948	0.300681	2.002195
10	1	0	3.471823	-1.720741	2.421925
11	1	0	3.540916	-2.544892	-1.796277
12	1	0	4.195074	-3.149137	0.522826
13	6	0	1.134366	1.219198	-0.369962
14	1	0	1.125575	1.442361	-1.450633
15	8	0	1.580567	2.346776	0.350118
16	1	0	-0.256140	0.785663	1.035015
17	6	0	2.852194	2.812219	-0.065049
18	1	0	3.048039	3.731573	0.487307
19	1	0	2.854085	3.028790	-1.141753
20	1	0	3.641223	2.082555	0.153198
21	6	0	-0.920134	-0.037082	-0.712853
22	1	0	-0.435733	-1.021237	-0.612162
23	1	0	-0.861028	0.234661	-1.775974
24	6	0	-2.371547	-0.160844	-0.305472
25	6	0	-5.080887	-0.409310	0.384382
26	6	0	-2.964404	-1.420834	-0.193147
27	6	0	-3.148958	0.976260	-0.061630
28	6	0	-4.494158	0.853134	0.281510
29	6	0	-4.312052	-1.547212	0.145832
30	1	0	-2.366082	-2.311297	-0.370663
31	1	0	-2.686808	1.955885	-0.138216
32	1	0	-5.085910	1.743952	0.470429
33	1	0	-4.757282	-2.533855	0.231447
34	1	0	-6.128387	-0.504206	0.653546

1e.2MeOH-ts

Zero-point correction=	0.337026
(Hartree/Particle)	
Thermal correction to Energy=	0.356958
Thermal correction to Enthalpy=	0.357902
Thermal correction to Gibbs Free Energy=	0.286325
Sum of electronic and zero-point Energies=	-826.830582
Sum of electronic and thermal Energies=	-826.810650
Sum of electronic and thermal Enthalpies=	-826.809706
Sum of electronic and thermal Free Energies=	-826.881283

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.458181	-0.160762	-0.452431
2	6	0	1.822817	-0.963498	-0.162972
3	6	0	4.195570	-1.527673	1.186348
4	6	0	2.896323	-1.552840	-0.842033
5	6	0	1.938830	-0.663377	1.202072
6	6	0	3.124823	-0.944075	1.869259
7	6	0	4.080892	-1.835003	-0.168636
8	1	0	2.803955	-1.774512	-1.901838
9	1	0	1.119387	-0.194071	1.736869
10	1	0	3.217412	-0.706556	2.923944
11	1	0	4.911248	-2.289094	-0.698831
12	1	0	5.119126	-1.743459	1.714222
13	6	0	0.628117	-0.660905	-0.939533
14	1	0	0.602400	-0.982778	-1.977983
15	8	0	1.509721	1.547247	-1.525992
16	1	0	0.998808	1.854347	-0.438631
17	1	0	-0.369548	0.368943	0.430238
18	8	0	0.462268	2.032567	0.591743
19	6	0	1.271412	2.756716	1.473473
20	1	0	2.043681	2.125601	1.948733
21	1	0	0.668941	3.200258	2.278433
22	1	0	1.795725	3.582472	0.965833
23	6	0	2.892185	1.708983	-1.447072
24	1	0	3.199913	2.760490	-1.585757
25	1	0	3.409900	1.118459	-2.220528
26	1	0	3.299633	1.381203	-0.471195
27	6	0	-1.610467	0.211878	-1.276975
28	1	0	-1.536979	-0.335377	-2.220054
29	1	0	-1.524406	1.283239	-1.485443
30	6	0	-2.902561	-0.094977	-0.559598
31	6	0	-5.273969	-0.674868	0.804782
32	6	0	-3.389082	-1.405049	-0.517224
33	6	0	-3.608809	0.920817	0.086698
34	6	0	-4.792148	0.632380	0.767653
35	6	0	-4.570386	-1.694960	0.161122
36	1	0	-2.841725	-2.198439	-1.020781
37	1	0	-3.231824	1.939845	0.055622
38	1	0	-5.335532	1.428723	1.266291
39	1	0	-4.944373	-2.713662	0.185654
40	1	0	-6.195676	-0.900101	1.332026

1e.3MeOH-ts

Zero-point correction=	0.391348
(Hartree/Particle)	
Thermal correction to Energy=	0.414624
Thermal correction to Enthalpy=	0.415568
Thermal correction to Gibbs Free Energy=	0.336353
Sum of electronic and zero-point Energies=	-942.477289
Sum of electronic and thermal Energies=	-942.454012
Sum of electronic and thermal Enthalpies=	-942.453068
Sum of electronic and thermal Free Energies=	-942.532284

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.514741	-1.046530	-0.807107
2	6	0	-3.360895	-2.908488	0.145156
3	6	0	-2.728153	-1.236524	-1.478097
4	6	0	-1.219378	-1.810245	0.326358
5	6	0	-2.145524	-2.734282	0.804527
6	6	0	-3.648158	-2.163348	-1.000871
7	1	0	-2.951147	-0.630073	-2.349768
8	1	0	-0.261214	-1.700123	0.825858
9	1	0	-1.911858	-3.322606	1.686068
10	1	0	-4.592634	-2.301837	-1.516834
11	1	0	-4.081553	-3.629372	0.518276
12	6	0	-0.530448	-0.083778	-1.339046
13	1	0	-0.443355	0.033013	-2.416602
14	8	0	-1.959030	1.539410	-1.451838
15	8	0	-2.353957	1.477070	0.922396
16	6	0	-2.850178	2.719659	1.351306
17	1	0	-2.060876	3.338961	1.807539
18	1	0	-3.649013	2.594539	2.095356
19	1	0	-3.270595	3.291518	0.509467
20	6	0	-1.216303	2.714405	-1.650327
21	1	0	-1.871464	3.567617	-1.873283
22	1	0	-0.525093	2.595336	-2.497350
23	1	0	-0.623229	2.972168	-0.757643
24	7	0	0.459617	0.330618	-0.605515
25	1	0	-2.199397	1.488816	-0.330269
26	8	0	-0.184713	0.852796	1.922267
27	1	0	-1.135823	1.133758	1.556503
28	6	0	-0.321101	0.060402	3.082180
29	1	0	0.615093	-0.480682	3.259067
30	1	0	-1.129686	-0.675209	2.974392
31	1	0	-0.531997	0.678326	3.964148
32	1	0	0.336276	0.326424	0.439009
33	6	0	1.645008	1.029263	-1.103022
34	1	0	1.605431	2.068275	-0.759649
35	1	0	1.622609	1.024653	-2.195581
36	6	0	2.891149	0.352760	-0.576417
37	6	0	5.163027	-0.925130	0.439807
38	6	0	3.795050	-0.266027	-1.439954
39	6	0	3.129858	0.328866	0.802607
40	6	0	4.258859	-0.310271	1.308489
41	6	0	4.930953	-0.900276	-0.933946
42	1	0	3.612642	-0.252365	-2.511322
43	1	0	2.423931	0.808159	1.479323
44	1	0	4.436813	-0.325479	2.379292
45	1	0	5.631013	-1.375513	-1.614018

46	1	0	6.045257	-1.419579	0.834171

2.8.3 M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

IMINE 1e

Zero-point correction= 0.233817
(Hartree/Particle)
Thermal correction to Energy= 0.246073
Thermal correction to Enthalpy= 0.247017
Thermal correction to Gibbs Free Energy= 0.192631
Sum of electronic and zero-point Energies= -595.599811
Sum of electronic and thermal Energies= -595.587555
Sum of electronic and thermal Enthalpies= -595.586611
Sum of electronic and thermal Free Energies= -595.640997

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.007349	-0.103870	-1.018283
2	6	0	0.958442	-0.830532	-0.624764
3	1	0	0.874005	-1.927459	-0.588597
4	6	0	2.257174	-0.274664	-0.192106
5	6	0	4.739427	0.712614	0.633128
6	6	0	3.269617	-1.152869	0.206742
7	6	0	2.495350	1.106165	-0.175026
8	6	0	3.730421	1.595342	0.235571
9	6	0	4.508315	-0.661830	0.618261
10	1	0	3.085120	-2.224243	0.193967
11	1	0	1.704081	1.780831	-0.486198
12	1	0	3.911341	2.665624	0.247610
13	1	0	5.288844	-1.349921	0.927010
14	1	0	5.702033	1.098062	0.954587
15	6	0	-1.237530	-0.782665	-1.413112
16	1	0	-1.130993	-1.876384	-1.360017
17	1	0	-1.449064	-0.509470	-2.452424
18	6	0	-2.385150	-0.333677	-0.535003
19	6	0	-4.461084	0.528886	1.139883
20	6	0	-2.634086	-0.982905	0.677530
21	6	0	-3.184466	0.752639	-0.899770
22	6	0	-4.217341	1.183979	-0.067365
23	6	0	-3.666841	-0.556862	1.511655
24	1	0	-2.015979	-1.829791	0.967374
25	1	0	-2.997814	1.261398	-1.842367
26	1	0	-4.832877	2.028248	-0.362462
27	1	0	-3.853559	-1.072226	2.448856
28	1	0	-5.267181	0.860699	1.786886

1e.MeOH-ts

Zero-point correction=	0.286453
(Hartree/Particle)	
Thermal correction to Energy=	0.302503
Thermal correction to Enthalpy=	0.303447
Thermal correction to Gibbs Free Energy=	0.240919
Sum of electronic and zero-point Energies=	-711.168248
Sum of electronic and thermal Energies=	-711.152198
Sum of electronic and thermal Enthalpies=	-711.151254
Sum of electronic and thermal Free Energies=	-711.213781

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.141622	-0.996228	-1.144583
2	6	0	-1.791634	-0.595546	0.276770
3	6	0	-4.482724	-0.226926	0.914505
4	6	0	-2.165545	-0.239620	1.578341
5	6	0	-2.776750	-0.772851	-0.706862
6	6	0	-4.114352	-0.591061	-0.385079
7	6	0	-3.508606	-0.046751	1.894383
8	1	0	-1.401377	-0.108491	2.339389
9	1	0	-2.507512	-1.062986	-1.717834
10	1	0	-4.874987	-0.735027	-1.145074
11	1	0	-3.791815	0.234643	2.903014
12	1	0	-5.530858	-0.086683	1.159061
13	6	0	-0.376726	-0.796522	0.017315
14	1	0	0.296984	-0.861647	0.871201
15	8	0	-0.644984	1.504086	-1.198819
16	6	0	-1.688628	2.382086	-1.062767
17	1	0	-2.468282	2.014682	-0.350605
18	1	0	-2.240380	2.581897	-2.009538
19	1	0	-1.392434	3.386742	-0.682981
20	1	0	-0.432924	-0.722082	-1.939172
21	6	0	1.560546	-1.278987	-1.412378
22	1	0	1.734284	-0.975230	-2.447146
23	1	0	1.714019	-2.360175	-1.352909
24	6	0	2.501821	-0.550105	-0.481134
25	6	0	4.311590	0.814718	1.150322
26	6	0	3.582386	-1.226467	0.085395
27	6	0	2.316850	0.814354	-0.224296
28	6	0	3.221813	1.488433	0.592987
29	6	0	4.490600	-0.543706	0.896797
30	1	0	3.717827	-2.287753	-0.106728
31	1	0	1.441653	1.320255	-0.640666
32	1	0	3.077115	2.545207	0.797124
33	1	0	5.329564	-1.075408	1.334798
34	1	0	5.013794	1.346679	1.784901

1e.MeOH-pf

```
 Zero-point correction=                           0.290655
(Hartree/Particle)
 Thermal correction to Energy=                    0.305939
 Thermal correction to Enthalpy=                  0.306883
 Thermal correction to Gibbs Free Energy=         0.245403
 Sum of electronic and zero-point Energies=           -711.237014
 Sum of electronic and thermal Energies=              -711.221729
 Sum of electronic and thermal Enthalpies=            -711.220785
 Sum of electronic and thermal Free Energies=         -711.282266
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.267544	0.999883	-0.106968
2	6	0	-2.023460	0.038168	0.129179
3	6	0	-3.620312	-2.246337	-0.125631
4	6	0	-2.504226	-0.614900	1.262939
5	6	0	-2.349347	-0.457133	-1.137686
6	6	0	-3.144450	-1.592728	-1.265753
7	6	0	-3.299419	-1.756781	1.138537
8	1	0	-2.256797	-0.228999	2.249725
9	1	0	-1.987814	0.059340	-2.024220
10	1	0	-3.397521	-1.968414	-2.252527
11	1	0	-3.668542	-2.258843	2.027620
12	1	0	-4.240734	-3.131712	-0.224867
13	6	0	-1.114269	1.253698	0.259544
14	1	0	-1.120164	1.584294	1.312003
15	8	0	-1.538501	2.307651	-0.577780
16	1	0	0.295852	0.688700	-1.078230
17	6	0	-2.814179	2.820393	-0.234520
18	1	0	-2.995573	3.677348	-0.883720
19	1	0	-2.831938	3.148229	0.813225
20	1	0	-3.603113	2.074872	-0.388699
21	6	0	0.916869	0.000058	0.743065
22	1	0	0.416003	-0.979881	0.708560
23	1	0	0.849961	0.358751	1.778420
24	6	0	2.365908	-0.167861	0.351501
25	6	0	5.058117	-0.462774	-0.380119
26	6	0	2.845152	-1.394909	-0.110709
27	6	0	3.249493	0.914062	0.441523
28	6	0	4.586245	0.769739	0.079890
29	6	0	4.185481	-1.544561	-0.474507
30	1	0	2.165224	-2.239912	-0.186722
31	1	0	2.877737	1.871878	0.796201
32	1	0	5.262608	1.615732	0.156638
33	1	0	4.544200	-2.504525	-0.833103
34	1	0	6.100198	-0.576058	-0.662807

1e.2MeOH-ts

Zero-point correction=	0.337186
(Hartree/Particle)	
Thermal correction to Energy=	0.357105
Thermal correction to Enthalpy=	0.358050
Thermal correction to Gibbs Free Energy=	0.285758
Sum of electronic and zero-point Energies=	-826.833559
Sum of electronic and thermal Energies=	-826.813639
Sum of electronic and thermal Enthalpies=	-826.812695
Sum of electronic and thermal Free Energies=	-826.884986

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.465601	-0.103696	-0.465428
2	6	0	1.804501	-0.952445	-0.231617
3	6	0	4.181669	-1.613281	1.063802
4	6	0	2.872670	-1.497652	-0.954931
5	6	0	1.927008	-0.748024	1.150750
6	6	0	3.115267	-1.076940	1.791179
7	6	0	4.060133	-1.826880	-0.308583
8	1	0	2.773425	-1.648751	-2.026357
9	1	0	1.109776	-0.320909	1.723246
10	1	0	3.213098	-0.915272	2.859623
11	1	0	4.886865	-2.245331	-0.872706
12	1	0	5.106921	-1.866700	1.571594
13	6	0	0.608346	-0.598573	-0.981130
14	1	0	0.574347	-0.858488	-2.036709
15	8	0	1.548396	1.686884	-1.414936
16	1	0	1.016858	1.907771	-0.274629
17	1	0	-0.378822	0.350206	0.455557
18	8	0	0.493465	2.018798	0.737311
19	6	0	1.332022	2.652653	1.664001
20	1	0	2.097955	1.968829	2.068638
21	1	0	0.748067	3.033920	2.512197
22	1	0	1.861754	3.509322	1.217863
23	6	0	2.932435	1.801776	-1.308967
24	1	0	3.275542	2.851300	-1.361022
25	1	0	3.448662	1.258050	-2.118200
26	1	0	3.319949	1.388392	-0.356874
27	6	0	-1.626673	0.311215	-1.254790
28	1	0	-1.551295	-0.169053	-2.233831
29	1	0	-1.556698	1.394891	-1.392472
30	6	0	-2.912723	-0.057918	-0.554593
31	6	0	-5.288530	-0.751517	0.747577
32	6	0	-3.256063	-1.403121	-0.383652
33	6	0	-3.763138	0.934982	-0.067562
34	6	0	-4.950745	0.589779	0.579975
35	6	0	-4.438251	-1.749310	0.265312
36	1	0	-2.594561	-2.179187	-0.761630
37	1	0	-3.497773	1.981132	-0.195622
38	1	0	-5.607831	1.368413	0.954196
39	1	0	-4.698737	-2.795301	0.392950
40	1	0	-6.210757	-1.021280	1.252560

1e.3MeOH-ts

Zero-point correction=	0.391315
(Hartree/Particle)	
Thermal correction to Energy=	0.414660
Thermal correction to Enthalpy=	0.415605
Thermal correction to Gibbs Free Energy=	0.336383
Sum of electronic and zero-point Energies=	-942.480221
Sum of electronic and thermal Energies=	-942.456876
Sum of electronic and thermal Enthalpies=	-942.455931
Sum of electronic and thermal Free Energies=	-942.535153

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.497910	1.073306	-0.783960
2	6	0	3.347520	2.918390	0.196282
3	6	0	2.692601	1.304006	-1.475744
4	6	0	1.221964	1.789237	0.385064
5	6	0	2.149941	2.704723	0.876804
6	6	0	3.614646	2.222042	-0.984941
7	1	0	2.898995	0.738903	-2.378819
8	1	0	0.277505	1.651217	0.903263
9	1	0	1.930838	3.256789	1.785107
10	1	0	4.543353	2.393596	-1.519292
11	1	0	4.068499	3.633721	0.579230
12	6	0	0.515601	0.117736	-1.332458
13	1	0	0.419334	0.031617	-2.411889
14	8	0	1.947986	-1.489080	-1.492868
15	8	0	2.394814	-1.488135	0.872053
16	6	0	2.901693	-2.744639	1.247311
17	1	0	2.120131	-3.386352	1.685363
18	1	0	3.705846	-2.644459	1.989289
19	1	0	3.317837	-3.281024	0.380379
20	6	0	1.210942	-2.665794	-1.708080
21	1	0	1.870146	-3.509896	-1.952543
22	1	0	0.511409	-2.535185	-2.545903
23	1	0	0.627937	-2.945003	-0.815290
24	7	0	-0.468042	-0.321845	-0.603799
25	1	0	2.208336	-1.465682	-0.369877
26	8	0	0.215834	-0.926940	1.923070
27	1	0	1.157956	-1.179657	1.539327
28	6	0	0.360894	-0.175645	3.110239
29	1	0	-0.582228	0.337994	3.324638
30	1	0	1.150970	0.581269	3.013811
31	1	0	0.602903	-0.821034	3.963996
32	1	0	-0.342159	-0.338909	0.434767
33	6	0	-1.654471	-1.011853	-1.112309
34	1	0	-1.614207	-2.056819	-0.787889
35	1	0	-1.632279	-0.987279	-2.204251
36	6	0	-2.900514	-0.344601	-0.573911
37	6	0	-5.174392	0.914682	0.461593
38	6	0	-3.805675	0.285295	-1.428290
39	6	0	-3.138986	-0.341020	0.805372
40	6	0	-4.268822	0.288970	1.321201
41	6	0	-4.942610	0.910103	-0.912631
42	1	0	-3.623216	0.287573	-2.499669
43	1	0	-2.433091	-0.829517	1.475521
44	1	0	-4.446189	0.288719	2.392178
45	1	0	-5.643563	1.394106	-1.585573

46	1	0	-6.057292	1.401843	0.863423

2.8.4 M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

IMINE 1e

Zero-point correction= 0.233817
(Hartree/Particle)
Thermal correction to Energy= 0.246072
Thermal correction to Enthalpy= 0.247017
Thermal correction to Gibbs Free Energy= 0.192635
Sum of electronic and zero-point Energies= -595.599761
Sum of electronic and thermal Energies= -595.587505
Sum of electronic and thermal Enthalpies= -595.586561
Sum of electronic and thermal Free Energies= -595.640943

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.007259	-0.102527	-1.018884
2	6	0	0.958196	-0.829679	-0.625504
3	1	0	0.873477	-1.926627	-0.590210
4	6	0	2.256954	-0.274498	-0.192086
5	6	0	4.739388	0.711532	0.634068
6	6	0	3.269231	-1.153265	0.205929
7	6	0	2.495342	1.106291	-0.173603
8	6	0	3.730506	1.594831	0.237459
9	6	0	4.508047	-0.662854	0.617851
10	1	0	3.084507	-2.224594	0.192192
11	1	0	1.704104	1.781353	-0.483991
12	1	0	3.911583	2.665071	0.250659
13	1	0	5.288461	-1.351389	0.925912
14	1	0	5.702055	1.096498	0.955898
15	6	0	-1.237499	-0.780697	-1.414442
16	1	0	-1.131092	-1.874527	-1.362966
17	1	0	-1.449084	-0.505964	-2.453341
18	6	0	-2.384977	-0.332822	-0.535615
19	6	0	-4.460943	0.527479	1.140422
20	6	0	-2.635516	-0.985227	0.674894
21	6	0	-3.182630	0.755613	-0.897680
22	6	0	-4.215551	1.185771	-0.064767
23	6	0	-3.668320	-0.560342	1.509546
24	1	0	-2.018594	-1.833641	0.962778
25	1	0	-2.994636	1.266971	-1.838592
26	1	0	-4.829898	2.031585	-0.357893
27	1	0	-3.856323	-1.078207	2.445102
28	1	0	-5.267116	0.858363	1.787805

1e.MeOH-ts

```
 Zero-point correction=                           0.286449
(Hartree/Particle)
 Thermal correction to Energy=                    0.302506
 Thermal correction to Enthalpy=                  0.303450
 Thermal correction to Gibbs Free Energy=         0.240893
 Sum of electronic and zero-point Energies=           -711.168121
 Sum of electronic and thermal Energies=              -711.152064
 Sum of electronic and thermal Enthalpies=            -711.151119
 Sum of electronic and thermal Free Energies=         -711.213677
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.141545	-0.999485	-1.141831
2	6	0	-1.791964	-0.594510	0.278194
3	6	0	-4.483143	-0.223934	0.914588
4	6	0	-2.166102	-0.235758	1.578904
5	6	0	-2.776928	-0.773580	-0.705280
6	6	0	-4.114540	-0.590774	-0.384184
7	6	0	-3.509211	-0.041995	1.894284
8	1	0	-1.402059	-0.103094	2.339810
9	1	0	-2.507463	-1.065629	-1.715639
10	1	0	-4.875036	-0.735962	-1.144088
11	1	0	-3.792567	0.241595	2.902258
12	1	0	-5.531293	-0.082875	1.158604
13	6	0	-0.377020	-0.796156	0.019437
14	1	0	0.296471	-0.859184	0.873654
15	8	0	-0.644445	1.499166	-1.201147
16	6	0	-1.687815	2.378043	-1.069001
17	1	0	-2.463919	2.017308	-0.349535
18	1	0	-2.244111	2.567841	-2.015151
19	1	0	-1.390466	3.386589	-0.700715
20	1	0	-0.432488	-0.726107	-1.937069
21	6	0	1.560495	-1.283147	-1.408407
22	1	0	1.734499	-0.982653	-2.444086
23	1	0	1.713947	-2.364160	-1.345548
24	6	0	2.501824	-0.551486	-0.479353
25	6	0	4.311872	0.818225	1.147683
26	6	0	3.582949	-1.225967	0.088387
27	6	0	2.316432	0.813542	-0.225945
28	6	0	3.221545	1.490049	0.589162
29	6	0	4.491309	-0.540776	0.897563
30	1	0	3.718745	-2.287689	-0.101106
31	1	0	1.440868	1.318034	-0.643251
32	1	0	3.076509	2.547286	0.790641
33	1	0	5.330713	-1.071017	1.336490
34	1	0	5.014174	1.352122	1.780525

1e.MeOH-pf

```
 Zero-point correction=                           0.290657
(Hartree/Particle)
 Thermal correction to Energy=                    0.305941
 Thermal correction to Enthalpy=                  0.306885
 Thermal correction to Gibbs Free Energy=         0.245401
 Sum of electronic and zero-point Energies=           -711.236955
 Sum of electronic and thermal Energies=              -711.221671
 Sum of electronic and thermal Enthalpies=            -711.220727
 Sum of electronic and thermal Free Energies=         -711.282211
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.267439	1.000409	-0.106259
2	6	0	-2.023398	0.038140	0.129209
3	6	0	-3.619520	-2.246803	-0.126359
4	6	0	-2.504231	-0.615278	1.262734
5	6	0	-2.348915	-0.457005	-1.137814
6	6	0	-3.143641	-1.592809	-1.266256
7	6	0	-3.299039	-1.757376	1.137961
8	1	0	-2.257084	-0.229526	2.249650
9	1	0	-1.987362	0.059788	-2.024151
10	1	0	-3.396412	-1.968380	-2.253150
11	1	0	-3.668164	-2.259755	2.026865
12	1	0	-4.239639	-3.132359	-0.225888
13	6	0	-1.114482	1.253843	0.260010
14	1	0	-1.120679	1.584171	1.312568
15	8	0	-1.538719	2.307888	-0.577134
16	1	0	0.296144	0.690226	-1.077823
17	6	0	-2.814596	2.820246	-0.234132
18	1	0	-2.995875	3.677510	-0.882954
19	1	0	-2.832834	3.147577	0.813779
20	1	0	-3.603366	2.074678	-0.388966
21	6	0	0.916658	-0.000040	0.743077
22	1	0	0.415761	-0.979943	0.707913
23	1	0	0.849723	0.357935	1.778697
24	6	0	2.365704	-0.167823	0.351446
25	6	0	5.057932	-0.462552	-0.380168
26	6	0	2.845296	-1.395141	-0.109621
27	6	0	3.248966	0.914468	0.440351
28	6	0	4.585720	0.770207	0.078729
29	6	0	4.185625	-1.544711	-0.473420
30	1	0	2.165649	-2.240436	-0.184791
31	1	0	2.876936	1.872499	0.794147
32	1	0	5.261794	1.616502	0.154610
33	1	0	4.544598	-2.504894	-0.831194
34	1	0	6.100009	-0.575769	-0.662898

1e.2MeOH-ts

Zero-point correction=	0.337150
(Hartree/Particle)	
Thermal correction to Energy=	0.357075
Thermal correction to Enthalpy=	0.358020
Thermal correction to Gibbs Free Energy=	0.285730
Sum of electronic and zero-point Energies=	-826.833484
Sum of electronic and thermal Energies=	-826.813559
Sum of electronic and thermal Enthalpies=	-826.812614
Sum of electronic and thermal Free Energies=	-826.884904

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.465298	-0.104679	-0.465090
2	6	0	1.805285	-0.952192	-0.231333
3	6	0	4.182663	-1.612003	1.064229
4	6	0	2.873723	-1.496960	-0.954568
5	6	0	1.927644	-0.747665	1.151024
6	6	0	3.116009	-1.076074	1.791521
7	6	0	4.061285	-1.825690	-0.308154
8	1	0	2.774620	-1.648067	-2.026008
9	1	0	1.110219	-0.320769	1.723408
10	1	0	3.213733	-0.914287	2.859958
11	1	0	4.888232	-2.243780	-0.872230
12	1	0	5.108004	-1.865004	1.572069
13	6	0	0.609002	-0.598753	-0.980901
14	1	0	0.575183	-0.858662	-2.036487
15	8	0	1.546901	1.685751	-1.415194
16	1	0	1.016162	1.906947	-0.276354
17	1	0	-0.378329	0.350097	0.455562
18	8	0	0.492273	2.017869	0.736713
19	6	0	1.329980	2.652554	1.663461
20	1	0	2.096296	1.969424	2.068654
21	1	0	0.745582	3.033812	2.511401
22	1	0	1.859368	3.509433	1.217267
23	6	0	2.930886	1.802281	-1.309680
24	1	0	3.272642	2.852169	-1.362420
25	1	0	3.447316	1.258723	-2.118844
26	1	0	3.319090	1.389832	-0.357499
27	6	0	-1.626206	0.310243	-1.254681
28	1	0	-1.550844	-0.170271	-2.233610
29	1	0	-1.555914	1.393870	-1.392601
30	6	0	-2.912411	-0.058462	-0.554556
31	6	0	-5.288478	-0.751262	0.747578
32	6	0	-3.256556	-1.403530	-0.384206
33	6	0	-3.762173	0.934706	-0.066937
34	6	0	-4.949902	0.589903	0.580578
35	6	0	-4.438864	-1.749332	0.264736
36	1	0	-2.595582	-2.179837	-0.762622
37	1	0	-3.496147	1.980748	-0.194494
38	1	0	-5.606476	1.368754	0.955246
39	1	0	-4.699972	-2.795228	0.391894
40	1	0	-6.210814	-1.020710	1.252532

1e.3MeOH-ts

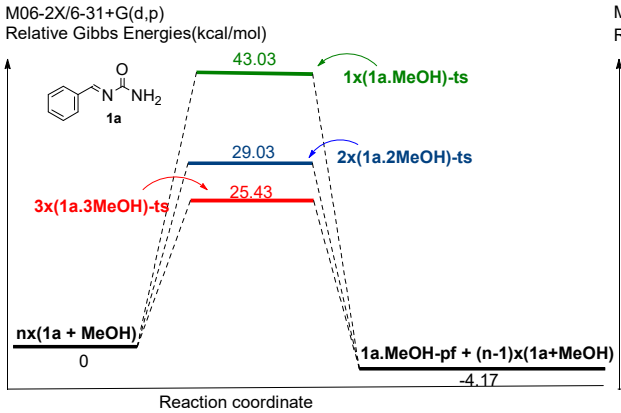
Zero-point correction=	0.391322
(Hartree/Particle)	
Thermal correction to Energy=	0.414662
Thermal correction to Enthalpy=	0.415606
Thermal correction to Gibbs Free Energy=	0.336405
Sum of electronic and zero-point Energies=	-942.480112
Sum of electronic and thermal Energies=	-942.456772
Sum of electronic and thermal Enthalpies=	-942.455827
Sum of electronic and thermal Free Energies=	-942.535028

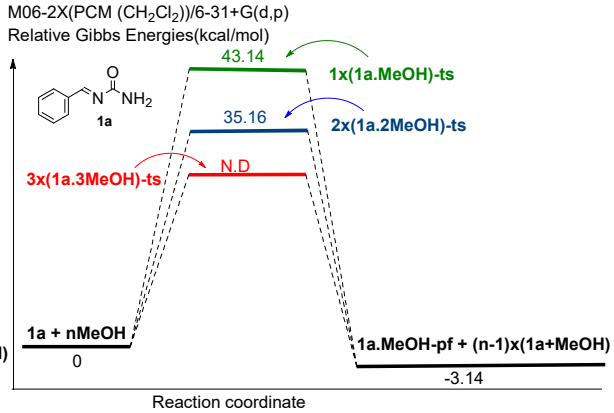
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.498271	1.072477	-0.784722
2	6	0	3.347399	2.918581	0.194436
3	6	0	2.693559	1.301972	-1.475862
4	6	0	1.221540	1.790046	0.383114
5	6	0	2.149269	2.706050	0.874321
6	6	0	3.615348	2.220538	-0.985592
7	1	0	2.900660	0.735434	-2.377870
8	1	0	0.276634	1.652836	0.900717
9	1	0	1.929559	3.259374	1.781710
10	1	0	4.544564	2.391101	-1.519371
11	1	0	4.068227	3.634278	0.576988
12	6	0	0.515999	0.116537	-1.332618
13	1	0	0.419982	0.029383	-2.411995
14	8	0	1.948495	-1.490770	-1.491644
15	8	0	2.393599	-1.487710	0.873647
16	6	0	2.900459	-2.743652	1.250669
17	1	0	2.118818	-3.384851	1.689346
18	1	0	3.704424	-2.642461	1.992721
19	1	0	3.316879	-3.281114	0.384534
20	6	0	1.211345	-2.667485	-1.706282
21	1	0	1.870472	-3.511860	-1.950014
22	1	0	0.512087	-2.537314	-2.544424
23	1	0	0.628013	-2.946006	-0.813492
24	7	0	-0.467725	-0.322385	-0.603721
25	1	0	2.208171	-1.466433	-0.368752
26	8	0	0.214975	-0.924717	1.923240
27	1	0	1.157392	-1.178256	1.539954
28	6	0	0.359813	-0.172088	3.109547
29	1	0	-0.583278	0.341978	3.323139
30	1	0	1.150081	0.584545	3.012490
31	1	0	0.601457	-0.816546	3.964112
32	1	0	-0.341866	-0.338720	0.435027
33	6	0	-1.654113	-1.012753	-1.111790
34	1	0	-1.613872	-2.057476	-0.786582
35	1	0	-1.631893	-0.988998	-2.203761
36	6	0	-2.900156	-0.345088	-0.573899
37	6	0	-5.173921	0.915076	0.460760
38	6	0	-3.805250	0.284335	-1.428688
39	6	0	-3.138643	-0.340601	0.805378
40	6	0	-4.268426	0.289824	1.320775
41	6	0	-4.942128	0.909588	-0.913452
42	1	0	-3.622790	0.285901	-2.500070
43	1	0	-2.432774	-0.828720	1.475827
44	1	0	-4.445816	0.290265	2.391750
45	1	0	-5.643032	1.393215	-1.586713

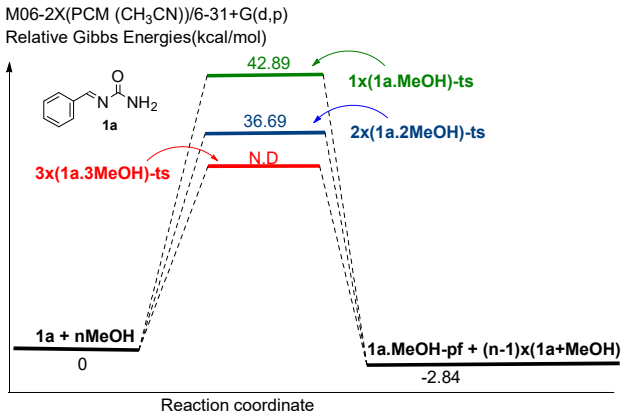
46	1	0	-6.056778	1.402584	0.862263

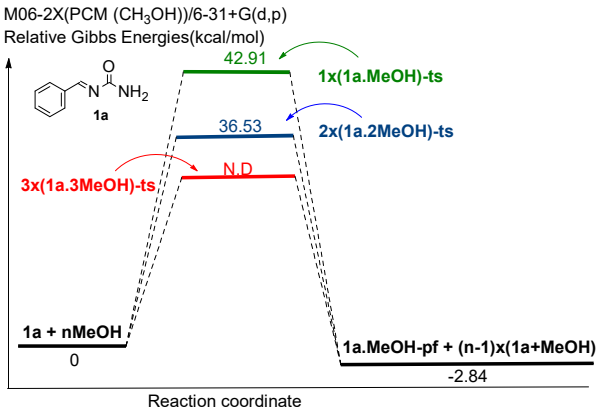
3.- Computational data on the addition of methanol (2a) to imine derivatives 1 in clusters

3.1.-Energy profiles of the addition of methanol (2a) to imine derivative 1a in clusters 1x(1a+2a), 2x(1a+2a), and 3x(1a+2a) in gas phase, CH_2Cl_2, CH_3CN and CH_3OH.









N.D.=Not determined

3.2.- Computacional data of the addition of methanol (2a) to imine 1a in clusters 1x(1a+2a), 2x(1a+2a), and 3x(1a+2a)

3.2.1 M06-2X/6-31+G(d,p) calculations

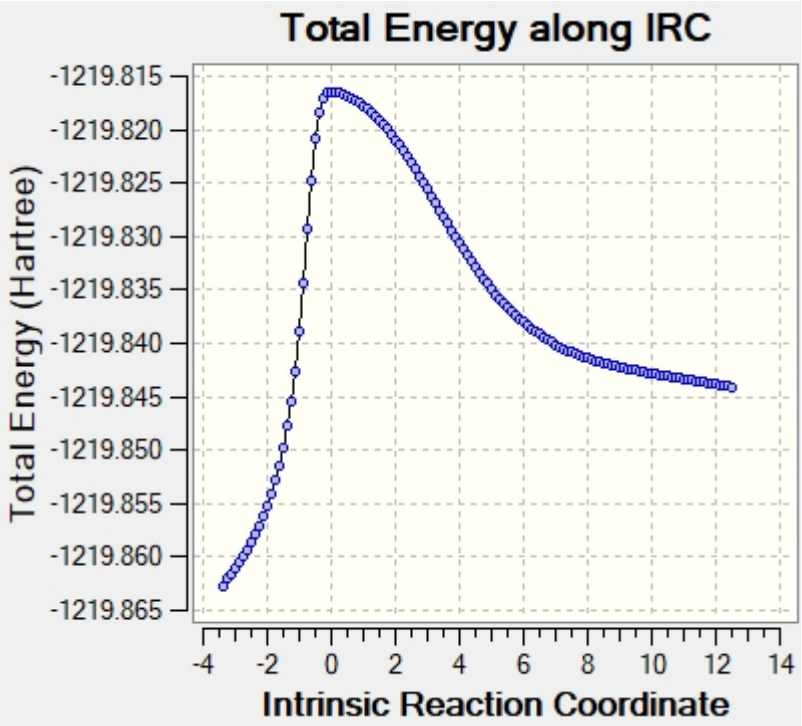
2x(1a+MeOH)-ts

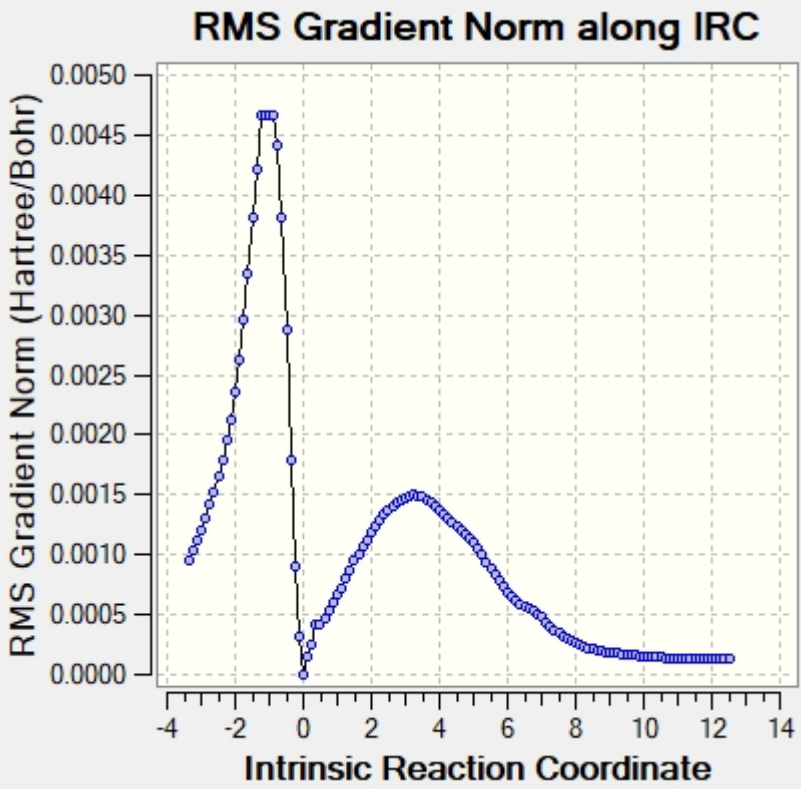
```
 Zero-point correction=                           0.411093
(Hartree/Particle)
 Thermal correction to Energy=                    0.437418
 Thermal correction to Enthalpy=                  0.438362
 Thermal correction to Gibbs Free Energy=         0.352565
 Sum of electronic and zero-point Energies=          -1219.405345
 Sum of electronic and thermal Energies=             -1219.379021
 Sum of electronic and thermal Enthalpies=           -1219.378076
 Sum of electronic and thermal Free Energies=        -1219.463873
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.922315	-0.919778	-0.509997
2	7	0	-4.695625	-1.605375	0.408646
3	8	0	-4.072163	-1.101163	-1.719517
4	6	0	-1.610178	1.878248	-0.331196
5	6	0	-0.722748	4.402753	0.491249
6	6	0	-0.539605	2.497929	-0.985098
7	6	0	-2.234310	2.533160	0.731499
8	6	0	-1.787557	3.787903	1.145252
9	6	0	-0.102954	3.756229	-0.579238
10	1	0	-0.046302	1.989592	-1.809318
11	1	0	-3.072690	2.047335	1.219097
12	1	0	-2.279136	4.288247	1.973814
13	1	0	0.717645	4.236992	-1.103916
14	1	0	-0.381110	5.383672	0.806949
15	6	0	-2.133970	0.541656	-0.806149
16	8	0	-0.806462	-0.315111	-0.951973
17	6	0	-0.963328	-1.489477	-1.779351
18	1	0	0.025218	-1.938118	-1.872923
19	1	0	-1.348399	-1.167799	-2.746774
20	1	0	-1.668896	-2.184502	-1.319243
21	7	0	-2.995395	-0.090214	0.080181
22	1	0	-0.662851	-0.637934	0.090681
23	1	0	-5.524084	-2.031971	0.022116
24	1	0	-4.783723	-1.200417	1.328121
25	8	0	-1.062347	-0.917595	1.368991
26	6	0	-0.387374	-0.210873	2.404237
27	1	0	-0.873430	-0.401192	3.365079
28	1	0	-0.384826	0.867914	2.206235
29	1	0	-2.055557	-0.563977	1.106239
30	1	0	-2.491178	0.563761	-1.840769
31	1	0	0.642710	-0.576334	2.437150
32	7	0	1.541387	-2.031699	0.275748
33	6	0	1.208066	-3.432502	0.357124
34	7	0	-0.021595	-3.597513	0.888279
35	1	0	-0.363969	-4.536360	1.014860

36	1	0	-0.557415	-2.790626	1.194629
37	8	0	1.931914	-4.339053	-0.017067
38	6	0	2.769386	-1.800136	0.009871
39	1	0	3.467769	-2.633840	-0.136740
40	6	0	3.310136	-0.439984	-0.100450
41	6	0	4.422312	2.112941	-0.268077
42	6	0	4.680905	-0.280997	-0.329923
43	6	0	2.492927	0.691288	0.034160
44	6	0	3.051013	1.960758	-0.044097
45	6	0	5.237268	0.992754	-0.415447
46	1	0	5.309629	-1.161487	-0.436771
47	1	0	1.425694	0.561703	0.192773
48	1	0	2.415066	2.832712	0.070923
49	1	0	6.301299	1.110821	-0.592925
50	1	0	4.853541	3.107572	-0.328961

2x(1a+MeOH)-ts IRC





3x(1a+MeOH)-ts

Zero-point correction=	0.616372
(Hartree/Particle)	
Thermal correction to Energy=	0.657774
Thermal correction to Enthalpy=	0.658718
Thermal correction to Gibbs Free Energy=	0.538378
Sum of electronic and zero-point Energies=	-1829.146708
Sum of electronic and thermal Energies=	-1829.105306
Sum of electronic and thermal Enthalpies=	-1829.104361
Sum of electronic and thermal Free Energies=	-1829.224702

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.355420	2.242682	0.323270
2	7	0	2.319717	2.498691	1.279585
3	8	0	0.951619	3.147553	-0.414748
4	6	0	-0.170413	-0.698490	-1.168544
5	6	0	-0.272202	-3.206579	-2.401110
6	6	0	-1.104960	-0.955654	-2.177832
7	6	0	0.709053	-1.706892	-0.780434
8	6	0	0.664479	-2.957849	-1.399149
9	6	0	-1.163033	-2.203447	-2.789406
10	1	0	-1.782450	-0.161678	-2.485220
11	1	0	1.451371	-1.513064	-0.013969
12	1	0	1.381996	-3.714435	-1.097226
13	1	0	-1.905825	-2.398909	-3.556019
14	1	0	-0.309209	-4.177796	-2.886049
15	6	0	-0.119361	0.682880	-0.563826
16	1	0	-0.230963	1.462431	-1.324994
17	8	0	-1.522291	0.788878	0.144809
18	8	0	-1.488371	-0.939918	1.851638
19	6	0	-2.440919	-0.807728	2.908485
20	1	0	-2.524935	0.237061	3.229571
21	1	0	-2.127715	-1.418505	3.759004
22	6	0	-1.727115	2.056701	0.800749
23	1	0	-2.754056	2.060844	1.170517
24	1	0	-1.573154	2.845698	0.064534
25	1	0	-1.010122	2.172996	1.619016
26	7	0	0.914774	0.939790	0.323717
27	1	0	-1.584074	-0.033977	0.901372
28	1	0	2.858994	3.333374	1.096599
29	1	0	2.855288	1.706697	1.606790
30	8	0	0.810085	-0.412856	2.460391
31	1	0	-0.489827	-0.813412	2.207702
32	6	0	1.843257	-1.348448	2.707938
33	1	0	1.725325	-2.259434	2.105791
34	1	0	1.831949	-1.618267	3.767572
35	1	0	0.966978	0.154201	1.555497
36	1	0	2.819453	-0.903983	2.477452
37	7	0	4.674174	-1.138610	0.548030
38	6	0	4.265622	-2.492357	0.743206
39	7	0	4.917265	-3.041637	1.796257
40	1	0	4.764016	-4.013566	2.011295
41	1	0	5.645277	-2.521645	2.258187
42	8	0	3.423074	-3.088033	0.090374
43	6	0	4.115855	-0.540782	-0.438605
44	1	0	3.387387	-1.063072	-1.071004

45	6	0	4.400503	0.861424	-0.752677
46	6	0	4.802249	3.566529	-1.280685
47	6	0	3.602158	1.518745	-1.693468
48	6	0	5.417051	1.560990	-0.085812
49	6	0	5.618851	2.907885	-0.355111
50	6	0	3.794379	2.874300	-1.948555
51	1	0	2.801012	0.974960	-2.189002
52	1	0	6.028550	1.031878	0.638280
53	1	0	6.407472	3.451279	0.156198
54	1	0	3.141364	3.392146	-2.642183
55	1	0	4.951611	4.623979	-1.476895
56	1	0	-3.402346	-1.160080	2.531386
57	7	0	-3.952195	-1.463269	0.064352
58	6	0	-3.488866	-2.674111	-0.543122
59	7	0	-2.482482	-3.229616	0.175529
60	1	0	-1.986944	-2.629202	0.827794
61	1	0	-1.956938	-3.952315	-0.294198
62	8	0	-3.973958	-3.148279	-1.555149
63	6	0	-4.262626	-0.540494	-0.756196
64	1	0	-4.167548	-0.691799	-1.839367
65	6	0	-4.732655	0.775587	-0.293060
66	6	0	-5.493402	3.311095	0.591588
67	6	0	-4.641272	1.875685	-1.149657
68	6	0	-5.228326	0.946571	1.005813
69	6	0	-5.611390	2.209354	1.443318
70	6	0	-5.009874	3.143982	-0.705066
71	1	0	-4.261590	1.738518	-2.159357
72	1	0	-5.310889	0.078272	1.652209
73	1	0	-6.004783	2.339444	2.446648
74	1	0	-4.922462	3.998408	-1.368479
75	1	0	-5.787014	4.297262	0.937428

3.2.2 M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

2x(1a+MeOH)-ts

Zero-point correction=	0.409547
(Hartree/Particle)	
Thermal correction to Energy=	0.436275
Thermal correction to Enthalpy=	0.437219
Thermal correction to Gibbs Free Energy=	0.349601
Sum of electronic and zero-point Energies=	-1219.426489
Sum of electronic and thermal Energies=	-1219.399761
Sum of electronic and thermal Enthalpies=	-1219.398817
Sum of electronic and thermal Free Energies=	-1219.486435

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.970114	-0.922692	-0.488748
2	7	0	-4.688033	-1.674590	0.420865
3	8	0	-4.228256	-1.001881	-1.701938
4	6	0	-1.645185	1.844329	-0.310353

5	6	0	-0.787093	4.373011	0.529836
6	6	0	-0.619017	2.505496	-0.995418
7	6	0	-2.239733	2.458754	0.792440
8	6	0	-1.808057	3.717208	1.214505
9	6	0	-0.195851	3.765366	-0.579907
10	1	0	-0.150862	2.028911	-1.852910
11	1	0	-3.041810	1.943285	1.309966
12	1	0	-2.275291	4.186127	2.074865
13	1	0	0.592580	4.276798	-1.124165
14	1	0	-0.455392	5.354583	0.853693
15	6	0	-2.141186	0.500724	-0.798500
16	8	0	-0.820055	-0.324546	-0.950235
17	6	0	-0.957257	-1.482406	-1.802919
18	1	0	0.023305	-1.954574	-1.846040
19	1	0	-1.265835	-1.136106	-2.789052
20	1	0	-1.702853	-2.166475	-1.390386
21	7	0	-2.994601	-0.160594	0.085127
22	1	0	-0.659650	-0.664575	0.096832
23	1	0	-5.570873	-2.030184	0.084323
24	1	0	-4.672900	-1.371148	1.383695
25	8	0	-1.019113	-0.972266	1.354415
26	6	0	-0.343034	-0.273521	2.401715
27	1	0	-0.826005	-0.485482	3.357945
28	1	0	-0.351549	0.806317	2.216969
29	1	0	-2.009917	-0.646077	1.137664
30	1	0	-2.504755	0.539391	-1.830015
31	1	0	0.688262	-0.633331	2.420147
32	7	0	1.599056	-2.028451	0.232502
33	6	0	1.303687	-3.430059	0.321296
34	7	0	0.087625	-3.633369	0.857720
35	1	0	-0.237653	-4.578765	0.989376
36	1	0	-0.470854	-2.841942	1.163367
37	8	0	2.052233	-4.324513	-0.058756
38	6	0	2.829739	-1.756045	0.013432
39	1	0	3.565836	-2.561899	-0.089815
40	6	0	3.330327	-0.382674	-0.100328
41	6	0	4.374805	2.197371	-0.290216
42	6	0	4.702895	-0.189840	-0.296661
43	6	0	2.477553	0.727458	-0.006533
44	6	0	3.002136	2.010751	-0.097269
45	6	0	5.225292	1.097941	-0.393391
46	1	0	5.359194	-1.053070	-0.370327
47	1	0	1.410666	0.572088	0.130414
48	1	0	2.341805	2.868215	-0.018734
49	1	0	6.289722	1.242961	-0.545877
50	1	0	4.778599	3.202593	-0.361181

3.2.3 M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

2x(1a+MeOH)-ts

```
 Zero-point correction=                           0.409809
(Hartree/Particle)
 Thermal correction to Energy=                    0.436409
 Thermal correction to Enthalpy=                  0.437354
 Thermal correction to Gibbs Free Energy=         0.350513
 Sum of electronic and zero-point Energies=          -1219.429809
 Sum of electronic and thermal Energies=             -1219.403208
 Sum of electronic and thermal Enthalpies=           -1219.402263
 Sum of electronic and thermal Free Energies=        -1219.489104
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.114901	-0.518970	-0.104494
2	7	0	-4.796462	-1.148801	0.917831
3	8	0	-4.548652	-0.581591	-1.269699
4	6	0	-1.452972	1.915137	-0.370403
5	6	0	-0.163656	4.337488	0.174190
6	6	0	-0.575102	2.474760	-1.306703
7	6	0	-1.683054	2.576183	0.835808
8	6	0	-1.033460	3.781903	1.110101
9	6	0	0.062781	3.681887	-1.039033
10	1	0	-0.393084	1.958927	-2.246332
11	1	0	-2.376710	2.143880	1.549815
12	1	0	-1.214649	4.288502	2.052947
13	1	0	0.739449	4.110246	-1.772258
14	1	0	0.335807	5.278168	0.384885
15	6	0	-2.168173	0.627052	-0.708871
16	8	0	-0.986860	-0.358462	-0.976582
17	6	0	-1.359058	-1.498148	-1.781146
18	1	0	-0.461441	-2.102944	-1.900539
19	1	0	-1.704994	-1.126737	-2.745456
20	1	0	-2.150082	-2.065428	-1.284354
21	7	0	-2.976333	0.108042	0.305343
22	1	0	-0.742354	-0.707014	0.058866
23	1	0	-5.759155	-1.379440	0.719676
24	1	0	-4.601626	-0.842245	1.859998
25	8	0	-0.994039	-0.987396	1.338855
26	6	0	-0.151305	-0.395727	2.331362
27	1	0	-0.576539	-0.569214	3.321895
28	1	0	-0.045048	0.680686	2.158784
29	1	0	-1.948987	-0.534304	1.234895
30	1	0	-2.655201	0.674951	-1.687953
31	1	0	0.827793	-0.873720	2.258932
32	7	0	1.423690	-2.145212	-0.019834
33	6	0	1.059805	-3.527758	-0.013205
34	7	0	-0.119495	-3.719152	0.604726
35	1	0	-0.481657	-4.656149	0.694961
36	1	0	-0.606615	-2.933288	1.023695
37	8	0	1.726243	-4.420069	-0.529836
38	6	0	2.680974	-1.919103	-0.089083
39	1	0	3.394859	-2.750131	-0.139609
40	6	0	3.242887	-0.564274	-0.074796
41	6	0	4.391376	1.976000	0.031514

42	6	0	4.634761	-0.420797	-0.038388
43	6	0	2.424349	0.575788	-0.068627
44	6	0	3.000022	1.839188	-0.012557
45	6	0	5.209445	0.847317	0.014240
46	1	0	5.264771	-1.306253	-0.045585
47	1	0	1.344446	0.460384	-0.115125
48	1	0	2.365737	2.719717	-0.003607
49	1	0	6.288725	0.954068	0.045123
50	1	0	4.834915	2.965784	0.078519

3.2.4 M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

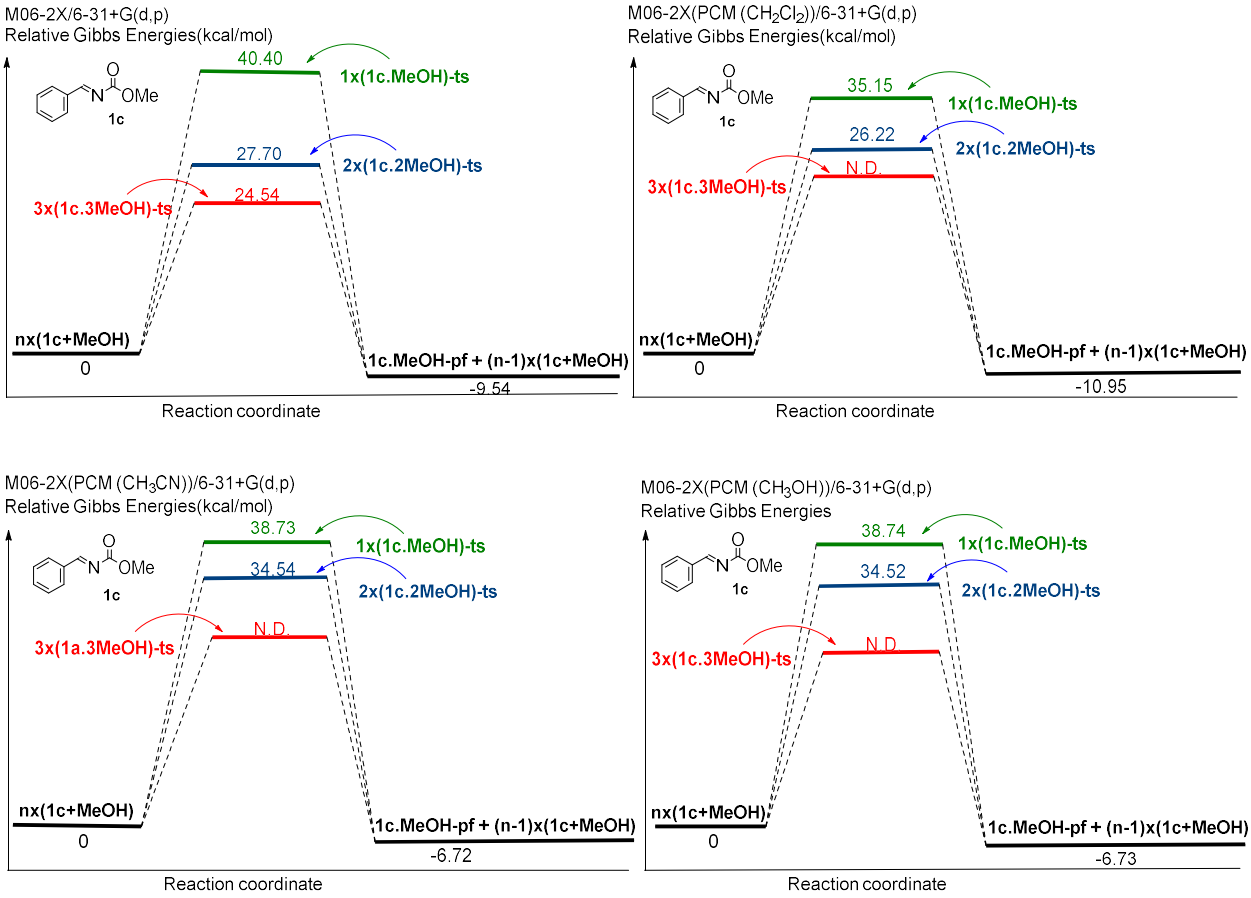
2x(1a+MeOH)-ts

Zero-point correction= 0.409818
(Hartree/Particle)
Thermal correction to Energy= 0.436418
Thermal correction to Enthalpy= 0.437362
Thermal correction to Gibbs Free Energy= 0.350529
Sum of electronic and zero-point Energies= -1219.429687
Sum of electronic and thermal Energies= -1219.403087
Sum of electronic and thermal Enthalpies= -1219.402143
Sum of electronic and thermal Free Energies= -1219.488976

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.114587	-0.519976	-0.103772
2	7	0	-4.795907	-1.149338	0.919027
3	8	0	-4.547944	-0.583947	-1.268966
4	6	0	-1.453537	1.915258	-0.370746
5	6	0	-0.164371	4.337873	0.173095
6	6	0	-0.574430	2.473829	-1.306520
7	6	0	-1.684964	2.577534	0.834532
8	6	0	-1.035474	3.783384	1.108448
9	6	0	0.063384	3.681073	-1.039220
10	1	0	-0.391342	1.957066	-2.245424
11	1	0	-2.379529	2.145998	1.548110
12	1	0	-1.217750	4.290973	2.050555
13	1	0	0.740970	4.108609	-1.772080
14	1	0	0.334999	5.278672	0.383485
15	6	0	-2.168726	0.627047	-0.708765
16	8	0	-0.987250	-0.358426	-0.976728
17	6	0	-1.359501	-1.498368	-1.780920
18	1	0	-0.461579	-2.102540	-1.901193
19	1	0	-1.706664	-1.127209	-2.744879
20	1	0	-2.149703	-2.066132	-1.283382
21	7	0	-2.976461	0.108195	0.305798
22	1	0	-0.742378	-0.706549	0.058589
23	1	0	-5.758340	-1.380934	0.720728
24	1	0	-4.601707	-0.841463	1.860888
25	8	0	-0.993664	-0.986143	1.339158

26	6	0	-0.150530	-0.393108	2.330452
27	1	0	-0.574964	-0.565730	3.321496
28	1	0	-0.044818	0.683178	2.156691
29	1	0	-1.948818	-0.533212	1.235010
30	1	0	-2.656082	0.674588	-1.687703
31	1	0	0.828740	-0.870732	2.257851
32	7	0	1.423453	-2.144897	-0.019827
33	6	0	1.058955	-3.527308	-0.013151
34	7	0	-0.120204	-3.718176	0.605282
35	1	0	-0.482792	-4.655006	0.695486
36	1	0	-0.606749	-2.932081	1.024489
37	8	0	1.724785	-4.419840	-0.530085
38	6	0	2.680822	-1.919369	-0.089155
39	1	0	3.394327	-2.750730	-0.139634
40	6	0	3.243326	-0.564757	-0.074836
41	6	0	4.392964	1.974993	0.032043
42	6	0	4.635225	-0.421937	-0.036912
43	6	0	2.425341	0.575733	-0.070019
44	6	0	3.001603	1.838853	-0.013679
45	6	0	5.210485	0.845900	0.016047
46	1	0	5.264804	-1.307709	-0.043182
47	1	0	1.345415	0.461011	-0.118059
48	1	0	2.367731	2.719693	-0.005807
49	1	0	6.289784	0.952116	0.048150
50	1	0	4.836945	2.964570	0.079281

3.3.-Energy profiles of the addition of methanol (2a) to imine derivative 1c in clusters 1x(1c+2a), 2x(1c+2a), and 3x(1c+2a) in gas phase, CH_2Cl_2, CH_3CN and CH_3OH.



N.D.=Not determined

3.4.- Computacional data of the addition of methanol (2a) to imine 1c in clusters 1x(1c+2a), 2x(1c+2a), and 3x(1c+2a)

3.4.1 M06-2X/6-31+G(d,p) calculations

2x(1c+MeOH)-ts

```
 Zero-point correction=                           0.443320
(Hartree/Particle)
 Thermal correction to Energy=                    0.472518
 Thermal correction to Enthalpy=                  0.473462
 Thermal correction to Gibbs Free Energy=         0.380433
 Sum of electronic and zero-point Energies=          -1337.656152
 Sum of electronic and thermal Energies=             -1337.626954
 Sum of electronic and thermal Enthalpies=           -1337.626009
 Sum of electronic and thermal Free Energies=        -1337.719038
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.478364	2.783932	0.369084
2	8	0	2.641941	3.321183	1.604265
3	8	0	2.577724	3.469705	-0.644111
4	6	0	2.405469	-0.602494	-0.857353
5	6	0	3.341723	-3.222405	-1.141295
6	6	0	2.350509	-1.241978	-2.099657
7	6	0	2.930213	-1.281447	0.241392
8	6	0	3.385987	-2.593113	0.101247
9	6	0	2.823736	-2.542960	-2.245940
10	1	0	1.944640	-0.709621	-2.956831
11	1	0	3.005013	-0.758857	1.190230
12	1	0	3.796714	-3.115005	0.960358
13	1	0	2.792674	-3.025438	-3.218087
14	1	0	3.717549	-4.234967	-1.253354
15	6	0	1.941893	0.829802	-0.745001
16	8	0	0.370706	0.689038	-0.915199
17	6	0	-0.269943	1.940084	-1.254738
18	1	0	-1.337335	1.736550	-1.326830
19	1	0	0.139970	2.273410	-2.208769
20	1	0	-0.059705	2.684177	-0.482880
21	7	0	2.208457	1.455267	0.463988
22	1	0	0.067370	0.422529	0.115410
23	8	0	0.133958	0.487886	1.463920
24	6	0	0.119245	-0.599067	2.380966
25	1	0	0.756810	-0.359890	3.237015
26	1	0	0.471293	-1.525198	1.911208
27	1	0	1.086652	0.931168	1.369282
28	1	0	2.204448	1.418514	-1.630238
29	1	0	-0.904438	-0.743095	2.733007
30	7	0	-3.045989	0.063663	-0.462190
31	6	0	-4.092734	1.015144	-0.429578
32	8	0	-3.702867	2.117019	-1.077518
33	8	0	-5.182982	0.884297	0.078551
34	6	0	-3.200804	-0.916897	0.347484
35	1	0	-4.073658	-0.958394	1.011254
36	6	0	-2.234392	-2.012583	0.439321
37	6	0	-0.370138	-4.063764	0.725043

38	6	0	-2.389418	-2.967871	1.450715
39	6	0	-1.149340	-2.100469	-0.443923
40	6	0	-0.219785	-3.121822	-0.296592
41	6	0	-1.456468	-3.991322	1.596226
42	1	0	-3.236421	-2.898623	2.129085
43	1	0	-1.040730	-1.357188	-1.227593
44	1	0	0.631614	-3.177246	-0.966497
45	1	0	-1.575006	-4.727055	2.384995
46	1	0	0.365975	-4.853991	0.839750
47	6	0	-4.671248	3.167777	-1.121236
48	1	0	-4.939171	3.476023	-0.108704
49	1	0	-5.568856	2.830031	-1.643364
50	1	0	-4.193912	3.983674	-1.660481
51	6	0	2.948182	4.709726	1.618293
52	1	0	2.157886	5.287008	1.131824
53	1	0	3.891388	4.903146	1.101331
54	1	0	3.027820	4.983155	2.670273

3x(1c+MeOH)-ts

Zero-point correction= 0.667629
(Hartree/Particle)
Thermal correction to Energy= 0.713180
Thermal correction to Enthalpy= 0.714124
Thermal correction to Gibbs Free Energy= 0.582853
Sum of electronic and zero-point Energies= -2006.520296
Sum of electronic and thermal Energies= -2006.474745
Sum of electronic and thermal Enthalpies= -2006.473801
Sum of electronic and thermal Free Energies= -2006.605072

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.742616	1.859579	-0.556172
2	8	0	-1.698531	2.157043	-1.465947
3	8	0	-0.041499	2.723926	-0.043349
4	6	0	-0.113859	-1.158793	1.340061
5	6	0	-0.697850	-3.441834	2.838042
6	6	0	0.653626	-1.478473	2.463460
7	6	0	-1.174579	-1.989113	0.970670
8	6	0	-1.469664	-3.124902	1.719579
9	6	0	0.366190	-2.619219	3.208628
10	1	0	1.492968	-0.847003	2.742954
11	1	0	-1.788461	-1.735080	0.113287
12	1	0	-2.317676	-3.739593	1.435905
13	1	0	0.977268	-2.866187	4.070747
14	1	0	-0.930688	-4.325083	3.425200
15	6	0	0.201286	0.082802	0.562606
16	1	0	0.687726	0.862428	1.158987
17	8	0	1.593768	-0.420435	-0.257641
18	8	0	0.886974	-2.292121	-1.705514
19	6	0	1.753008	-2.483621	-2.823327
20	1	0	1.617449	-1.684173	-3.560114
21	1	0	1.543401	-3.448062	-3.295788

22	6	0	2.050985	0.555680	-1.208480
23	1	0	2.966952	0.168921	-1.661278
24	1	0	2.249998	1.485305	-0.671654
25	1	0	1.283351	0.725123	-1.970701
26	7	0	-0.733381	0.512991	-0.326327
27	1	0	1.323151	-1.290145	-0.817735
28	8	0	-1.184374	-1.026114	-2.405608
29	1	0	-0.014212	-1.960442	-2.032408
30	6	0	-2.541913	-1.373670	-2.607303
31	1	0	-2.866170	-2.140674	-1.890181
32	1	0	-2.655081	-1.770688	-3.619296
33	1	0	-1.113125	-0.386910	-1.613920
34	1	0	-3.182902	-0.491046	-2.502058
35	7	0	-4.861356	0.103272	-0.185820
36	6	0	-4.861143	-1.293523	-0.346851
37	8	0	-5.599530	-1.620359	-1.412855
38	8	0	-4.313960	-2.115096	0.359949
39	6	0	-3.918898	0.565824	0.549927
40	1	0	-3.148460	-0.089678	0.973054
41	6	0	-3.837238	1.992121	0.881839
42	6	0	-3.673020	4.683354	1.588365
43	6	0	-2.797720	2.440829	1.701886
44	6	0	-4.795301	2.900014	0.407958
45	6	0	-4.713066	4.239199	0.765187
46	6	0	-2.711924	3.786935	2.051081
47	1	0	-2.051034	1.732494	2.053814
48	1	0	-5.590229	2.531093	-0.232435
49	1	0	-5.455381	4.943384	0.402532
50	1	0	-1.891747	4.132923	2.671023
51	1	0	-3.609961	5.732562	1.861073
52	1	0	2.780495	-2.481135	-2.453638
53	7	0	4.556701	-1.168515	0.104846
54	6	0	3.781132	-2.144013	0.771670
55	8	0	3.241119	-2.965925	-0.128346
56	8	0	3.636329	-2.245676	1.968683
57	6	0	4.601893	-0.038664	0.699031
58	1	0	4.060925	0.121836	1.641350
59	6	0	5.335029	1.107422	0.149391
60	6	0	6.660109	3.332791	-0.879140
61	6	0	5.240101	2.343600	0.796343
62	6	0	6.098463	0.988289	-1.019990
63	6	0	6.760247	2.098336	-1.528003
64	6	0	5.900327	3.456602	0.281867
65	1	0	4.642313	2.430489	1.700432
66	1	0	6.158765	0.020474	-1.508494
67	1	0	7.354381	2.009069	-2.431976
68	1	0	5.819492	4.415895	0.782356
69	1	0	7.175488	4.198756	-1.283168
70	6	0	-5.734493	-3.020021	-1.652228
71	1	0	-6.207333	-3.506273	-0.795897
72	1	0	-4.757133	-3.477728	-1.824871
73	1	0	-6.360168	-3.105879	-2.538871
74	6	0	-1.907839	3.547089	-1.690962
75	1	0	-2.701108	3.608313	-2.435673
76	1	0	-0.994769	4.020662	-2.060096
77	1	0	-2.218584	4.037659	-0.764116
78	6	0	2.356659	-3.964991	0.395625
79	1	0	2.112875	-4.607185	-0.448825
80	1	0	1.449231	-3.494326	0.781766
81	1	0	2.854288	-4.524074	1.190281

3.4.2 M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

2x(1c+MeOH)-ts

```
 Zero-point correction=                           0.442791
(Hartree/Particle)
 Thermal correction to Energy=                    0.472066
 Thermal correction to Enthalpy=                  0.473010
 Thermal correction to Gibbs Free Energy=         0.379794
 Sum of electronic and zero-point Energies=          -1337.674570
 Sum of electronic and thermal Energies=             -1337.645295
 Sum of electronic and thermal Enthalpies=           -1337.644351
 Sum of electronic and thermal Free Energies=        -1337.737567
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.610023	2.705216	0.342187
2	8	0	2.748976	3.272521	1.571339
3	8	0	2.842357	3.354422	-0.681064
4	6	0	2.380112	-0.676248	-0.824808
5	6	0	3.241843	-3.326992	-1.052743
6	6	0	2.397433	-1.308254	-2.072268
7	6	0	2.796821	-1.377278	0.306994
8	6	0	3.216140	-2.703745	0.193913
9	6	0	2.833836	-2.625628	-2.189678
10	1	0	2.078391	-0.759434	-2.955351
11	1	0	2.812840	-0.871734	1.267562
12	1	0	3.535692	-3.245120	1.079127
13	1	0	2.857992	-3.104073	-3.163814
14	1	0	3.583219	-4.353840	-1.141105
15	6	0	1.939516	0.765517	-0.744148
16	8	0	0.386501	0.670024	-0.902048
17	6	0	-0.220558	1.919969	-1.308164
18	1	0	-1.298336	1.765133	-1.286706
19	1	0	0.125944	2.140027	-2.318018
20	1	0	0.077389	2.714399	-0.619623
21	7	0	2.223167	1.418565	0.457971
22	1	0	0.057373	0.445947	0.128706
23	8	0	0.086111	0.538651	1.477979
24	6	0	0.016855	-0.564924	2.384137
25	1	0	0.695477	-0.389172	3.222358
26	1	0	0.284220	-1.501690	1.883002
27	1	0	1.041207	0.937826	1.404587
28	1	0	2.224353	1.323782	-1.641531
29	1	0	-1.005393	-0.635812	2.758937
30	7	0	-3.076022	0.138484	-0.477074
31	6	0	-4.093577	1.115197	-0.432191
32	8	0	-3.658795	2.229891	-1.018995
33	8	0	-5.206005	0.987018	0.035442
34	6	0	-3.225730	-0.830814	0.349698
35	1	0	-4.070540	-0.845599	1.048624
36	6	0	-2.284852	-1.948764	0.418144
37	6	0	-0.463749	-4.044567	0.661019
38	6	0	-2.434529	-2.894821	1.439793
39	6	0	-1.226888	-2.066916	-0.495261
40	6	0	-0.320267	-3.111460	-0.370729
41	6	0	-1.522435	-3.940347	1.563365

42	1	0	-3.257446	-2.800161	2.143639
43	1	0	-1.119008	-1.330930	-1.285645
44	1	0	0.507081	-3.194624	-1.067642
45	1	0	-1.634971	-4.668142	2.360059
46	1	0	0.254513	-4.853250	0.758854
47	6	0	-4.593873	3.315728	-1.057610
48	1	0	-4.870191	3.608573	-0.043320
49	1	0	-5.486698	3.020215	-1.611187
50	1	0	-4.077946	4.127604	-1.564990
51	6	0	3.163899	4.635521	1.577207
52	1	0	2.446198	5.261863	1.042256
53	1	0	4.147368	4.744345	1.114361
54	1	0	3.207977	4.925976	2.626196

3.4.3 M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

2x(1c+MeOH)-ts

Zero-point correction= 0.442644
(Hartree/Particle)
Thermal correction to Energy= 0.471917
Thermal correction to Enthalpy= 0.472861
Thermal correction to Gibbs Free Energy= 0.379603
Sum of electronic and zero-point Energies= -1337.677776
Sum of electronic and thermal Energies= -1337.648502
Sum of electronic and thermal Enthalpies= -1337.647558
Sum of electronic and thermal Free Energies= -1337.740816

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.636804	2.688095	0.336154
2	8	0	2.780155	3.262069	1.562250
3	8	0	2.884995	3.328210	-0.690457
4	6	0	2.376405	-0.691853	-0.817804
5	6	0	3.221341	-3.348912	-1.037054
6	6	0	2.408147	-1.321929	-2.066022
7	6	0	2.770593	-1.398056	0.319204
8	6	0	3.181822	-2.727370	0.210245
9	6	0	2.836317	-2.642570	-2.178936
10	1	0	2.105851	-0.769708	-2.952806
11	1	0	2.773243	-0.897048	1.282288
12	1	0	3.482124	-3.273178	1.099385
13	1	0	2.870808	-3.119901	-3.153268
14	1	0	3.554446	-4.378753	-1.121536
15	6	0	1.939447	0.751438	-0.742239
16	8	0	0.391275	0.664661	-0.893923
17	6	0	-0.210274	1.913200	-1.313427
18	1	0	-1.288892	1.766043	-1.280837
19	1	0	0.128446	2.115643	-2.329532
20	1	0	0.098158	2.715210	-0.638316
21	7	0	2.230533	1.409789	0.458159
22	1	0	0.059666	0.449927	0.141369

23	8	0	0.084737	0.547867	1.484029
24	6	0	0.003235	-0.560747	2.385463
25	1	0	0.685537	-0.397748	3.222950
26	1	0	0.258622	-1.496882	1.877472
27	1	0	1.041460	0.938719	1.413856
28	1	0	2.227368	1.304170	-1.641973
29	1	0	-1.019404	-0.620458	2.760574
30	7	0	-3.084427	0.156254	-0.478437
31	6	0	-4.095744	1.138259	-0.431719
32	8	0	-3.650907	2.255002	-1.005706
33	8	0	-5.212815	1.011713	0.026643
34	6	0	-3.235266	-0.812435	0.349362
35	1	0	-4.075974	-0.822873	1.053107
36	6	0	-2.299552	-1.934799	0.412900
37	6	0	-0.486584	-4.038927	0.646545
38	6	0	-2.449296	-2.880996	1.434567
39	6	0	-1.245559	-2.056815	-0.504923
40	6	0	-0.343120	-3.105506	-0.385107
41	6	0	-1.541194	-3.930662	1.553321
42	1	0	-3.268005	-2.782778	2.142658
43	1	0	-1.136868	-1.320654	-1.294998
44	1	0	0.480909	-3.191983	-1.085656
45	1	0	-1.653297	-4.658258	2.350185
46	1	0	0.228442	-4.850851	0.740957
47	6	0	-4.579193	3.347323	-1.044269
48	1	0	-4.858589	3.637276	-0.030042
49	1	0	-5.470295	3.060101	-1.604774
50	1	0	-4.055384	4.158236	-1.544874
51	6	0	3.214991	4.619480	1.562978
52	1	0	2.507994	5.253607	1.023073
53	1	0	4.201976	4.711847	1.103989
54	1	0	3.259478	4.914497	2.610571

3.4.4 M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

2x(1c+MeOH)-ts

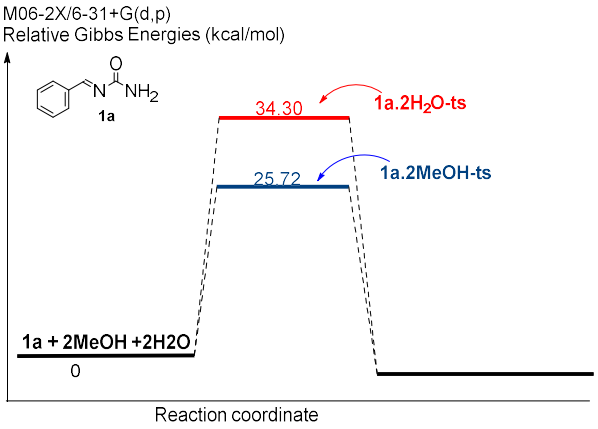
Zero-point correction= (Hartree/Particle)	0.442648
Thermal correction to Energy=	0.471921
Thermal correction to Enthalpy=	0.472865
Thermal correction to Gibbs Free Energy=	0.379620
Sum of electronic and zero-point Energies=	-1337.677669
Sum of electronic and thermal Energies=	-1337.648395
Sum of electronic and thermal Enthalpies=	-1337.647451
Sum of electronic and thermal Free Energies=	-1337.740697

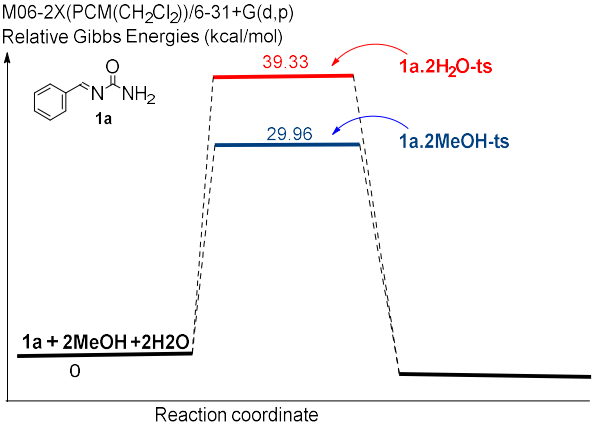
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

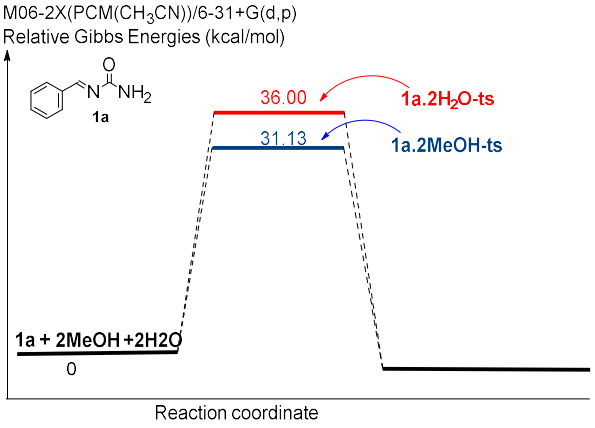
1	6	0	2.638514	2.686540	0.336324
2	8	0	2.782685	3.260001	1.562549
3	8	0	2.886725	3.326774	-0.690167
4	6	0	2.375647	-0.692916	-0.818446
5	6	0	3.219124	-3.350366	-1.038590
6	6	0	2.406074	-1.322902	-2.066742
7	6	0	2.770408	-1.399397	0.318183
8	6	0	3.180898	-2.728907	0.208788
9	6	0	2.833508	-2.643739	-2.180111
10	1	0	2.103371	-0.770447	-2.953244
11	1	0	2.774207	-0.898365	1.281250
12	1	0	3.481710	-3.274912	1.097638
13	1	0	2.867006	-3.121002	-3.154512
14	1	0	3.551718	-4.380345	-1.123431
15	6	0	1.939688	0.750645	-0.742398
16	8	0	0.391286	0.664865	-0.893869
17	6	0	-0.209453	1.914010	-1.312679
18	1	0	-1.288194	1.767793	-1.279680
19	1	0	0.129016	2.116537	-2.328854
20	1	0	0.099961	2.715526	-0.637434
21	7	0	2.231385	1.408437	0.458080
22	1	0	0.059825	0.450031	0.141387
23	8	0	0.085332	0.547852	1.484165
24	6	0	0.003092	-0.560343	2.385959
25	1	0	0.684833	-0.397072	3.223857
26	1	0	0.258649	-1.496777	1.878597
27	1	0	1.042387	0.938058	1.413738
28	1	0	2.227745	1.303453	-1.642043
29	1	0	-1.019808	-0.619759	2.760418
30	7	0	-3.084300	0.157762	-0.478104
31	6	0	-4.095231	1.140167	-0.431775
32	8	0	-3.649924	2.256611	-1.006112
33	8	0	-5.212366	1.014151	0.026527
34	6	0	-3.235595	-0.810664	0.349909
35	1	0	-4.076338	-0.820550	1.053628
36	6	0	-2.300459	-1.933514	0.413624
37	6	0	-0.488729	-4.038706	0.647295
38	6	0	-2.450753	-2.879617	1.435302
39	6	0	-1.246521	-2.056124	-0.504174
40	6	0	-0.344714	-3.105366	-0.384369
41	6	0	-1.543260	-3.929804	1.554076
42	1	0	-3.269445	-2.780949	2.143356
43	1	0	-1.137421	-1.320018	-1.294235
44	1	0	0.479254	-3.192424	-1.084901
45	1	0	-1.655802	-4.657343	2.350932
46	1	0	0.225808	-4.851064	0.741690
47	6	0	-4.577858	3.349192	-1.045183
48	1	0	-4.857406	3.639521	-0.031105
49	1	0	-5.468938	3.062077	-1.605781
50	1	0	-4.053696	4.159806	-1.545912
51	6	0	3.218914	4.616944	1.563480
52	1	0	2.512443	5.251933	1.023896
53	1	0	4.205857	4.708395	1.104214
54	1	0	3.263995	4.911664	2.611136

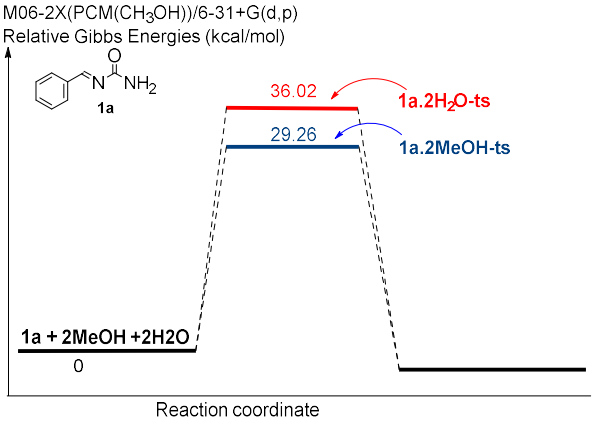
4.- Computational data on the addition of water to imines 1

4.1.-Comparative energy profiles for the addition of 2 water molecules vs. 2 methanol (2a) molecules to imine derivative 1a in gas phase, CH_2Cl_2, CH_3CN and CH_3OH.









4.2.-Computacional data for the addition of water to imine 1a

4.2.1 M06-2X/6-31+G(d,p) calculations

H_2O

```
Zero-point correction=                           0.021636
(Hartree/Particle)
 Thermal correction to Energy=                    0.024472
 Thermal correction to Enthalpy=                  0.025416
 Thermal correction to Gibbs Free Energy=         0.003999
 Sum of electronic and zero-point Energies=           -76.373328
 Sum of electronic and thermal Energies=              -76.370492
 Sum of electronic and thermal Enthalpies=            -76.369548
 Sum of electronic and thermal Free Energies=         -76.390965
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.768747	-0.462228
2	8	0	0.000000	0.000000	0.115557
3	1	0	0.000000	-0.768747	-0.462228

1a.2H_2O-ts

```
 Zero-point correction=                           0.200743
(Hartree/Particle)
 Thermal correction to Energy=                    0.213586
 Thermal correction to Enthalpy=                  0.214531
 Thermal correction to Gibbs Free Energy=         0.161437
 Sum of electronic and zero-point Energies=          -646.800506
 Sum of electronic and thermal Energies=             -646.787662
 Sum of electronic and thermal Enthalpies=           -646.786718
 Sum of electronic and thermal Free Energies=        -646.839812
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.241954	-0.270980	-0.672795
2	6	0	2.612704	-0.691649	-0.433333
3	7	0	3.442749	0.363052	-0.476749
4	8	0	2.863222	-1.861451	-0.249586
5	1	0	4.400936	0.174006	-0.223167
6	6	0	-1.105015	-0.399989	-0.037908
7	6	0	-3.807108	0.205299	-0.289189
8	6	0	-2.068976	-1.349286	0.313487
9	6	0	-1.491980	0.867015	-0.497012
10	6	0	-2.843488	1.162503	-0.618105
11	6	0	-3.421910	-1.049083	0.178290
12	1	0	-1.757244	-2.322674	0.682268
13	1	0	-0.734305	1.622347	-0.697205
14	1	0	-3.151059	2.144347	-0.962627

15	1	0	-4.170647	-1.789322	0.440282
16	1	0	-4.861444	0.443260	-0.390743
17	6	0	0.302806	-0.781036	0.078358
18	1	0	0.565421	-1.695798	0.603588
19	8	0	0.808005	0.459535	1.813534
20	1	0	1.076605	1.321453	1.205685
21	1	0	0.130713	0.713101	2.449311
22	1	0	1.127160	0.716330	-0.961337
23	1	0	3.009872	1.281211	-0.259434
24	8	0	1.461106	2.136391	0.150601
25	1	0	1.450219	3.088793	0.276271

4.2.2 M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

H_2O

Zero-point correction= 0.021545
(Hartree/Particle)
Thermal correction to Energy= 0.024381
Thermal correction to Enthalpy= 0.025325
Thermal correction to Gibbs Free Energy= 0.003901
Sum of electronic and zero-point Energies= -76.380586
Sum of electronic and thermal Energies= -76.377750
Sum of electronic and thermal Enthalpies= -76.376806
Sum of electronic and thermal Free Energies= -76.398230

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.766675	-0.466365
2	8	0	0.000000	0.000000	0.116591
3	1	0	0.000000	-0.766675	-0.466365

1a.2H_2O-ts

Zero-point correction= 0.199123
(Hartree/Particle)
Thermal correction to Energy= 0.212322
Thermal correction to Enthalpy= 0.213267
Thermal correction to Gibbs Free Energy= 0.158942
Sum of electronic and zero-point Energies= -646.816755
Sum of electronic and thermal Energies= -646.803555
Sum of electronic and thermal Enthalpies= -646.802611
Sum of electronic and thermal Free Energies= -646.856936

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

1	7	0	1.255723	-0.229008	-0.691821
2	6	0	2.619210	-0.651270	-0.470407
3	7	0	3.452757	0.396728	-0.439898
4	8	0	2.879519	-1.834204	-0.357514
5	1	0	4.419152	0.200865	-0.220631
6	6	0	-1.100895	-0.396970	-0.091102
7	6	0	-3.810111	0.209674	-0.276673
8	6	0	-2.055330	-1.290242	0.411345
9	6	0	-1.505403	0.810231	-0.680141
10	6	0	-2.858814	1.108551	-0.768379
11	6	0	-3.410222	-0.988732	0.312855
12	1	0	-1.732586	-2.219380	0.872452
13	1	0	-0.771225	1.524985	-1.039764
14	1	0	-3.176740	2.043180	-1.218009
15	1	0	-4.148987	-1.684288	0.695921
16	1	0	-4.866215	0.448517	-0.352194
17	6	0	0.301563	-0.779749	0.019404
18	1	0	0.552355	-1.719914	0.502187
19	8	0	0.775601	0.347627	1.853602
20	1	0	1.059905	1.255486	1.275347
21	1	0	-0.001004	0.545952	2.390391
22	1	0	1.136926	0.762171	-0.941127
23	1	0	3.034280	1.305875	-0.179979
24	8	0	1.481890	2.133185	0.356098
25	1	0	1.358704	3.060687	0.578529

4.2.3 M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

H_2O

Zero-point correction=	0.021517
(Hartree/Particle)	
Thermal correction to Energy=	0.024353
Thermal correction to Enthalpy=	0.025297
Thermal correction to Gibbs Free Energy=	0.003871
Sum of electronic and zero-point Energies=	-76.381674
Sum of electronic and thermal Energies=	-76.378838
Sum of electronic and thermal Enthalpies=	-76.377894
Sum of electronic and thermal Free Energies=	-76.399320

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.766046	-0.467698
2	8	0	0.000000	0.000000	0.116924
3	1	0	0.000000	-0.766046	-0.467698

1a.2H_2O-ts

Zero-point correction=	0.198777
(Hartree/Particle)	
Thermal correction to Energy=	0.211398
Thermal correction to Enthalpy=	0.212343
Thermal correction to Gibbs Free Energy=	0.158590
Sum of electronic and zero-point Energies=	-646.826043
Sum of electronic and thermal Energies=	-646.813421
Sum of electronic and thermal Enthalpies=	-646.812477
Sum of electronic and thermal Free Energies=	-646.866229

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.359486	0.164313	-0.364622
2	6	0	2.554530	-0.463456	-0.599670
3	7	0	3.479484	0.337028	-1.226216
4	8	0	2.826978	-1.649623	-0.347257
5	1	0	4.435477	0.016475	-1.221597
6	6	0	-1.025348	-0.318600	-0.034299
7	6	0	-3.720722	0.184735	-0.587060
8	6	0	-2.012570	-1.216712	0.384770
9	6	0	-1.394352	0.825943	-0.745108
10	6	0	-2.738400	1.077446	-1.016611
11	6	0	-3.356109	-0.966527	0.111721
12	1	0	-1.729225	-2.121193	0.918996
13	1	0	-0.624504	1.503280	-1.100367
14	1	0	-3.018517	1.967101	-1.571798
15	1	0	-4.114243	-1.671586	0.437513
16	1	0	-4.766119	0.380519	-0.804132
17	6	0	0.416044	-0.603297	0.303655
18	1	0	0.639206	-1.671296	0.335235
19	8	0	0.560032	-0.222229	1.855649
20	1	0	0.794440	0.888550	1.823458
21	1	0	-0.253498	-0.412280	2.351009
22	1	0	1.374892	1.474847	0.399829
23	1	0	3.326667	1.333735	-1.250837
24	8	0	1.251593	1.993063	1.325937
25	1	0	0.615366	2.715575	1.239544

4.2.4 M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

H_2O

```
 Zero-point correction=                           0.021518
(Hartree/Particle)
 Thermal correction to Energy=                    0.024353
 Thermal correction to Enthalpy=                  0.025298
 Thermal correction to Gibbs Free Energy=         0.003871
 Sum of electronic and zero-point Energies=            -76.381639
 Sum of electronic and thermal Energies=               -76.378803
 Sum of electronic and thermal Enthalpies=             -76.377859
 Sum of electronic and thermal Free Energies=          -76.399285
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.766046	-0.467698
2	8	0	0.000000	0.000000	0.116924
3	1	0	0.000000	-0.766046	-0.467698

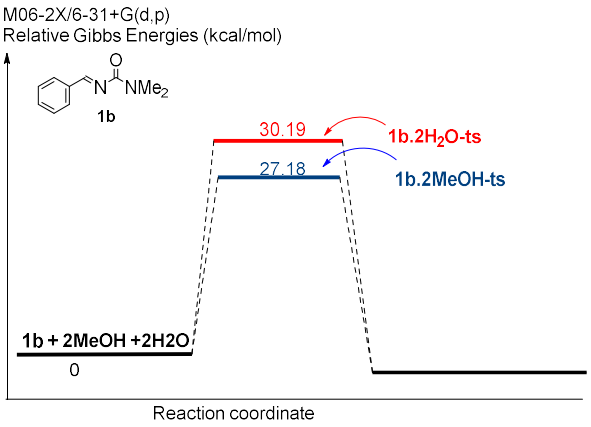
1a.2H_2O-ts

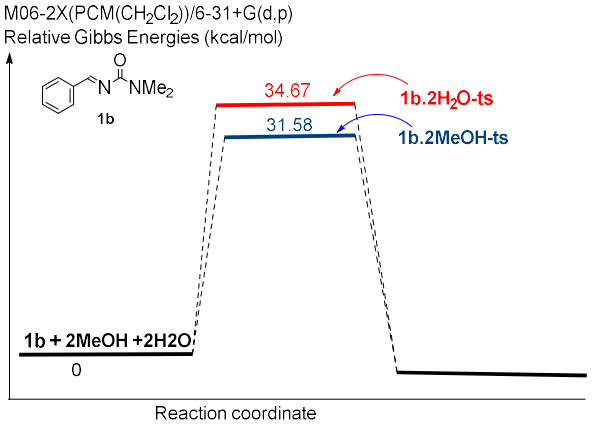
```
 Zero-point correction=                           0.198784
(Hartree/Particle)
 Thermal correction to Energy=                    0.211400
 Thermal correction to Enthalpy=                  0.212344
 Thermal correction to Gibbs Free Energy=         0.158627
 Sum of electronic and zero-point Energies=           -646.825912
 Sum of electronic and thermal Energies=              -646.813296
 Sum of electronic and thermal Enthalpies=            -646.812352
 Sum of electronic and thermal Free Energies=         -646.866070
```

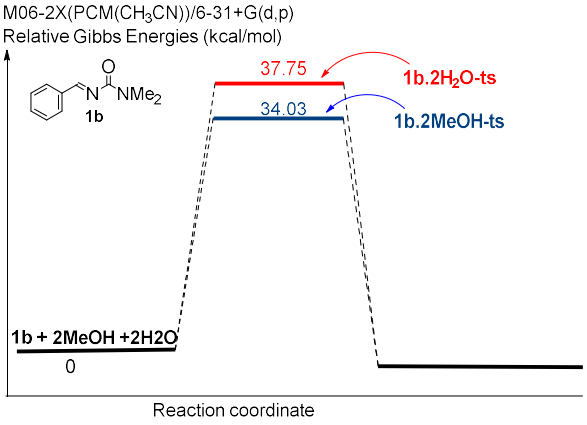
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.359441	0.166386	-0.363909
2	6	0	2.554845	-0.460063	-0.601588
3	7	0	3.479784	0.343636	-1.223821
4	8	0	2.827343	-1.647271	-0.354580
5	1	0	4.435740	0.023010	-1.221469
6	6	0	-1.025356	-0.318458	-0.036312
7	6	0	-3.720772	0.187841	-0.586191
8	6	0	-2.012992	-1.216448	0.382131
9	6	0	-1.393981	0.827329	-0.745251
10	6	0	-2.738074	1.080306	-1.015301
11	6	0	-3.356528	-0.964763	0.110591

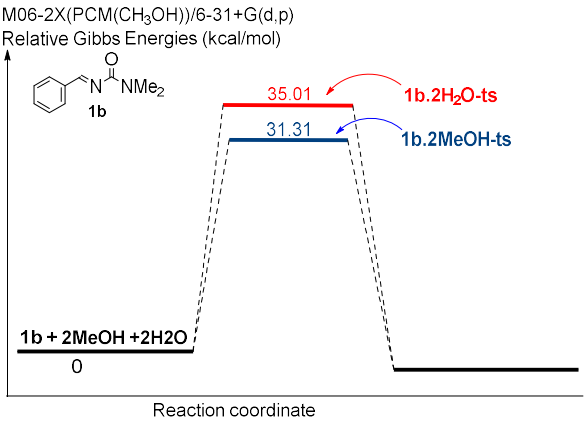
12	1	0	-1.729946	-2.122109	0.914558
13	1	0	-0.623771	1.504388	-1.100245
14	1	0	-3.017913	1.970920	-1.569093
15	1	0	-4.114973	-1.669718	0.435889
16	1	0	-4.766184	0.384772	-0.802146
17	6	0	0.416069	-0.604898	0.299998
18	1	0	0.639485	-1.672982	0.325969
19	8	0	0.559714	-0.232161	1.854461
20	1	0	0.794496	0.878767	1.827972
21	1	0	-0.254241	-0.424149	2.348328
22	1	0	1.374451	1.472167	0.407247
23	1	0	3.326533	1.340337	-1.244827
24	8	0	1.251385	1.985784	1.336296
25	1	0	0.614933	2.708554	1.254057

4.3.-Comparative energy profiles for the addition of 2 water molecules vs. 2 methanol (2a) molecules to imine derivative 1b in gas phase, CH_2Cl_2, CH_3CN and CH_3OH.









4.4.-Computacional data for the addition of water to imine 1b

4.4.1 M06-2X/6-31+G(d,p) calculations

1b.2H_2O-ts

```
 Zero-point correction=                           0.254919
(Hartree/Particle)
 Thermal correction to Energy=                    0.270467
 Thermal correction to Enthalpy=                  0.271411
 Thermal correction to Gibbs Free Energy=         0.211296
 Sum of electronic and zero-point Energies=           -725.322009
 Sum of electronic and thermal Energies=              -725.306462
 Sum of electronic and thermal Enthalpies=            -725.305517
 Sum of electronic and thermal Free Energies=         -725.365633
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.781420	0.040884	-0.121512
2	6	0	2.002700	-0.572819	-0.434223
3	7	0	3.055830	0.300074	-0.510265
4	8	0	2.129438	-1.775452	-0.655822
5	6	0	-1.634229	-0.309169	-0.202687
6	6	0	-4.236158	0.619389	-0.633341
7	6	0	-2.718122	-1.192391	-0.154443
8	6	0	-1.860075	1.038280	-0.490031
9	6	0	-3.157850	1.500481	-0.699392
10	6	0	-4.014764	-0.731670	-0.366138
11	1	0	-2.540735	-2.249912	0.033539
12	1	0	-1.008164	1.706215	-0.574278
13	1	0	-3.327889	2.548296	-0.926778
14	1	0	-4.848986	-1.425262	-0.333404
15	1	0	-5.245304	0.981331	-0.803382
16	6	0	-0.249483	-0.827477	0.049787
17	1	0	-0.064560	-1.848924	-0.285129
18	8	0	-0.297882	-1.131103	1.752041
19	1	0	-0.001363	-0.107460	2.120932
20	1	0	-1.193668	-1.358237	2.039166
21	1	0	0.731800	0.857475	0.957555
22	8	0	0.528497	1.085293	2.069116
23	1	0	-0.063553	1.834255	2.199118
24	6	0	4.397247	-0.226097	-0.666701
25	1	0	4.906285	0.281611	-1.493383
26	1	0	4.331562	-1.291413	-0.879478
27	1	0	4.982809	-0.074140	0.249575
28	6	0	2.942957	1.713335	-0.202551
29	1	0	3.026743	1.910927	0.874534
30	1	0	1.991105	2.104913	-0.562893
31	1	0	3.749410	2.242543	-0.717606

4.4.2 M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

1b.2H_2O-ts

```
 Zero-point correction=                           0.254966
(Hartree/Particle)
 Thermal correction to Energy=                    0.270620
 Thermal correction to Enthalpy=                  0.271564
 Thermal correction to Gibbs Free Energy=         0.210294
 Sum of electronic and zero-point Energies=           -725.338622
 Sum of electronic and thermal Energies=              -725.322968
 Sum of electronic and thermal Enthalpies=            -725.322024
 Sum of electronic and thermal Free Energies=         -725.383294
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.791167	0.027354	-0.059214
2	6	0	1.989691	-0.551054	-0.428440
3	7	0	3.024757	0.340112	-0.565910
4	8	0	2.151798	-1.762334	-0.660053
5	6	0	-1.630957	-0.302614	-0.192811
6	6	0	-4.207870	0.677234	-0.663121
7	6	0	-2.717776	-1.180097	-0.270170
8	6	0	-1.839716	1.067029	-0.369496
9	6	0	-3.125259	1.554611	-0.599406
10	6	0	-4.002503	-0.693450	-0.502618
11	1	0	-2.555818	-2.250782	-0.160785
12	1	0	-0.987386	1.739066	-0.347380
13	1	0	-3.281383	2.619925	-0.737938
14	1	0	-4.838727	-1.382295	-0.566889
15	1	0	-5.207008	1.059418	-0.847590
16	6	0	-0.258060	-0.856253	0.086451
17	1	0	-0.093328	-1.845734	-0.342290
18	8	0	-0.301847	-1.236449	1.674520
19	1	0	-0.022555	-0.251111	2.153552
20	1	0	-1.184576	-1.534255	1.946512
21	1	0	0.753457	0.821127	1.168573
22	8	0	0.532321	0.924766	2.232528
23	1	0	-0.067313	1.664397	2.395732
24	6	0	4.377731	-0.151257	-0.743722
25	1	0	4.879122	0.418134	-1.532866
26	1	0	4.341835	-1.201784	-1.023656
27	1	0	4.958527	-0.044249	0.182348
28	6	0	2.899340	1.745966	-0.224819
29	1	0	3.073610	1.926727	0.844927
30	1	0	1.908394	2.112609	-0.490978
31	1	0	3.645779	2.307979	-0.792448

4.4.3 M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

1b.2H_2O-ts

```
 Zero-point correction=                           0.255154
(Hartree/Particle)
 Thermal correction to Energy=                    0.270708
 Thermal correction to Enthalpy=                  0.271653
 Thermal correction to Gibbs Free Energy=         0.211162
 Sum of electronic and zero-point Energies=           -725.341654
 Sum of electronic and thermal Energies=              -725.326099
 Sum of electronic and thermal Enthalpies=            -725.325155
 Sum of electronic and thermal Free Energies=         -725.385646
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.791242	0.026581	-0.057474
2	6	0	1.985270	-0.553175	-0.424817
3	7	0	3.018718	0.337058	-0.587656
4	8	0	2.152262	-1.770099	-0.637413
5	6	0	-1.632400	-0.303616	-0.184643
6	6	0	-4.207694	0.671534	-0.674352
7	6	0	-2.716022	-1.183625	-0.275932
8	6	0	-1.843511	1.066722	-0.354758
9	6	0	-3.128234	1.551795	-0.594637
10	6	0	-3.999988	-0.699335	-0.518421
11	1	0	-2.552839	-2.254057	-0.167632
12	1	0	-0.995136	1.743076	-0.317864
13	1	0	-3.286146	2.617609	-0.727007
14	1	0	-4.833589	-1.390321	-0.592851
15	1	0	-5.206159	1.051913	-0.866115
16	6	0	-0.260517	-0.857100	0.104627
17	1	0	-0.100338	-1.848638	-0.321518
18	8	0	-0.296624	-1.220273	1.681867
19	1	0	-0.014708	-0.232634	2.161167
20	1	0	-1.176435	-1.522406	1.960194
21	1	0	0.761146	0.841668	1.185267
22	8	0	0.545755	0.936191	2.240422
23	1	0	-0.051403	1.677295	2.408682
24	6	0	4.373544	-0.155664	-0.750901
25	1	0	4.885754	0.421455	-1.526938
26	1	0	4.341859	-1.203164	-1.042354
27	1	0	4.942846	-0.058872	0.183581
28	6	0	2.894516	1.745499	-0.254265
29	1	0	3.074330	1.932300	0.813587
30	1	0	1.901948	2.110234	-0.516379
31	1	0	3.638228	2.304306	-0.828317

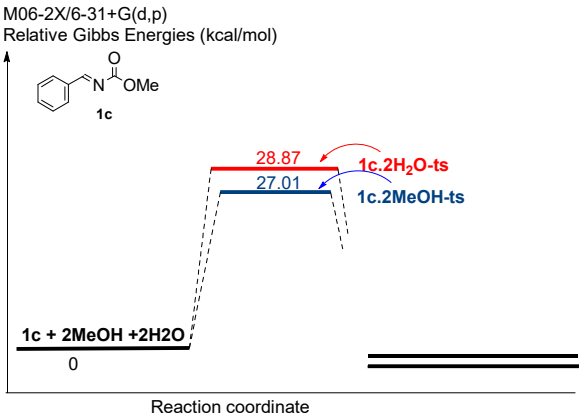
4.4.4 M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

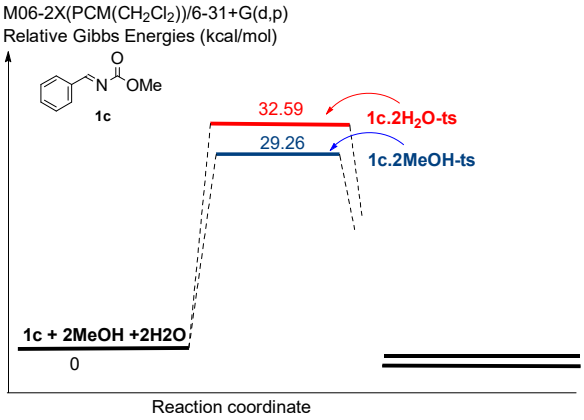
1b.2H_2O-ts

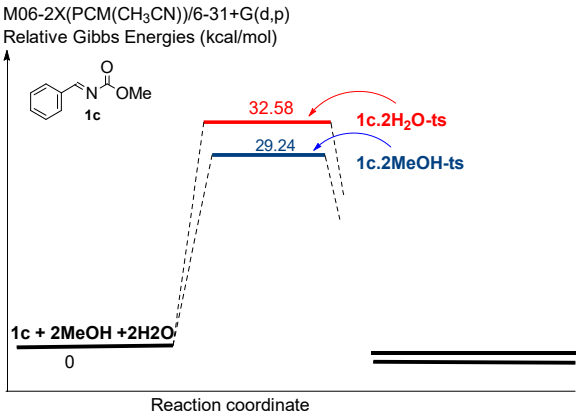
```
 Zero-point correction=                           0.255150
(Hartree/Particle)
 Thermal correction to Energy=                    0.270706
 Thermal correction to Enthalpy=                  0.271650
 Thermal correction to Gibbs Free Energy=         0.211149
 Sum of electronic and zero-point Energies=           -725.341547
 Sum of electronic and thermal Energies=              -725.325990
 Sum of electronic and thermal Enthalpies=            -725.325046
 Sum of electronic and thermal Free Energies=         -725.385548
```

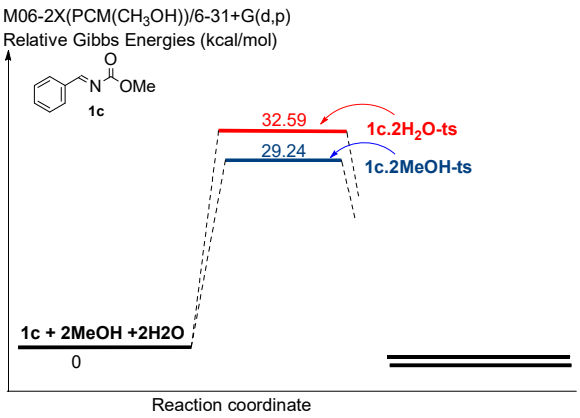
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.791273	0.026590	-0.057504
2	6	0	1.985423	-0.553205	-0.424859
3	7	0	3.018883	0.337053	-0.587215
4	8	0	2.152253	-1.770003	-0.637753
5	6	0	-1.632328	-0.303636	-0.184739
6	6	0	-4.207696	0.671534	-0.673996
7	6	0	-2.715979	-1.183630	-0.275810
8	6	0	-1.843454	1.066691	-0.354889
9	6	0	-3.128209	1.551778	-0.594537
10	6	0	-3.999981	-0.699331	-0.518069
11	1	0	-2.552763	-2.254068	-0.167598
12	1	0	-0.995008	1.742973	-0.318272
13	1	0	-3.286126	2.617582	-0.726992
14	1	0	-4.833603	-1.390304	-0.592375
15	1	0	-5.206188	1.051917	-0.865615
16	6	0	-0.260403	-0.857066	0.104289
17	1	0	-0.100089	-1.848610	-0.321774
18	8	0	-0.296707	-1.220446	1.681917
19	1	0	-0.015017	-0.232749	2.160987
20	1	0	-1.176554	-1.522569	1.960087
21	1	0	0.760916	0.841217	1.184524
22	8	0	0.545226	0.936382	2.239915
23	1	0	-0.051978	1.677537	2.407694
24	6	0	4.373653	-0.155634	-0.750901
25	1	0	4.885471	0.421132	-1.527469
26	1	0	4.341829	-1.203275	-1.041840
27	1	0	4.943368	-0.058386	0.183276
28	6	0	2.894601	1.745474	-0.253862
29	1	0	3.073924	1.932268	0.814073
30	1	0	1.902179	2.110271	-0.516476
31	1	0	3.638604	2.304243	-0.827578

4.5.-Comparative energy profiles for the addition of 2 water molecules vs. 2 methanol (2a) molecules to imine derivative 1c in gas phase, CH_2Cl_2, CH_3CN and CH_3OH.









4.6.-Computacional data for the addition of water to imine 1c

4.6.1 M06-2X/6-31+G(d,p) calculations

1c.2H_2O-ts

```
 Zero-point correction=                           0.215523
(Hartree/Particle)
 Thermal correction to Energy=                    0.229223
 Thermal correction to Enthalpy=                  0.230168
 Thermal correction to Gibbs Free Energy=         0.174015
 Sum of electronic and zero-point Energies=           -705.933469
 Sum of electronic and thermal Energies=              -705.919769
 Sum of electronic and thermal Enthalpies=            -705.918824
 Sum of electronic and thermal Free Energies=         -705.974977
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.004622	0.159633	-0.195062
2	6	0	2.224436	-0.468369	-0.240101
3	8	0	3.152482	0.367533	-0.754911
4	8	0	2.490018	-1.610873	0.095091
5	6	0	-1.381439	-0.334988	0.000464
6	6	0	-4.025513	0.028040	-0.829201
7	6	0	-2.412360	-1.086158	0.575179
8	6	0	-1.679222	0.582615	-1.007880
9	6	0	-2.998940	0.765317	-1.417231
10	6	0	-3.730416	-0.904279	0.165464
11	1	0	-2.179144	-1.832049	1.333704
12	1	0	-0.862772	1.120484	-1.479620
13	1	0	-3.224686	1.476224	-2.206075
14	1	0	-4.523658	-1.495554	0.611958
15	1	0	-5.051455	0.168189	-1.154909
16	6	0	0.031976	-0.528967	0.475852
17	1	0	0.281237	-1.559598	0.737212
18	8	0	-0.007201	0.142208	2.014329
19	1	0	0.237776	1.225828	1.774775
20	1	0	-0.890616	0.057679	2.402062
21	1	0	0.953180	1.524024	0.304411
22	8	0	0.715783	2.225603	1.110994
23	1	0	0.107262	2.911771	0.815014
24	6	0	4.461282	-0.183334	-0.860023
25	1	0	5.077035	0.603416	-1.294318
26	1	0	4.456356	-1.066376	-1.503080
27	1	0	4.839655	-0.466493	0.125139

4.6.2 M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

1c.2H_2O-ts

```
 Zero-point correction=                           0.215823
(Hartree/Particle)
 Thermal correction to Energy=                    0.229531
 Thermal correction to Enthalpy=                  0.230475
 Thermal correction to Gibbs Free Energy=         0.174156
 Sum of electronic and zero-point Energies=           -705.950635
 Sum of electronic and thermal Energies=              -705.936928
 Sum of electronic and thermal Enthalpies=            -705.935983
 Sum of electronic and thermal Free Energies=         -705.992302
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.011040	0.138651	-0.207520
2	6	0	2.207822	-0.494444	-0.141470
3	8	0	3.138123	0.181839	-0.863204
4	8	0	2.493752	-1.537722	0.444273
5	6	0	-1.385511	-0.313725	0.071232
6	6	0	-4.023112	-0.150300	-0.839205
7	6	0	-2.400701	-1.028265	0.716339
8	6	0	-1.694892	0.471264	-1.041460
9	6	0	-3.011505	0.554316	-1.492240
10	6	0	-3.716120	-0.946122	0.264961
11	1	0	-2.159139	-1.661501	1.567729
12	1	0	-0.896681	0.993298	-1.559101
13	1	0	-3.247490	1.162582	-2.359734
14	1	0	-4.497352	-1.507332	0.767532
15	1	0	-5.046344	-0.088026	-1.196076
16	6	0	0.022067	-0.400601	0.603402
17	1	0	0.255328	-1.381911	1.022568
18	8	0	0.015528	0.498665	1.930101
19	1	0	0.242425	1.533930	1.544029
20	1	0	-0.840188	0.456848	2.387442
21	1	0	0.969252	1.670110	0.065096
22	8	0	0.740954	2.440409	0.747366
23	1	0	0.118485	3.066952	0.355123
24	6	0	4.437921	-0.403180	-0.890193
25	1	0	5.047021	0.258864	-1.504062
26	1	0	4.402399	-1.401444	-1.332340
27	1	0	4.852350	-0.472127	0.117948

4.6.3 M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

1c.2H_2O-ts

```
 Zero-point correction=                           0.215575
(Hartree/Particle)
 Thermal correction to Energy=                    0.229351
 Thermal correction to Enthalpy=                  0.230295
 Thermal correction to Gibbs Free Energy=         0.173728
 Sum of electronic and zero-point Energies=           -705.954086
 Sum of electronic and thermal Energies=              -705.940309
 Sum of electronic and thermal Enthalpies=            -705.939365
 Sum of electronic and thermal Free Energies=         -705.995932
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.008179	0.137258	-0.215116
2	6	0	2.204147	-0.492160	-0.152395
3	8	0	3.133190	0.186442	-0.875885
4	8	0	2.497178	-1.535625	0.433260
5	6	0	-1.390066	-0.312625	0.065449
6	6	0	-4.030097	-0.131901	-0.835593
7	6	0	-2.400081	-1.056199	0.685141
8	6	0	-1.706106	0.511992	-1.016422
9	6	0	-3.023716	0.603327	-1.462696
10	6	0	-3.716679	-0.965656	0.238217
11	1	0	-2.154763	-1.716173	1.514723
12	1	0	-0.913938	1.061243	-1.514815
13	1	0	-3.264336	1.242969	-2.306017
14	1	0	-4.493726	-1.549123	0.721586
15	1	0	-5.054188	-0.062477	-1.188675
16	6	0	0.018080	-0.410494	0.595773
17	1	0	0.247260	-1.402922	0.990414
18	8	0	0.026385	0.456796	1.928091
19	1	0	0.261872	1.503855	1.569187
20	1	0	-0.824290	0.408766	2.395029
21	1	0	0.975893	1.681319	0.091598
22	8	0	0.764813	2.424384	0.800251
23	1	0	0.142365	3.070995	0.440735
24	6	0	4.435966	-0.392601	-0.905309
25	1	0	5.042436	0.275301	-1.515354
26	1	0	4.406039	-1.388260	-1.353725
27	1	0	4.850915	-0.464366	0.102389

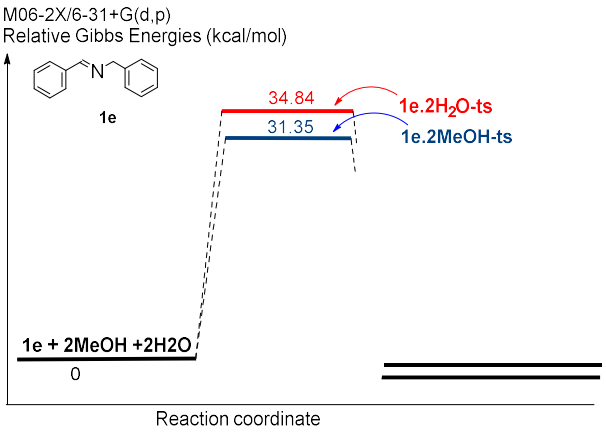
4.6.4 M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

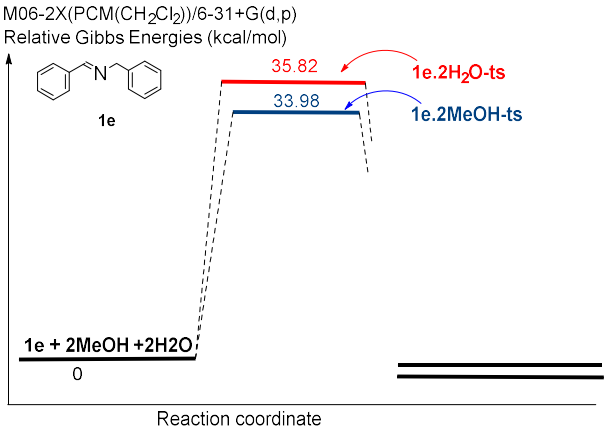
1c.2H_2O-ts

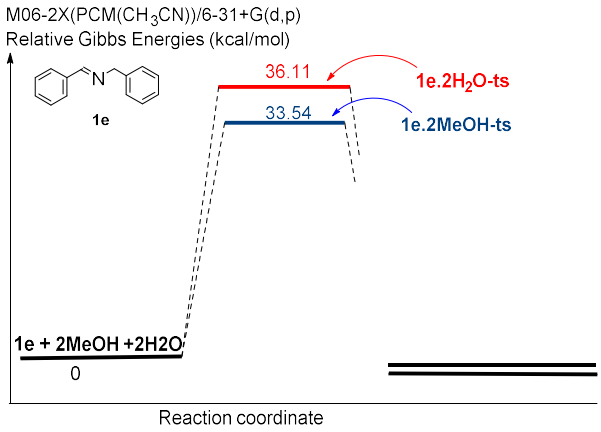
```
 Zero-point correction=                           0.215582
(Hartree/Particle)
 Thermal correction to Energy=                    0.229356
 Thermal correction to Enthalpy=                  0.230300
 Thermal correction to Gibbs Free Energy=         0.173748
 Sum of electronic and zero-point Energies=           -705.953968
 Sum of electronic and thermal Energies=              -705.940195
 Sum of electronic and thermal Enthalpies=            -705.939250
 Sum of electronic and thermal Free Energies=         -705.995802
```

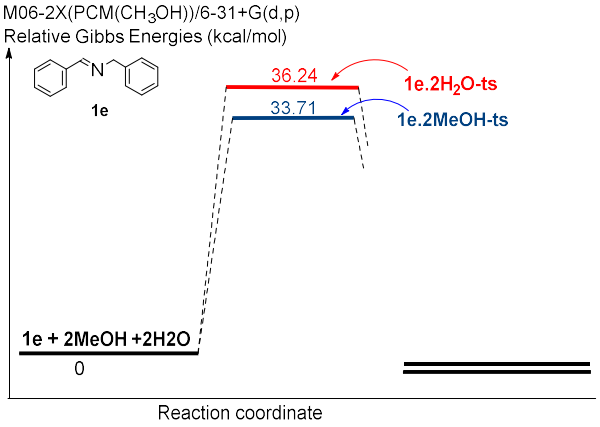
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.008179	0.137287	-0.215088
2	6	0	2.204199	-0.492253	-0.152475
3	8	0	3.133357	0.186743	-0.875351
4	8	0	2.496936	-1.536044	0.432609
5	6	0	-1.390051	-0.312648	0.065366
6	6	0	-4.030116	-0.131778	-0.835496
7	6	0	-2.400223	-1.055479	0.685715
8	6	0	-1.705935	0.511204	-1.017124
9	6	0	-3.023573	0.602620	-1.463302
10	6	0	-3.716842	-0.964835	0.238901
11	1	0	-2.154970	-1.715055	1.515644
12	1	0	-0.913577	1.059706	-1.516044
13	1	0	-3.264096	1.241628	-2.307130
14	1	0	-4.494017	-1.547725	0.722759
15	1	0	-5.054222	-0.062315	-1.188526
16	6	0	0.018128	-0.410595	0.595513
17	1	0	0.247400	-1.402921	0.990350
18	8	0	0.026129	0.456920	1.928269
19	1	0	0.261900	1.503713	1.569231
20	1	0	-0.824859	0.409325	2.394653
21	1	0	0.975893	1.680630	0.091458
22	8	0	0.764917	2.424192	0.799932
23	1	0	0.142722	3.070859	0.440128
24	6	0	4.436102	-0.392352	-0.904721
25	1	0	5.042686	0.275660	-1.514536
26	1	0	4.406170	-1.387926	-1.353322
27	1	0	4.850877	-0.464380	0.103029

4.7.-Comparative energy profiles for the addition of 2 water molecules vs. 2 methanol (2a) molecules to imine derivative 1e in gas phase, CH_2Cl_2, CH_3CN and CH_3OH.









4.8.-Computacional data for the addition of water to imine 1e

4.8.1 M06-2X/6-31+G(d,p) calculations

1e.2H_2O-ts

```
 Zero-point correction=                           0.282509
(Hartree/Particle)
 Thermal correction to Energy=                    0.298740
 Thermal correction to Enthalpy=                  0.299684
 Thermal correction to Gibbs Free Energy=         0.237631
 Sum of electronic and zero-point Energies=           -748.314649
 Sum of electronic and thermal Energies=              -748.298419
 Sum of electronic and thermal Enthalpies=            -748.297474
 Sum of electronic and thermal Free Energies=         -748.359527
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.113752	-0.254639	0.410308
2	6	0	-2.294790	-0.454042	0.131949
3	6	0	-4.671214	-0.387659	-1.312653
4	6	0	-3.314182	-1.366648	0.419692
5	6	0	-2.471067	0.514401	-0.866077
6	6	0	-3.662351	0.540036	-1.581589
7	6	0	-4.500093	-1.339406	-0.309297
8	1	0	-3.175963	-2.101610	1.208359
9	1	0	-1.701410	1.270832	-1.017689
10	1	0	-3.810738	1.294945	-2.346905
11	1	0	-5.287255	-2.054048	-0.092555
12	1	0	-5.596738	-0.360527	-1.879516
13	6	0	-1.046955	-0.557488	0.893566
14	1	0	-1.062574	-1.104829	1.832760
15	8	0	-1.195061	1.381373	2.091035
16	1	0	-0.720883	1.934462	1.219672
17	1	0	0.136102	0.447500	-0.345414
18	8	0	-0.093211	2.272471	0.126845
19	6	0	1.313416	-0.218565	1.257595
20	1	0	1.265621	-1.064308	1.949093
21	1	0	1.251582	0.716145	1.826103
22	6	0	2.562213	-0.264170	0.414898
23	6	0	4.856825	-0.311397	-1.177254
24	6	0	3.404608	-1.375631	0.429696
25	6	0	2.872154	0.830159	-0.400317
26	6	0	4.013992	0.800694	-1.196914
27	6	0	4.553018	-1.398861	-0.361387
28	1	0	3.164740	-2.226164	1.063276
29	1	0	2.201213	1.688981	-0.396603
30	1	0	4.251817	1.650348	-1.829582
31	1	0	5.205975	-2.265854	-0.341822
32	1	0	5.749291	-0.328476	-1.795182
33	1	0	-2.054407	1.766658	2.288221
34	1	0	0.000085	3.219134	-0.008862

4.8.2 M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

1e.2H_2O-ts

```
 Zero-point correction=                           0.279550
(Hartree/Particle)
 Thermal correction to Energy=                    0.296706
 Thermal correction to Enthalpy=                  0.297650
 Thermal correction to Gibbs Free Energy=         0.233434
 Sum of electronic and zero-point Energies=           -748.332893
 Sum of electronic and thermal Energies=              -748.315737
 Sum of electronic and thermal Enthalpies=            -748.314793
 Sum of electronic and thermal Free Energies=         -748.379009
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.118545	-0.256368	0.444510
2	6	0	-2.280069	-0.490892	0.139043
3	6	0	-4.673919	-0.465436	-1.280075
4	6	0	-3.371629	-1.240881	0.593200
5	6	0	-2.393096	0.290140	-1.020647
6	6	0	-3.590865	0.298386	-1.724428
7	6	0	-4.566729	-1.232348	-0.120863
8	1	0	-3.281702	-1.829909	1.501736
9	1	0	-1.568970	0.926700	-1.331458
10	1	0	-3.686148	0.908437	-2.616578
11	1	0	-5.410826	-1.817937	0.227379
12	1	0	-5.606031	-0.453708	-1.836119
13	6	0	-1.043448	-0.559934	0.909797
14	1	0	-1.076895	-1.001747	1.902204
15	8	0	-1.243995	1.676019	1.989143
16	1	0	-0.679563	2.081589	0.967963
17	1	0	0.164634	0.303340	-0.411715
18	8	0	-0.060686	2.310383	-0.021524
19	6	0	1.314752	-0.160051	1.291845
20	1	0	1.267399	-0.957329	2.036789
21	1	0	1.244497	0.810055	1.796479
22	6	0	2.565195	-0.248605	0.454075
23	6	0	4.856524	-0.374911	-1.141024
24	6	0	3.404340	-1.361899	0.519123
25	6	0	2.877387	0.805471	-0.411961
26	6	0	4.016970	0.738436	-1.210331
27	6	0	4.550716	-1.423225	-0.274459
28	1	0	3.164607	-2.181430	1.191773
29	1	0	2.210654	1.666052	-0.448769
30	1	0	4.255025	1.557733	-1.881722
31	1	0	5.201595	-2.290052	-0.216900
32	1	0	5.747525	-0.423064	-1.759350
33	1	0	-2.174626	1.923701	1.953132
34	1	0	-0.160316	3.235425	-0.267141

4.8.3 M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

1e.2H_2O-ts

```
 Zero-point correction=                           0.280223
(Hartree/Particle)
 Thermal correction to Energy=                    0.297267
 Thermal correction to Enthalpy=                  0.298211
 Thermal correction to Gibbs Free Energy=         0.233898
 Sum of electronic and zero-point Energies=           -748.335769
 Sum of electronic and thermal Energies=              -748.318725
 Sum of electronic and thermal Enthalpies=            -748.317781
 Sum of electronic and thermal Free Energies=         -748.382094
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.121352	-0.051365	-0.449881
2	6	0	2.259764	-0.465166	-0.219175
3	6	0	4.659191	-0.787718	1.151123
4	6	0	3.279246	-1.252054	-0.768489
5	6	0	2.449281	0.181232	1.011983
6	6	0	3.650331	0.016317	1.690391
7	6	0	4.476122	-1.419757	-0.078216
8	1	0	3.129059	-1.736595	-1.729006
9	1	0	1.681914	0.845367	1.402299
10	1	0	3.807836	0.521016	2.637730
11	1	0	5.262705	-2.036676	-0.499156
12	1	0	5.594229	-0.912446	1.688096
13	6	0	1.014021	-0.360153	-0.968523
14	1	0	1.013668	-0.650079	-2.016405
15	8	0	1.309094	2.112946	-1.646879
16	1	0	0.705435	2.338966	-0.531318
17	1	0	-0.136535	0.361659	0.487363
18	8	0	0.086211	2.406760	0.430387
19	6	0	-1.319896	0.224107	-1.249956
20	1	0	-1.249297	-0.357849	-2.171038
21	1	0	-1.277030	1.291427	-1.491358
22	6	0	-2.567126	-0.111643	-0.472916
23	6	0	-4.853096	-0.729796	1.010589
24	6	0	-3.270999	-1.290190	-0.726741
25	6	0	-3.010986	0.758379	0.528118
26	6	0	-4.149757	0.447764	1.269762
27	6	0	-4.414029	-1.597781	0.011188
28	1	0	-2.927230	-1.966428	-1.505177
29	1	0	-2.452460	1.673077	0.718019
30	1	0	-4.492322	1.126427	2.044692
31	1	0	-4.959859	-2.513164	-0.194523
32	1	0	-5.742673	-0.968987	1.584841
33	1	0	2.256389	2.255734	-1.540554
34	1	0	0.260801	3.249207	0.861768

4.8.4 M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

1e.2H_2O-ts

```
 Zero-point correction=                           0.280150
(Hartree/Particle)
 Thermal correction to Energy=                    0.297220
 Thermal correction to Enthalpy=                  0.298164
 Thermal correction to Gibbs Free Energy=         0.233810
 Sum of electronic and zero-point Energies=           -748.335717
 Sum of electronic and thermal Energies=              -748.318647
 Sum of electronic and thermal Enthalpies=            -748.317703
 Sum of electronic and thermal Free Energies=         -748.382056
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.120822	-0.053387	-0.448933
2	6	0	2.260686	-0.465094	-0.218428
3	6	0	4.660604	-0.784188	1.151743
4	6	0	3.279997	-1.253261	-0.766207
5	6	0	2.450596	0.184362	1.011026
6	6	0	3.651934	0.021172	1.689366
7	6	0	4.477113	-1.419271	-0.075956
8	1	0	3.129472	-1.740103	-1.725509
9	1	0	1.683287	0.849473	1.399834
10	1	0	3.809838	0.528279	2.635355
11	1	0	5.263551	-2.037227	-0.495643
12	1	0	5.595846	-0.907537	1.688684
13	6	0	1.014619	-0.362049	-0.967523
14	1	0	1.014070	-0.653637	-2.014941
15	8	0	1.303781	2.108222	-1.651508
16	1	0	0.703344	2.336453	-0.536858
17	1	0	-0.135886	0.361835	0.487397
18	8	0	0.085199	2.405660	0.427271
19	6	0	-1.319279	0.220915	-1.249571
20	1	0	-1.248853	-0.362922	-2.169492
21	1	0	-1.275755	1.287713	-1.493142
22	6	0	-2.566734	-0.112865	-0.472083
23	6	0	-4.853489	-0.727494	1.011661
24	6	0	-3.271686	-1.290973	-0.724876
25	6	0	-3.009875	0.758534	0.528099
26	6	0	-4.149067	0.449646	1.269823
27	6	0	-4.415092	-1.596841	0.013166
28	1	0	-2.928453	-1.968241	-1.502658
29	1	0	-2.450373	1.672833	0.717176
30	1	0	-4.491154	1.129360	2.044050
31	1	0	-4.961735	-2.511916	-0.191764
32	1	0	-5.743396	-0.965286	1.585987
33	1	0	2.250404	2.257963	-1.549128
34	1	0	0.257734	3.250062	0.855634

Supporting information 3 (SI3): Computational data on the addition of R_2NH to imine derivatives 1

Contents:

1.- Computational methods: general information

All calculations were performed within the density functional theory (DFT)[13] for which purpose we used the Gaussian 09 (Revision B.01) software package.[14] Computations were executed at the University of the Balearic Islands computational center. Truhlar's M06-2X functional has been employed throughout.[15] In some cases simplified models of imine derivatives **1** have been employed in computation, as follows. Authentic **1a** and **1e** were used for computational studies, as well as the *N,N*-dimethyl derivative (instead of the *N,N*-diethyl analog) of **1b**, and the methoxycarbonyl derivative (instead of the *tert*-butoxycarbonyl analog) of **1c**. Our model for **3a** (diethylamine) in computations was dimethylamine. The numbering system has not been changed though, to avoid confusion. Stationary points were optimized at the M06-2X/6-31+G(d,p) level of theory. The nature (local minimum or first-order saddle point) of these stationary points was determined by frequency analysis: local minima showed no imaginary frequencies, whereas saddle points showed the existence of a single imaginary frequency. Solvation effects were taken in consideration by means of full optimizations carried out at the M06-2X(PCM=solvent)/6-31+G(d,p) level of theory using the PCM(IEFPCM) method of Tomasi et al.[16] Gibbs energies of stationary points obtained with M06-2X/6-31+G(d,p) and M06-2X(PCM=solvent)/6-31+G(d,p) are provided, as well as their Cartesian coordinates. Absolute energies are given in Hartrees, whereas relative energies are reported in kcal/mol.

[13] R.G.Y. Parr, W. Yang, "*Density Functional Theory of Atoms and Molecules"*, Oxford University Press, Oxford, **1989**.

[14] M. J. Frisch, G. W. Trucks, H.B. Schlegel, G. E. Scuseria,M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Menucci, 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. Zakrezwski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J.Fox, Gaussian 09, Revision B.01, Gaussian, Inc., Wallingford CT, **2010**.

[15] Y. Zhao, D.G. Truhlar, *Theor. Chem. Account.* **2008**, *120*, 215-241.

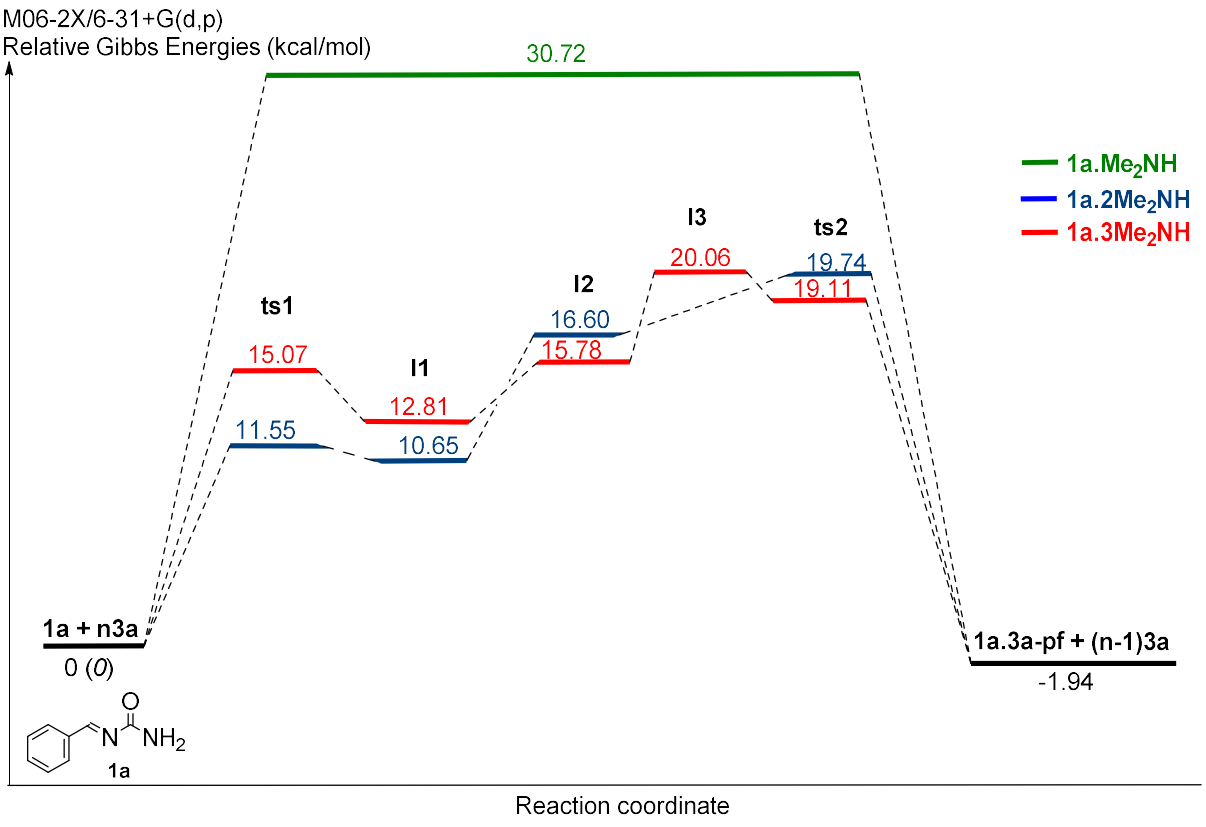
[16] a) E. Cancès, B. Mennucci, J. Tomasi, *J. Chem. Phys.* **1997**, *107*, 3032-3047; b) J. Tomasi, B. Mennucci, E. Cancès , *J. Mol. Struct. (Teochem)* **1999**, *464*, 211-226.

2.- Computational data on the addition of dimethylamine to imine derivatives 1

2.1.-Computational data (includes IRC where appropriate) for the addition of n dimethylamine (3a) molecules (n=1-3) to imine derivative 1a in gas phase, Et_2NH, CH_2Cl_2, CH_3CN and CH_3OH

2.1.1.-M06-2X/6-31+G(d,p) calculations

Energy profiles for the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1a** in gas phase.



3a [Me_2NH]

Zero-point correction= (Hartree/Particle)	0.093145
Thermal correction to Energy=	0.097570
Thermal correction to Enthalpy=	0.098514
Thermal correction to Gibbs Free Energy=	0.067641
Sum of electronic and zero-point Energies=	-135.004940
Sum of electronic and thermal Energies=	-135.000516
Sum of electronic and thermal Enthalpies=	-134.999572
Sum of electronic and thermal Free Energies=	-135.030445

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000014	0.567501	-0.147897
2	1	0	-0.000045	1.341159	0.508248
3	6	0	-1.207452	-0.224048	0.020453
4	1	0	-2.087172	0.418981	-0.060058
5	1	0	-1.252541	-0.763955	0.982339
6	1	0	-1.261947	-0.967541	-0.781480
7	6	0	1.207457	-0.224032	0.020472
8	1	0	1.253393	-0.762581	0.983072
9	1	0	2.087273	0.418636	-0.061972
10	1	0	1.260910	-0.968732	-0.780421

1a.Me_2NH-ts

Zero-point correction= (Hartree/Particle)	0.244728
Thermal correction to Energy=	0.258102
Thermal correction to Enthalpy=	0.259047
Thermal correction to Gibbs Free Energy=	0.204225
Sum of electronic and zero-point Energies=	-629.053517
Sum of electronic and thermal Energies=	-629.040142
Sum of electronic and thermal Enthalpies=	-629.039198
Sum of electronic and thermal Free Energies=	-629.094020

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.364627	-0.623931	-0.462362
2	6	0	2.466267	-1.051478	0.234408
3	7	0	3.419438	-1.652474	-0.573026
4	8	0	2.670859	-0.901739	1.442839
5	6	0	-1.003477	-0.188705	0.207386
6	6	0	-3.721674	-0.823340	0.039290
7	6	0	-1.921377	0.393463	1.085877
8	6	0	-1.451629	-1.104536	-0.745295
9	6	0	-2.807276	-1.418182	-0.829315
10	6	0	-3.276283	0.081573	1.002569
11	1	0	-1.568145	1.086192	1.847712

12	1	0	-0.719493	-1.568393	-1.398852
13	1	0	-3.151145	-2.134298	-1.569547
14	1	0	-3.981213	0.532926	1.693931
15	1	0	-4.776213	-1.073337	-0.024884
16	6	0	0.451143	0.197725	0.291841
17	1	0	0.753265	0.346229	1.334934
18	1	0	1.379686	0.611223	-1.111048
19	6	0	-0.332687	2.254640	-1.113253
20	1	0	0.101610	3.024820	-1.754355
21	1	0	-0.954728	2.728473	-0.345524
22	1	0	-0.954801	1.588760	-1.711364
23	7	0	0.762777	1.494340	-0.501280
24	6	0	1.706963	2.346947	0.240798
25	1	0	2.139580	3.084186	-0.438904
26	1	0	2.496131	1.713593	0.653832
27	1	0	1.190316	2.862386	1.057677
28	1	0	3.085990	-2.049760	-1.438180
29	1	0	4.104570	-2.193265	-0.067295

1a.Me$_2$NH-pf

Zero-point correction= 0.248708
(Hartree/Particle)
Thermal correction to Energy= 0.262508
Thermal correction to Enthalpy= 0.263452
Thermal correction to Gibbs Free Energy= 0.207895
Sum of electronic and zero-point Energies= -629.105265
Sum of electronic and thermal Energies= -629.091466
Sum of electronic and thermal Enthalpies= -629.090521
Sum of electronic and thermal Free Energies= -629.146079

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.386753	-0.743059	0.217392
2	6	0	-2.662560	-0.824429	-0.320498
3	7	0	-3.395852	-1.895524	0.165252
4	8	0	-3.092787	-0.056610	-1.159436
5	6	0	0.953429	-0.183104	-0.212414
6	6	0	3.663305	-0.903448	-0.061304
7	6	0	1.821492	0.075931	-1.275942
8	6	0	1.463890	-0.805238	0.932962
9	6	0	2.807324	-1.166719	1.007232
10	6	0	3.167222	-0.279368	-1.203629
11	1	0	1.434265	0.554021	-2.172704
12	1	0	0.811689	-1.003547	1.780612
13	1	0	3.187029	-1.650080	1.902214
14	1	0	3.825488	-0.073823	-2.042142
15	1	0	4.710111	-1.184714	-0.003607
16	6	0	-0.493975	0.278048	-0.307130
17	1	0	-0.739673	0.442572	-1.363047
18	1	0	-0.964191	-1.626243	0.470296
19	6	0	-0.444841	1.597754	1.767512

20	1	0	-0.890953	2.498420	2.199491
21	1	0	0.641486	1.621816	1.966507
22	1	0	-0.879069	0.729272	2.270480
23	7	0	-0.770484	1.551199	0.354946
24	6	0	-0.219171	2.682035	-0.366064
25	1	0	-0.601111	3.606400	0.076565
26	1	0	-0.545577	2.645406	-1.409918
27	1	0	0.885483	2.719563	-0.340339
28	1	0	-3.229575	-2.181000	1.119231
29	1	0	-4.368163	-1.862268	-0.105617

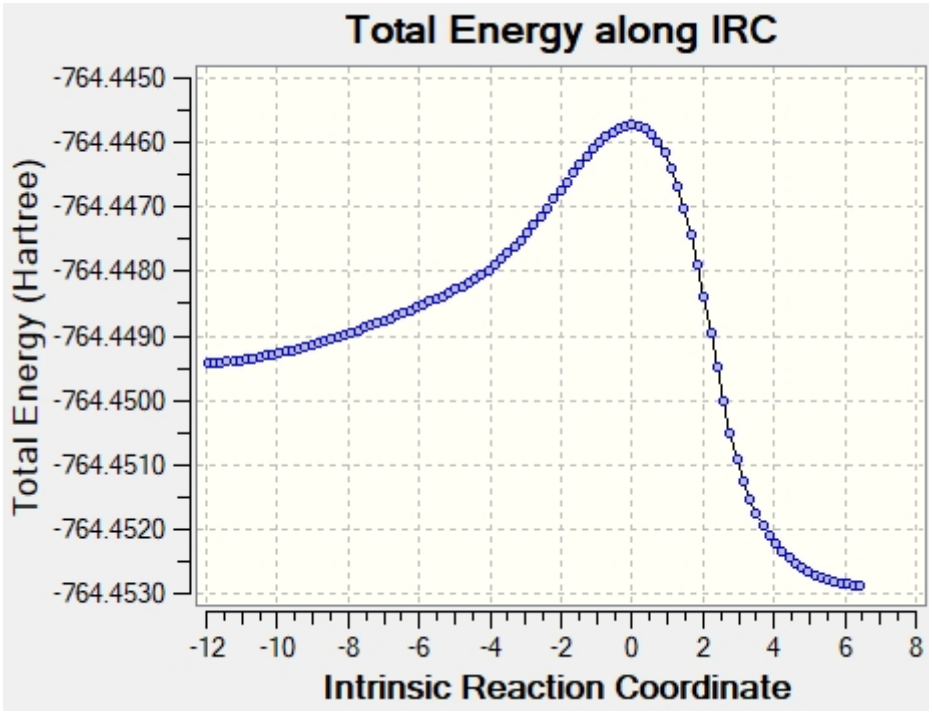
1a.2Me$_2$NH-ts1

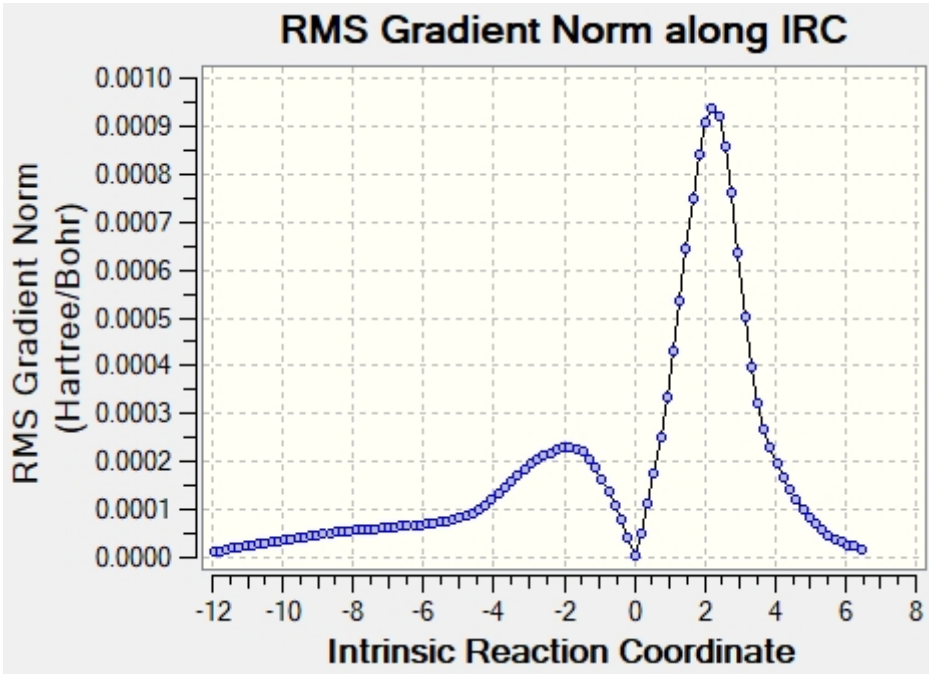
Zero-point correction=	0.341757
(Hartree/Particle)	
Thermal correction to Energy=	0.361634
Thermal correction to Enthalpy=	0.362578
Thermal correction to Gibbs Free Energy=	0.290717
Sum of electronic and zero-point Energies=	-764.103971
Sum of electronic and thermal Energies=	-764.084094
Sum of electronic and thermal Enthalpies=	-764.083150
Sum of electronic and thermal Free Energies=	-764.155010

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.029732	1.617347	-0.008338
2	6	0	1.274542	1.949425	-0.516412
3	7	0	1.799066	3.075027	0.063069
4	8	0	1.917659	1.309256	-1.356394
5	6	0	-1.973514	0.310571	-0.304533
6	6	0	-4.617666	-0.334673	0.339530
7	6	0	-2.745435	-0.461759	-1.176853
8	6	0	-2.540034	0.770629	0.888980
9	6	0	-3.853810	0.444191	1.210881
10	6	0	-4.063616	-0.783525	-0.858157
11	6	0	-0.568165	0.636597	-0.648438
12	7	0	3.316084	-0.849027	-0.023446
13	1	0	-0.237895	0.355916	-1.653978
14	1	0	1.175963	3.666114	0.589965
15	1	0	2.604808	3.486352	-0.379961
16	1	0	3.288629	-0.206164	-0.813100
17	1	0	-2.311365	-0.805501	-2.113168
18	1	0	-4.657955	-1.379210	-1.544090
19	1	0	-5.644448	-0.583530	0.589969
20	1	0	-4.287751	0.803145	2.139235
21	1	0	-1.933739	1.391353	1.541325
22	7	0	0.306426	-1.129838	0.054217
23	1	0	1.294822	-0.947361	-0.170563
24	6	0	4.324588	-1.878673	-0.217702
25	1	0	4.241731	-2.625451	0.579616
26	1	0	5.354898	-1.485318	-0.203446
27	1	0	4.159595	-2.384248	-1.172497

28	6	0	-0.106806	-2.368270	-0.586954
29	1	0	-1.160374	-2.562751	-0.361236
30	1	0	0.490518	-3.226621	-0.247614
31	1	0	0.008257	-2.271375	-1.670913
32	6	0	3.536434	-0.079309	1.193585
33	1	0	2.799529	0.726697	1.261465
34	1	0	4.542335	0.369926	1.244994
35	1	0	3.415458	-0.732552	2.065663
36	6	0	0.165011	-1.145626	1.501444
37	1	0	0.352224	-0.134555	1.880124
38	1	0	0.871477	-1.843304	1.971916
39	1	0	-0.856301	-1.437636	1.766711

1a.2Me$_2$NH-ts1





1a.2Me$_2$NH-I1

Zero-point correction=	0.344781
(Hartree/Particle)	
Thermal correction to Energy=	0.364168
Thermal correction to Enthalpy=	0.365112
Thermal correction to Gibbs Free Energy=	0.295636
Sum of electronic and zero-point Energies=	-764.107319
Sum of electronic and thermal Energies=	-764.087932
Sum of electronic and thermal Enthalpies=	-764.086988
Sum of electronic and thermal Free Energies=	-764.156464

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.236912	1.757970	-0.071006
2	6	0	1.015494	2.135183	-0.340527
3	7	0	1.332969	3.439579	0.011517
4	8	0	1.934847	1.405240	-0.817317
5	6	0	-1.970584	0.065853	-0.285386
6	6	0	-4.625769	-0.696565	0.177890
7	6	0	-2.594461	-0.871174	-1.112061
8	6	0	-2.696146	0.637277	0.763192
9	6	0	-4.014088	0.252907	0.997035
10	6	0	-3.915806	-1.254009	-0.883480
11	6	0	-0.529455	0.462078	-0.516521
12	7	0	3.384424	-0.816567	0.211164
13	1	0	-0.242087	0.266173	-1.564232
14	1	0	0.545711	4.066990	0.080711
15	1	0	2.152542	3.802775	-0.450599
16	1	0	-2.049879	-1.292268	-1.954884
17	1	0	-4.391236	-1.976631	-1.539684
18	1	0	-5.656139	-0.988468	0.356983
19	1	0	-4.570898	0.705249	1.812250
20	1	0	-2.213687	1.404767	1.360554
21	7	0	0.406459	-0.580034	0.225000
22	6	0	3.637621	-1.220674	-1.166720
23	1	0	3.400086	-2.284958	-1.288453
24	1	0	4.686599	-1.075443	-1.472338
25	1	0	2.999816	-0.629493	-1.829356
26	6	0	0.360198	-1.955851	-0.298499
27	1	0	-0.587205	-2.423085	-0.022859
28	1	0	1.203366	-2.506556	0.125063
29	1	0	0.459163	-1.923331	-1.385863
30	6	0	4.303599	-1.437551	1.152097
31	1	0	4.124046	-1.050762	2.158896
32	1	0	5.364019	-1.272679	0.899416
33	1	0	4.131287	-2.519975	1.169708
34	6	0	0.270054	-0.543501	1.694443
35	1	0	0.245552	0.502917	2.002381
36	1	0	1.133263	-1.053028	2.127921
37	1	0	-0.657148	-1.043510	1.982782
38	1	0	3.444038	0.199804	0.252967
39	1	0	1.347484	-0.200887	-0.008325

1a.2Me$_2$NH-I2

Zero-point correction=	0.344909
(Hartree/Particle)	
Thermal correction to Energy=	0.364059
Thermal correction to Enthalpy=	0.365003
Thermal correction to Gibbs Free Energy=	0.297099
Sum of electronic and zero-point Energies=	-764.099162
Sum of electronic and thermal Energies=	-764.080013
Sum of electronic and thermal Enthalpies=	-764.079069
Sum of electronic and thermal Free Energies=	-764.146973

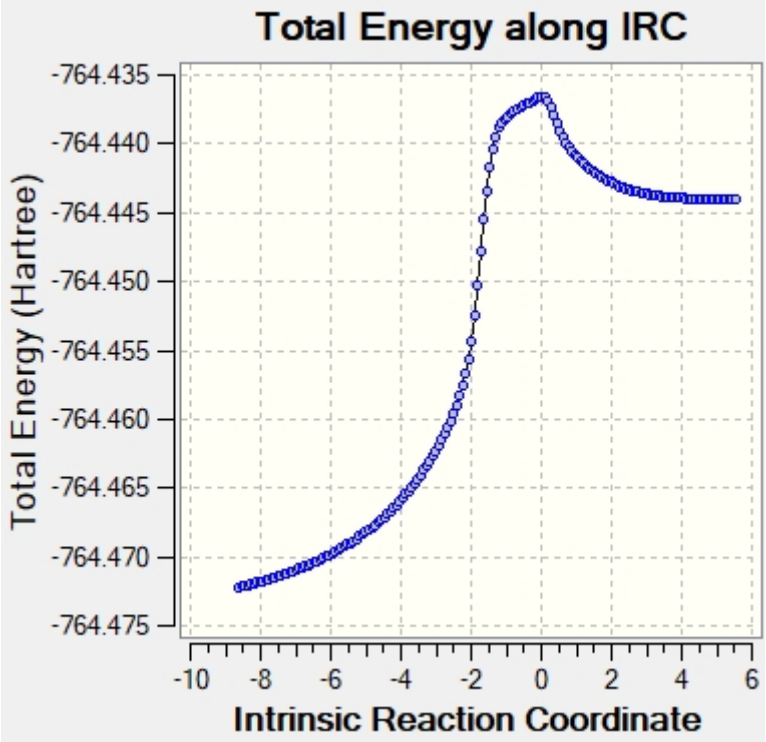
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.841669	-0.757662	-0.833453
2	6	0	1.769525	-1.736185	-0.932208
3	7	0	2.675403	-1.534159	-1.979844
4	8	0	1.922357	-2.719236	-0.183663
5	6	0	-1.476849	-0.487581	-0.139416
6	6	0	-4.080611	0.372105	-0.727118
7	6	0	-2.583038	-1.166547	0.375132
8	6	0	-1.688675	0.610292	-0.977336
9	6	0	-2.980818	1.044599	-1.261379
10	6	0	-3.879348	-0.742703	0.083716
11	1	0	-2.428038	-2.041723	1.002690
12	1	0	-0.830864	1.094590	-1.432734
13	1	0	-3.132680	1.898901	-1.914596
14	1	0	-4.729591	-1.286228	0.484488
15	1	0	-5.088117	0.705518	-0.955914
16	6	0	-0.072906	-0.936527	0.210564
17	6	0	2.961397	1.999017	0.026183
18	1	0	3.309689	0.962752	0.032482
19	1	0	3.255027	2.483998	0.963726
20	1	0	3.462904	2.522934	-0.801277
21	6	0	-0.608537	0.235685	2.478280
22	1	0	-0.143485	0.792966	3.294593
23	1	0	-1.007138	-0.707091	2.862465
24	1	0	-1.418248	0.819972	2.042949
25	7	0	1.506068	2.011900	-0.108024
26	6	0	0.976262	3.345163	-0.363663
27	1	0	1.413037	3.812029	-1.259719
28	1	0	1.193176	3.992520	0.492402
29	1	0	-0.109404	3.296428	-0.486556
30	7	0	0.412860	-0.051363	1.451071
31	6	0	1.618966	-0.656644	2.064784
32	1	0	2.038838	0.049030	2.785935
33	1	0	2.340329	-0.888647	1.284706
34	1	0	1.336709	-1.588001	2.560814
35	1	0	-0.087247	-1.953278	0.633451
36	1	0	1.260851	1.346978	-0.849768
37	1	0	0.731401	0.852151	0.991152
38	1	0	2.307814	-0.997742	-2.752712
39	1	0	3.161968	-2.379237	-2.242751

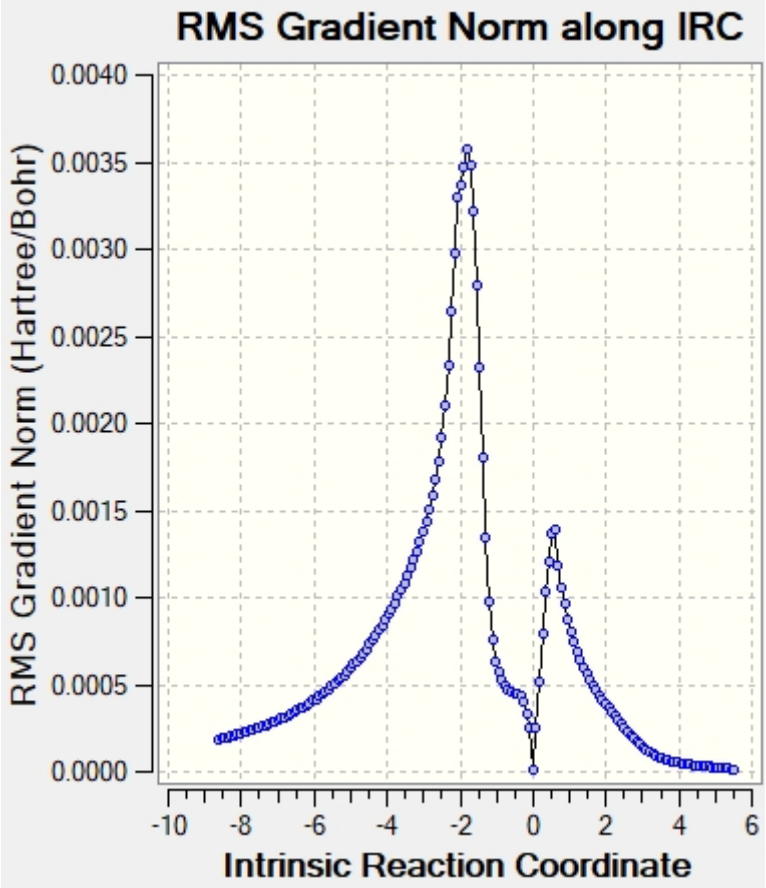
1a.2Me$_2$NH-ts2

Zero-point correction=	0.340538
(Hartree/Particle)	
Thermal correction to Energy=	0.358864
Thermal correction to Enthalpy=	0.359808
Thermal correction to Gibbs Free Energy=	0.294582
Sum of electronic and zero-point Energies=	-764.096009
Sum of electronic and thermal Energies=	-764.077684
Sum of electronic and thermal Enthalpies=	-764.076740
Sum of electronic and thermal Free Energies=	-764.141966

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.857333	-0.727579	-0.766679
2	6	0	1.791134	-1.696770	-0.822835
3	7	0	2.682438	-1.540622	-1.903265
4	8	0	1.976074	-2.632819	-0.025892
5	6	0	-1.467094	-0.469744	-0.077704
6	6	0	-4.103202	0.206988	-0.775180
7	6	0	-2.552893	-1.068557	0.566264
8	6	0	-1.720509	0.446088	-1.102051
9	6	0	-3.027029	0.791765	-1.442231
10	6	0	-3.862282	-0.734858	0.223662
11	1	0	-2.370025	-1.811001	1.339805
12	1	0	-0.881879	0.850710	-1.660607
13	1	0	-3.206955	1.504661	-2.241701
14	1	0	-4.693070	-1.216457	0.730480
15	1	0	-5.121735	0.468342	-1.045273
16	6	0	-0.045345	-0.812487	0.334591
17	6	0	2.988541	1.817352	-0.101781
18	1	0	3.348617	0.788666	-0.025374
19	1	0	3.269025	2.380489	0.792786
20	1	0	3.448160	2.285050	-0.978409
21	6	0	-0.604626	0.626737	2.374463
22	1	0	-0.133362	1.283062	3.112316
23	1	0	-1.068355	-0.215666	2.905662
24	1	0	-1.384747	1.180031	1.849828
25	7	0	1.525994	1.786017	-0.240853
26	6	0	0.917638	3.079486	-0.558388
27	1	0	1.279695	3.457628	-1.519775
28	1	0	1.168287	3.804367	0.221464
29	1	0	-0.168187	2.967120	-0.601423
30	7	0	0.424251	0.168246	1.435050
31	6	0	1.541417	-0.439996	2.179939
32	1	0	2.011422	0.321489	2.811472
33	1	0	2.267707	-0.859546	1.483793
34	1	0	1.179723	-1.260117	2.813860
35	1	0	-0.035390	-1.809381	0.803111
36	1	0	1.282963	0.993810	-0.903594
37	1	0	0.994400	1.187470	0.678396
38	1	0	3.178760	-2.398668	-2.102263
39	1	0	2.261741	-1.117974	-2.719681

1a.2Me$_2$NH-ts2





1a.3Me$_2$NH-ts1

Zero-point correction=	0.436240
(Hartree/Particle)	
Thermal correction to Energy=	0.462077
Thermal correction to Enthalpy=	0.463021
Thermal correction to Gibbs Free Energy=	0.378147
Sum of electronic and zero-point Energies=	-899.121756
Sum of electronic and thermal Energies=	-899.095919
Sum of electronic and thermal Enthalpies=	-899.094975
Sum of electronic and thermal Free Energies=	-899.179849

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.773299	1.444300	-1.081840
2	6	0	0.545916	1.637241	-1.461606
3	7	0	0.800157	2.925671	-1.843927
4	8	0	1.450030	0.794152	-1.429892
5	6	0	-2.478039	-0.165414	-0.515503
6	6	0	-5.130538	-0.893222	-0.013506
7	6	0	-2.860234	-1.509379	-0.545357
8	6	0	-3.436836	0.815832	-0.241880
9	6	0	-4.755548	0.451489	0.012424
10	6	0	-4.181840	-1.874310	-0.297251
11	6	0	-1.067749	0.203055	-0.777441
12	7	0	2.554950	0.485403	1.368569
13	1	0	-0.405365	-0.612598	-1.084287
14	1	0	0.014863	3.533193	-2.014176
15	1	0	1.678983	3.113779	-2.298395
16	1	0	-2.115860	-2.270904	-0.767583
17	1	0	-4.471156	-2.920236	-0.327381
18	1	0	-6.161237	-1.173684	0.181219
19	1	0	-5.496717	1.216275	0.223981
20	1	0	-3.126064	1.856144	-0.245834
21	7	0	-0.342536	-0.079548	1.210812
22	6	0	3.251419	-0.185645	2.454384
23	1	0	2.732696	0.005154	3.401665
24	1	0	4.297092	0.145410	2.569413
25	1	0	3.251145	-1.264622	2.274760
26	6	0	-0.592278	-1.369423	1.833726
27	1	0	-1.670317	-1.508543	1.968727
28	1	0	-0.101093	-1.458050	2.814228
29	1	0	-0.219320	-2.170096	1.187121
30	6	0	2.622205	1.935749	1.472836
31	1	0	2.125336	2.387477	0.609546
32	1	0	3.656129	2.316821	1.522836
33	1	0	2.103011	2.264164	2.381285
34	6	0	-0.842235	1.040048	1.991735
35	1	0	-0.719948	1.958930	1.408132
36	1	0	-0.306901	1.145812	2.946320
37	1	0	-1.908009	0.896120	2.200884
38	1	0	0.677873	0.052091	1.081547
39	7	0	3.444118	-1.273574	-1.042212
40	6	0	4.552213	-1.970338	-1.672814
41	1	0	5.016214	-2.647819	-0.947533
42	1	0	5.310192	-1.250584	-1.991897
43	1	0	4.250383	-2.571892	-2.547636
44	6	0	2.364597	-2.170464	-0.665709
45	1	0	1.537192	-1.573551	-0.272427

46	1	0	2.709802	-2.854416	0.119404
47	1	0	1.988188	-2.781570	-1.504890
48	1	0	3.064518	-0.554762	-1.654136
49	1	0	2.958085	0.181664	0.480194

1a.3Me$_2$NH-I1

Zero-point correction= 0.440061
(Hartree/Particle)
Thermal correction to Energy= 0.464943
Thermal correction to Enthalpy= 0.465887
Thermal correction to Gibbs Free Energy= 0.383336
Sum of electronic and zero-point Energies= -899.126727
Sum of electronic and thermal Energies= -899.101844
Sum of electronic and thermal Enthalpies= -899.100900
Sum of electronic and thermal Free Energies= -899.183451

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.751392	1.465928	-0.496846
2	6	0	-0.521157	1.809643	-0.278668
3	7	0	-0.988771	2.867947	-1.060794
4	8	0	-1.338298	1.241087	0.494658
5	6	0	2.666940	0.256512	0.394814
6	6	0	5.450246	-0.053484	0.506094
7	6	0	3.274213	-0.319373	1.513547
8	6	0	3.470589	0.702630	-0.658214
9	6	0	4.852814	0.541769	-0.605759
10	6	0	4.658800	-0.477299	1.571237
11	6	0	1.161631	0.406063	0.325763
12	7	0	-2.152182	-1.208672	-0.912577
13	1	0	0.732559	0.432603	1.339289
14	1	0	-0.262671	3.472509	-1.418060
15	1	0	-1.781622	3.345076	-0.656399
16	1	0	2.661787	-0.628121	2.358321
17	1	0	5.117283	-0.918944	2.450737
18	1	0	6.528767	-0.171300	0.548409
19	1	0	5.468658	0.892046	-1.428726
20	1	0	2.988676	1.199685	-1.494307
21	7	0	0.551278	-0.940747	-0.224303
22	6	0	-2.721607	-2.547909	-0.990464
23	1	0	-2.165521	-3.151395	-1.718614
24	1	0	-3.779713	-2.541532	-1.297363
25	1	0	-2.653277	-3.034152	-0.013338
26	6	0	0.675908	-2.092691	0.687385
27	1	0	1.720809	-2.400182	0.759233
28	1	0	0.068375	-2.912068	0.295031
29	1	0	0.299916	-1.801571	1.670505
30	6	0	-2.330911	-0.462817	-2.156270
31	1	0	-1.934607	0.550411	-2.040762
32	1	0	-3.389028	-0.395769	-2.456638
33	1	0	-1.785823	-0.961574	-2.966976
34	6	0	1.023737	-1.266346	-1.585870
35	1	0	0.990024	-0.348440	-2.175699
36	1	0	0.350564	-2.015417	-2.010014

37	1	0	2.044019	-1.652740	-1.540289
38	1	0	-0.493590	-0.792311	-0.328463
39	7	0	-3.863171	0.186312	1.269540
40	6	0	-4.538018	1.029768	0.295035
41	1	0	-5.328315	0.459326	-0.208270
42	1	0	-3.809768	1.359216	-0.451870
43	1	0	-5.002399	1.924808	0.744160
44	6	0	-4.709648	-0.138339	2.403923
45	1	0	-4.136810	-0.695964	3.149708
46	1	0	-5.541266	-0.771083	2.074273
47	1	0	-5.141552	0.751919	2.893303
48	1	0	-3.007963	0.658135	1.557921
49	1	0	-2.622176	-0.705996	-0.152817

1a.3Me_2NH-I2

Zero-point correction= 0.439771
(Hartree/Particle)
Thermal correction to Energy= 0.464667
Thermal correction to Enthalpy= 0.465611
Thermal correction to Gibbs Free Energy= 0.384537
Sum of electronic and zero-point Energies= -899.123488
Sum of electronic and thermal Energies= -899.098592
Sum of electronic and thermal Enthalpies= -899.097648
Sum of electronic and thermal Free Energies= -899.178722

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.173825	0.471528	1.658834
2	1	0	0.107752	-0.511783	1.346700
3	1	0	1.094960	-1.995256	0.131588
4	1	0	1.464842	-0.209238	-1.261763
5	7	0	1.983566	-1.085025	-1.431847
6	7	0	0.713334	-2.126095	1.081966
7	6	0	1.814649	-2.440777	1.988376
8	1	0	2.264065	-3.424298	1.783130
9	1	0	1.453592	-2.446594	3.023788
10	1	0	2.594433	-1.680079	1.899136
11	6	0	-0.306942	-3.170571	1.087331
12	1	0	0.101415	-4.160021	0.831016
13	1	0	-1.098377	-2.920610	0.376290
14	1	0	-0.755292	-3.240819	2.085005
15	6	0	-1.298117	0.333736	2.606195
16	1	0	-1.621662	1.327513	2.928106
17	1	0	-0.965579	-0.240700	3.474039
18	1	0	-2.124896	-0.182148	2.118496
19	6	0	1.017826	1.045857	2.328324
20	1	0	0.815354	2.082936	2.601104
21	1	0	1.849603	1.026404	1.625160
22	1	0	1.249535	0.438017	3.206373
23	6	0	1.876690	-1.477834	-2.827738
24	1	0	2.385071	-0.776726	-3.511853
25	1	0	0.823529	-1.533189	-3.119295
26	1	0	2.323797	-2.467645	-2.975854
27	6	0	3.366644	-0.880149	-1.023257
28	1	0	3.929038	-0.233724	-1.716578

29	1	0	3.889550	-1.842130	-0.952671
30	1	0	3.386962	-0.396512	-0.041677
31	7	0	0.560863	1.342595	-0.499345
32	6	0	-0.542775	1.293487	0.361683
33	6	0	-1.737432	0.607949	-0.270228
34	6	0	-3.942153	-0.662747	-1.445356
35	6	0	-3.016552	1.152406	-0.150414
36	6	0	-1.568323	-0.574269	-0.997020
37	6	0	-2.663928	-1.209128	-1.575505
38	6	0	-4.115856	0.523189	-0.736237
39	1	0	-3.151796	2.082742	0.396668
40	1	0	-0.566913	-0.979695	-1.118977
41	1	0	-2.520829	-2.127241	-2.138769
42	1	0	-5.104127	0.962666	-0.641594
43	1	0	-4.794494	-1.154400	-1.903983
44	6	0	1.307498	2.463510	-0.373709
45	8	0	1.162228	3.385662	0.448201
46	7	0	2.392269	2.506113	-1.259003
47	1	0	-0.828853	2.274966	0.772371
48	1	0	2.774887	3.435520	-1.360279
49	1	0	2.245785	2.014969	-2.130181

1a.3Me$_2$NH-I3

Zero-point correction=	0.439675
(Hartree/Particle)	
Thermal correction to Energy=	0.463740
Thermal correction to Enthalpy=	0.464685
Thermal correction to Gibbs Free Energy=	0.387208
Sum of electronic and zero-point Energies=	-899.119436
Sum of electronic and thermal Energies=	-899.095370
Sum of electronic and thermal Enthalpies=	-899.094426
Sum of electronic and thermal Free Energies=	-899.171903

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.851966	-1.750956	0.890316
2	1	0	-0.745092	-0.080059	1.558564
3	1	0	-0.205252	1.491398	1.098658
4	1	0	0.072266	1.491848	-0.758138
5	7	0	0.371722	2.337526	-0.235155
6	7	0	-0.789961	0.947000	1.830380
7	6	0	-2.184929	1.416896	1.683220
8	1	0	-2.229938	2.480183	1.933160
9	1	0	-2.835846	0.853423	2.356078
10	1	0	-2.481603	1.254642	0.643698
11	6	0	-0.239511	1.146529	3.181292
12	1	0	-0.292790	2.205433	3.443411
13	1	0	0.803256	0.826007	3.193345
14	1	0	-0.812283	0.562644	3.905419
15	6	0	-0.287342	-3.039885	1.305170
16	1	0	-0.590000	-3.840361	0.611000
17	1	0	-0.656245	-3.294882	2.303351
18	1	0	0.801517	-3.009973	1.333083
19	6	0	-2.313341	-1.916473	0.841939

20	1	0	-2.608180	-2.694355	0.124570
21	1	0	-2.794633	-0.990534	0.529720
22	1	0	-2.663870	-2.186724	1.844101
23	6	0	1.788581	2.613596	-0.442135
24	1	0	2.007727	2.900872	-1.481873
25	1	0	2.376145	1.726717	-0.197255
26	1	0	2.105765	3.435577	0.209953
27	6	0	-0.471881	3.460932	-0.628760
28	1	0	-0.268393	3.797853	-1.657735
29	1	0	-0.301953	4.312883	0.039754
30	1	0	-1.525844	3.173858	-0.563098
31	7	0	-0.954013	-0.133854	-0.915245
32	6	0	-0.313138	-1.330381	-0.447546
33	6	0	1.188457	-1.055509	-0.356064
34	6	0	3.951806	-0.493634	-0.373293
35	6	0	1.897887	-0.962016	-1.559411
36	6	0	1.886496	-0.841197	0.835014
37	6	0	3.257274	-0.567571	0.830289
38	6	0	3.261855	-0.687890	-1.572521
39	1	0	1.358072	-1.107189	-2.492231
40	1	0	1.365547	-0.926661	1.785134
41	1	0	3.779719	-0.419010	1.771261
42	1	0	3.791071	-0.629458	-2.519064
43	1	0	5.017614	-0.287649	-0.380368
44	6	0	-1.979161	-0.344274	-1.759728
45	8	0	-2.450302	-1.423056	-2.155006
46	1	0	-0.474543	-2.170402	-1.149696
47	7	0	-2.615205	0.855722	-2.169218
48	1	0	-1.977485	1.631209	-2.294208
49	1	0	-3.194698	0.694366	-2.982882

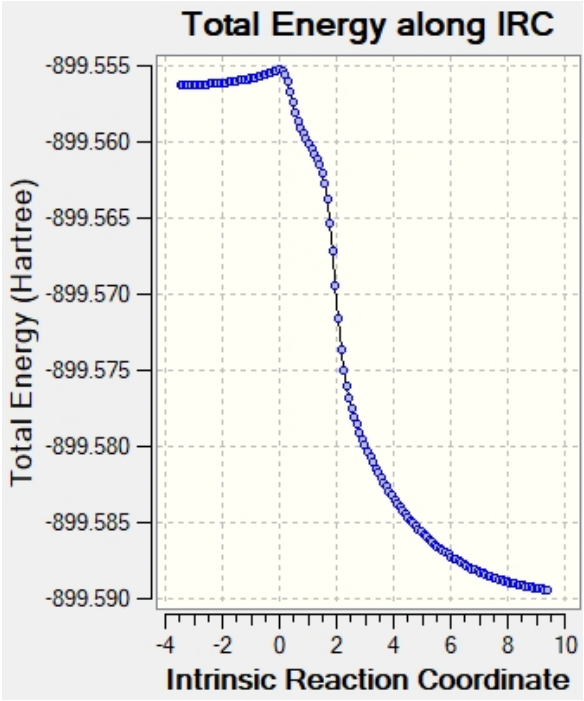
1a.3Me$_2$NH-ts2

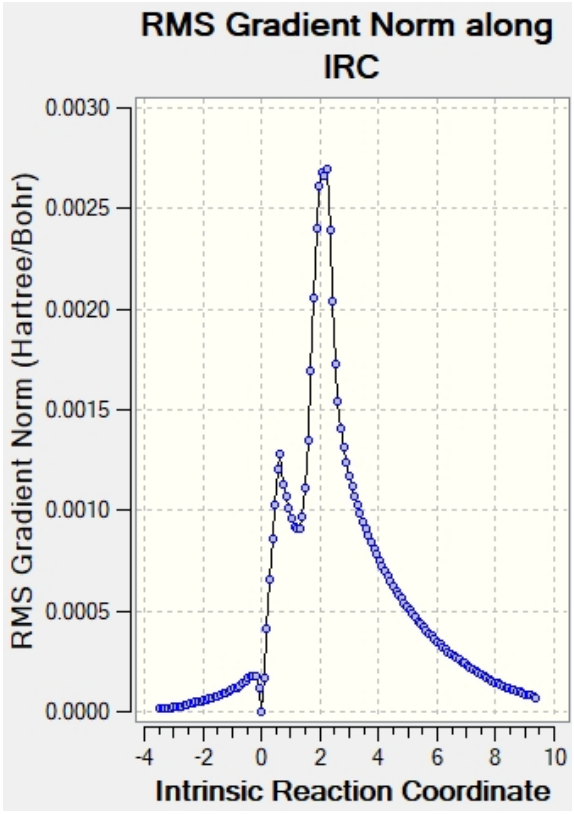
Zero-point correction= 0.434789
(Hartree/Particle)
Thermal correction to Energy= 0.458625
Thermal correction to Enthalpy= 0.459569
Thermal correction to Gibbs Free Energy= 0.381837
Sum of electronic and zero-point Energies= -899.120470
Sum of electronic and thermal Energies= -899.096634
Sum of electronic and thermal Enthalpies= -899.095690
Sum of electronic and thermal Free Energies= -899.173422

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.202202	0.412137	1.672912
2	1	0	0.476508	-1.074559	1.215672
3	1	0	1.526630	-1.591853	-0.117010
4	1	0	1.404950	-0.046978	-1.115224
5	7	0	2.046763	-0.896250	-1.221857
6	7	0	1.051120	-1.945202	0.936155
7	6	0	2.125945	-2.128746	1.921734
8	1	0	2.759784	-2.971541	1.630249
9	1	0	1.709166	-2.324897	2.915642
10	1	0	2.732915	-1.222401	1.964139

11	6	0	0.183227	-3.124387	0.822153
12	1	0	0.762767	-3.979755	0.462080
13	1	0	-0.627221	-2.914250	0.122266
14	1	0	-0.251238	-3.376429	1.795529
15	6	0	-1.304396	0.241316	2.619588
16	1	0	-1.740640	1.208937	2.920176
17	1	0	-0.928800	-0.254830	3.520591
18	1	0	-2.093493	-0.375433	2.184469
19	6	0	0.895767	1.126163	2.337180
20	1	0	0.594485	2.137573	2.644243
21	1	0	1.736326	1.231874	1.648891
22	1	0	1.210003	0.555562	3.218494
23	6	0	1.919627	-1.516816	-2.537078
24	1	0	2.256541	-0.841820	-3.335213
25	1	0	0.875131	-1.778489	-2.727528
26	1	0	2.522729	-2.430357	-2.585673
27	6	0	3.418260	-0.470585	-0.930528
28	1	0	3.829450	0.144461	-1.739110
29	1	0	4.063404	-1.344449	-0.777689
30	1	0	3.414979	0.146173	-0.027708
31	7	0	0.453056	1.242944	-0.512773
32	6	0	-0.620496	1.166086	0.430277
33	6	0	-1.820350	0.468147	-0.191662
34	6	0	-4.030163	-0.850484	-1.324546
35	6	0	-3.116754	0.942139	0.013194
36	6	0	-1.645759	-0.663188	-0.992123
37	6	0	-2.736924	-1.324933	-1.548960
38	6	0	-4.215919	0.290643	-0.547725
39	1	0	-3.265711	1.834631	0.616826
40	1	0	-0.633841	-0.998071	-1.202458
41	1	0	-2.581081	-2.201022	-2.173390
42	1	0	-5.216345	0.679201	-0.382117
43	1	0	-4.882856	-1.357757	-1.765276
44	6	0	1.112813	2.414633	-0.530297
45	8	0	1.000868	3.378539	0.244061
46	7	0	2.092651	2.477737	-1.555460
47	1	0	-0.928895	2.173899	0.763232
48	1	0	2.405910	3.431024	-1.685581
49	1	0	1.782534	2.053772	-2.421081

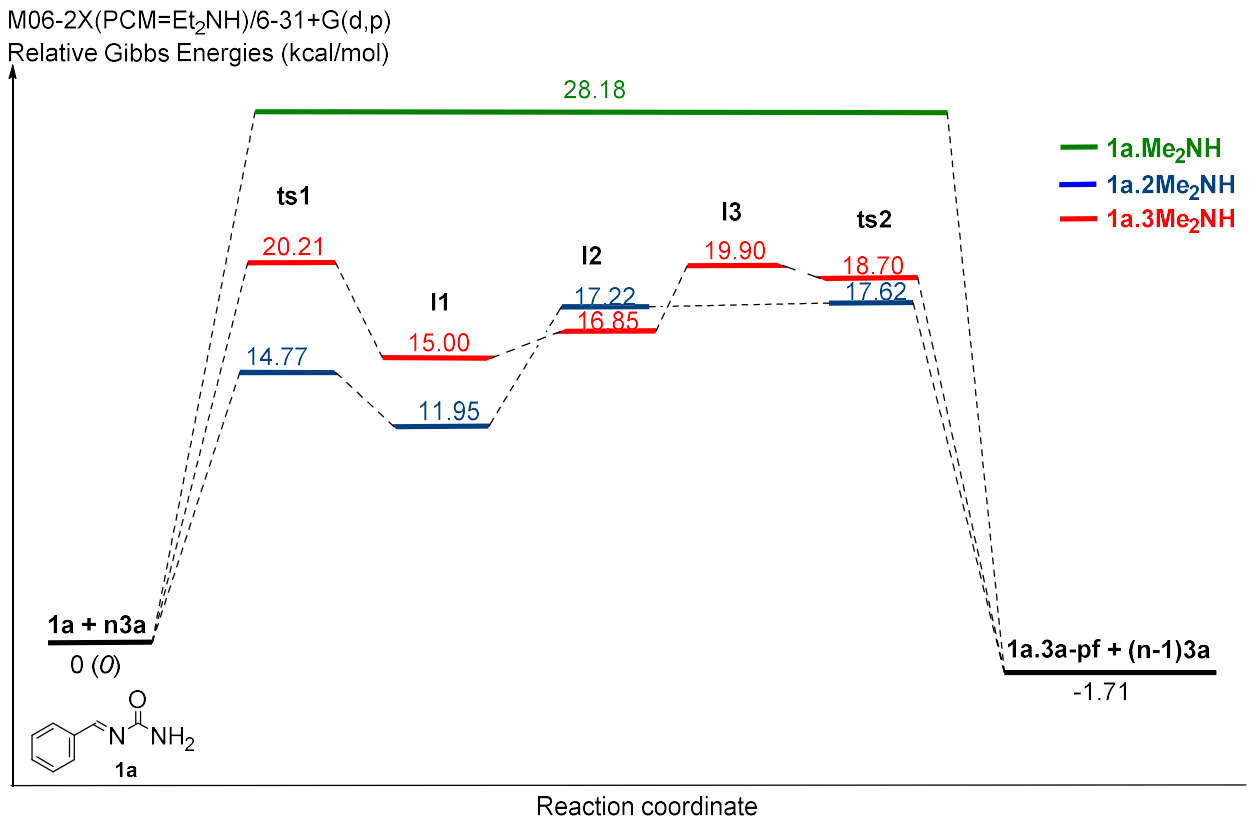
1a.3Me$_2$NH-ts2





2.1.2.-M06-2X(PCM=Diethylamine)/6-31+G(d,p) calculations

Energy profiles for the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1a** in diethylamine.



1a

Zero-point correction= 0.150745
(Hartree/Particle)
Thermal correction to Energy= 0.160365
Thermal correction to Enthalpy= 0.161309
Thermal correction to Gibbs Free Energy= 0.114656
Sum of electronic and zero-point Energies= -494.084284
Sum of electronic and thermal Energies= -494.074664
Sum of electronic and thermal Enthalpies= -494.073720
Sum of electronic and thermal Free Energies= -494.120373

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.621127	-0.497973	-0.000008
2	7	0	-1.512091	0.419717	-0.000023
3	6	0	0.815634	-0.201837	-0.000001
4	6	0	-2.862249	-0.059313	-0.000041
5	7	0	-3.734367	0.969330	0.000009
6	8	0	-3.196411	-1.236419	0.000002
7	1	0	-4.724582	0.781719	0.000047
8	6	0	3.560804	0.293410	0.000016
9	6	0	1.723238	-1.266885	0.000007
10	6	0	1.290507	1.117325	-0.000001
11	6	0	2.657953	1.361304	0.000008
12	6	0	3.094512	-1.020088	0.000016
13	1	0	1.350789	-2.288132	0.000007
14	1	0	0.574675	1.932954	-0.000006
15	1	0	3.026504	2.382090	0.000008
16	1	0	3.795292	-1.848511	0.000022
17	1	0	4.628738	0.488598	0.000023
18	1	0	-0.913887	-1.554700	-0.000010
19	1	0	-3.396657	1.918353	0.000013

Me_2NH

Zero-point correction= 0.093107
(Hartree/Particle)
Thermal correction to Energy= 0.097516
Thermal correction to Enthalpy= 0.098460
Thermal correction to Gibbs Free Energy= 0.067615
Sum of electronic and zero-point Energies= -135.007342
Sum of electronic and thermal Energies= -135.002933
Sum of electronic and thermal Enthalpies= -135.001989
Sum of electronic and thermal Free Energies= -135.032834

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.571823	-0.151875
2	1	0	0.000000	1.332021	0.521119
3	6	0	-1.206828	-0.225013	0.020361
4	1	0	-2.088952	0.415388	-0.053728
5	1	0	-1.242638	-0.763028	0.982918

6	1	0	-1.262200	-0.969676	-0.780354
7	6	0	1.206828	-0.225013	0.020361
8	1	0	1.242644	-0.763019	0.982923
9	1	0	2.088953	0.415386	-0.053742
10	1	0	1.262193	-0.969684	-0.780346

1a.Me_2NH-ts

Zero-point correction= (Hartree/Particle)	0.243947
Thermal correction to Energy=	0.257527
Thermal correction to Enthalpy=	0.258471
Thermal correction to Gibbs Free Energy=	0.202689
Sum of electronic and zero-point Energies=	-629.067034
Sum of electronic and thermal Energies=	-629.053453
Sum of electronic and thermal Enthalpies=	-629.052509
Sum of electronic and thermal Free Energies=	-629.108291

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.593421	-0.242129	0.428678
2	6	0	-2.319849	-1.193055	-0.209121
3	7	0	-3.480699	-1.564848	0.454210
4	8	0	-2.032617	-1.696286	-1.306354
5	6	0	0.863465	-0.133658	-0.184727
6	6	0	3.489696	-1.057116	0.088172
7	6	0	1.861464	0.306625	-1.058832
8	6	0	1.184868	-1.048476	0.817912
9	6	0	2.493725	-1.509282	0.953558
10	6	0	3.171445	-0.148126	-0.921325
11	1	0	1.609223	1.000078	-1.858686
12	1	0	0.396266	-1.397505	1.477960
13	1	0	2.735037	-2.226809	1.731954
14	1	0	3.939180	0.197117	-1.606875
15	1	0	4.507493	-1.420150	0.192197
16	6	0	-0.541024	0.397390	-0.332999
17	1	0	-0.782073	0.487167	-1.399908
18	1	0	-1.719176	1.072220	0.748928
19	6	0	0.184437	2.171613	1.346587
20	1	0	-0.201970	3.063178	1.843307
21	1	0	1.166191	2.386397	0.911678
22	1	0	0.282997	1.364254	2.073969
23	7	0	-0.774601	1.772064	0.306809
24	6	0	-1.052990	2.845503	-0.654329
25	1	0	-1.384397	3.732527	-0.111722
26	1	0	-1.843532	2.521464	-1.333570
27	1	0	-0.152772	3.089623	-1.228745
28	1	0	-3.506930	-1.386473	1.447539
29	1	0	-3.854977	-2.456927	0.165550

1a.Me_2NH-pf

Zero-point correction= (Hartree/Particle)	0.248794
Thermal correction to Energy=	0.262529
Thermal correction to Enthalpy=	0.263473
Thermal correction to Gibbs Free Energy=	0.208363
Sum of electronic and zero-point Energies=	-629.115499
Sum of electronic and thermal Energies=	-629.101764
Sum of electronic and thermal Enthalpies=	-629.100820
Sum of electronic and thermal Free Energies=	-629.155931

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.404743	-0.706201	0.221441
2	6	0	-2.671247	-0.826908	-0.305221
3	7	0	-3.389020	-1.896063	0.187542
4	8	0	-3.117961	-0.075636	-1.162681
5	6	0	0.942964	-0.186631	-0.209735
6	6	0	3.642914	-0.941934	-0.046517
7	6	0	1.809221	0.023909	-1.285787
8	6	0	1.449138	-0.778575	0.953746
9	6	0	2.788062	-1.156886	1.034288
10	6	0	3.150317	-0.349245	-1.207630
11	1	0	1.426805	0.479371	-2.196278
12	1	0	0.801175	-0.942704	1.811955
13	1	0	3.164466	-1.615600	1.943438
14	1	0	3.807592	-0.181238	-2.055233
15	1	0	4.685929	-1.235936	0.016308
16	6	0	-0.498127	0.293606	-0.314034
17	1	0	-0.738789	0.439266	-1.373156
18	1	0	-0.998082	-1.537745	0.626695
19	6	0	-0.453064	1.647157	1.741069
20	1	0	-0.868720	2.573091	2.148701
21	1	0	0.629178	1.631867	1.958433
22	1	0	-0.929431	0.806005	2.251972
23	7	0	-0.752233	1.589904	0.320553
24	6	0	-0.121301	2.683242	-0.398765
25	1	0	-0.481274	3.631887	0.008963
26	1	0	-0.397873	2.638108	-1.456586
27	1	0	0.980809	2.672037	-0.322806
28	1	0	-3.179491	-2.235349	1.115313
29	1	0	-4.369893	-1.877856	-0.051518

1a.2Me$_2$NH-ts1

Zero-point correction=	0.340870
(Hartree/Particle)	
Thermal correction to Energy=	0.361012
Thermal correction to Enthalpy=	0.361956
Thermal correction to Gibbs Free Energy=	0.290307
Sum of electronic and zero-point Energies=	-764.111934
Sum of electronic and thermal Energies=	-764.091792
Sum of electronic and thermal Enthalpies=	-764.090847
Sum of electronic and thermal Free Energies=	-764.162497

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.052470	1.625363	0.016765
2	6	0	1.299156	1.970791	-0.496459
3	7	0	1.833129	3.062849	0.117973
4	8	0	1.918093	1.364847	-1.381059
5	6	0	-1.963052	0.339237	-0.304251
6	6	0	-4.614172	-0.315973	0.301486
7	6	0	-2.726668	-0.416677	-1.199118
8	6	0	-2.539905	0.773735	0.894619
9	6	0	-3.857515	0.442894	1.197242
10	6	0	-4.048543	-0.742467	-0.899690
11	6	0	-0.561022	0.672897	-0.640009
12	7	0	3.313929	-0.868070	-0.049278
13	1	0	-0.213661	0.372584	-1.632433
14	1	0	1.254267	3.610731	0.734319
15	1	0	2.672410	3.468556	-0.264283
16	1	0	3.263419	-0.199607	-0.815697
17	1	0	-2.281985	-0.746953	-2.135180
18	1	0	-4.635817	-1.325549	-1.602204
19	1	0	-5.643529	-0.568424	0.537216
20	1	0	-4.299081	0.780927	2.129807
21	1	0	-1.941829	1.374001	1.572893
22	7	0	0.290878	-1.194551	0.079120
23	1	0	1.285756	-1.041033	-0.132309
24	6	0	4.390152	-1.824005	-0.267292
25	1	0	4.346656	-2.602558	0.501861
26	1	0	5.391491	-1.364386	-0.225209
27	1	0	4.268434	-2.303057	-1.241704
28	6	0	-0.154644	-2.417076	-0.571219
29	1	0	-1.223047	-2.562794	-0.379882
30	1	0	0.387500	-3.303083	-0.209676
31	1	0	-0.001854	-2.332132	-1.651235
32	6	0	3.474763	-0.131679	1.197975
33	1	0	2.673577	0.606938	1.299644
34	1	0	4.440635	0.395483	1.268156
35	1	0	3.407727	-0.827220	2.042065
36	6	0	0.115823	-1.207046	1.521943
37	1	0	0.316039	-0.202343	1.911276
38	1	0	0.788073	-1.922910	2.015899
39	1	0	-0.919028	-1.472874	1.761732

1a.2Me$_2$NH-I1

Zero-point correction=	0.344886
(Hartree/Particle)	
Thermal correction to Energy=	0.363935
Thermal correction to Enthalpy=	0.364880
Thermal correction to Gibbs Free Energy=	0.296302
Sum of electronic and zero-point Energies=	-764.118437
Sum of electronic and thermal Energies=	-764.099388
Sum of electronic and thermal Enthalpies=	-764.098443
Sum of electronic and thermal Free Energies=	-764.167021

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.064736	1.557421	0.157510
2	6	0	1.206401	1.993268	-0.386044
3	7	0	1.711214	3.167901	0.183545
4	8	0	1.883781	1.441680	-1.294789
5	6	0	-1.876435	0.128871	-0.229654
6	6	0	-4.626003	-0.308585	0.105940
7	6	0	-2.603630	-0.590453	-1.181787
8	6	0	-2.545148	0.645618	0.884297
9	6	0	-3.909601	0.423215	1.054617
10	6	0	-3.971688	-0.810567	-1.017361
11	6	0	-0.388886	0.351166	-0.410623
12	7	0	3.154750	-0.658185	0.137949
13	1	0	-0.118030	0.230795	-1.469738
14	1	0	1.017210	3.737311	0.647992
15	1	0	2.321820	3.681193	-0.436654
16	1	0	-2.100060	-0.969202	-2.068787
17	1	0	-4.524545	-1.363905	-1.770278
18	1	0	-5.691049	-0.474872	0.236099
19	1	0	-4.418397	0.830738	1.923117
20	1	0	-1.982316	1.239276	1.597623
21	7	0	0.383018	-0.847006	0.243918
22	6	0	3.560624	-1.298156	-1.112145
23	1	0	3.318627	-2.365977	-1.072419
24	1	0	4.639239	-1.200441	-1.303414
25	1	0	3.011289	-0.833613	-1.934406
26	6	0	0.176119	-2.145053	-0.428400
27	1	0	-0.843901	-2.494684	-0.258312
28	1	0	0.887624	-2.866603	-0.019295
29	1	0	0.355285	-2.021940	-1.498406
30	6	0	3.910574	-1.137437	1.290671
31	1	0	3.615599	-0.579323	2.182469
32	1	0	4.997604	-1.037480	1.155382
33	1	0	3.686341	-2.196766	1.456074
34	6	0	0.157895	-0.949779	1.702231
35	1	0	0.255090	0.049948	2.126705
36	1	0	0.913752	-1.616631	2.122907
37	1	0	-0.839357	-1.350368	1.893580
38	1	0	3.263025	0.348266	0.018560
39	1	0	1.427535	-0.632733	0.138601

1a.2Me$_2$NH-I2

Zero-point correction=	0.345448
(Hartree/Particle)	
Thermal correction to Energy=	0.364258
Thermal correction to Enthalpy=	0.365202
Thermal correction to Gibbs Free Energy=	0.298601
Sum of electronic and zero-point Energies=	-764.111746
Sum of electronic and thermal Energies=	-764.092936
Sum of electronic and thermal Enthalpies=	-764.091992
Sum of electronic and thermal Free Energies=	-764.158593

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.745406	-0.794365	-0.759456
2	6	0	1.602446	-1.823325	-0.800390
3	7	0	2.514214	-1.749541	-1.865371
4	8	0	1.711864	-2.780444	0.004365
5	6	0	-1.558809	-0.389050	-0.063608
6	6	0	-4.157898	0.416435	-0.736037
7	6	0	-2.665471	-0.992479	0.536900
8	6	0	-1.764860	0.608575	-1.020590
9	6	0	-3.055692	1.015696	-1.349201
10	6	0	-3.960707	-0.594977	0.202416
11	1	0	-2.514197	-1.783394	1.268022
12	1	0	-0.901965	1.042976	-1.513492
13	1	0	-3.204593	1.792198	-2.093561
14	1	0	-4.812592	-1.078078	0.671107
15	1	0	-5.164355	0.727772	-0.998405
16	6	0	-0.155863	-0.810709	0.324045
17	6	0	1.386526	2.569277	-1.167992
18	1	0	0.432561	3.089145	-1.045326
19	1	0	1.217917	1.641271	-1.722683
20	1	0	2.071078	3.211124	-1.740989
21	6	0	-0.597682	0.767703	2.336546
22	1	0	-0.071302	1.410619	3.044732
23	1	0	-1.098462	-0.039556	2.875994
24	1	0	-1.333811	1.349043	1.783381
25	7	0	1.929767	2.207958	0.143633
26	6	0	3.225207	1.533530	-0.000560
27	1	0	3.932919	2.121648	-0.602555
28	1	0	3.061621	0.569132	-0.493310
29	1	0	3.666000	1.358199	0.983916
30	7	0	0.393636	0.192975	1.399797
31	6	0	1.509002	-0.435229	2.151350
32	1	0	2.027280	0.339192	2.721141
33	1	0	2.185185	-0.916317	1.446984
34	1	0	1.099900	-1.187335	2.829204
35	1	0	-0.194825	-1.767531	0.865583
36	1	0	2.051862	3.051991	0.697951
37	1	0	0.843207	0.984130	0.846459
38	1	0	2.181323	-1.218201	-2.658373
39	1	0	2.911991	-2.646344	-2.108195

1a.2Me$_2$NH-ts2

Zero-point correction=	0.340655
(Hartree/Particle)	
Thermal correction to Energy=	0.359219
Thermal correction to Enthalpy=	0.360163
Thermal correction to Gibbs Free Energy=	0.293946
Sum of electronic and zero-point Energies=	-764.111248
Sum of electronic and thermal Energies=	-764.092684
Sum of electronic and thermal Enthalpies=	-764.091740
Sum of electronic and thermal Free Energies=	-764.157956

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.879029	-0.829433	-0.709777
2	6	0	1.741048	-1.850385	-0.724424
3	7	0	2.651345	-1.805437	-1.801347
4	8	0	1.865861	-2.782358	0.105447
5	6	0	-1.441770	-0.478021	-0.031097
6	6	0	-4.082206	0.146474	-0.765251
7	6	0	-2.524885	-1.064218	0.629112
8	6	0	-1.699966	0.404649	-1.083606
9	6	0	-3.008093	0.723578	-1.443731
10	6	0	-3.836574	-0.757242	0.267491
11	1	0	-2.338338	-1.772314	1.433207
12	1	0	-0.867541	0.814558	-1.647455
13	1	0	-3.190498	1.411560	-2.264152
14	1	0	-4.664872	-1.228702	0.787764
15	1	0	-5.101859	0.387373	-1.049858
16	6	0	-0.019977	-0.796398	0.402737
17	6	0	2.937255	1.918198	-0.258844
18	1	0	3.310680	0.893502	-0.208340
19	1	0	3.192954	2.453962	0.657826
20	1	0	3.388525	2.428340	-1.114024
21	6	0	-0.533406	0.767788	2.333690
22	1	0	-0.050524	1.479106	3.009366
23	1	0	-0.957140	-0.050030	2.933419
24	1	0	-1.343229	1.272688	1.805619
25	7	0	1.471391	1.867171	-0.404096
26	6	0	0.840754	3.175596	-0.630516
27	1	0	1.207561	3.627222	-1.555791
28	1	0	1.077106	3.833193	0.208777
29	1	0	-0.241768	3.046458	-0.689987
30	7	0	0.470279	0.271479	1.384477
31	6	0	1.632578	-0.248959	2.124326
32	1	0	2.110592	0.569237	2.671816
33	1	0	2.342412	-0.694459	1.427277
34	1	0	1.320214	-1.023489	2.837010
35	1	0	-0.028632	-1.744701	0.963680
36	1	0	1.250787	1.168788	-1.131894
37	1	0	0.987067	1.259509	0.504965
38	1	0	3.045262	-2.713691	-2.007585
39	1	0	2.291494	-1.332081	-2.619333

1a.3Me$_2$NH-ts1

Zero-point correction=	0.435606
(Hartree/Particle)	
Thermal correction to Energy=	0.461645
Thermal correction to Enthalpy=	0.462589
Thermal correction to Gibbs Free Energy=	0.377309
Sum of electronic and zero-point Energies=	-899.128366
Sum of electronic and thermal Energies=	-899.102327
Sum of electronic and thermal Enthalpies=	-899.101383
Sum of electronic and thermal Free Energies=	-899.186663

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.736957	-1.331551	-1.273419
2	6	0	-0.588641	-1.492939	-1.667411
3	7	0	-0.836924	-2.735661	-2.166613
4	8	0	-1.491025	-0.651985	-1.564243
5	6	0	2.419943	0.221254	-0.505540
6	6	0	5.054363	0.951218	0.084056
7	6	0	2.769576	1.569433	-0.384043
8	6	0	3.401577	-0.762121	-0.336962
9	6	0	4.711168	-0.397260	-0.038208
10	6	0	4.082549	1.935694	-0.093636
11	6	0	1.018755	-0.142275	-0.806250
12	7	0	-2.572385	-0.672118	1.262257
13	1	0	0.324284	0.689051	-0.956394
14	1	0	-0.061025	-3.349762	-2.356428
15	1	0	-1.726549	-2.910271	-2.606476
16	1	0	2.007120	2.333256	-0.519575
17	1	0	4.346379	2.985081	-0.006518
18	1	0	6.077677	1.232477	0.313264
19	1	0	5.468889	-1.163111	0.096078
20	1	0	3.118634	-1.804718	-0.446080
21	7	0	0.345663	-0.172375	1.276717
22	6	0	-3.300620	-0.088899	2.378122
23	1	0	-2.841739	-0.404023	3.322592
24	1	0	-4.363184	-0.381808	2.403235
25	1	0	-3.245344	1.001814	2.316673
26	6	0	0.672806	0.980489	2.100790
27	1	0	1.761081	1.062880	2.198863
28	1	0	0.236353	0.910254	3.108492
29	1	0	0.302134	1.894377	1.625882
30	6	0	-2.692087	-2.122061	1.206748
31	1	0	-2.173110	-2.495167	0.318941
32	1	0	-3.738944	-2.467045	1.173126
33	1	0	-2.222632	-2.564400	2.093224
34	6	0	0.827435	-1.425587	1.832547
35	1	0	0.649569	-2.227226	1.107759
36	1	0	0.325335	-1.678894	2.777589
37	1	0	1.904992	-1.355741	2.018422
38	1	0	-0.680785	-0.248396	1.159490
39	7	0	-3.324513	1.549443	-0.860598
40	6	0	-4.281327	2.441949	-1.497112
41	1	0	-4.753300	3.071980	-0.735359
42	1	0	-5.066166	1.858996	-1.985233
43	1	0	-3.823041	3.109133	-2.246986
44	6	0	-2.214593	2.272597	-0.260041

45	1	0	-1.501405	1.551282	0.148398
46	1	0	-2.583657	2.898875	0.560945
47	1	0	-1.682021	2.927807	-0.971687
48	1	0	-2.944402	0.891215	-1.536888
49	1	0	-2.913951	-0.265163	0.391827

1a.3Me$_2$NH-I1

Zero-point correction= (Hartree/Particle)	0.439115
Thermal correction to Energy=	0.464149
Thermal correction to Enthalpy=	0.465093
Thermal correction to Gibbs Free Energy=	0.381908
Sum of electronic and zero-point Energies=	-899.137761
Sum of electronic and thermal Energies=	-899.112726
Sum of electronic and thermal Enthalpies=	-899.111782
Sum of electronic and thermal Free Energies=	-899.194968

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.635513	-1.233386	-0.716998
2	6	0	0.587750	-1.680564	-0.422144
3	7	0	1.128854	-2.567141	-1.362996
4	8	0	1.307864	-1.358363	0.560817
5	6	0	-2.647607	-0.311671	0.319067
6	6	0	-5.448236	-0.275371	0.477237
7	6	0	-3.288944	-0.018635	1.525509
8	6	0	-3.425171	-0.605442	-0.805629
9	6	0	-4.815857	-0.581802	-0.729019
10	6	0	-4.681667	0.000706	1.607774
11	6	0	-1.133559	-0.328431	0.244613
12	7	0	2.054813	1.332874	-0.632969
13	1	0	-0.716319	-0.486506	1.248765
14	1	0	0.438291	-3.045917	-1.925086
15	1	0	1.838664	-3.173834	-0.975856
16	1	0	-2.695112	0.179324	2.415390
17	1	0	-5.164872	0.220040	2.554993
18	1	0	-6.532220	-0.265672	0.537893
19	1	0	-5.408452	-0.814572	-1.608685
20	1	0	-2.920873	-0.874341	-1.728358
21	7	0	-0.622582	1.107951	-0.089018
22	6	0	2.587393	2.683127	-0.467124
23	1	0	2.017027	3.386397	-1.084472
24	1	0	3.645532	2.752176	-0.761064
25	1	0	2.499288	2.988579	0.578697
26	6	0	-0.836808	2.089673	0.992320
27	1	0	-1.903562	2.290668	1.109433
28	1	0	-0.314197	3.013646	0.734241
29	1	0	-0.427650	1.687119	1.920926
30	6	0	2.245646	0.835764	-1.996784
31	1	0	1.867782	-0.187873	-2.072823
32	1	0	3.304449	0.846725	-2.296753
33	1	0	1.689231	1.468209	-2.697891
34	6	0	-1.123841	1.611587	-1.385615

35	1	0	-0.995842	0.819836	-2.125050
36	1	0	-0.535449	2.488851	-1.665351
37	1	0	-2.177292	1.884591	-1.297158
38	1	0	0.452856	1.047216	-0.219935
39	7	0	3.982486	-0.412374	1.087458
40	6	0	4.548473	-1.137746	-0.040869
41	1	0	5.341220	-0.541179	-0.507667
42	1	0	3.764030	-1.317871	-0.782192
43	1	0	4.982821	-2.111174	0.245654
44	6	0	4.919426	-0.291521	2.192875
45	1	0	4.436580	0.206460	3.037518
46	1	0	5.774447	0.319835	1.883846
47	1	0	5.311128	-1.263412	2.538229
48	1	0	3.132223	-0.895896	1.372429
49	1	0	2.554956	0.711979	0.012183

1a.3Me$_2$NH-I2

Zero-point correction= 0.439865
(Hartree/Particle)
Thermal correction to Energy= 0.464619
Thermal correction to Enthalpy= 0.465563
Thermal correction to Gibbs Free Energy= 0.384588
Sum of electronic and zero-point Energies= -899.136738
Sum of electronic and thermal Energies= -899.111984
Sum of electronic and thermal Enthalpies= -899.111040
Sum of electronic and thermal Free Energies= -899.192015

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.163218	0.419820	1.673072
2	1	0	0.159500	-0.550466	1.336642
3	1	0	1.158424	-2.022535	0.117417
4	1	0	1.479204	-0.196524	-1.269274
5	7	0	1.987644	-1.062654	-1.495246
6	7	0	0.773311	-2.126526	1.066801
7	6	0	1.864221	-2.411394	1.997955
8	1	0	2.320227	-3.396897	1.823328
9	1	0	1.484020	-2.392473	3.025781
10	1	0	2.640337	-1.647713	1.903847
11	6	0	-0.246408	-3.173290	1.094841
12	1	0	0.170040	-4.169679	0.885897
13	1	0	-1.024257	-2.954681	0.359155
14	1	0	-0.711983	-3.202393	2.086236
15	6	0	-1.286688	0.203190	2.611026
16	1	0	-1.655289	1.169785	2.964254
17	1	0	-0.929160	-0.385044	3.458520
18	1	0	-2.086639	-0.334146	2.102717
19	6	0	0.997664	1.022899	2.371004
20	1	0	0.739110	2.034111	2.689707
21	1	0	1.835038	1.067373	1.675795
22	1	0	1.252560	0.397524	3.228704
23	6	0	1.825852	-1.390517	-2.903896
24	1	0	2.301380	-0.654617	-3.574485
25	1	0	0.762329	-1.443075	-3.154886

26	1	0	2.274291	-2.368471	-3.112503
27	6	0	3.387519	-0.882818	-1.134392
28	1	0	3.920282	-0.189911	-1.807123
29	1	0	3.910999	-1.846019	-1.159178
30	1	0	3.454741	-0.477632	-0.120209
31	7	0	0.551695	1.372178	-0.442626
32	6	0	-0.557273	1.264034	0.421802
33	6	0	-1.734961	0.579454	-0.243999
34	6	0	-3.907781	-0.687998	-1.480695
35	6	0	-3.019194	1.115734	-0.141895
36	6	0	-1.544453	-0.593630	-0.980802
37	6	0	-2.624249	-1.227451	-1.590277
38	6	0	-4.102587	0.488128	-0.759625
39	1	0	-3.173131	2.034337	0.419532
40	1	0	-0.540444	-0.998566	-1.082714
41	1	0	-2.464344	-2.139718	-2.158270
42	1	0	-5.095342	0.919891	-0.677615
43	1	0	-4.747942	-1.178866	-1.962064
44	6	0	1.238797	2.521988	-0.333651
45	8	0	1.022477	3.478946	0.443968
46	7	0	2.357451	2.589242	-1.175835
47	1	0	-0.871466	2.224961	0.856258
48	1	0	2.672757	3.534355	-1.344776
49	1	0	2.294016	2.021120	-2.009972

1a.3Me$_2$NH-I3

Zero-point correction=	0.439698
(Hartree/Particle)	
Thermal correction to Energy=	0.463952
Thermal correction to Enthalpy=	0.464896
Thermal correction to Gibbs Free Energy=	0.386528
Sum of electronic and zero-point Energies=	-899.134297
Sum of electronic and thermal Energies=	-899.110043
Sum of electronic and thermal Enthalpies=	-899.109099
Sum of electronic and thermal Free Energies=	-899.187467

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.883357	-1.662894	1.036758
2	1	0	-0.724698	0.072997	1.611575
3	1	0	-0.188523	1.590391	1.017959
4	1	0	0.077283	1.453594	-0.871977
5	7	0	0.381209	2.323616	-0.404739
6	7	0	-0.754328	1.112929	1.802611
7	6	0	-2.154207	1.572493	1.664960
8	1	0	-2.193015	2.651228	1.831168
9	1	0	-2.780975	1.064830	2.401169
10	1	0	-2.484556	1.329285	0.653031
11	6	0	-0.163050	1.419116	3.119220
12	1	0	-0.217294	2.494759	3.296181
13	1	0	0.881367	1.105372	3.124418
14	1	0	-0.711520	0.891732	3.901749
15	6	0	-0.331589	-2.912964	1.569361
16	1	0	-0.626649	-3.771049	0.943483
17	1	0	-0.717447	-3.077987	2.579468

18	1	0	0.756662	-2.883703	1.612975
19	6	0	-2.344600	-1.811146	1.002168
20	1	0	-2.647188	-2.670609	0.385983
21	1	0	-2.808396	-0.918344	0.583728
22	1	0	-2.705990	-1.959443	2.024806
23	6	0	1.795513	2.581925	-0.652510
24	1	0	1.995046	2.824952	-1.707309
25	1	0	2.381891	1.701649	-0.381530
26	1	0	2.129187	3.427897	-0.041417
27	6	0	-0.465062	3.427580	-0.847607
28	1	0	-0.294862	3.690421	-1.903253
29	1	0	-0.262709	4.318625	-0.243287
30	1	0	-1.519137	3.161926	-0.721777
31	7	0	-0.988983	-0.220725	-0.902300
32	6	0	-0.345571	-1.371940	-0.329337
33	6	0	1.159099	-1.100565	-0.274466
34	6	0	3.925202	-0.562724	-0.366007
35	6	0	1.859544	-1.129232	-1.486274
36	6	0	1.867481	-0.780920	0.887006
37	6	0	3.239744	-0.517641	0.844887
38	6	0	3.225431	-0.866168	-1.536778
39	1	0	1.313976	-1.361678	-2.398110
40	1	0	1.356094	-0.769821	1.845758
41	1	0	3.770326	-0.281853	1.763073
42	1	0	3.747440	-0.902177	-2.488428
43	1	0	4.991808	-0.363498	-0.400289
44	6	0	-1.949885	-0.489020	-1.791312
45	8	0	-2.367164	-1.601111	-2.188061
46	1	0	-0.509598	-2.272116	-0.951843
47	7	0	-2.598404	0.665938	-2.288922
48	1	0	-2.010757	1.489169	-2.316142
49	1	0	-3.061713	0.487541	-3.170382

1a.3Me$_2$NH-ts2

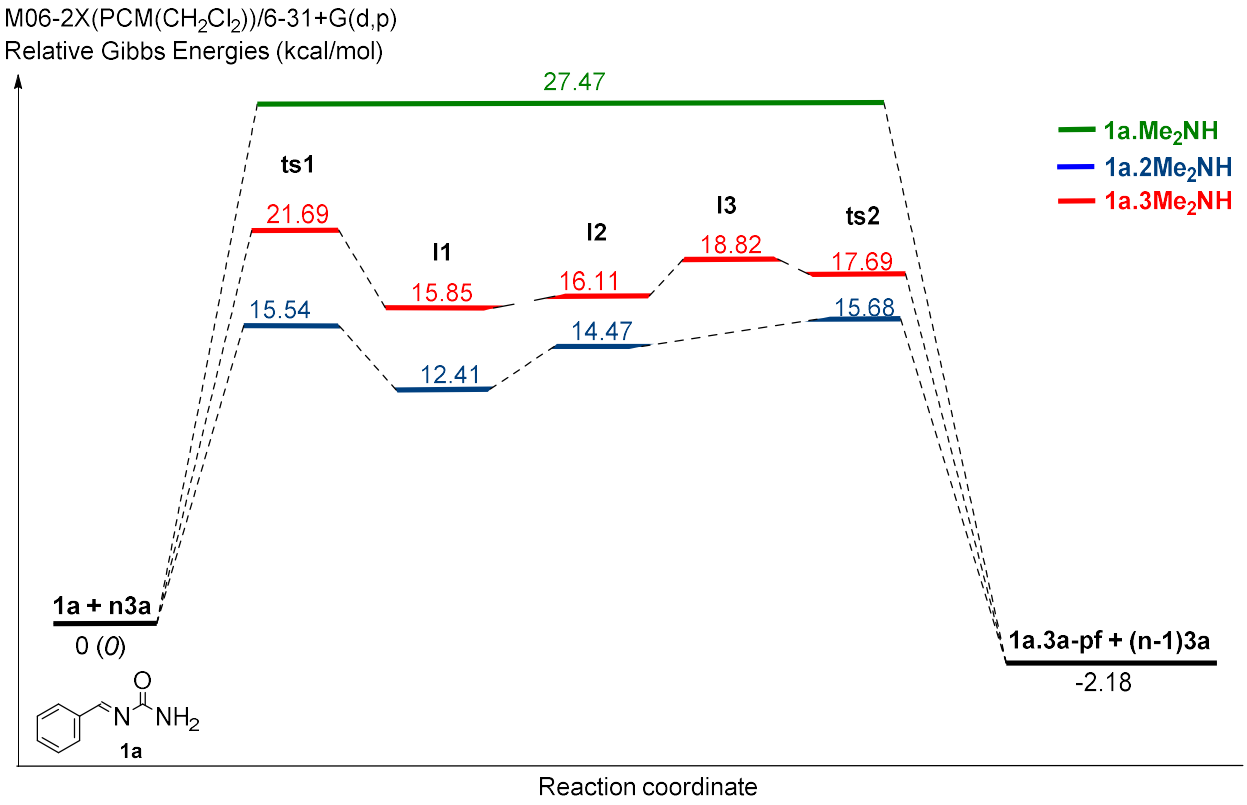
Zero-point correction= 0.435053
(Hartree/Particle)
Thermal correction to Energy= 0.458986
Thermal correction to Enthalpy= 0.459930
Thermal correction to Gibbs Free Energy= 0.382093
Sum of electronic and zero-point Energies= -899.136116
Sum of electronic and thermal Energies= -899.112182
Sum of electronic and thermal Enthalpies= -899.111238
Sum of electronic and thermal Free Energies= -899.189075

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.194467	0.356573	1.686927
2	1	0	0.599629	-1.190935	1.197041
3	1	0	1.652652	-1.499999	-0.185655
4	1	0	1.376421	0.062360	-1.135310
5	7	0	2.042036	-0.749636	-1.277653
6	7	0	1.255575	-1.959174	0.877865
7	6	0	2.380457	-2.045506	1.823315
8	1	0	3.110038	-2.773326	1.458548

9	1	0	2.031495	-2.355542	2.813431
10	1	0	2.858969	-1.067710	1.903211
11	6	0	0.549572	-3.239237	0.721757
12	1	0	1.237089	-3.986216	0.316482
13	1	0	-0.288992	-3.112518	0.035040
14	1	0	0.169187	-3.591347	1.685503
15	6	0	-1.261323	0.086920	2.650673
16	1	0	-1.742735	1.016187	3.001209
17	1	0	-0.838050	-0.426721	3.519381
18	1	0	-2.026083	-0.553830	2.206840
19	6	0	0.875911	1.105772	2.351500
20	1	0	0.521136	2.081341	2.717760
21	1	0	1.691236	1.286158	1.647738
22	1	0	1.250559	0.521739	3.198718
23	6	0	1.855301	-1.386869	-2.581333
24	1	0	2.096529	-0.700412	-3.402600
25	1	0	0.816856	-1.709135	-2.693253
26	1	0	2.505260	-2.264009	-2.662991
27	6	0	3.413948	-0.272750	-1.076498
28	1	0	3.742068	0.368145	-1.903172
29	1	0	4.097961	-1.124457	-0.994909
30	1	0	3.456952	0.317229	-0.157538
31	7	0	0.346320	1.340115	-0.461333
32	6	0	-0.697784	1.134127	0.502136
33	6	0	-1.852725	0.376602	-0.131360
34	6	0	-3.969551	-1.064296	-1.288972
35	6	0	-3.169474	0.816319	0.003516
36	6	0	-1.609152	-0.787157	-0.865850
37	6	0	-2.653490	-1.509161	-1.436062
38	6	0	-4.223488	0.103747	-0.572987
39	1	0	-3.372467	1.723976	0.567045
40	1	0	-0.580549	-1.108433	-1.003963
41	1	0	-2.444125	-2.411665	-2.004166
42	1	0	-5.242262	0.462956	-0.461898
43	1	0	-4.787404	-1.619482	-1.738036
44	6	0	0.874908	2.567168	-0.488536
45	8	0	0.627911	3.545317	0.252835
46	7	0	1.881615	2.726164	-1.471114
47	1	0	-1.078356	2.097869	0.886255
48	1	0	2.046557	3.702978	-1.675820
49	1	0	1.720936	2.179895	-2.308195

2.1.3.-M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

Energy profiles for the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1a** in dichloromethane.



3a [Me_2NH]

Zero-point correction=	0.093094
(Hartree/Particle)	
Thermal correction to Energy=	0.097499
Thermal correction to Enthalpy=	0.098443
Thermal correction to Gibbs Free Energy=	0.067604
Sum of electronic and zero-point Energies=	-135.008304
Sum of electronic and thermal Energies=	-135.003898
Sum of electronic and thermal Enthalpies=	-135.002954
Sum of electronic and thermal Free Energies=	-135.033793

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000000	0.573143	-0.153449
2	1	0	-0.000002	1.328661	0.525178
3	6	0	-1.206730	-0.225316	0.020308
4	1	0	-2.089463	0.414655	-0.049351
5	1	0	-1.238145	-0.763388	0.982532
6	1	0	-1.263756	-0.969705	-0.780546
7	6	0	1.206730	-0.225315	0.020308
8	1	0	1.238180	-0.763331	0.982564
9	1	0	2.089468	0.414641	-0.049429
10	1	0	1.263713	-0.969754	-0.780503

1a.Me_2NH-ts

Zero-point correction=	0.243887
(Hartree/Particle)	
Thermal correction to Energy=	0.257458
Thermal correction to Enthalpy=	0.258402
Thermal correction to Gibbs Free Energy=	0.202702
Sum of electronic and zero-point Energies=	-629.072094
Sum of electronic and thermal Energies=	-629.058523
Sum of electronic and thermal Enthalpies=	-629.057579
Sum of electronic and thermal Free Energies=	-629.113279

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.597288	-0.238306	0.415114
2	6	0	-2.307349	-1.208270	-0.205539
3	7	0	-3.478149	-1.568924	0.443571
4	8	0	-1.996012	-1.743003	-1.284794
5	6	0	0.863060	-0.126522	-0.185156
6	6	0	3.488312	-1.052248	0.096422
7	6	0	1.861583	0.302872	-1.064365
8	6	0	1.183886	-1.030825	0.827819
9	6	0	2.492075	-1.492709	0.967929
10	6	0	3.170927	-0.153332	-0.922587
11	1	0	1.611287	0.990811	-1.869350
12	1	0	0.397210	-1.370484	1.495114
13	1	0	2.732910	-2.200305	1.755463
14	1	0	3.939118	0.184748	-1.611153

15	1	0	4.505729	-1.415135	0.204429
16	6	0	-0.540495	0.405927	-0.340029
17	1	0	-0.775909	0.495833	-1.407998
18	1	0	-1.734209	1.059445	0.739693
19	6	0	0.169067	2.179993	1.342395
20	1	0	-0.223589	3.070372	1.835789
21	1	0	1.151378	2.399776	0.911173
22	1	0	0.268101	1.375164	2.072574
23	7	0	-0.784365	1.775606	0.299189
24	6	0	-1.064107	2.849476	-0.661910
25	1	0	-1.404284	3.732121	-0.118035
26	1	0	-1.849317	2.522425	-1.345843
27	1	0	-0.162880	3.101591	-1.230970
28	1	0	-3.532459	-1.351145	1.428243
29	1	0	-3.838126	-2.475995	0.184234

1a.Me_2NH-pf

Zero-point correction= 0.248647
(Hartree/Particle)
Thermal correction to Energy= 0.262427
Thermal correction to Enthalpy= 0.263371
Thermal correction to Gibbs Free Energy= 0.208146
Sum of electronic and zero-point Energies= -629.120021
Sum of electronic and thermal Energies= -629.106241
Sum of electronic and thermal Enthalpies= -629.105297
Sum of electronic and thermal Free Energies= -629.160522

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.407616	-0.703538	0.208007
2	6	0	-2.674419	-0.825512	-0.305856
3	7	0	-3.394314	-1.887262	0.190613
4	8	0	-3.124729	-0.074036	-1.167006
5	6	0	0.942848	-0.187497	-0.210607
6	6	0	3.641372	-0.947235	-0.043424
7	6	0	1.810905	0.021378	-1.285823
8	6	0	1.445942	-0.780162	0.953911
9	6	0	2.784397	-1.160502	1.036325
10	6	0	3.151448	-0.354170	-1.205757
11	1	0	1.431294	0.478011	-2.196904
12	1	0	0.798034	-0.944806	1.811965
13	1	0	3.158297	-1.619870	1.946119
14	1	0	3.810190	-0.187296	-2.052425
15	1	0	4.683804	-1.242914	0.021165
16	6	0	-0.497181	0.295428	-0.318483
17	1	0	-0.732955	0.442109	-1.378342
18	1	0	-1.015565	-1.505761	0.680446
19	6	0	-0.461620	1.644707	1.740664
20	1	0	-0.871578	2.573308	2.147786
21	1	0	0.618662	1.619887	1.964785
22	1	0	-0.947626	0.806199	2.246705
23	7	0	-0.750256	1.594111	0.316392
24	6	0	-0.096908	2.682791	-0.392347
25	1	0	-0.454484	3.634624	0.009906

26	1	0	-0.353676	2.640107	-1.455264
27	1	0	1.003139	2.660906	-0.296981
28	1	0	-3.166504	-2.253958	1.103670
29	1	0	-4.378594	-1.866789	-0.033285

1a.2Me$_2$NH-ts1

Zero-point correction=	0.345095
(Hartree/Particle)	
Thermal correction to Energy=	0.363999
Thermal correction to Enthalpy=	0.364944
Thermal correction to Gibbs Free Energy=	0.297408
Sum of electronic and zero-point Energies=	-764.123383
Sum of electronic and thermal Energies=	-764.104478
Sum of electronic and thermal Enthalpies=	-764.103534
Sum of electronic and thermal Free Energies=	-764.171070

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.095244	1.531285	0.194925
2	6	0	1.214098	1.995352	-0.369209
3	7	0	1.733770	3.149441	0.231813
4	8	0	1.864215	1.489789	-1.324664
5	6	0	-1.862892	0.129249	-0.219975
6	6	0	-4.621761	-0.274401	0.087328
7	6	0	-2.596023	-0.548981	-1.197612
8	6	0	-2.529914	0.619899	0.907182
9	6	0	-3.898885	0.414441	1.063268
10	6	0	-3.968579	-0.751860	-1.047481
11	6	0	-0.370928	0.333400	-0.390084
12	7	0	3.133408	-0.643735	0.125968
13	1	0	-0.101553	0.229773	-1.450859
14	1	0	1.056236	3.694883	0.747116
15	1	0	2.315317	3.696808	-0.387680
16	1	0	-2.093091	-0.911091	-2.091751
17	1	0	-4.524827	-1.274308	-1.819641
18	1	0	-5.689900	-0.428110	0.206988
19	1	0	-4.405434	0.799583	1.943197
20	1	0	-1.963952	1.176820	1.647255
21	7	0	0.383746	-0.875504	0.246475
22	6	0	3.548259	-1.265023	-1.131674
23	1	0	3.305761	-2.332736	-1.108185
24	1	0	4.628017	-1.163913	-1.312365
25	1	0	3.003677	-0.790270	-1.951052
26	6	0	0.168169	-2.159191	-0.452685
27	1	0	-0.855434	-2.503619	-0.293912
28	1	0	0.870384	-2.894495	-0.052911
29	1	0	0.353694	-2.018162	-1.519228
30	6	0	3.871208	-1.155226	1.278235
31	1	0	3.569516	-0.614295	2.178213
32	1	0	4.959949	-1.061192	1.156872
33	1	0	3.634715	-2.215466	1.416026
34	6	0	0.149053	-1.007837	1.701513
35	1	0	0.263001	-0.021992	2.152798
36	1	0	0.889278	-1.699278	2.109041

37	1	0	-0.855861	-1.394972	1.879202
38	1	0	3.256696	0.363181	0.030762
39	1	0	1.436075	-0.664803	0.150327

1a.2Me$_2$NH-I1

Zero-point correction=	0.345095
(Hartree/Particle)	
Thermal correction to Energy=	0.363999
Thermal correction to Enthalpy=	0.364944
Thermal correction to Gibbs Free Energy=	0.297408
Sum of electronic and zero-point Energies=	-764.123383
Sum of electronic and thermal Energies=	-764.104478
Sum of electronic and thermal Enthalpies=	-764.103534
Sum of electronic and thermal Free Energies=	-764.171070

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.095244	1.531285	0.194925
2	6	0	1.214098	1.995352	-0.369209
3	7	0	1.733770	3.149441	0.231813
4	8	0	1.864215	1.489789	-1.324664
5	6	0	-1.862892	0.129249	-0.219975
6	6	0	-4.621761	-0.274401	0.087328
7	6	0	-2.596023	-0.548981	-1.197612
8	6	0	-2.529914	0.619899	0.907182
9	6	0	-3.898885	0.414441	1.063268
10	6	0	-3.968579	-0.751860	-1.047481
11	6	0	-0.370928	0.333400	-0.390084
12	7	0	3.133408	-0.643735	0.125968
13	1	0	-0.101553	0.229773	-1.450859
14	1	0	1.056236	3.694883	0.747116
15	1	0	2.315317	3.696808	-0.387680
16	1	0	-2.093091	-0.911091	-2.091751
17	1	0	-4.524827	-1.274308	-1.819641
18	1	0	-5.689900	-0.428110	0.206988
19	1	0	-4.405434	0.799583	1.943197
20	1	0	-1.963952	1.176820	1.647255
21	7	0	0.383746	-0.875504	0.246475
22	6	0	3.548259	-1.265023	-1.131674
23	1	0	3.305761	-2.332736	-1.108185
24	1	0	4.628017	-1.163913	-1.312365
25	1	0	3.003677	-0.790270	-1.951052
26	6	0	0.168169	-2.159191	-0.452685
27	1	0	-0.855434	-2.503619	-0.293912
28	1	0	0.870384	-2.894495	-0.052911
29	1	0	0.353694	-2.018162	-1.519228
30	6	0	3.871208	-1.155226	1.278235
31	1	0	3.569516	-0.614295	2.178213
32	1	0	4.959949	-1.061192	1.156872
33	1	0	3.634715	-2.215466	1.416026
34	6	0	0.149053	-1.007837	1.701513
35	1	0	0.263001	-0.021992	2.152798
36	1	0	0.889278	-1.699278	2.109041
37	1	0	-0.855861	-1.394972	1.879202

38	1	0	3.256696	0.363181	0.030762
39	1	0	1.436075	-0.664803	0.150327

1a.2Me$_2$NH-I2

Zero-point correction=	0.344623
(Hartree/Particle)	
Thermal correction to Energy=	0.363835
Thermal correction to Enthalpy=	0.364779
Thermal correction to Gibbs Free Energy=	0.296310
Sum of electronic and zero-point Energies=	-764.119475
Sum of electronic and thermal Energies=	-764.100263
Sum of electronic and thermal Enthalpies=	-764.099318
Sum of electronic and thermal Free Energies=	-764.167788

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.871044	-0.900093	-0.756127
2	6	0	1.702759	-1.947684	-0.811195
3	7	0	2.620175	-1.888646	-1.870878
4	8	0	1.782662	-2.920743	-0.019757
5	6	0	-1.433263	-0.509306	-0.046232
6	6	0	-4.049182	0.249443	-0.715754
7	6	0	-2.528970	-1.137954	0.549417
8	6	0	-1.660965	0.488633	-0.998450
9	6	0	-2.959057	0.873785	-1.325352
10	6	0	-3.831594	-0.764209	0.216118
11	1	0	-2.363421	-1.926717	1.279438
12	1	0	-0.812784	0.942793	-1.500090
13	1	0	-3.121252	1.652450	-2.064561
14	1	0	-4.673493	-1.265569	0.683505
15	1	0	-5.061481	0.543641	-0.975060
16	6	0	-0.021256	-0.904682	0.341578
17	6	0	2.870451	2.254401	-0.143059
18	1	0	3.336665	1.268794	-0.065120
19	1	0	3.059761	2.806577	0.782818
20	1	0	3.342308	2.800226	-0.972420
21	6	0	-0.461851	0.515898	2.438023
22	1	0	0.038859	1.177077	3.146761
23	1	0	-0.814474	-0.378666	2.957732
24	1	0	-1.304280	1.033778	1.982271
25	7	0	1.428154	2.094497	-0.330506
26	6	0	0.757418	3.366391	-0.589756
27	1	0	1.169782	3.888745	-1.464782
28	1	0	0.873790	4.016853	0.282353
29	1	0	-0.310607	3.197642	-0.749600
30	7	0	0.508675	0.123398	1.391363
31	6	0	1.762904	-0.376417	2.005256
32	1	0	2.209856	0.426123	2.594614
33	1	0	2.442762	-0.688169	1.214783
34	1	0	1.529593	-1.230156	2.644822
35	1	0	-0.042176	-1.853989	0.896383
36	1	0	1.277427	1.433826	-1.095080
37	1	0	0.778960	0.982693	0.808456

38	1	0	2.320414	-1.321759	-2.652419
39	1	0	2.981804	-2.794142	-2.137279

1a.2Me$_2$NH-ts2

Zero-point correction=	0.340453
(Hartree/Particle)	
Thermal correction to Energy=	0.359104
Thermal correction to Enthalpy=	0.360048
Thermal correction to Gibbs Free Energy=	0.293005
Sum of electronic and zero-point Energies=	-764.118409
Sum of electronic and thermal Energies=	-764.099758
Sum of electronic and thermal Enthalpies=	-764.098814
Sum of electronic and thermal Free Energies=	-764.165857

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.908842	-0.882730	-0.684376
2	6	0	1.729083	-1.933053	-0.687809
3	7	0	2.642933	-1.940396	-1.762210
4	8	0	1.818107	-2.866635	0.151635
5	6	0	-1.408305	-0.498860	0.000169
6	6	0	-4.055610	0.088210	-0.739154
7	6	0	-2.484596	-1.052305	0.699092
8	6	0	-1.676710	0.330838	-1.092114
9	6	0	-2.988428	0.631772	-1.455323
10	6	0	-3.799946	-0.763942	0.334640
11	1	0	-2.290348	-1.716999	1.537820
12	1	0	-0.849280	0.713922	-1.681016
13	1	0	-3.178899	1.280001	-2.305725
14	1	0	-4.623266	-1.208068	0.885997
15	1	0	-5.078019	0.315745	-1.024877
16	6	0	0.018644	-0.796260	0.433830
17	6	0	2.854124	2.134534	-0.318344
18	1	0	3.331508	1.157303	-0.227943
19	1	0	3.037220	2.718854	0.585770
20	1	0	3.265351	2.664720	-1.181123
21	6	0	-0.457387	0.828496	2.316511
22	1	0	0.031508	1.584071	2.936859
23	1	0	-0.833743	0.028635	2.969205
24	1	0	-1.299030	1.286837	1.795942
25	7	0	1.402209	1.934570	-0.477460
26	6	0	0.652263	3.184071	-0.685231
27	1	0	0.980382	3.685658	-1.599004
28	1	0	0.823888	3.842177	0.168982
29	1	0	-0.413162	2.956699	-0.753148
30	7	0	0.523017	0.313391	1.351617
31	6	0	1.720021	-0.158271	2.067921
32	1	0	2.187396	0.682631	2.587921
33	1	0	2.425345	-0.587978	1.356174
34	1	0	1.449190	-0.929080	2.801226
35	1	0	0.012115	-1.715764	1.040797
36	1	0	1.248112	1.251497	-1.229234
37	1	0	0.969859	1.279660	0.439540
38	1	0	2.979608	-2.869013	-1.978963

39	1	0	2.321476	-1.433649	-2.576421

1a.3Me$_2$NH-ts1

Zero-point correction= 0.435646
(Hartree/Particle)
Thermal correction to Energy= 0.461594
Thermal correction to Enthalpy= 0.462538
Thermal correction to Gibbs Free Energy= 0.376767
Sum of electronic and zero-point Energies= -899.131293
Sum of electronic and thermal Energies= -899.105345
Sum of electronic and thermal Enthalpies= -899.104401
Sum of electronic and thermal Free Energies= -899.190172

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.638284	-1.355111	-1.365883
2	6	0	-0.678668	-1.545023	-1.765107
3	7	0	-0.880716	-2.753736	-2.355147
4	8	0	-1.619699	-0.753088	-1.599332
5	6	0	2.252347	0.172642	-0.420391
6	6	0	4.856251	0.959089	0.230502
7	6	0	2.541341	1.516097	-0.162285
8	6	0	3.279587	-0.775913	-0.360519
9	6	0	4.574191	-0.384113	-0.030142
10	6	0	3.838952	1.910577	0.158733
11	6	0	0.863227	-0.224510	-0.739502
12	7	0	-2.746364	-0.473108	1.212944
13	1	0	0.130932	0.587202	-0.782352
14	1	0	-0.086691	-3.331320	-2.581978
15	1	0	-1.769483	-2.939287	-2.792659
16	1	0	1.743276	2.253580	-0.212459
17	1	0	4.055358	2.956171	0.354155
18	1	0	5.867105	1.262248	0.485311
19	1	0	5.366720	-1.124386	0.022240
20	1	0	3.047244	-1.813926	-0.577582
21	7	0	0.230407	-0.553769	1.300544
22	6	0	-3.523544	0.202339	2.242643
23	1	0	-3.206289	-0.149387	3.230631
24	1	0	-4.607074	0.022963	2.150905
25	1	0	-3.346951	1.280031	2.188530
26	6	0	0.758685	0.366343	2.297922
27	1	0	1.846324	0.252660	2.361427
28	1	0	0.329165	0.184921	3.293603
29	1	0	0.541628	1.397836	2.005673
30	6	0	-3.024758	-1.902461	1.153900
31	1	0	-2.476265	-2.343822	0.317047
32	1	0	-4.096417	-2.127430	1.028430
33	1	0	-2.687779	-2.378573	2.081975
34	6	0	0.546331	-1.942845	1.588849
35	1	0	0.160832	-2.577219	0.785840
36	1	0	0.117687	-2.274283	2.544743
37	1	0	1.634616	-2.065897	1.632978
38	1	0	-0.796161	-0.443499	1.226713

39	7	0	-2.663052	1.952651	-0.846762
40	6	0	-3.120582	2.905103	-1.848666
41	1	0	-3.714762	3.688056	-1.364906
42	1	0	-3.757577	2.398755	-2.577986
43	1	0	-2.294413	3.397385	-2.389187
44	6	0	-1.737921	2.560861	0.096610
45	1	0	-1.382180	1.801162	0.800032
46	1	0	-2.254854	3.338248	0.670851
47	1	0	-0.862784	3.030404	-0.387479
48	1	0	-2.205856	1.163401	-1.302149
49	1	0	-2.940301	-0.048889	0.307151

1a.3Me$_2$NH-I1

Zero-point correction=	0.438830
(Hartree/Particle)	
Thermal correction to Energy=	0.463912
Thermal correction to Enthalpy=	0.464856
Thermal correction to Gibbs Free Energy=	0.381861
Sum of electronic and zero-point Energies=	-899.142408
Sum of electronic and thermal Energies=	-899.117326
Sum of electronic and thermal Enthalpies=	-899.116382
Sum of electronic and thermal Free Energies=	-899.199376

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.615367	-1.181415	-0.763595
2	6	0	0.596580	-1.656371	-0.467726
3	7	0	1.147436	-2.499841	-1.442403
4	8	0	1.300462	-1.398817	0.546943
5	6	0	-2.641020	-0.321096	0.304382
6	6	0	-5.441067	-0.347118	0.484607
7	6	0	-3.278169	-0.095821	1.527786
8	6	0	-3.422459	-0.575808	-0.827428
9	6	0	-4.812866	-0.583663	-0.739753
10	6	0	-4.670469	-0.107756	1.620895
11	6	0	-1.127072	-0.304874	0.221250
12	7	0	2.036952	1.360529	-0.562695
13	1	0	-0.704042	-0.481826	1.219440
14	1	0	0.466022	-2.943151	-2.043594
15	1	0	1.844954	-3.133291	-1.075966
16	1	0	-2.681346	0.076810	2.420868
17	1	0	-5.149433	0.060746	2.580515
18	1	0	-6.524489	-0.361026	0.553414
19	1	0	-5.407974	-0.784491	-1.625592
20	1	0	-2.924136	-0.785288	-1.768645
21	7	0	-0.644850	1.142659	-0.080449
22	6	0	2.565147	2.699869	-0.307368
23	1	0	2.013361	3.435151	-0.903231
24	1	0	3.631554	2.781269	-0.565224
25	1	0	2.443116	2.948065	0.749972
26	6	0	-0.883676	2.095093	1.023152
27	1	0	-1.955298	2.263283	1.146908
28	1	0	-0.389247	3.038994	0.783526
29	1	0	-0.461114	1.685240	1.942449

30	6	0	2.257809	0.942484	-1.948628
31	1	0	1.881371	-0.074894	-2.088260
32	1	0	3.322846	0.969194	-2.223528
33	1	0	1.716194	1.614031	-2.624006
34	6	0	-1.150683	1.667849	-1.367340
35	1	0	-1.015242	0.894087	-2.123871
36	1	0	-0.571573	2.556671	-1.628186
37	1	0	-2.206407	1.929931	-1.273796
38	1	0	0.435892	1.098917	-0.205207
39	7	0	3.998918	-0.469562	1.060077
40	6	0	4.559696	-1.123346	-0.114149
41	1	0	5.345424	-0.495374	-0.550286
42	1	0	3.771722	-1.263546	-0.860363
43	1	0	5.001418	-2.109539	0.110398
44	6	0	4.943819	-0.416267	2.164944
45	1	0	4.467169	0.028456	3.042219
46	1	0	5.796568	0.213076	1.887714
47	1	0	5.337997	-1.407432	2.446658
48	1	0	3.152176	-0.972080	1.321121
49	1	0	2.523787	0.702916	0.054707

1a.3Me$_2$NH-I2

Zero-point correction=	0.439318
(Hartree/Particle)	
Thermal correction to Energy=	0.464268
Thermal correction to Enthalpy=	0.465212
Thermal correction to Gibbs Free Energy=	0.383215
Sum of electronic and zero-point Energies=	-899.142861
Sum of electronic and thermal Energies=	-899.117911
Sum of electronic and thermal Enthalpies=	-899.116967
Sum of electronic and thermal Free Energies=	-899.198964

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.176948	0.367012	1.689340
2	1	0	0.175651	-0.588507	1.329784
3	1	0	1.201973	-2.017661	0.083460
4	1	0	1.500948	-0.158725	-1.256370
5	7	0	2.017130	-1.007651	-1.521940
6	7	0	0.815906	-2.133583	1.030113
7	6	0	1.908157	-2.414033	1.962458
8	1	0	2.384315	-3.386427	1.770531
9	1	0	1.521263	-2.422943	2.987533
10	1	0	2.668595	-1.632554	1.888332
11	6	0	-0.189792	-3.195276	1.044117
12	1	0	0.242096	-4.182782	0.826046
13	1	0	-0.967848	-2.980161	0.307588
14	1	0	-0.657470	-3.240513	2.033615
15	6	0	-1.307527	0.094238	2.605797
16	1	0	-1.718410	1.040992	2.965602
17	1	0	-0.940953	-0.491907	3.450261
18	1	0	-2.077448	-0.466206	2.076548
19	6	0	0.958199	0.977854	2.421876

20	1	0	0.657974	1.959362	2.793262
21	1	0	1.796875	1.085265	1.735202
22	1	0	1.232112	0.322512	3.250413
23	6	0	1.850894	-1.273694	-2.943445
24	1	0	2.316655	-0.504493	-3.582798
25	1	0	0.786546	-1.325842	-3.191060
26	1	0	2.307139	-2.237169	-3.197032
27	6	0	3.417532	-0.833794	-1.159346
28	1	0	3.941859	-0.105631	-1.801065
29	1	0	3.947685	-1.790403	-1.234057
30	1	0	3.487533	-0.480853	-0.125901
31	7	0	0.537826	1.386427	-0.390254
32	6	0	-0.576715	1.236842	0.466388
33	6	0	-1.739794	0.556880	-0.230309
34	6	0	-3.885468	-0.704709	-1.519483
35	6	0	-3.031379	1.074964	-0.126077
36	6	0	-1.527978	-0.595059	-0.994909
37	6	0	-2.594401	-1.226231	-1.630561
38	6	0	-4.101286	0.450201	-0.770246
39	1	0	-3.203453	1.974232	0.460789
40	1	0	-0.519134	-0.988592	-1.094926
41	1	0	-2.417972	-2.122906	-2.217973
42	1	0	-5.100249	0.866643	-0.684888
43	1	0	-4.715495	-1.194228	-2.019397
44	6	0	1.185333	2.555240	-0.283905
45	8	0	0.929075	3.517913	0.479374
46	7	0	2.313580	2.652755	-1.111437
47	1	0	-0.909339	2.181129	0.922369
48	1	0	2.590089	3.606104	-1.302372
49	1	0	2.288761	2.063706	-1.933381

1a.3Me$_2$NH-I3

Zero-point correction=	0.439704
(Hartree/Particle)	
Thermal correction to Energy=	0.464058
Thermal correction to Enthalpy=	0.465003
Thermal correction to Gibbs Free Energy=	0.385636
Sum of electronic and zero-point Energies=	-899.140568
Sum of electronic and thermal Energies=	-899.116214
Sum of electronic and thermal Enthalpies=	-899.115269
Sum of electronic and thermal Free Energies=	-899.194636

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.888619	-1.555955	1.168478
2	1	0	-0.721850	0.214606	1.619712
3	1	0	-0.190930	1.684039	0.916006
4	1	0	0.056747	1.397986	-0.984540
5	7	0	0.363593	2.292872	-0.574318
6	7	0	-0.748856	1.264896	1.737508
7	6	0	-2.151373	1.712057	1.584851
8	1	0	-2.191530	2.799682	1.671978
9	1	0	-2.767144	1.257354	2.363478
10	1	0	-2.495312	1.396389	0.598123

11	6	0	-0.146158	1.660051	3.026339
12	1	0	-0.212400	2.743682	3.135789
13	1	0	0.901851	1.359123	3.039622
14	1	0	-0.680461	1.175285	3.845017
15	6	0	-0.338668	-2.750385	1.817511
16	1	0	-0.628027	-3.662851	1.270286
17	1	0	-0.731075	-2.822644	2.835582
18	1	0	0.749077	-2.714373	1.866067
19	6	0	-2.349319	-1.704709	1.144430
20	1	0	-2.651250	-2.616656	0.606926
21	1	0	-2.810467	-0.850992	0.649005
22	1	0	-2.713852	-1.763139	2.174461
23	6	0	1.776200	2.533374	-0.849659
24	1	0	1.963802	2.730092	-1.916280
25	1	0	2.361818	1.662816	-0.547070
26	1	0	2.120392	3.403135	-0.279562
27	6	0	-0.484309	3.371827	-1.073526
28	1	0	-0.322044	3.573286	-2.143533
29	1	0	-0.275486	4.294384	-0.521366
30	1	0	-1.537864	3.117689	-0.923242
31	7	0	-1.003940	-0.309595	-0.897145
32	6	0	-0.350234	-1.395960	-0.216438
33	6	0	1.153920	-1.117368	-0.190740
34	6	0	3.919916	-0.590782	-0.334150
35	6	0	1.853563	-1.259253	-1.395148
36	6	0	1.862864	-0.691843	0.935560
37	6	0	3.235041	-0.433903	0.868031
38	6	0	3.219546	-1.001116	-1.471512
39	1	0	1.307987	-1.575944	-2.281615
40	1	0	1.354061	-0.590472	1.889858
41	1	0	3.765653	-0.113668	1.760231
42	1	0	3.740137	-1.124792	-2.416513
43	1	0	4.986353	-0.394954	-0.387543
44	6	0	-1.924475	-0.665608	-1.792493
45	8	0	-2.290000	-1.817918	-2.138340
46	1	0	-0.509295	-2.352580	-0.749502
47	7	0	-2.600258	0.427705	-2.380534
48	1	0	-2.061982	1.284292	-2.400501
49	1	0	-2.999423	0.194811	-3.280419

1a.3Me$_2$NH-ts2

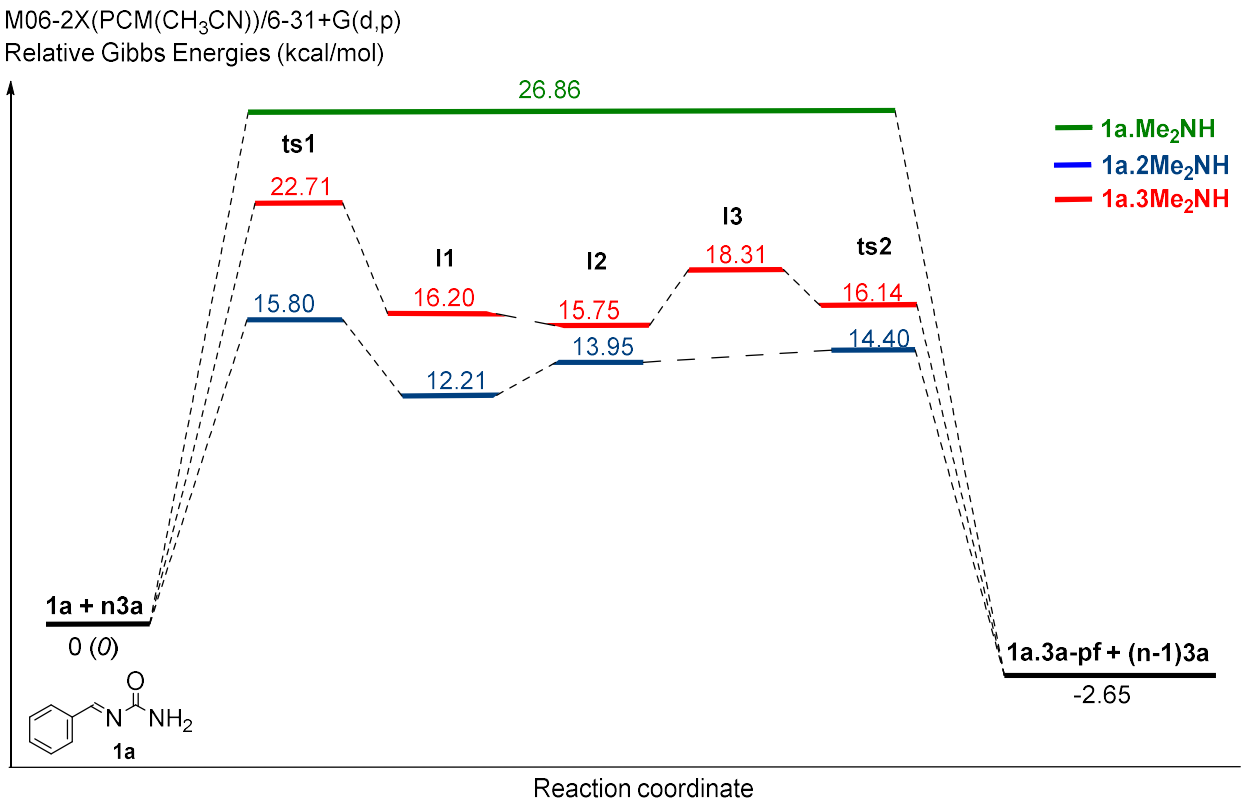
Zero-point correction= 0.434865
(Hartree/Particle)
Thermal correction to Energy= 0.458919
Thermal correction to Enthalpy= 0.459863
Thermal correction to Gibbs Free Energy= 0.381730
Sum of electronic and zero-point Energies= -899.143312
Sum of electronic and thermal Energies= -899.119258
Sum of electronic and thermal Enthalpies= -899.118314
Sum of electronic and thermal Free Energies= -899.196448

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

1	7	0	-0.181843	0.335863	1.683688
2	1	0	0.670361	-1.232258	1.190475
3	1	0	1.709406	-1.450867	-0.225154
4	1	0	1.349004	0.101988	-1.153242
5	7	0	2.035175	-0.686672	-1.297750
6	7	0	1.349887	-1.959795	0.850734
7	6	0	2.494507	-2.014610	1.774976
8	1	0	3.243741	-2.707938	1.384657
9	1	0	2.177296	-2.352278	2.766601
10	1	0	2.937398	-1.020554	1.860482
11	6	0	0.697176	-3.266820	0.683843
12	1	0	1.404110	-3.969864	0.236269
13	1	0	-0.169014	-3.163114	0.027904
14	1	0	0.366328	-3.660684	1.649792
15	6	0	-1.221883	0.014744	2.660657
16	1	0	-1.726385	0.921723	3.037456
17	1	0	-0.767109	-0.502417	3.510661
18	1	0	-1.973950	-0.641599	2.218013
19	6	0	0.877514	1.102334	2.343319
20	1	0	0.500363	2.059681	2.736984
21	1	0	1.676494	1.317459	1.630360
22	1	0	1.284329	0.514455	3.172390
23	6	0	1.847123	-1.347853	-2.591336
24	1	0	2.047586	-0.662534	-3.423489
25	1	0	0.820282	-1.711603	-2.677728
26	1	0	2.528184	-2.200508	-2.671291
27	6	0	3.394159	-0.159882	-1.126901
28	1	0	3.681856	0.483716	-1.966341
29	1	0	4.107804	-0.986653	-1.054098
30	1	0	3.433656	0.435562	-0.211553
31	7	0	0.289053	1.381942	-0.448666
32	6	0	-0.732128	1.117094	0.528057
33	6	0	-1.868051	0.332050	-0.105842
34	6	0	-3.947514	-1.156797	-1.270029
35	6	0	-3.194310	0.744836	0.020736
36	6	0	-1.595844	-0.831000	-0.832184
37	6	0	-2.621521	-1.576092	-1.406556
38	6	0	-4.230156	0.008166	-0.559393
39	1	0	-3.420206	1.647965	0.582838
40	1	0	-0.561232	-1.138658	-0.955802
41	1	0	-2.389790	-2.477781	-1.966843
42	1	0	-5.257131	0.344971	-0.453558
43	1	0	-4.751143	-1.731175	-1.720598
44	6	0	0.766606	2.626349	-0.471426
45	8	0	0.469481	3.599485	0.265774
46	7	0	1.778843	2.831645	-1.437210
47	1	0	-1.143765	2.058076	0.936900
48	1	0	1.882240	3.809444	-1.674828
49	1	0	1.691560	2.243583	-2.256540

2.1.4.-M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

Energy profiles for the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1a** in acetonitrile.



3a [Me_2NH]

```
 Zero-point correction=                           0.093082
(Hartree/Particle)
 Thermal correction to Energy=                    0.097486
 Thermal correction to Enthalpy=                  0.098431
 Thermal correction to Gibbs Free Energy=         0.067594
 Sum of electronic and zero-point Energies=           -135.008899
 Sum of electronic and thermal Energies=              -135.004495
 Sum of electronic and thermal Enthalpies=            -135.003550
 Sum of electronic and thermal Free Energies=         -135.034387

Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0        0.189374   -0.567970    0.414779
      2          1           0        1.132678   -0.629644    0.786074
      3          6           0        0.250206   -0.568038   -1.041633
      4          1           0        0.791946   -1.449892   -1.391649
      5          1           0        0.737370    0.330222   -1.456018
      6          1           0       -0.766874   -0.612274   -1.444688
      7          6           0       -0.446538    0.638718    0.928932
      8          1           0        0.023423    1.566819    0.563314
      9          1           0       -0.414734    0.639969    2.021016
     10          1           0       -1.496855    0.652090    0.619873
 ---------------------------------------------------------------------
```

1a.Me_2NH-ts

```
 Zero-point correction=                           0.243782
(Hartree/Particle)
 Thermal correction to Energy=                    0.257383
 Thermal correction to Enthalpy=                  0.258327
 Thermal correction to Gibbs Free Energy=         0.202495
 Sum of electronic and zero-point Energies=           -629.075241
 Sum of electronic and thermal Energies=              -629.061641
 Sum of electronic and thermal Enthalpies=            -629.060696
 Sum of electronic and thermal Free Energies=         -629.116529

Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -1.602331   -0.232484    0.402060
      2          6           0       -2.292374   -1.223018   -0.203698
      3          7           0       -3.470308   -1.580504    0.432163
      4          8           0       -1.956055   -1.782782   -1.265116
      5          6           0        0.860592   -0.118614   -0.185568
      6          6           0        3.483543   -1.049683    0.104146
      7          6           0        1.860879    0.302107   -1.067123
      8          6           0        1.178733   -1.016504    0.834422
      9          6           0        2.485671   -1.480966    0.978669
     10          6           0        3.169042   -0.156925   -0.921304
     11          1           0        1.613506    0.986742   -1.875699
     12          1           0        0.392024   -1.348703    1.505557
     13          1           0        2.724480   -2.182254    1.772404
```

14	1	0	3.938705	0.175404	-1.610999
15	1	0	4.500078	-1.413893	0.215774
16	6	0	-0.541879	0.415273	-0.346518
17	1	0	-0.771710	0.506400	-1.415591
18	1	0	-1.747821	1.055252	0.729726
19	6	0	0.153917	2.187023	1.340979
20	1	0	-0.243652	3.075981	1.832675
21	1	0	1.137524	2.410399	0.914548
22	1	0	0.251294	1.382640	2.071917
23	7	0	-0.793609	1.781183	0.292871
24	6	0	-1.071481	2.856343	-0.667804
25	1	0	-1.418148	3.735812	-0.123131
26	1	0	-1.851834	2.528244	-1.356769
27	1	0	-0.168223	3.113677	-1.231101
28	1	0	-3.550519	-1.330225	1.407523
29	1	0	-3.813386	-2.500811	0.197233

1a.Me_2NH-pf

Zero-point correction= 0.248514
(Hartree/Particle)
Thermal correction to Energy= 0.262347
Thermal correction to Enthalpy= 0.263292
Thermal correction to Gibbs Free Energy= 0.207903
Sum of electronic and zero-point Energies= -629.122970
Sum of electronic and thermal Energies= -629.109136
Sum of electronic and thermal Enthalpies= -629.108192
Sum of electronic and thermal Free Energies= -629.163580

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.409424	-0.700219	0.203489
2	6	0	-2.675162	-0.827479	-0.304063
3	7	0	-3.396452	-1.882006	0.199459
4	8	0	-3.126095	-0.082157	-1.174014
5	6	0	0.942619	-0.187503	-0.209208
6	6	0	3.639664	-0.952272	-0.039886
7	6	0	1.809755	0.011402	-1.287225
8	6	0	1.445576	-0.772705	0.959263
9	6	0	2.783460	-1.155309	1.042637
10	6	0	3.149628	-0.366907	-1.206244
11	1	0	1.430551	0.462622	-2.201179
12	1	0	0.799613	-0.930896	1.819948
13	1	0	3.157199	-1.608839	1.955370
14	1	0	3.807605	-0.208017	-2.055031
15	1	0	4.681446	-1.250015	0.025640
16	6	0	-0.496914	0.296567	-0.320482
17	1	0	-0.730266	0.438696	-1.381348
18	1	0	-1.031687	-1.470879	0.735984
19	6	0	-0.469459	1.652428	1.735358
20	1	0	-0.875678	2.584797	2.137471
21	1	0	0.609181	1.622189	1.965310
22	1	0	-0.962524	0.818354	2.241871
23	7	0	-0.749599	1.599702	0.308568
24	6	0	-0.080504	2.681581	-0.397467

25	1	0	-0.435255	3.637541	-0.002646
26	1	0	-0.324460	2.636236	-1.463348
27	1	0	1.017922	2.652049	-0.289532
28	1	0	-3.155927	-2.265305	1.102426
29	1	0	-4.382613	-1.862429	-0.015530

1a.2Me$_2$NH-ts1

Zero-point correction=	0.340084
(Hartree/Particle)	
Thermal correction to Energy=	0.360553
Thermal correction to Enthalpy=	0.361498
Thermal correction to Gibbs Free Energy=	0.288640
Sum of electronic and zero-point Energies=	-764.117126
Sum of electronic and thermal Energies=	-764.096657
Sum of electronic and thermal Enthalpies=	-764.095713
Sum of electronic and thermal Free Energies=	-764.168571

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.057962	1.630281	0.030163
2	6	0	1.308513	1.981562	-0.478931
3	7	0	1.847786	3.050877	0.157409
4	8	0	1.911810	1.403566	-1.394997
5	6	0	-1.957444	0.345696	-0.308276
6	6	0	-4.620622	-0.302684	0.251383
7	6	0	-2.709614	-0.402444	-1.219989
8	6	0	-2.550735	0.772773	0.885879
9	6	0	-3.874560	0.445585	1.165393
10	6	0	-4.037736	-0.724078	-0.943732
11	6	0	-0.553242	0.679637	-0.627762
12	7	0	3.313771	-0.879600	-0.085967
13	1	0	-0.188188	0.358598	-1.606516
14	1	0	1.327762	3.527998	0.876244
15	1	0	2.735719	3.416783	-0.147387
16	1	0	3.238372	-0.196920	-0.837530
17	1	0	-2.251174	-0.730958	-2.149899
18	1	0	-4.615524	-1.301183	-1.658813
19	1	0	-5.654342	-0.552676	0.469751
20	1	0	-4.328502	0.776307	2.094564
21	1	0	-1.962088	1.360748	1.583004
22	7	0	0.283181	-1.222200	0.133760
23	1	0	1.280936	-1.089369	-0.074926
24	6	0	4.417446	-1.796929	-0.338439
25	1	0	4.411725	-2.589637	0.417075
26	1	0	5.403077	-1.304777	-0.303469
27	1	0	4.295647	-2.262022	-1.319493
28	6	0	-0.182282	-2.445880	-0.501071
29	1	0	-1.258895	-2.556104	-0.332914
30	1	0	0.322416	-3.340363	-0.107284
31	1	0	-0.003220	-2.389695	-1.578753
32	6	0	3.473589	-0.162598	1.173662
33	1	0	2.647857	0.543647	1.306934
34	1	0	4.420704	0.397955	1.235282

35	1	0	3.448120	-0.876701	2.004057
36	6	0	0.090697	-1.207054	1.574279
37	1	0	0.307784	-0.201594	1.952373
38	1	0	0.737366	-1.930229	2.091263
39	1	0	-0.952996	-1.445360	1.804475

1a.2Me$_2$NH-I1

Zero-point correction= (Hartree/Particle)	0.345025
Thermal correction to Energy=	0.363917
Thermal correction to Enthalpy=	0.364861
Thermal correction to Gibbs Free Energy=	0.297466
Sum of electronic and zero-point Energies=	-764.126717
Sum of electronic and thermal Energies=	-764.107826
Sum of electronic and thermal Enthalpies=	-764.106881
Sum of electronic and thermal Free Energies=	-764.174277

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.111798	1.517080	0.210885
2	6	0	1.219450	1.994508	-0.362445
3	7	0	1.751384	3.133655	0.257222
4	8	0	1.852525	1.514472	-1.343003
5	6	0	-1.857280	0.130682	-0.215273
6	6	0	-4.620439	-0.254511	0.081576
7	6	0	-2.594085	-0.528959	-1.203028
8	6	0	-2.522670	0.610847	0.917703
9	6	0	-3.893742	0.414767	1.068438
10	6	0	-3.968670	-0.722485	-1.058125
11	6	0	-0.363143	0.323892	-0.381925
12	7	0	3.123745	-0.634996	0.122922
13	1	0	-0.096322	0.228018	-1.443924
14	1	0	1.087261	3.665476	0.803488
15	1	0	2.320133	3.699430	-0.357852
16	1	0	-2.092267	-0.885936	-2.099774
17	1	0	-4.527049	-1.231807	-1.837439
18	1	0	-5.689852	-0.401849	0.197617
19	1	0	-4.398405	0.790285	1.953567
20	1	0	-1.954953	1.150115	1.669435
21	7	0	0.382634	-0.890890	0.244815
22	6	0	3.542453	-1.248120	-1.138039
23	1	0	3.300333	-2.315760	-1.121083
24	1	0	4.622523	-1.144876	-1.314611
25	1	0	2.998961	-0.770040	-1.956190
26	6	0	0.162760	-2.166260	-0.469644
27	1	0	-0.863289	-2.506761	-0.318584
28	1	0	0.858485	-2.909667	-0.074312
29	1	0	0.353504	-2.015332	-1.533792
30	6	0	3.853997	-1.161505	1.274318
31	1	0	3.549363	-0.628911	2.178214
32	1	0	4.943300	-1.069757	1.158505
33	1	0	3.612183	-2.221875	1.399210
34	6	0	0.142064	-1.040166	1.697716

35	1	0	0.263303	-0.062498	2.164303
36	1	0	0.874583	-1.743751	2.097657
37	1	0	-0.866388	-1.421347	1.867425
38	1	0	3.255011	0.371719	0.039370
39	1	0	1.438277	-0.680735	0.154260

1a.2Me$_2$NH-I2

Zero-point correction= 0.344804
(Hartree/Particle)
Thermal correction to Energy= 0.364123
Thermal correction to Enthalpy= 0.365067
Thermal correction to Gibbs Free Energy= 0.295570
Sum of electronic and zero-point Energies= -764.122267
Sum of electronic and thermal Energies= -764.102948
Sum of electronic and thermal Enthalpies= -764.102004
Sum of electronic and thermal Free Energies= -764.171501

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.786546	-1.065029	-0.766125
2	6	0	1.553867	-2.159426	-0.762208
3	7	0	2.424894	-2.248938	-1.858752
4	8	0	1.614182	-3.069308	0.106204
5	6	0	-1.450867	-0.477609	0.010449
6	6	0	-4.049460	0.352780	-0.630322
7	6	0	-2.553638	-1.058423	0.639216
8	6	0	-1.659995	0.513766	-0.952338
9	6	0	-2.949979	0.934326	-1.266234
10	6	0	-3.849327	-0.649228	0.318061
11	1	0	-2.400268	-1.833963	1.385913
12	1	0	-0.801554	0.939595	-1.461065
13	1	0	-3.099636	1.709020	-2.012289
14	1	0	-4.699296	-1.112687	0.809369
15	1	0	-5.056056	0.674786	-0.878637
16	6	0	-0.043787	-0.912639	0.368216
17	6	0	0.842944	3.084572	-1.134712
18	1	0	-0.212523	3.274236	-0.926471
19	1	0	0.914176	2.342265	-1.935751
20	1	0	1.310668	4.013686	-1.489002
21	6	0	-0.296639	0.618742	2.392659
22	1	0	0.256583	1.322992	3.015308
23	1	0	-0.592912	-0.247417	2.988799
24	1	0	-1.179399	1.105093	1.980731
25	7	0	1.500317	2.553232	0.061258
26	6	0	2.925192	2.306812	-0.183284
27	1	0	3.434278	3.185242	-0.603881
28	1	0	3.026102	1.476938	-0.889941
29	1	0	3.420713	2.028630	0.749255
30	7	0	0.584862	0.170595	1.288065
31	6	0	1.886527	-0.301970	1.822240
32	1	0	2.342649	0.506293	2.395709
33	1	0	2.527233	-0.580439	0.987313
34	1	0	1.711847	-1.167198	2.464321

35	1	0	-0.085474	-1.802616	1.012744
36	1	0	1.411244	3.237881	0.809256
37	1	0	0.809069	1.019635	0.686387
38	1	0	2.133244	-1.721073	-2.670367
39	1	0	2.710507	-3.195666	-2.068913

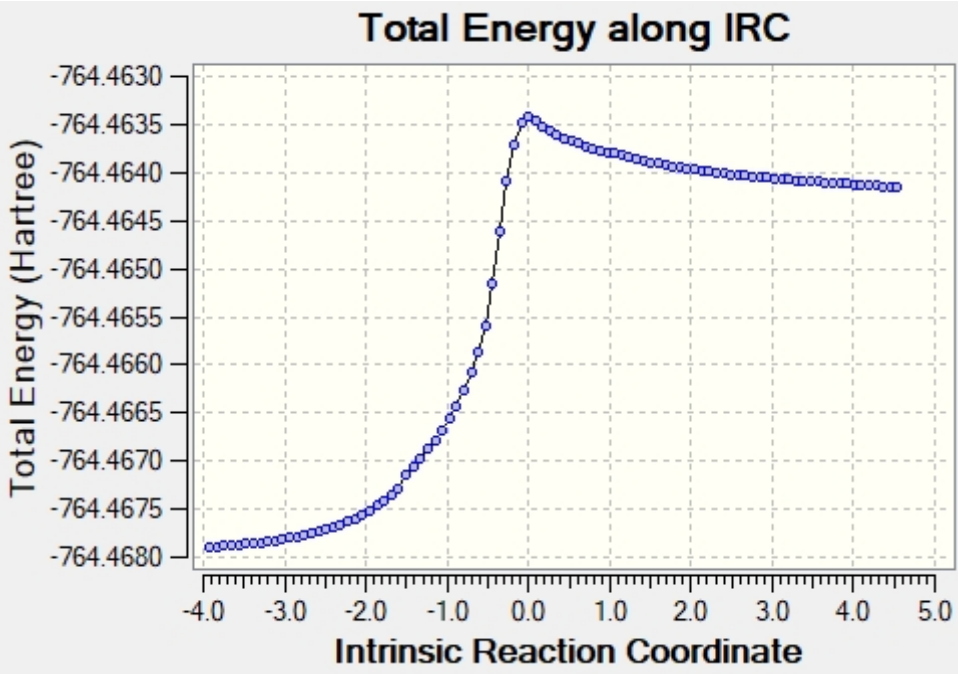
1a.2Me$_2$NH-ts2

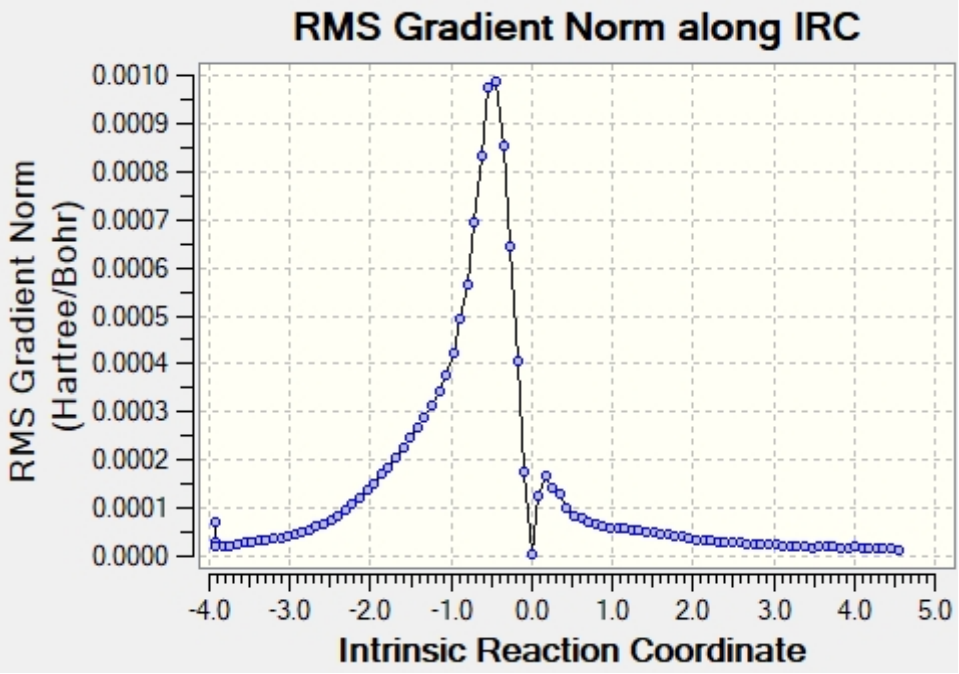
Zero-point correction= (Hartree/Particle)	0.340255
Thermal correction to Energy=	0.359027
Thermal correction to Enthalpy=	0.359971
Thermal correction to Gibbs Free Energy=	0.292639
Sum of electronic and zero-point Energies=	-764.123172
Sum of electronic and thermal Energies=	-764.104399
Sum of electronic and thermal Enthalpies=	-764.103455
Sum of electronic and thermal Free Energies=	-764.170787

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.923685	-0.925757	-0.650696
2	6	0	1.681845	-2.018736	-0.648127
3	7	0	2.615204	-2.072404	-1.703859
4	8	0	1.701807	-2.966662	0.184486
5	6	0	-1.389565	-0.493139	0.027357
6	6	0	-4.036807	0.071095	-0.727932
7	6	0	-2.465148	-1.014370	0.751769
8	6	0	-1.658131	0.293863	-1.096424
9	6	0	-2.970156	0.583234	-1.468018
10	6	0	-3.780842	-0.737241	0.379278
11	1	0	-2.270347	-1.642983	1.617822
12	1	0	-0.831368	0.654001	-1.700679
13	1	0	-3.161274	1.198843	-2.342092
14	1	0	-4.603972	-1.154667	0.951399
15	1	0	-5.059322	0.290373	-1.019613
16	6	0	0.037961	-0.781649	0.465758
17	6	0	2.830253	2.202569	-0.383758
18	1	0	3.337395	1.239244	-0.306588
19	1	0	2.995463	2.777465	0.529694
20	1	0	3.225247	2.758015	-1.238107
21	6	0	-0.401995	0.910744	2.290306
22	1	0	0.098064	1.688650	2.872209
23	1	0	-0.763500	0.133073	2.976678
24	1	0	-1.253609	1.349976	1.769640
25	7	0	1.384080	1.963102	-0.543588
26	6	0	0.601395	3.196987	-0.726698
27	1	0	0.922881	3.731662	-1.623804
28	1	0	0.747421	3.835588	0.146824
29	1	0	-0.456669	2.942236	-0.810400
30	7	0	0.560102	0.361812	1.324547
31	6	0	1.776074	-0.076592	2.030107
32	1	0	2.248097	0.785105	2.509320
33	1	0	2.469299	-0.520741	1.314736
34	1	0	1.527282	-0.822847	2.795968

35	1	0	0.025592	-1.671624	1.114930
36	1	0	1.245277	1.301066	-1.313398
37	1	0	0.971339	1.289756	0.384245
38	1	0	2.886008	-3.017593	-1.941149
39	1	0	2.355439	-1.519160	-2.510056

1a.2Me$_2$NH-ts2





1a.3Me$_2$NH-ts1

Zero-point correction=	0.435348
(Hartree/Particle)	
Thermal correction to Energy=	0.461371
Thermal correction to Enthalpy=	0.462316
Thermal correction to Gibbs Free Energy=	0.376854
Sum of electronic and zero-point Energies=	-899.133438
Sum of electronic and thermal Energies=	-899.107416
Sum of electronic and thermal Enthalpies=	-899.106471
Sum of electronic and thermal Free Energies=	-899.191933

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.617127	-1.332062	-1.394107
2	6	0	-0.701676	-1.514744	-1.795154
3	7	0	-0.909575	-2.721460	-2.382408
4	8	0	-1.636183	-0.712139	-1.639791
5	6	0	2.233079	0.177271	-0.421167
6	6	0	4.837412	0.962830	0.230285
7	6	0	2.516758	1.516261	-0.134473
8	6	0	3.265544	-0.767105	-0.387958
9	6	0	4.560416	-0.376033	-0.057336
10	6	0	3.814708	1.910328	0.186065
11	6	0	0.843924	-0.218334	-0.739972
12	7	0	-2.734588	-0.475575	1.209176
13	1	0	0.106187	0.589268	-0.747698
14	1	0	-0.126554	-3.326025	-2.573886
15	1	0	-1.805475	-2.919641	-2.799288
16	1	0	1.714514	2.250359	-0.160819
17	1	0	4.027002	2.952404	0.403471
18	1	0	5.848288	1.265532	0.485464
19	1	0	5.356694	-1.113425	-0.025132
20	1	0	3.038105	-1.802211	-0.623101
21	7	0	0.237684	-0.610937	1.309775
22	6	0	-3.500101	0.186263	2.256638
23	1	0	-3.185752	-0.193939	3.234834
24	1	0	-4.586268	0.024586	2.163371
25	1	0	-3.307093	1.262132	2.229202
26	6	0	0.801126	0.263307	2.328854
27	1	0	1.890236	0.146096	2.349814
28	1	0	0.406201	0.036838	3.329610
29	1	0	0.575751	1.306880	2.091311
30	6	0	-3.032468	-1.899463	1.117597
31	1	0	-2.492034	-2.328679	0.269179
32	1	0	-4.107348	-2.107079	0.990272
33	1	0	-2.699146	-2.401584	2.033073
34	6	0	0.537674	-2.014105	1.540289
35	1	0	0.119701	-2.614113	0.727195
36	1	0	0.129785	-2.372763	2.495389
37	1	0	1.624571	-2.156495	1.550255
38	1	0	-0.787598	-0.480559	1.256050
39	7	0	-2.631730	1.993881	-0.808448
40	6	0	-3.071478	2.963525	-1.802897
41	1	0	-3.657516	3.749211	-1.313884
42	1	0	-3.711131	2.473946	-2.541420
43	1	0	-2.235701	3.450257	-2.333114
44	6	0	-1.704599	2.582210	0.146982
45	1	0	-1.354437	1.809825	0.839471

46	1	0	-2.217866	3.353902	0.731810
47	1	0	-0.826598	3.053152	-0.329476
48	1	0	-2.178640	1.206854	-1.271873
49	1	0	-2.922754	-0.027801	0.313812

1a.3Me$_2$NH-I1

Zero-point correction= 0.438742
(Hartree/Particle)
Thermal correction to Energy= 0.463820
Thermal correction to Enthalpy= 0.464764
Thermal correction to Gibbs Free Energy= 0.381807
Sum of electronic and zero-point Energies= -899.145368
Sum of electronic and thermal Energies= -899.120290
Sum of electronic and thermal Enthalpies= -899.119346
Sum of electronic and thermal Free Energies= -899.202302

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.600906	-1.149221	-0.787970
2	6	0	0.606087	-1.635797	-0.492096
3	7	0	1.165793	-2.452660	-1.483887
4	8	0	1.299410	-1.413111	0.539108
5	6	0	-2.639106	-0.331568	0.294075
6	6	0	-5.438681	-0.395597	0.480398
7	6	0	-3.275607	-0.150981	1.525443
8	6	0	-3.421122	-0.559640	-0.843279
9	6	0	-4.811210	-0.586588	-0.752448
10	6	0	-4.667537	-0.181888	1.621493
11	6	0	-1.125332	-0.292466	0.210143
12	7	0	2.022059	1.380570	-0.516620
13	1	0	-0.701258	-0.480982	1.205681
14	1	0	0.492967	-2.878657	-2.106951
15	1	0	1.861692	-3.095536	-1.130996
16	1	0	-2.678588	0.003623	2.421663
17	1	0	-5.145407	-0.045841	2.586741
18	1	0	-6.521705	-0.423010	0.551154
19	1	0	-5.406404	-0.764570	-1.643110
20	1	0	-2.926270	-0.730125	-1.794169
21	7	0	-0.662173	1.162457	-0.068910
22	6	0	2.538088	2.712075	-0.199394
23	1	0	1.997149	3.465651	-0.781578
24	1	0	3.609840	2.806871	-0.428095
25	1	0	2.388072	2.921266	0.862757
26	6	0	-0.915399	2.093742	1.050363
27	1	0	-1.989462	2.242433	1.177559
28	1	0	-0.437461	3.049378	0.825210
29	1	0	-0.485315	1.676833	1.962923
30	6	0	2.266932	1.018659	-1.914496
31	1	0	1.903557	0.003067	-2.096392
32	1	0	3.335412	1.066730	-2.172228
33	1	0	1.727287	1.709403	-2.571474
34	6	0	-1.171896	1.703633	-1.348050
35	1	0	-1.031487	0.943279	-2.116888
36	1	0	-0.599505	2.600441	-1.595109

37	1	0	-2.229125	1.957647	-1.250439
38	1	0	0.420890	1.128960	-0.190752
39	7	0	4.019895	-0.500731	1.035083
40	6	0	4.564130	-1.113813	-0.169101
41	1	0	5.352386	-0.477343	-0.587633
42	1	0	3.768751	-1.217316	-0.913379
43	1	0	4.997727	-2.111992	0.013797
44	6	0	4.975498	-0.504185	2.132809
45	1	0	4.510474	-0.097141	3.034224
46	1	0	5.830354	0.130981	1.876399
47	1	0	5.364685	-1.510130	2.364395
48	1	0	3.171357	-1.006362	1.284032
49	1	0	2.502357	0.700904	0.080751

1a.3Me$_2$NH-I2

Zero-point correction= 0.439133
(Hartree/Particle)
Thermal correction to Energy= 0.464139
Thermal correction to Enthalpy= 0.465084
Thermal correction to Gibbs Free Energy= 0.382730
Sum of electronic and zero-point Energies= -899.146623
Sum of electronic and thermal Energies= -899.121616
Sum of electronic and thermal Enthalpies= -899.120672
Sum of electronic and thermal Free Energies= -899.203025

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.178717	0.357044	1.699414
2	1	0	0.190887	-0.594279	1.338165
3	1	0	1.225099	-2.015443	0.084095
4	1	0	1.504868	-0.156061	-1.251316
5	7	0	2.014186	-0.999166	-1.545258
6	7	0	0.847799	-2.121655	1.034669
7	6	0	1.950627	-2.378740	1.962316
8	1	0	2.437885	-3.346352	1.775282
9	1	0	1.570592	-2.382831	2.989709
10	1	0	2.699522	-1.587475	1.875938
11	6	0	-0.146083	-3.194754	1.068948
12	1	0	0.295528	-4.179094	0.857298
13	1	0	-0.932462	-2.996284	0.336565
14	1	0	-0.604135	-3.234173	2.062923
15	6	0	-1.311416	0.064858	2.608522
16	1	0	-1.743364	1.004337	2.962458
17	1	0	-0.939933	-0.512022	3.456843
18	1	0	-2.065912	-0.511998	2.074680
19	6	0	0.942625	0.982801	2.440942
20	1	0	0.623900	1.957732	2.814649
21	1	0	1.784429	1.103957	1.760246
22	1	0	1.220923	0.329933	3.269625
23	6	0	1.816212	-1.230256	-2.969175
24	1	0	2.268067	-0.445558	-3.599557
25	1	0	0.746447	-1.277266	-3.193801
26	1	0	2.266154	-2.187094	-3.256403
27	6	0	3.422797	-0.837233	-1.209159

28	1	0	3.933608	-0.089041	-1.838790
29	1	0	3.949655	-1.790968	-1.327531
30	1	0	3.517186	-0.521089	-0.165708
31	7	0	0.531158	1.388936	-0.373844
32	6	0	-0.584917	1.224621	0.482094
33	6	0	-1.740173	0.539111	-0.222300
34	6	0	-3.871303	-0.729956	-1.528200
35	6	0	-3.033976	1.054013	-0.129474
36	6	0	-1.518770	-0.613981	-0.982839
37	6	0	-2.578042	-1.248872	-1.626941
38	6	0	-4.096643	0.425458	-0.782272
39	1	0	-3.214292	1.952048	0.456714
40	1	0	-0.508774	-1.007075	-1.072794
41	1	0	-2.394103	-2.146745	-2.210054
42	1	0	-5.097614	0.838591	-0.704932
43	1	0	-4.695933	-1.222707	-2.033787
44	6	0	1.158580	2.567206	-0.277179
45	8	0	0.881380	3.537480	0.472158
46	7	0	2.291926	2.675464	-1.096988
47	1	0	-0.927965	2.164671	0.938724
48	1	0	2.548315	3.630959	-1.305535
49	1	0	2.288800	2.071462	-1.908618

1a.3Me$_2$NH-I3

Zero-point correction= 0.439361
(Hartree/Particle)
Thermal correction to Energy= 0.463825
Thermal correction to Enthalpy= 0.464769
Thermal correction to Gibbs Free Energy= 0.385419
Sum of electronic and zero-point Energies= -899.145001
Sum of electronic and thermal Energies= -899.120538
Sum of electronic and thermal Enthalpies= -899.119594
Sum of electronic and thermal Free Energies= -899.198943

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.860768	-1.516619	1.232562
2	1	0	-0.731973	0.285208	1.615520
3	1	0	-0.231919	1.736669	0.860342
4	1	0	0.002481	1.370943	-1.039955
5	7	0	0.303280	2.283214	-0.667568
6	7	0	-0.782258	1.336534	1.694597
7	6	0	-2.194750	1.744695	1.523475
8	1	0	-2.260641	2.833306	1.570341
9	1	0	-2.800582	1.304181	2.317668
10	1	0	-2.530022	1.385265	0.548814
11	6	0	-0.193504	1.789927	2.971631
12	1	0	-0.289826	2.874108	3.045032
13	1	0	0.862121	1.517939	2.996525
14	1	0	-0.717430	1.316861	3.803555
15	6	0	-0.284150	-2.660047	1.946611
16	1	0	-0.547581	-3.608230	1.448589
17	1	0	-0.679231	-2.686375	2.965621
18	1	0	0.802007	-2.593074	1.997839

19	6	0	-2.316610	-1.701684	1.210881
20	1	0	-2.592922	-2.643804	0.711164
21	1	0	-2.796781	-0.880009	0.680369
22	1	0	-2.684018	-1.727167	2.240842
23	6	0	1.711440	2.522802	-0.966769
24	1	0	1.885183	2.687612	-2.041233
25	1	0	2.305482	1.665379	-0.643626
26	1	0	2.057146	3.411385	-0.427798
27	6	0	-0.556317	3.336754	-1.200932
28	1	0	-0.408713	3.493574	-2.280437
29	1	0	-0.345094	4.281836	-0.689683
30	1	0	-1.606903	3.086225	-1.026340
31	7	0	-1.000421	-0.378558	-0.888605
32	6	0	-0.322039	-1.415877	-0.155738
33	6	0	1.175980	-1.106091	-0.142395
34	6	0	3.931228	-0.530623	-0.300767
35	6	0	1.887563	-1.308384	-1.330970
36	6	0	1.867496	-0.598195	0.960207
37	6	0	3.234256	-0.315915	0.885709
38	6	0	3.248705	-1.025754	-1.414789
39	1	0	1.357773	-1.693644	-2.199924
40	1	0	1.349789	-0.448996	1.903078
41	1	0	3.750111	0.071002	1.759829
42	1	0	3.779080	-1.196724	-2.346905
43	1	0	4.993486	-0.314705	-0.359728
44	6	0	-1.888472	-0.792776	-1.788203
45	8	0	-2.197463	-1.969367	-2.118210
46	1	0	-0.459313	-2.400717	-0.641596
47	7	0	-2.604190	0.254343	-2.410174
48	1	0	-2.121008	1.143446	-2.411977
49	1	0	-2.955448	-0.001956	-3.323631

1a.3Me$_2$NH-ts2

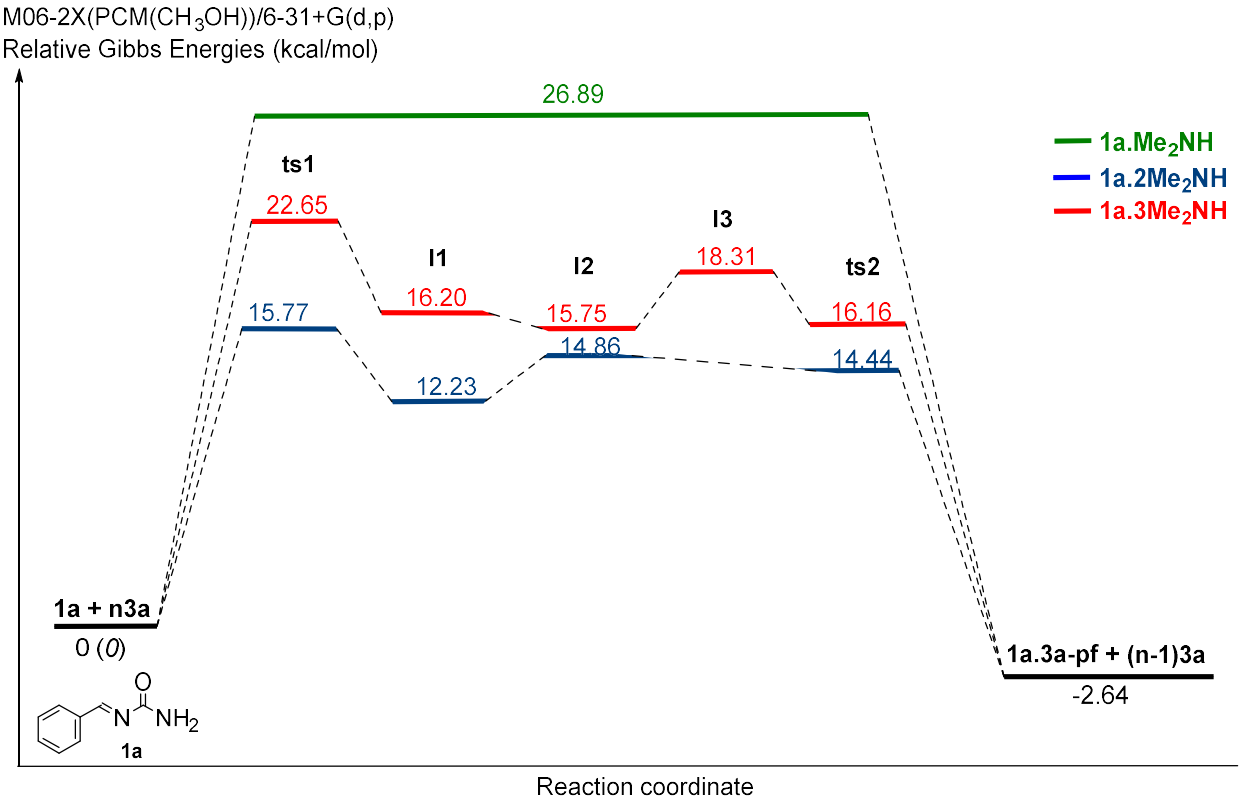
Zero-point correction= 0.434663
(Hartree/Particle)
Thermal correction to Energy= 0.458935
Thermal correction to Enthalpy= 0.459879
Thermal correction to Gibbs Free Energy= 0.380448
Sum of electronic and zero-point Energies= -899.148192
Sum of electronic and thermal Energies= -899.123920
Sum of electronic and thermal Enthalpies= -899.122976
Sum of electronic and thermal Free Energies= -899.202408

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.143368	0.243492	1.688805
2	1	0	0.792134	-1.293126	1.141607
3	1	0	1.797002	-1.368337	-0.306703
4	1	0	1.318496	0.212566	-1.142969
5	7	0	2.036612	-0.531763	-1.337403
6	7	0	1.502203	-1.959031	0.754131
7	6	0	2.672839	-1.988214	1.647079
8	1	0	3.444986	-2.626351	1.210384

9	1	0	2.400033	-2.378856	2.632409
10	1	0	3.067710	-0.976756	1.759413
11	6	0	0.922341	-3.294184	0.543029
12	1	0	1.659649	-3.933873	0.052091
13	1	0	0.038637	-3.215628	-0.092812
14	1	0	0.635931	-3.746606	1.497445
15	6	0	-1.128584	-0.192967	2.677789
16	1	0	-1.663437	0.660603	3.130348
17	1	0	-0.617153	-0.738872	3.475845
18	1	0	-1.863179	-0.858216	2.219394
19	6	0	0.895004	1.026320	2.360087
20	1	0	0.475920	1.921570	2.848869
21	1	0	1.645096	1.347651	1.634042
22	1	0	1.377176	0.407485	3.123337
23	6	0	1.838491	-1.144135	-2.654468
24	1	0	1.984500	-0.413980	-3.459045
25	1	0	0.825893	-1.548285	-2.727077
26	1	0	2.552621	-1.961448	-2.789889
27	6	0	3.373243	0.055899	-1.183955
28	1	0	3.604678	0.742422	-2.006575
29	1	0	4.127627	-0.736518	-1.162715
30	1	0	3.411880	0.615964	-0.246440
31	7	0	0.194159	1.434303	-0.387451
32	6	0	-0.777220	1.054766	0.604460
33	6	0	-1.885988	0.244871	-0.045440
34	6	0	-3.908803	-1.273442	-1.268742
35	6	0	-3.224224	0.618252	0.074850
36	6	0	-1.572629	-0.895538	-0.791720
37	6	0	-2.570002	-1.654792	-1.396229
38	6	0	-4.232307	-0.133341	-0.535483
39	1	0	-3.482137	1.501724	0.654182
40	1	0	-0.529088	-1.177139	-0.902700
41	1	0	-2.306795	-2.538436	-1.970926
42	1	0	-5.269597	0.172010	-0.434725
43	1	0	-4.690949	-1.859265	-1.741710
44	6	0	0.567799	2.711444	-0.390865
45	8	0	0.194883	3.648622	0.363889
46	7	0	1.554847	3.017479	-1.354838
47	1	0	-1.230166	1.945233	1.078941
48	1	0	1.561664	3.998704	-1.601341
49	1	0	1.540880	2.415786	-2.168843

2.1.5.- M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

Energy profiles for the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1a** in methanol.



3a [Me_2NH]

```
 Zero-point correction=                           0.093083
(Hartree/Particle)
 Thermal correction to Energy=                    0.097487
 Thermal correction to Enthalpy=                  0.098431
 Thermal correction to Gibbs Free Energy=         0.067595
 Sum of electronic and zero-point Energies=           -135.008878
 Sum of electronic and thermal Energies=              -135.004474
 Sum of electronic and thermal Enthalpies=            -135.003530
 Sum of electronic and thermal Free Energies=         -135.034367

Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0        0.000000    0.573514   -0.154177
      2          1           0       -0.000001    1.327247    0.526538
      3          6           0       -1.206735   -0.225353    0.020283
      4          1           0       -2.089848    0.414240   -0.048220
      5          1           0       -1.236577   -0.762561    0.982796
      6          1           0       -1.264321   -0.970482   -0.779923
      7          6           0        1.206735   -0.225353    0.020284
      8          1           0        1.236598   -0.762526    0.982815
      9          1           0        2.089851    0.414231   -0.048268
     10          1           0        1.264295   -0.970512   -0.779896
 ---------------------------------------------------------------------
```

1a.Me_2NH-ts

```
 Zero-point correction=                           0.243788
(Hartree/Particle)
 Thermal correction to Energy=                    0.257387
 Thermal correction to Enthalpy=                  0.258331
 Thermal correction to Gibbs Free Energy=         0.202510
 Sum of electronic and zero-point Energies=           -629.075132
 Sum of electronic and thermal Energies=              -629.061534
 Sum of electronic and thermal Enthalpies=            -629.060589
 Sum of electronic and thermal Free Energies=         -629.116410

Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -1.602057   -0.232820    0.402640
      2          6           0       -2.292968   -1.222486   -0.203729
      3          7           0       -3.470575   -1.580116    0.432728
      4          8           0       -1.957731   -1.781205   -1.265949
      5          6           0        0.860739   -0.118924   -0.185545
      6          6           0        3.483828   -1.049672    0.103824
      7          6           0        1.860895    0.302042   -1.067128
      8          6           0        1.179076   -1.016910    0.834283
      9          6           0        2.486085   -1.481215    0.978357
     10          6           0        3.169125   -0.156826   -0.921482
     11          1           0        1.613344    0.986696   -1.875637
     12          1           0        0.392427   -1.349327    1.505374
     13          1           0        2.725040   -2.182628    1.771938
```

14	1	0	3.938679	0.175655	-1.611227
15	1	0	4.500414	-1.413787	0.215297
16	6	0	-0.541799	0.414855	-0.346242
17	1	0	-0.771883	0.505876	-1.415267
18	1	0	-1.747244	1.055231	0.730263
19	6	0	0.154571	2.186896	1.340869
20	1	0	-0.242840	3.075904	1.832612
21	1	0	1.138034	2.410217	0.914078
22	1	0	0.252228	1.382579	2.071842
23	7	0	-0.793299	1.780908	0.293135
24	6	0	-1.071566	2.855926	-0.667569
25	1	0	-1.418023	3.735492	-0.122910
26	1	0	-1.852180	2.527713	-1.356185
27	1	0	-0.168526	3.113168	-1.231262
28	1	0	-3.549675	-1.331164	1.408511
29	1	0	-3.814337	-2.499912	0.196816

1a.Me_2NH-pf

Zero-point correction= 0.248517
(Hartree/Particle)
Thermal correction to Energy= 0.262350
Thermal correction to Enthalpy= 0.263294
Thermal correction to Gibbs Free Energy= 0.207910
Sum of electronic and zero-point Energies= -629.122869
Sum of electronic and thermal Energies= -629.109036
Sum of electronic and thermal Enthalpies= -629.108092
Sum of electronic and thermal Free Energies= -629.163476

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.409424	-0.700219	0.203489
2	6	0	-2.675162	-0.827479	-0.304063
3	7	0	-3.396452	-1.882006	0.199459
4	8	0	-3.126095	-0.082157	-1.174014
5	6	0	0.942619	-0.187503	-0.209208
6	6	0	3.639664	-0.952272	-0.039886
7	6	0	1.809755	0.011402	-1.287225
8	6	0	1.445576	-0.772705	0.959263
9	6	0	2.783460	-1.155309	1.042637
10	6	0	3.149628	-0.366907	-1.206244
11	1	0	1.430551	0.462622	-2.201179
12	1	0	0.799613	-0.930896	1.819948
13	1	0	3.157199	-1.608839	1.955370
14	1	0	3.807605	-0.208017	-2.055031
15	1	0	4.681446	-1.250015	0.025640
16	6	0	-0.496914	0.296567	-0.320482
17	1	0	-0.730266	0.438696	-1.381348
18	1	0	-1.031687	-1.470879	0.735984
19	6	0	-0.469459	1.652428	1.735358
20	1	0	-0.875678	2.584797	2.137471
21	1	0	0.609181	1.622189	1.965310
22	1	0	-0.962524	0.818354	2.241871
23	7	0	-0.749599	1.599702	0.308568
24	6	0	-0.080504	2.681581	-0.397467

25	1	0	-0.435255	3.637541	-0.002646
26	1	0	-0.324460	2.636236	-1.463348
27	1	0	1.017922	2.652049	-0.289532
28	1	0	-3.155927	-2.265305	1.102426
29	1	0	-4.382613	-1.862429	-0.015530

1a.2Me$_2$NH-ts1

Zero-point correction= 0.340092
(Hartree/Particle)
Thermal correction to Energy= 0.360557
Thermal correction to Enthalpy= 0.361501
Thermal correction to Gibbs Free Energy= 0.288652
Sum of electronic and zero-point Energies= -764.117061
Sum of electronic and thermal Energies= -764.096597
Sum of electronic and thermal Enthalpies= -764.095653
Sum of electronic and thermal Free Energies= -764.168501

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.058151	1.630187	0.030116
2	6	0	1.308556	1.981610	-0.479150
3	7	0	1.847772	3.051159	0.157092
4	8	0	1.912198	1.403229	-1.394708
5	6	0	-1.957375	0.345821	-0.308128
6	6	0	-4.620280	-0.302798	0.252565
7	6	0	-2.709919	-0.402140	-1.219668
8	6	0	-2.550184	0.772672	0.886338
9	6	0	-3.873865	0.445358	1.166373
10	6	0	-4.037899	-0.723904	-0.942892
11	6	0	-0.553248	0.679786	-0.628004
12	7	0	3.313591	-0.879395	-0.085084
13	1	0	-0.188606	0.359267	-1.607090
14	1	0	1.325504	3.531105	0.872415
15	1	0	2.733739	3.419407	-0.150623
16	1	0	3.238876	-0.196650	-0.836668
17	1	0	-2.251874	-0.730418	-2.149856
18	1	0	-4.615977	-1.300878	-1.657845
19	1	0	-5.653893	-0.552889	0.471329
20	1	0	-4.327430	0.775918	2.095786
21	1	0	-1.961242	1.360611	1.583241
22	7	0	0.283256	-1.222146	0.132208
23	1	0	1.281047	-1.089310	-0.076366
24	6	0	4.416691	-1.797506	-0.337097
25	1	0	4.410096	-2.590196	0.418436
26	1	0	5.402673	-1.306075	-0.301747
27	1	0	4.294940	-2.262551	-1.318181
28	6	0	-0.182322	-2.445488	-0.503189
29	1	0	-1.258859	-2.555940	-0.334705
30	1	0	0.322640	-3.340143	-0.110129
31	1	0	-0.003631	-2.388643	-1.580901
32	6	0	3.473241	-0.162572	1.174648
33	1	0	2.648226	0.544649	1.307234
34	1	0	4.420958	0.396896	1.237006
35	1	0	3.446330	-0.876639	2.005033
36	6	0	0.090982	-1.207821	1.572769

37	1	0	0.308117	-0.202555	1.951360
38	1	0	0.737795	-1.931252	2.089220
39	1	0	-0.952669	-1.446286	1.803000

1a.2Me$_2$NH-I1

Zero-point correction= (Hartree/Particle)	0.345037
Thermal correction to Energy=	0.363926
Thermal correction to Enthalpy=	0.364870
Thermal correction to Gibbs Free Energy=	0.297489
Sum of electronic and zero-point Energies=	-764.126594
Sum of electronic and thermal Energies=	-764.107705
Sum of electronic and thermal Enthalpies=	-764.106761
Sum of electronic and thermal Free Energies=	-764.174142

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.111428	1.517024	0.210771
2	6	0	1.219086	1.994420	-0.362644
3	7	0	1.750428	3.134172	0.256334
4	8	0	1.852365	1.514043	-1.342863
5	6	0	-1.857186	0.130323	-0.215434
6	6	0	-4.620322	-0.254843	0.081398
7	6	0	-2.593887	-0.529833	-1.202909
8	6	0	-2.522672	0.611118	0.917179
9	6	0	-3.893734	0.415031	1.067919
10	6	0	-3.968465	-0.723346	-1.058025
11	6	0	-0.363046	0.323673	-0.381894
12	7	0	3.123890	-0.634894	0.122524
13	1	0	-0.095869	0.227422	-1.443784
14	1	0	1.085869	3.665914	0.802123
15	1	0	2.318956	3.699662	-0.359175
16	1	0	-2.092001	-0.887015	-2.099542
17	1	0	-4.526799	-1.232943	-1.837195
18	1	0	-5.689754	-0.402091	0.197405
19	1	0	-4.398501	0.791139	1.952742
20	1	0	-1.954951	1.151054	1.668430
21	7	0	0.382782	-0.890669	0.245531
22	6	0	3.542030	-1.248931	-1.138169
23	1	0	3.299990	-2.316598	-1.120331
24	1	0	4.622020	-1.145813	-1.315319
25	1	0	2.998201	-0.771340	-1.956368
26	6	0	0.163194	-2.166470	-0.468207
27	1	0	-0.862829	-2.507028	-0.317060
28	1	0	0.859045	-2.909550	-0.072423
29	1	0	0.354015	-2.016055	-1.532419
30	6	0	3.854668	-1.160426	1.273989
31	1	0	3.550366	-0.627153	2.177599
32	1	0	4.943933	-1.068698	1.157725
33	1	0	3.613072	-2.220756	1.399810
34	6	0	0.142230	-1.039039	1.698493
35	1	0	0.263360	-0.060946	2.164245
36	1	0	0.874813	-1.742276	2.098955

37	1	0	-0.866242	-1.420102	1.868428
38	1	0	3.254966	0.371779	0.038007
39	1	0	1.438350	-0.680434	0.154750

1a.2Me$_2$NH-I2

Zero-point correction= 0.345115
(Hartree/Particle)
Thermal correction to Energy= 0.364093
Thermal correction to Enthalpy= 0.365037
Thermal correction to Gibbs Free Energy= 0.297443
Sum of electronic and zero-point Energies= -764.122283
Sum of electronic and thermal Energies= -764.103306
Sum of electronic and thermal Enthalpies= -764.102362
Sum of electronic and thermal Free Energies= -764.169956

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.772422	-0.865332	-0.726138
2	6	0	1.549055	-1.949604	-0.774281
3	7	0	2.489849	-1.929882	-1.816838
4	8	0	1.568061	-2.937897	0.007791
5	6	0	-1.525449	-0.388077	-0.032943
6	6	0	-4.119244	0.415777	-0.728688
7	6	0	-2.636701	-0.989082	0.561981
8	6	0	-1.723934	0.608880	-0.992650
9	6	0	-3.012024	1.015246	-1.333464
10	6	0	-3.929467	-0.592584	0.214986
11	1	0	-2.491790	-1.771825	1.302912
12	1	0	-0.858993	1.051950	-1.474062
13	1	0	-3.154255	1.794017	-2.076618
14	1	0	-4.784931	-1.071222	0.681618
15	1	0	-5.123463	0.728124	-0.998141
16	6	0	-0.125775	-0.811208	0.367238
17	6	0	1.284872	2.690926	-1.205254
18	1	0	0.303169	3.149557	-1.064211
19	1	0	1.173237	1.794649	-1.823211
20	1	0	1.938360	3.400762	-1.731757
21	6	0	-0.519452	0.775890	2.353954
22	1	0	0.019960	1.434984	3.035853
23	1	0	-0.979491	-0.039669	2.916702
24	1	0	-1.286948	1.339073	1.825760
25	7	0	1.837148	2.284236	0.088243
26	6	0	3.166086	1.686297	-0.077742
27	1	0	3.837930	2.326220	-0.666921
28	1	0	3.049023	0.726073	-0.591754
29	1	0	3.619864	1.509744	0.900068
30	7	0	0.448560	0.217787	1.380943
31	6	0	1.608044	-0.374708	2.093493
32	1	0	2.120846	0.413810	2.646683
33	1	0	2.278789	-0.824204	1.363145
34	1	0	1.245617	-1.138718	2.784321
35	1	0	-0.182656	-1.744528	0.945840
36	1	0	1.910429	3.101759	0.689267

37	1	0	0.853302	1.021845	0.801068
38	1	0	2.245188	-1.322251	-2.587206
39	1	0	2.790402	-2.851145	-2.104950

1a.2Me$_2$NH-ts2

Zero-point correction= 0.340257
(Hartree/Particle)
Thermal correction to Energy= 0.359028
Thermal correction to Enthalpy= 0.359972
Thermal correction to Gibbs Free Energy= 0.292642
Sum of electronic and zero-point Energies= -764.123010
Sum of electronic and thermal Energies= -764.104239
Sum of electronic and thermal Enthalpies= -764.103295
Sum of electronic and thermal Free Energies= -764.170625

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.923811	-0.923991	-0.651927
2	6	0	1.684256	-2.015487	-0.649721
3	7	0	2.617224	-2.067149	-1.705916
4	8	0	1.706521	-2.963217	0.182884
5	6	0	-1.389696	-0.493785	0.026636
6	6	0	-4.037176	0.070262	-0.728043
7	6	0	-2.465098	-1.015541	0.750956
8	6	0	-1.658600	0.293527	-1.096822
9	6	0	-2.970734	0.582822	-1.468114
10	6	0	-3.780884	-0.738484	0.378794
11	1	0	-2.270064	-1.644599	1.616632
12	1	0	-0.831942	0.653789	-1.701138
13	1	0	-3.162099	1.198618	-2.342008
14	1	0	-4.603851	-1.156351	0.950831
15	1	0	-5.059779	0.289429	-1.019502
16	6	0	0.037955	-0.782222	0.464703
17	6	0	2.829051	2.203752	-0.381510
18	1	0	3.336901	1.240895	-0.303206
19	1	0	2.993637	2.779821	0.531320
20	1	0	3.223780	2.758550	-1.236400
21	6	0	-0.403145	0.907252	2.291922
22	1	0	0.096425	1.684630	2.874978
23	1	0	-0.764427	0.128561	2.977278
24	1	0	-1.254900	1.346760	1.771716
25	7	0	1.383110	1.962985	-0.541428
26	6	0	0.599379	3.195986	-0.725918
27	1	0	0.920340	3.729803	-1.623726
28	1	0	0.744966	3.835822	0.146772
29	1	0	-0.458477	2.940246	-0.809177
30	7	0	0.559373	0.360111	1.325627
31	6	0	1.775198	-0.079136	2.030907
32	1	0	2.246722	0.781835	2.511941
33	1	0	2.468913	-0.521845	1.315135
34	1	0	1.526390	-0.826953	2.795243
35	1	0	0.026092	-1.673341	1.112301
36	1	0	1.244968	1.299669	-1.310366

37	1	0	0.970802	1.289963	0.386106
38	1	0	2.890356	-3.011780	-1.942741
39	1	0	2.355414	-1.515146	-2.512296

1a.3Me$_2$NH-ts1

Zero-point correction=	0.435355
(Hartree/Particle)	
Thermal correction to Energy=	0.461377
Thermal correction to Enthalpy=	0.462321
Thermal correction to Gibbs Free Energy=	0.376819
Sum of electronic and zero-point Energies=	-899.133368
Sum of electronic and thermal Energies=	-899.107346
Sum of electronic and thermal Enthalpies=	-899.106401
Sum of electronic and thermal Free Energies=	-899.191904

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.618185	-1.333095	-1.393076
2	6	0	-0.700545	-1.516186	-1.794041
3	7	0	-0.908057	-2.722909	-2.381591
4	8	0	-1.635419	-0.714162	-1.638059
5	6	0	2.233881	0.177107	-0.421100
6	6	0	4.838089	0.962910	0.230518
7	6	0	2.517637	1.516312	-0.135507
8	6	0	3.266219	-0.767363	-0.386767
9	6	0	4.561025	-0.376160	-0.056058
10	6	0	3.815520	1.910496	0.185142
11	6	0	0.844793	-0.218652	-0.740065
12	7	0	-2.735189	-0.475188	1.209517
13	1	0	0.107191	0.589066	-0.749230
14	1	0	-0.124492	-3.326263	-2.574684
15	1	0	-1.803651	-2.920664	-2.799332
16	1	0	1.715496	2.250490	-0.162857
17	1	0	4.027878	2.952738	0.401695
18	1	0	5.848920	1.265712	0.485752
19	1	0	5.357213	-1.113611	-0.022989
20	1	0	3.038702	-1.802611	-0.621220
21	7	0	0.237227	-0.608721	1.309404
22	6	0	-3.500756	0.187238	2.256553
23	1	0	-3.185845	-0.191750	3.235043
24	1	0	-4.586854	0.024795	2.163815
25	1	0	-3.308466	1.263206	2.227915
26	6	0	0.799135	0.267362	2.327742
27	1	0	1.888154	0.149844	2.350953
28	1	0	0.402301	0.043061	3.328236
29	1	0	0.574566	1.310540	2.087704
30	6	0	-3.032284	-1.899324	1.119418
31	1	0	-2.491801	-2.329058	0.271297
32	1	0	-4.107077	-2.107682	0.992555
33	1	0	-2.698466	-2.400338	2.035326
34	6	0	0.537834	-2.011372	1.542243
35	1	0	0.120820	-2.612806	0.729715
36	1	0	0.129423	-2.368849	2.497568
37	1	0	1.624803	-2.153107	1.553219

38	1	0	-0.788103	-0.479083	1.254732
39	7	0	-2.633082	1.992101	-0.810345
40	6	0	-3.073425	2.960886	-1.805330
41	1	0	-3.659750	3.746611	-1.316714
42	1	0	-3.712978	2.470534	-2.543419
43	1	0	-2.237966	3.447672	-2.336016
44	6	0	-1.706012	2.581385	0.144506
45	1	0	-1.355766	1.809658	0.837675
46	1	0	-2.219374	3.353529	0.728662
47	1	0	-0.828041	3.052034	-0.332335
48	1	0	-2.179848	1.204859	-1.273262
49	1	0	-2.923892	-0.028370	0.313780

1a.3Me$_2$NH-I1

Zero-point correction=	0.438748
(Hartree/Particle)	
Thermal correction to Energy=	0.463824
Thermal correction to Enthalpy=	0.464769
Thermal correction to Gibbs Free Energy=	0.381820
Sum of electronic and zero-point Energies=	-899.145262
Sum of electronic and thermal Energies=	-899.120186
Sum of electronic and thermal Enthalpies=	-899.119242
Sum of electronic and thermal Free Energies=	-899.202191

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.601047	-1.150141	-0.786839
2	6	0	0.605934	-1.636513	-0.490555
3	7	0	1.165584	-2.454227	-1.481660
4	8	0	1.299230	-1.412923	0.540444
5	6	0	-2.639078	-0.331196	0.294414
6	6	0	-5.438685	-0.394397	0.480200
7	6	0	-3.275810	-0.148552	1.525348
8	6	0	-3.420866	-0.560951	-0.842752
9	6	0	-4.810973	-0.587486	-0.752192
10	6	0	-4.667766	-0.179039	1.621134
11	6	0	-1.125287	-0.292620	0.210643
12	7	0	2.022373	1.379845	-0.518113
13	1	0	-0.701306	-0.480504	1.206339
14	1	0	0.492689	-2.880441	-2.104493
15	1	0	1.861271	-3.096997	-1.128179
16	1	0	-2.678965	0.007265	2.421474
17	1	0	-5.145832	-0.041478	2.586071
18	1	0	-6.521729	-0.421536	0.550758
19	1	0	-5.406010	-0.766879	-1.642675
20	1	0	-2.925668	-0.733173	-1.793148
21	7	0	-0.661730	1.162040	-0.069453
22	6	0	2.538230	2.711869	-0.202846
23	1	0	1.996917	3.464568	-0.785845
24	1	0	3.609880	2.806603	-0.432063
25	1	0	2.388592	2.922430	0.859089
26	6	0	-0.914719	2.094277	1.049043
27	1	0	-1.988744	2.243345	1.176136

28	1	0	-0.436533	3.049612	0.823097
29	1	0	-0.484721	1.677996	1.961933
30	6	0	2.266929	1.016101	-1.915558
31	1	0	1.903426	0.000326	-2.096118
32	1	0	3.335365	1.063763	-2.173561
33	1	0	1.727222	1.706059	-2.573325
34	6	0	-1.171345	1.702291	-1.349018
35	1	0	-1.030926	0.941321	-2.117252
36	1	0	-0.598870	2.598881	-1.596709
37	1	0	-2.228578	1.956414	-1.251658
38	1	0	0.421330	1.128268	-0.191308
39	7	0	4.019296	-0.499632	1.035317
40	6	0	4.564248	-1.114541	-0.167577
41	1	0	5.352504	-0.478535	-0.586829
42	1	0	3.769223	-1.219511	-0.912026
43	1	0	4.998077	-2.112296	0.017130
44	6	0	4.974333	-0.500783	2.133495
45	1	0	4.508778	-0.092032	3.033866
46	1	0	5.829214	0.134023	1.876272
47	1	0	5.363582	-1.506195	2.367297
48	1	0	3.170703	-1.004978	1.284691
49	1	0	2.503058	0.701109	0.080052

1a.3Me$_2$NH-I2

Zero-point correction= 0.439137
(Hartree/Particle)
Thermal correction to Energy= 0.464142
Thermal correction to Enthalpy= 0.465086
Thermal correction to Gibbs Free Energy= 0.382736
Sum of electronic and zero-point Energies= -899.146496
Sum of electronic and thermal Energies= -899.121490
Sum of electronic and thermal Enthalpies= -899.120546
Sum of electronic and thermal Free Energies= -899.202897

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.178717	0.357044	1.699414
2	1	0	0.190887	-0.594279	1.338165
3	1	0	1.225099	-2.015443	0.084095
4	1	0	1.504868	-0.156061	-1.251316
5	7	0	2.014186	-0.999166	-1.545258
6	7	0	0.847799	-2.121655	1.034669
7	6	0	1.950627	-2.378740	1.962316
8	1	0	2.437885	-3.346352	1.775282
9	1	0	1.570592	-2.382831	2.989709
10	1	0	2.699522	-1.587475	1.875938
11	6	0	-0.146083	-3.194754	1.068948
12	1	0	0.295528	-4.179094	0.857298
13	1	0	-0.932462	-2.996284	0.336565
14	1	0	-0.604135	-3.234173	2.062923
15	6	0	-1.311416	0.064858	2.608522
16	1	0	-1.743364	1.004337	2.962458
17	1	0	-0.939933	-0.512022	3.456843

18	1	0	-2.065912	-0.511998	2.074680
19	6	0	0.942625	0.982801	2.440942
20	1	0	0.623900	1.957732	2.814649
21	1	0	1.784429	1.103957	1.760246
22	1	0	1.220923	0.329933	3.269625
23	6	0	1.816212	-1.230256	-2.969175
24	1	0	2.268067	-0.445558	-3.599557
25	1	0	0.746447	-1.277266	-3.193801
26	1	0	2.266154	-2.187094	-3.256403
27	6	0	3.422797	-0.837233	-1.209159
28	1	0	3.933608	-0.089041	-1.838790
29	1	0	3.949655	-1.790968	-1.327531
30	1	0	3.517186	-0.521089	-0.165708
31	7	0	0.531158	1.388936	-0.373844
32	6	0	-0.584917	1.224621	0.482094
33	6	0	-1.740173	0.539111	-0.222300
34	6	0	-3.871303	-0.729956	-1.528200
35	6	0	-3.033976	1.054013	-0.129474
36	6	0	-1.518770	-0.613981	-0.982839
37	6	0	-2.578042	-1.248872	-1.626941
38	6	0	-4.096643	0.425458	-0.782272
39	1	0	-3.214292	1.952048	0.456714
40	1	0	-0.508774	-1.007075	-1.072794
41	1	0	-2.394103	-2.146745	-2.210054
42	1	0	-5.097614	0.838591	-0.704932
43	1	0	-4.695933	-1.222707	-2.033787
44	6	0	1.158580	2.567206	-0.277179
45	8	0	0.881380	3.537480	0.472158
46	7	0	2.291926	2.675464	-1.096988
47	1	0	-0.927965	2.164671	0.938724
48	1	0	2.548315	3.630959	-1.305535
49	1	0	2.288800	2.071462	-1.908618

1a.3Me$_2$NH-I3

Zero-point correction=	0.439363
(Hartree/Particle)	
Thermal correction to Energy=	0.463826
Thermal correction to Enthalpy=	0.464770
Thermal correction to Gibbs Free Energy=	0.385401
Sum of electronic and zero-point Energies=	-899.144858
Sum of electronic and thermal Energies=	-899.120395
Sum of electronic and thermal Enthalpies=	-899.119451
Sum of electronic and thermal Free Energies=	-899.198820

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.861802	-1.517670	1.230756
2	1	0	-0.731492	0.283325	1.615608
3	1	0	-0.230363	1.735277	0.861869
4	1	0	0.004157	1.371905	-1.038434
5	7	0	0.305436	2.283557	-0.664843
6	7	0	-0.780854	1.334649	1.695875
7	6	0	-2.193015	1.744281	1.525625

8	1	0	-2.257906	2.832908	1.573700
9	1	0	-2.799040	1.303466	2.319516
10	1	0	-2.528878	1.386208	0.550671
11	6	0	-0.191286	1.786129	2.973179
12	1	0	-0.286684	2.870313	3.047849
13	1	0	0.864131	1.513269	2.997387
14	1	0	-0.715275	1.312589	3.804798
15	6	0	-0.286193	-2.662922	1.942714
16	1	0	-0.550787	-3.609954	1.443143
17	1	0	-0.681008	-2.690600	2.961800
18	1	0	0.800052	-2.597226	1.993698
19	6	0	-2.317840	-1.701404	1.208933
20	1	0	-2.595056	-2.642308	0.707481
21	1	0	-2.797347	-0.878384	0.679916
22	1	0	-2.685125	-1.728403	2.238908
23	6	0	1.713804	2.522766	-0.963350
24	1	0	1.887975	2.688589	-2.037583
25	1	0	2.307327	1.664717	-0.640931
26	1	0	2.059764	3.410635	-0.423355
27	6	0	-0.553483	3.338205	-1.197078
28	1	0	-0.405560	3.496295	-2.276355
29	1	0	-0.341868	4.282558	-0.684633
30	1	0	-1.604233	3.087970	-1.023033
31	7	0	-1.000762	-0.376276	-0.888825
32	6	0	-0.323166	-1.415183	-0.157526
33	6	0	1.175094	-1.106582	-0.143880
34	6	0	3.930792	-0.533179	-0.301942
35	6	0	1.886132	-1.307050	-1.333092
36	6	0	1.867377	-0.601460	0.959513
37	6	0	3.234366	-0.320210	0.885157
38	6	0	3.247484	-1.025456	-1.416748
39	1	0	1.355656	-1.689985	-2.202649
40	1	0	1.350079	-0.453730	1.902849
41	1	0	3.750870	0.064435	1.759903
42	1	0	3.777413	-1.194993	-2.349378
43	1	0	4.993229	-0.318110	-0.360785
44	6	0	-1.889930	-0.788759	-1.788239
45	8	0	-2.200699	-1.964650	-2.118683
46	1	0	-0.461285	-2.399186	-0.644820
47	7	0	-2.604475	0.259803	-2.409181
48	1	0	-2.119573	1.147962	-2.411486
49	1	0	-2.957199	0.004169	-3.322256

1a.3Me$_2$NH-ts2

Zero-point correction=	0.434646
(Hartree/Particle)	
Thermal correction to Energy=	0.458920
Thermal correction to Enthalpy=	0.459865
Thermal correction to Gibbs Free Energy=	0.380427
Sum of electronic and zero-point Energies=	-899.148040
Sum of electronic and thermal Energies=	-899.123766
Sum of electronic and thermal Enthalpies=	-899.122821
Sum of electronic and thermal Free Energies=	-899.202258

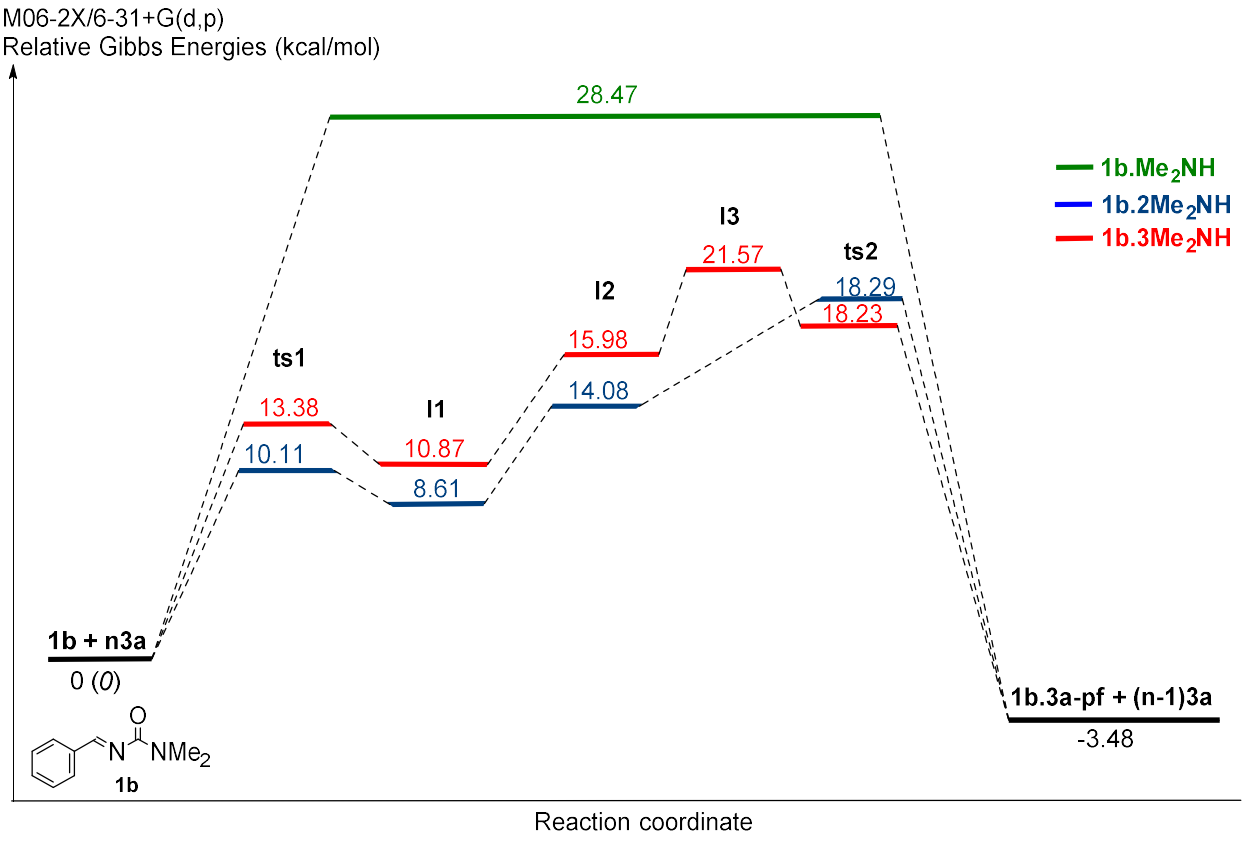
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.143871	0.244510	1.688765
2	1	0	0.789017	-1.292057	1.141863
3	1	0	1.794784	-1.370710	-0.305543
4	1	0	1.319251	0.210369	-1.143070
5	7	0	2.036628	-0.534989	-1.336811
6	7	0	1.498083	-1.959855	0.755320
7	6	0	2.668020	-1.990682	1.649103
8	1	0	3.439159	-2.630863	1.213599
9	1	0	2.393710	-2.379844	2.634607
10	1	0	3.064926	-0.979948	1.760786
11	6	0	0.915624	-3.293975	0.544925
12	1	0	1.651931	-3.935681	0.055095
13	1	0	0.032509	-3.214125	-0.091572
14	1	0	0.627576	-3.744988	1.499520
15	6	0	-1.130364	-0.189832	2.677412
16	1	0	-1.664326	0.664820	3.128954
17	1	0	-0.620210	-0.735811	3.476242
18	1	0	-1.865582	-0.854405	2.219035
19	6	0	0.895186	1.026354	2.360205
20	1	0	0.477073	1.922521	2.848083
21	1	0	1.646140	1.346209	1.634401
22	1	0	1.376010	0.407317	3.124154
23	6	0	1.838704	-1.147664	-2.653720
24	1	0	1.986053	-0.418033	-3.458539
25	1	0	0.825679	-1.550656	-2.726860
26	1	0	2.551988	-1.965852	-2.788406
27	6	0	3.373831	0.051124	-1.182594
28	1	0	3.606987	0.736516	-2.005673
29	1	0	4.127255	-0.742178	-1.159718
30	1	0	3.412136	0.612241	-0.245693
31	7	0	0.196783	1.433215	-0.388268
32	6	0	-0.775772	1.056004	0.603308
33	6	0	-1.885475	0.247331	-0.046512
34	6	0	-3.910107	-1.269059	-1.269214
35	6	0	-3.223325	0.621942	0.074218
36	6	0	-1.573434	-0.893285	-0.793008
37	6	0	-2.571709	-1.651605	-1.397199
38	6	0	-4.232298	-0.128678	-0.535811
39	1	0	-3.480197	1.505681	0.653597
40	1	0	-0.530167	-1.175648	-0.904602
41	1	0	-2.309522	-2.535419	-1.972112
42	1	0	-5.269264	0.177669	-0.434746
43	1	0	-4.692953	-1.854122	-1.741968
44	6	0	0.572938	2.709703	-0.391695
45	8	0	0.201910	3.647484	0.363064

46	7	0	1.560532	3.013702	-1.355784
47	1	0	-1.227511	1.947540	1.076885
48	1	0	1.569545	3.995021	-1.601832
49	1	0	1.544730	2.412417	-2.170054

2.2-Computational data (includes IRC where appropriate) for the addition of n dimethylamine (3a) molecules (n=1-3) to imine derivative 1b in gas phase, Et_2NH, CH_2Cl_2, CH_3CN and CH_3OH

2.2.1.-M06-2X/6-31+G(d,p) calculations

Energy profiles of the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1b** in the gas phase.



1b.Me_2NH-ts

Zero-point correction=	0.300405
(Hartree/Particle)	
Thermal correction to Energy=	0.317076
Thermal correction to Enthalpy=	0.318021
Thermal correction to Gibbs Free Energy=	0.254867
Sum of electronic and zero-point Energies=	-707.571349
Sum of electronic and thermal Energies=	-707.554677
Sum of electronic and thermal Enthalpies=	-707.553733
Sum of electronic and thermal Free Energies=	-707.616886

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.914338	-0.121779	0.285550
2	6	0	-2.048422	-0.166779	-0.493643
3	7	0	-3.169446	-0.665787	0.148082
4	8	0	-2.117756	0.230161	-1.665931
5	6	0	1.516307	-0.213980	-0.270279
6	6	0	3.976559	-1.536277	-0.127989
7	6	0	2.602575	0.229510	-1.029739
8	6	0	1.663708	-1.334898	0.547312
9	6	0	2.891015	-1.991839	0.619125
10	6	0	3.829936	-0.425537	-0.958518
11	1	0	2.481002	1.086826	-1.689669
12	1	0	0.798806	-1.681450	1.104400
13	1	0	2.998503	-2.865933	1.254380
14	1	0	4.666718	-0.077851	-1.556574
15	1	0	4.930488	-2.051836	-0.073452
16	6	0	0.209711	0.537156	-0.328975
17	1	0	0.012037	0.894637	-1.345628
18	1	0	-0.655820	0.984658	1.100082
19	6	0	-4.353735	-0.921616	-0.645594
20	1	0	-4.346053	-0.271827	-1.518502
21	1	0	-5.246287	-0.722856	-0.042807
22	1	0	-4.390688	-1.968011	-0.984289
23	6	0	-3.076565	-1.426619	1.376956
24	1	0	-2.204300	-1.114910	1.946579
25	1	0	-2.997559	-2.505989	1.174609
26	1	0	-3.978400	-1.256933	1.975289
27	6	0	1.407536	2.125011	1.365189
28	1	0	1.146941	2.891574	2.098293
29	1	0	2.167628	2.518486	0.681036
30	1	0	1.811240	1.250995	1.876773
31	7	0	0.190886	1.755105	0.633626
32	6	0	-0.468779	2.909634	0.000630
33	1	0	-0.739804	3.637769	0.768468
34	1	0	-1.366254	2.557572	-0.514372
35	1	0	0.205059	3.378401	-0.724834

1b.Me_2NH-pf

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 Zero-point correction=                           0.305287
(Hartree/Particle)
 Thermal correction to Energy=                    0.322130
 Thermal correction to Enthalpy=                  0.323075
 Thermal correction to Gibbs Free Energy=         0.260293
 Sum of electronic and zero-point Energies=           -707.622815
 Sum of electronic and thermal Energies=              -707.605971
 Sum of electronic and thermal Enthalpies=            -707.605027
 Sum of electronic and thermal Free Energies=         -707.667809

Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -0.929983   -0.227833    0.082731
      2          6           0       -2.185075    0.097764   -0.431425
      3          7           0       -3.198788   -0.741336   -0.033925
      4          8           0       -2.363576    1.064267   -1.158213
      5          6           0        1.482985   -0.168982   -0.273353
      6          6           0        3.938100   -1.533746   -0.244585
      7          6           0        2.428079    0.039700   -1.281060
      8          6           0        1.789215   -1.068301    0.755243
      9          6           0        3.004702   -1.748649    0.768381
     10          6           0        3.647678   -0.635381   -1.269147
     11          1           0        2.200595    0.733749   -2.086985
     12          1           0        1.076317   -1.235963    1.559543
     13          1           0        3.224447   -2.444767    1.572123
     14          1           0        4.367744   -0.464321   -2.063443
     15          1           0        4.885022   -2.064305   -0.235206
     16          6           0        0.185220    0.627000   -0.288998
     17          1           0        0.018379    1.007374   -1.303671
     18          6           0       -4.498842   -0.622227   -0.665148
     19          1           0       -5.276922   -0.492100    0.095038
     20          1           0       -4.730336   -1.518596   -1.254207
     21          1           0       -4.487530    0.247945   -1.318972
     22          6           0       -3.001027   -1.851414    0.874438
     23          1           0       -2.295200   -1.580014    1.663147
     24          1           0       -2.644881   -2.759481    0.364996
     25          1           0       -3.957248   -2.087978    1.348044
     26          6           0        0.468641    1.557474    1.970223
     27          1           0        0.224874    2.456979    2.543193
     28          1           0        1.524278    1.297995    2.167514
     29          1           0       -0.170040    0.744511    2.326864
     30          7           0        0.189703    1.809559    0.569726
     31          6           0        1.007599    2.880988    0.036976
     32          1           0        0.832846    3.787595    0.623621
     33          1           0        0.715589    3.084299   -0.997933
     34          1           0        2.090361    2.658133    0.063315
     35          1           0       -0.719855   -1.213272    0.159732
 ---------------------------------------------------------------------
```

1b.2Me$_2$NH-ts1

Zero-point correction=	0.398291
(Hartree/Particle)	
Thermal correction to Energy=	0.421103
Thermal correction to Enthalpy=	0.422047
Thermal correction to Gibbs Free Energy=	0.344293
Sum of electronic and zero-point Energies=	-842.622562
Sum of electronic and thermal Energies=	-842.599750
Sum of electronic and thermal Enthalpies=	-842.598805
Sum of electronic and thermal Free Energies=	-842.676560

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.000367	1.220334	-0.117824
2	6	0	1.286693	1.256259	-0.625639
3	7	0	2.058507	2.290287	-0.160807
4	8	0	1.761871	0.410965	-1.406188
5	6	0	-2.217022	0.292232	-0.340039
6	6	0	-4.934590	0.192135	0.319070
7	6	0	-3.123823	-0.370219	-1.171747
8	6	0	-2.683927	0.917265	0.820762
9	6	0	-4.035178	0.863103	1.149674
10	6	0	-4.477953	-0.421278	-0.846017
11	6	0	-0.774632	0.322865	-0.696086
12	7	0	2.799806	-1.829360	0.076649
13	1	0	-0.524100	-0.052729	-1.694158
14	1	0	2.861619	-1.267889	-0.771355
15	1	0	-2.764919	-0.839884	-2.084964
16	1	0	-5.175085	-0.932726	-1.502618
17	1	0	-5.989039	0.156220	0.575454
18	1	0	-4.391778	1.349801	2.052519
19	1	0	-1.970815	1.449293	1.443024
20	7	0	-0.223949	-1.480058	0.079846
21	1	0	0.777065	-1.470129	-0.155621
22	6	0	3.595425	-3.041702	-0.030126
23	1	0	3.403828	-3.680525	0.839134
24	1	0	4.680676	-2.848769	-0.072384
25	1	0	3.307134	-3.597173	-0.926085
26	6	0	-0.837015	-2.662168	-0.507120
27	1	0	-1.906469	-2.671555	-0.274804
28	1	0	-0.382637	-3.587391	-0.126462
29	1	0	-0.710997	-2.632676	-1.593616
30	6	0	3.196131	-1.001515	1.206859
31	1	0	2.610749	-0.076455	1.208447
32	1	0	4.266319	-0.733713	1.194345
33	1	0	2.995087	-1.537008	2.141928
34	6	0	-0.348513	-1.412693	1.527565
35	1	0	0.010926	-0.432212	1.859219
36	1	0	0.239303	-2.199194	2.019117
37	1	0	-1.400972	-1.517885	1.809170
38	6	0	1.562389	3.343334	0.700625
39	1	0	0.528969	3.136935	0.967492
40	1	0	1.619753	4.312789	0.188548
41	1	0	2.173301	3.401212	1.610644
42	6	0	3.432837	2.422171	-0.591178
43	1	0	3.571266	3.349485	-1.162201
44	1	0	3.693281	1.572836	-1.220136

45	1	0	4.099660	2.454458	0.280193

1b.2Me$_2$NH-I1

Zero-point correction=	0.400882
(Hartree/Particle)	
Thermal correction to Energy=	0.423380
Thermal correction to Enthalpy=	0.424324
Thermal correction to Gibbs Free Energy=	0.347656
Sum of electronic and zero-point Energies=	-842.625761
Sum of electronic and thermal Energies=	-842.603262
Sum of electronic and thermal Enthalpies=	-842.602318
Sum of electronic and thermal Free Energies=	-842.678987

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.015531	1.181100	-0.046699
2	6	0	1.239256	1.250369	-0.522327
3	7	0	2.013099	2.308721	-0.056321
4	8	0	1.773112	0.402988	-1.295670
5	6	0	-2.202890	0.135620	-0.273652
6	6	0	-4.935306	0.139841	0.346204
7	6	0	-3.123917	-0.490345	-1.117055
8	6	0	-2.665799	0.786802	0.872733
9	6	0	-4.023466	0.784218	1.183203
10	6	0	-4.484475	-0.492236	-0.810466
11	6	0	-0.726364	0.113350	-0.600031
12	7	0	2.778745	-1.828474	0.137075
13	1	0	-0.572489	-0.026014	-1.681946
14	1	0	2.930727	-1.283269	-0.711260
15	1	0	-2.777228	-0.961329	-2.034722
16	1	0	-5.190390	-0.973936	-1.480161
17	1	0	-5.994123	0.144944	0.586551
18	1	0	-4.374140	1.295707	2.074689
19	1	0	-1.942856	1.312834	1.488614
20	7	0	-0.116714	-1.254035	-0.051776
21	1	0	0.896826	-1.151639	-0.256185
22	6	0	3.470173	-3.107401	0.077140
23	1	0	3.191484	-3.714050	0.946300
24	1	0	4.567919	-3.007512	0.077679
25	1	0	3.172790	-3.650390	-0.824007
26	6	0	-0.552456	-2.467953	-0.764029
27	1	0	-1.599044	-2.674510	-0.532556
28	1	0	0.077735	-3.301986	-0.445631
29	1	0	-0.428906	-2.306325	-1.836855
30	6	0	3.206532	-1.017423	1.272271
31	1	0	2.727017	-0.034535	1.222133
32	1	0	4.298058	-0.868139	1.304303
33	1	0	2.909106	-1.507618	2.207192
34	6	0	-0.242977	-1.394083	1.412069
35	1	0	0.028186	-0.435958	1.859751
36	1	0	0.444298	-2.176779	1.741063
37	1	0	-1.273417	-1.652755	1.664109

38	6	0	1.381206	3.450270	0.573344
39	1	0	0.521358	3.118292	1.151502
40	1	0	1.038589	4.187149	-0.169769
41	1	0	2.104441	3.938640	1.235168
42	6	0	3.268728	2.587425	-0.720259
43	1	0	3.139237	3.285712	-1.562231
44	1	0	3.688513	1.659090	-1.104196
45	1	0	3.964733	3.038561	-0.005006

1b.2Me$_2$NH-I2

Zero-point correction=	0.400166
(Hartree/Particle)	
Thermal correction to Energy=	0.422727
Thermal correction to Enthalpy=	0.423672
Thermal correction to Gibbs Free Energy=	0.346779
Sum of electronic and zero-point Energies=	-842.616872
Sum of electronic and thermal Energies=	-842.594310
Sum of electronic and thermal Enthalpies=	-842.593366
Sum of electronic and thermal Free Energies=	-842.670258

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.376146	0.595906	1.622847
2	1	0	0.140872	1.399879	0.975661
3	1	0	-0.612154	1.526037	-0.845563
4	7	0	-0.634571	2.398139	-0.308417
5	6	0	1.650041	0.863819	2.320290
6	1	0	1.934487	-0.018347	2.899892
7	1	0	1.514657	1.713056	2.994025
8	1	0	2.430563	1.086116	1.593764
9	6	0	-0.742482	0.498457	2.590768
10	1	0	-0.537682	-0.315292	3.289806
11	1	0	-1.660287	0.268217	2.054936
12	1	0	-0.830912	1.448431	3.123925
13	6	0	0.022064	3.493458	-1.010171
14	1	0	-0.493468	3.770813	-1.942486
15	1	0	1.053077	3.216737	-1.247754
16	1	0	0.047145	4.377347	-0.364599
17	6	0	-2.038444	2.675585	-0.010205
18	1	0	-2.587915	3.043160	-0.890825
19	1	0	-2.113194	3.433098	0.777560
20	1	0	-2.518701	1.752821	0.329487
21	7	0	-0.718001	-0.529761	-0.231671
22	6	0	0.363498	-0.674519	0.641398
23	6	0	1.705145	-0.711804	-0.060918
24	6	0	4.217129	-0.752731	-1.307712
25	6	0	2.741021	-1.496345	0.450340
26	6	0	1.931647	0.029351	-1.223767
27	6	0	3.181431	0.017704	-1.837797
28	6	0	3.991050	-1.519919	-0.166978
29	1	0	2.562517	-2.103776	1.335072
30	1	0	1.106950	0.581630	-1.663079
31	1	0	3.345013	0.596577	-2.742019
32	1	0	4.783232	-2.142157	0.238062

33	1	0	5.188586	-0.768292	-1.792189
34	6	0	-1.821375	-1.221904	0.140903
35	8	0	-1.943507	-1.932711	1.160102
36	7	0	-2.924344	-1.049802	-0.705711
37	1	0	0.274566	-1.516146	1.345150
38	6	0	-2.733948	-0.513378	-2.038145
39	1	0	-2.213465	-1.218964	-2.704034
40	1	0	-2.149625	0.406518	-2.001465
41	1	0	-3.715760	-0.288547	-2.466254
42	6	0	-4.005783	-2.008406	-0.582796
43	1	0	-3.835614	-2.899844	-1.207504
44	1	0	-4.944602	-1.540894	-0.897039
45	1	0	-4.080794	-2.324071	0.456061

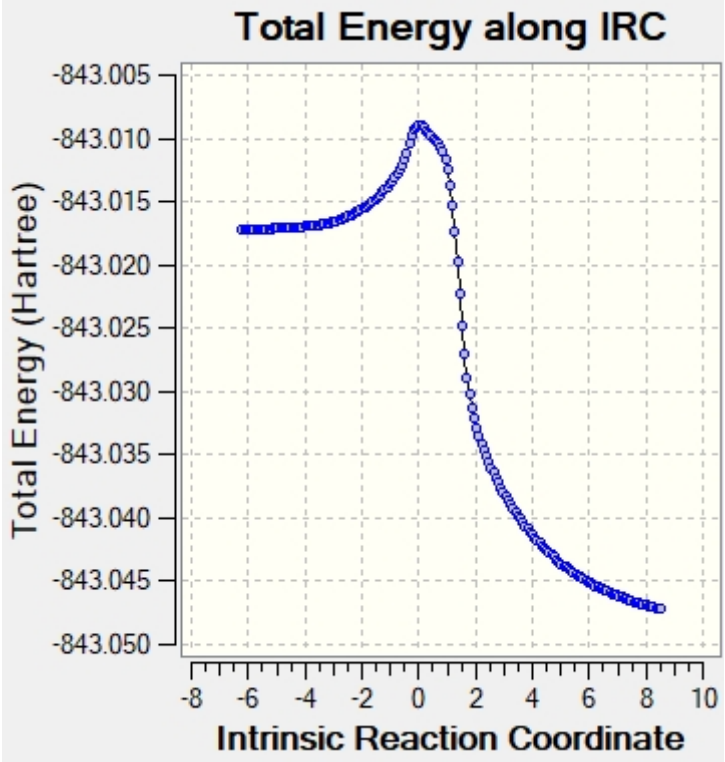
1b.2Me$_2$NH-ts2

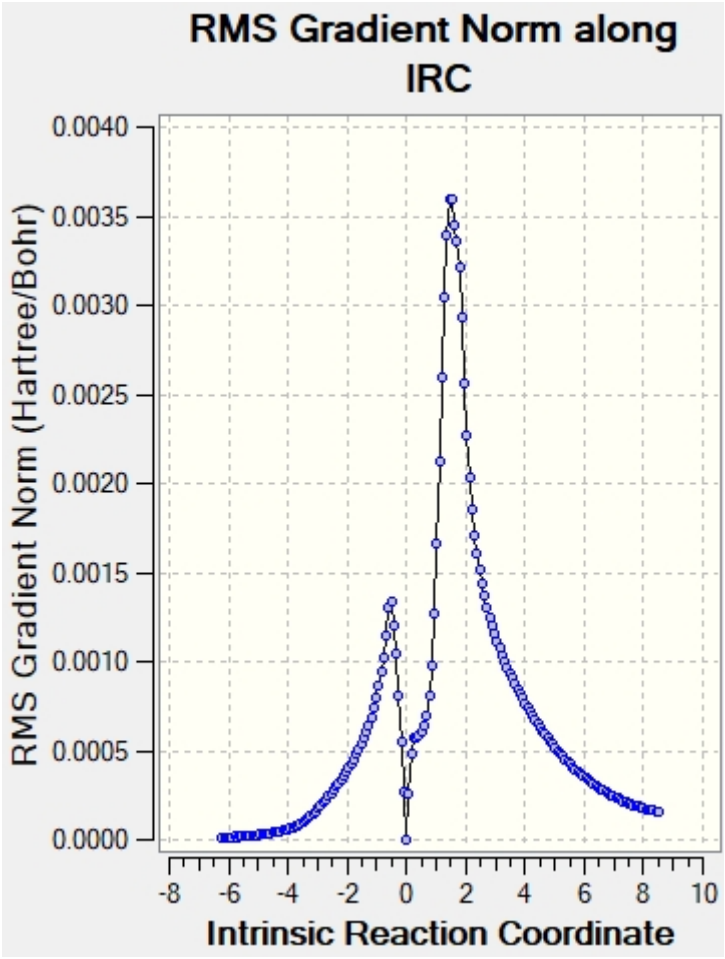
Zero-point correction= 0.395895
(Hartree/Particle)
Thermal correction to Energy= 0.417404
Thermal correction to Enthalpy= 0.418349
Thermal correction to Gibbs Free Energy= 0.345402
Sum of electronic and zero-point Energies= -842.613056
Sum of electronic and thermal Energies= -842.591547
Sum of electronic and thermal Enthalpies= -842.590603
Sum of electronic and thermal Free Energies= -842.663549

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.747636	-0.481759	-0.073857
2	6	0	1.849868	-1.061746	0.446820
3	7	0	2.941288	-1.128291	-0.443216
4	8	0	1.992877	-1.485634	1.609209
5	6	0	-1.672660	-0.661803	0.148960
6	6	0	-4.144681	-1.200183	-1.074438
7	6	0	-2.744236	-1.165667	0.891563
8	6	0	-1.845358	-0.469844	-1.224089
9	6	0	-3.074120	-0.725483	-1.830774
10	6	0	-3.972271	-1.432545	0.289205
11	1	0	-2.611083	-1.359968	1.953498
12	1	0	-0.990655	-0.167689	-1.821665
13	1	0	-3.190767	-0.573894	-2.900034
14	1	0	-4.790635	-1.829821	0.882137
15	1	0	-5.099345	-1.407670	-1.547973
16	6	0	-0.348747	-0.346582	0.827954
17	6	0	4.010368	-2.039949	-0.075289
18	1	0	4.934732	-1.732711	-0.574400
19	1	0	3.785181	-3.078858	-0.364777
20	1	0	4.146845	-2.007708	1.003828
21	6	0	2.691481	-1.044776	-1.869395
22	1	0	2.171687	-0.118914	-2.124630
23	1	0	2.083217	-1.883988	-2.240451
24	1	0	3.652957	-1.050442	-2.391222
25	6	0	1.970462	2.612462	-0.656771
26	1	0	2.561530	1.924406	-0.046692
27	1	0	1.917049	3.590154	-0.169008

28	1	0	2.459284	2.727287	-1.630453
29	6	0	-1.651071	1.585061	1.885893
30	1	0	-1.517169	2.606832	2.253337
31	1	0	-1.996900	0.959500	2.720124
32	1	0	-2.413940	1.582069	1.106087
33	7	0	0.624385	2.049309	-0.818216
34	6	0	-0.211128	2.748188	-1.796048
35	1	0	0.217158	2.673919	-2.801391
36	1	0	-0.290370	3.805213	-1.525313
37	1	0	-1.210588	2.306727	-1.799173
38	7	0	-0.368591	1.108248	1.356621
39	6	0	0.679769	1.264402	2.380899
40	1	0	0.801897	2.327814	2.611977
41	1	0	1.618193	0.846141	2.017654
42	1	0	0.407129	0.723157	3.295783
43	1	0	-0.238014	-0.984520	1.718342
44	1	0	0.733823	0.996651	-0.970165
45	1	0	0.076683	1.809634	0.254645

1b.2Me$_2$NH-ts2





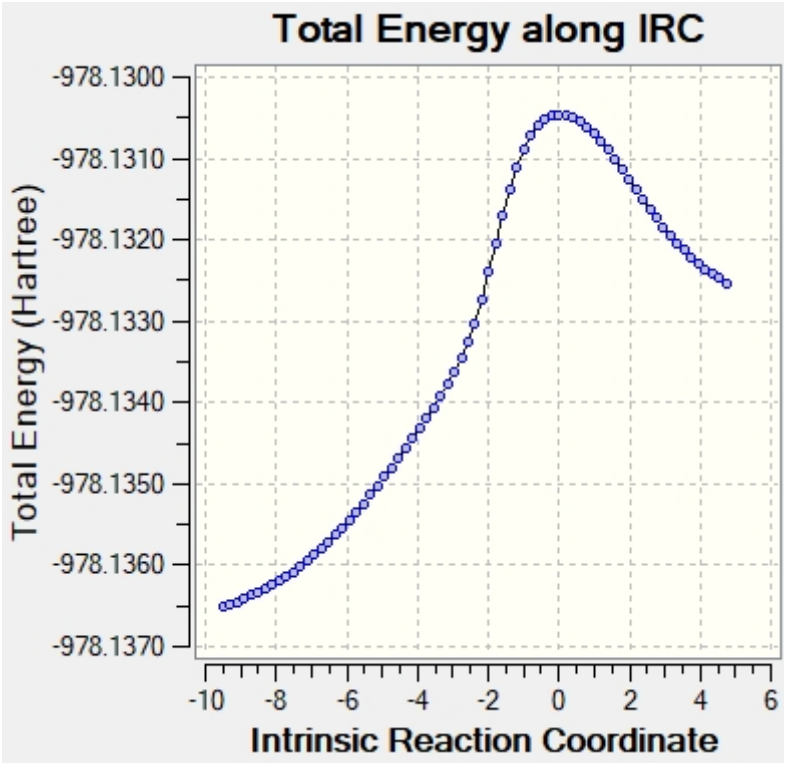
1b.3Me$_2$NH-ts1

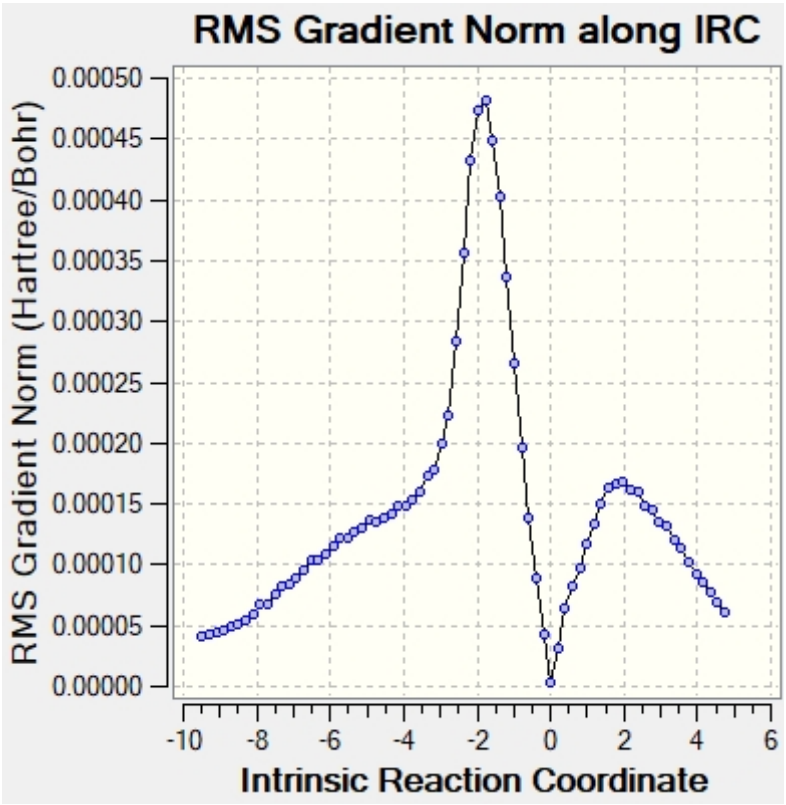
Zero-point correction= (Hartree/Particle)	0.493069
Thermal correction to Energy=	0.521818
Thermal correction to Enthalpy=	0.522762
Thermal correction to Gibbs Free Energy=	0.431505
Sum of electronic and zero-point Energies=	-977.640263
Sum of electronic and thermal Energies=	-977.611514
Sum of electronic and thermal Enthalpies=	-977.610570
Sum of electronic and thermal Free Energies=	-977.701827

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.779032	1.409704	-0.296965
2	6	0	0.567291	1.628860	-0.538773
3	7	0	0.992106	2.908931	-0.292739
4	8	0	1.375627	0.754833	-0.897357
5	6	0	-2.644606	-0.096186	-0.538002
6	6	0	-5.373979	-0.693441	-0.384948
7	6	0	-3.161516	-1.217777	-1.191985
8	6	0	-3.508600	0.733112	0.185022
9	6	0	-4.864911	0.432597	0.264519
10	6	0	-4.520698	-1.516736	-1.117683
11	6	0	-1.193375	0.203644	-0.614850
12	7	0	2.329035	-0.741376	1.523902
13	1	0	-0.609081	-0.418477	-1.301250
14	1	0	-2.494105	-1.855334	-1.767682
15	1	0	-4.913627	-2.387573	-1.633426
16	1	0	-6.433419	-0.923533	-0.325952
17	1	0	-5.529589	1.079427	0.829205
18	1	0	-3.094656	1.613115	0.667791
19	7	0	-0.567944	-1.038124	0.945111
20	6	0	3.035182	-1.827105	2.185338
21	1	0	2.524385	-2.087501	3.120100
22	1	0	4.081657	-1.578601	2.429413
23	1	0	3.035314	-2.708202	1.537505
24	6	0	-0.880982	-2.454938	0.837267
25	1	0	-1.964341	-2.597674	0.907230
26	1	0	-0.394612	-3.042599	1.629497
27	1	0	-0.541927	-2.834122	-0.131874
28	6	0	2.395009	0.503444	2.274922
29	1	0	1.874218	1.293503	1.724841
30	1	0	3.428887	0.836267	2.470077
31	1	0	1.898918	0.376917	3.244686
32	6	0	-1.031337	-0.439653	2.186880
33	1	0	-0.874301	0.643265	2.130739
34	1	0	-0.488244	-0.837896	3.055427
35	1	0	-2.100959	-0.636036	2.314960
36	1	0	0.458496	-0.910278	0.905359
37	7	0	3.390523	-1.241876	-1.355177
38	6	0	4.591836	-1.605548	-2.086354
39	1	0	4.998007	-2.537293	-1.677433
40	1	0	5.350727	-0.828531	-1.965042
41	1	0	4.418395	-1.761062	-3.165301
42	6	0	2.316100	-2.204749	-1.532977
43	1	0	1.415694	-1.814623	-1.050497
44	1	0	2.589028	-3.155897	-1.059175
45	1	0	2.083413	-2.409747	-2.592431

46	1	0	3.046467	-0.326220	-1.635162
47	1	0	2.736918	-0.605248	0.596823
48	6	0	0.090179	4.018735	-0.054631
49	1	0	-0.910776	3.637131	0.130701
50	1	0	0.066753	4.689705	-0.923978
51	1	0	0.432694	4.593754	0.813429
52	6	0	2.375951	3.256711	-0.537091
53	1	0	2.503255	3.727877	-1.521659
54	1	0	2.988458	2.356787	-0.496425
55	1	0	2.710873	3.963403	0.229504

1b.3Me$_2$NH-ts1





1b.3Me$_2$NH-I1

Zero-point correction= (Hartree/Particle)	0.495097
Thermal correction to Energy=	0.522778
Thermal correction to Enthalpy=	0.523722
Thermal correction to Gibbs Free Energy=	0.434768
Sum of electronic and zero-point Energies=	-977.645503
Sum of electronic and thermal Energies=	-977.617821
Sum of electronic and thermal Enthalpies=	-977.616877
Sum of electronic and thermal Free Energies=	-977.705831

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.784408	1.321150	-0.052626
2	6	0	0.512009	1.550421	-0.308313
3	7	0	0.987626	2.819819	0.014928
4	8	0	1.332318	0.700077	-0.755371
5	6	0	-2.675924	-0.151136	-0.457261
6	6	0	-5.456546	-0.500909	-0.521022
7	6	0	-3.250598	-1.136104	-1.264294
8	6	0	-3.510784	0.676742	0.298893
9	6	0	-4.891640	0.498820	0.271828
10	6	0	-4.633437	-1.314699	-1.296564
11	6	0	-1.172455	0.025546	-0.406752
12	7	0	2.125924	-0.986846	1.476329
13	1	0	-0.708423	-0.354194	-1.331086
14	1	0	-2.613049	-1.757430	-1.889831
15	1	0	-5.066173	-2.078437	-1.935547
16	1	0	-6.533770	-0.634239	-0.546134
17	1	0	-5.530996	1.148192	0.862400
18	1	0	-3.051930	1.471502	0.878951
19	7	0	-0.589284	-1.000261	0.654851
20	6	0	2.683721	-2.196576	2.066585
21	1	0	2.084535	-2.502477	2.933092
22	1	0	3.723674	-2.066217	2.405785
23	1	0	2.663977	-3.005349	1.329908
24	6	0	-0.734956	-2.421513	0.291135
25	1	0	-1.777928	-2.726567	0.395442
26	1	0	-0.099225	-3.016412	0.951969
27	1	0	-0.410867	-2.558071	-0.742634
28	6	0	2.247891	0.167298	2.363438
29	1	0	1.850743	1.056894	1.864419
30	1	0	3.291250	0.364241	2.656984
31	1	0	1.671231	-0.006391	3.280106
32	6	0	-1.080967	-0.738870	2.023420
33	1	0	-1.014264	0.336468	2.198648
34	1	0	-0.443586	-1.280799	2.726510
35	1	0	-2.116272	-1.075069	2.110778
36	1	0	0.452389	-0.825938	0.698250
37	7	0	3.618485	-0.890423	-1.242342
38	6	0	4.942638	-0.869186	-1.839021
39	1	0	5.469213	-1.799037	-1.596664
40	1	0	5.521644	-0.038857	-1.426557
41	1	0	4.924462	-0.770630	-2.938052
42	6	0	2.769618	-1.926780	-1.805925
43	1	0	1.764298	-1.816619	-1.388252
44	1	0	3.162864	-2.915626	-1.539276
45	1	0	2.690026	-1.878352	-2.905449

46	1	0	3.139573	0.002282	-1.357866
47	1	0	2.642732	-0.783176	0.615158
48	6	0	0.059482	3.922186	0.171789
49	1	0	-0.869797	3.550535	0.598268
50	1	0	-0.166162	4.404706	-0.792141
51	1	0	0.497663	4.671857	0.839020
52	6	0	2.309960	3.181313	-0.450722
53	1	0	2.318649	3.451103	-1.518541
54	1	0	2.995588	2.346431	-0.301759
55	1	0	2.662920	4.041673	0.125807

1b.3Me$_2$NH-I2

Zero-point correction=	0.496410
(Hartree/Particle)	
Thermal correction to Energy=	0.524184
Thermal correction to Enthalpy=	0.525128
Thermal correction to Gibbs Free Energy=	0.437761
Sum of electronic and zero-point Energies=	-977.639030
Sum of electronic and thermal Energies=	-977.611256
Sum of electronic and thermal Enthalpies=	-977.610312
Sum of electronic and thermal Free Energies=	-977.697679

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.744772	-0.027724	1.819749
2	1	0	0.841573	0.905182	1.314689
3	1	0	0.009057	2.270931	-0.013143
4	1	0	-1.109071	0.756191	-1.084923
5	7	0	-1.288924	1.732062	-1.360406
6	7	0	0.698773	2.557009	0.702429
7	6	0	0.045350	3.493858	1.613097
8	1	0	-0.230443	4.437231	1.116625
9	1	0	0.713985	3.734519	2.447658
10	1	0	-0.864283	3.043565	2.019826
11	6	0	1.847629	3.166458	0.040442
12	1	0	1.574971	4.073252	-0.520971
13	1	0	2.303365	2.451458	-0.648596
14	1	0	2.598445	3.443168	0.788756
15	6	0	1.991109	-0.269543	2.574147
16	1	0	1.921335	-1.237194	3.078912
17	1	0	2.118413	0.520964	3.316958
18	1	0	2.839215	-0.271575	1.890262
19	6	0	-0.404161	0.144340	2.740431
20	1	0	-0.597628	-0.795146	3.259625
21	1	0	-1.282847	0.397364	2.148329
22	1	0	-0.167427	0.950727	3.439244
23	6	0	-1.250602	1.888024	-2.804820
24	1	0	-2.076942	1.365451	-3.315736
25	1	0	-0.305994	1.498098	-3.196395
26	1	0	-1.313390	2.950329	-3.067386
27	6	0	-2.570710	2.125948	-0.791968
28	1	0	-3.427276	1.631938	-1.279364
29	1	0	-2.705332	3.210983	-0.879603

30	1	0	-2.594198	1.853538	0.267998
31	7	0	-0.720104	-0.851391	0.019100
32	6	0	0.445740	-1.144903	0.732554
33	6	0	1.661941	-1.199724	-0.170982
34	6	0	3.901517	-1.285452	-1.854672
35	6	0	2.608839	-2.215660	-0.039175
36	6	0	1.837607	-0.233961	-1.166659
37	6	0	2.953468	-0.270531	-1.997851
38	6	0	3.723214	-2.262508	-0.878189
39	1	0	2.468605	-2.982427	0.719437
40	1	0	1.076600	0.531750	-1.295255
41	1	0	3.079986	0.485971	-2.767288
42	1	0	4.448497	-3.063108	-0.770048
43	1	0	4.768163	-1.318307	-2.507534
44	6	0	-1.832055	-1.462076	0.496776
45	8	0	-1.937393	-2.065945	1.582852
46	7	0	-2.964032	-1.328181	-0.320618
47	6	0	-2.835559	-1.276170	-1.764492
48	1	0	-3.051263	-2.260449	-2.210071
49	1	0	-1.820398	-0.992788	-2.037566
50	1	0	-3.544253	-0.553649	-2.189541
51	6	0	-4.180375	-1.969582	0.135362
52	1	0	-5.036771	-1.488537	-0.349115
53	1	0	-4.264907	-1.869077	1.216171
54	1	0	-4.197251	-3.042640	-0.112037
55	1	0	0.375496	-2.053695	1.351477

1b.3Me$_2$NH-I3

Zero-point correction=	0.496238
(Hartree/Particle)	
Thermal correction to Energy=	0.523117
Thermal correction to Enthalpy=	0.524061
Thermal correction to Gibbs Free Energy=	0.440239
Sum of electronic and zero-point Energies=	-977.632772
Sum of electronic and thermal Energies=	-977.605893
Sum of electronic and thermal Enthalpies=	-977.604949
Sum of electronic and thermal Free Energies=	-977.688771

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.131022	-1.793792	1.294714
2	1	0	0.449263	-0.268799	1.887468
3	1	0	0.645438	1.366883	1.321982
4	1	0	-0.195445	1.622561	-0.403251
5	7	0	0.439921	2.362777	-0.060690
6	7	0	0.483357	0.773516	2.204996
7	6	0	-0.850868	1.126300	2.732372
8	1	0	-0.851940	2.169615	3.058477
9	1	0	-1.092829	0.479982	3.579763
10	1	0	-1.573114	0.969763	1.927569
11	6	0	1.566117	0.989472	3.178072
12	1	0	1.559636	2.029905	3.511693

13	1	0	2.525524	0.772752	2.706306
14	1	0	1.424563	0.331599	4.038966
15	6	0	0.972824	-2.990213	1.422320
16	1	0	0.503140	-3.848629	0.917757
17	1	0	1.094320	-3.238342	2.481335
18	1	0	1.958065	-2.836924	0.983815
19	6	0	-1.180819	-2.125767	1.879150
20	1	0	-1.641288	-2.978766	1.363232
21	1	0	-1.862623	-1.281145	1.785884
22	1	0	-1.039489	-2.368405	2.938191
23	6	0	1.474990	2.607514	-1.063040
24	1	0	1.069003	3.106798	-1.956364
25	1	0	1.926849	1.664790	-1.368212
26	1	0	2.255174	3.249434	-0.639064
27	6	0	-0.285547	3.593325	0.241527
28	1	0	-0.774655	4.023807	-0.646148
29	1	0	0.415570	4.337974	0.634573
30	1	0	-1.053685	3.417186	0.999132
31	7	0	-0.983269	-0.320133	-0.291276
32	6	0	-0.031061	-1.388834	-0.149007
33	6	0	1.307052	-0.970547	-0.753193
34	6	0	3.691211	-0.227442	-2.065304
35	6	0	1.374073	-0.912214	-2.151269
36	6	0	2.453473	-0.635391	-0.029518
37	6	0	3.636684	-0.266696	-0.675598
38	6	0	2.548615	-0.550447	-2.802631
39	1	0	0.480856	-1.157726	-2.720916
40	1	0	2.445314	-0.696947	1.054948
41	1	0	4.516776	-0.018665	-0.088902
42	1	0	2.577080	-0.522623	-3.887844
43	1	0	4.610778	0.049449	-2.571386
44	6	0	-2.192494	-0.773135	-0.696698
45	8	0	-2.512565	-1.956906	-0.927101
46	1	0	-0.371302	-2.288211	-0.691204
47	7	0	-3.188944	0.217208	-0.830485
48	6	0	-4.349947	-0.139948	-1.624888
49	1	0	-4.171470	-0.005637	-2.704436
50	1	0	-5.197268	0.488779	-1.332985
51	1	0	-4.589589	-1.185945	-1.445035
52	6	0	-2.800295	1.605079	-0.906314
53	1	0	-2.146472	1.825375	-1.768433
54	1	0	-2.273051	1.901632	0.001538
55	1	0	-3.701266	2.220359	-0.988331

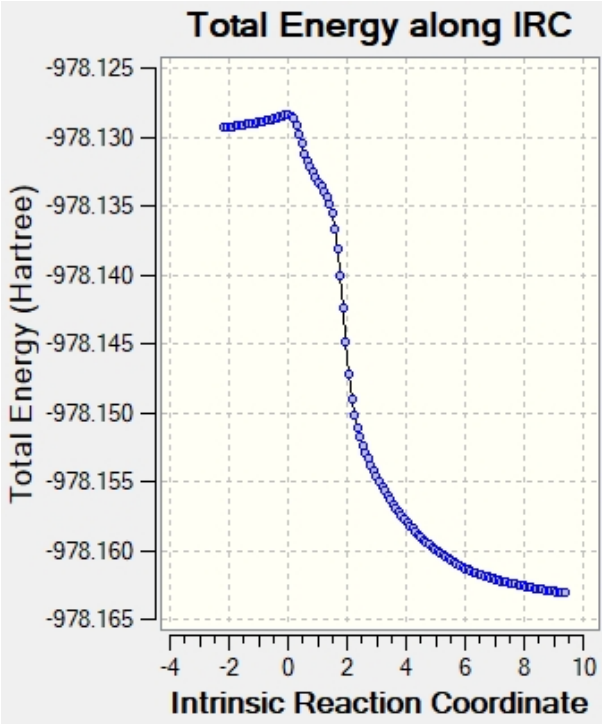
1b.3Me$_2$NH-ts2

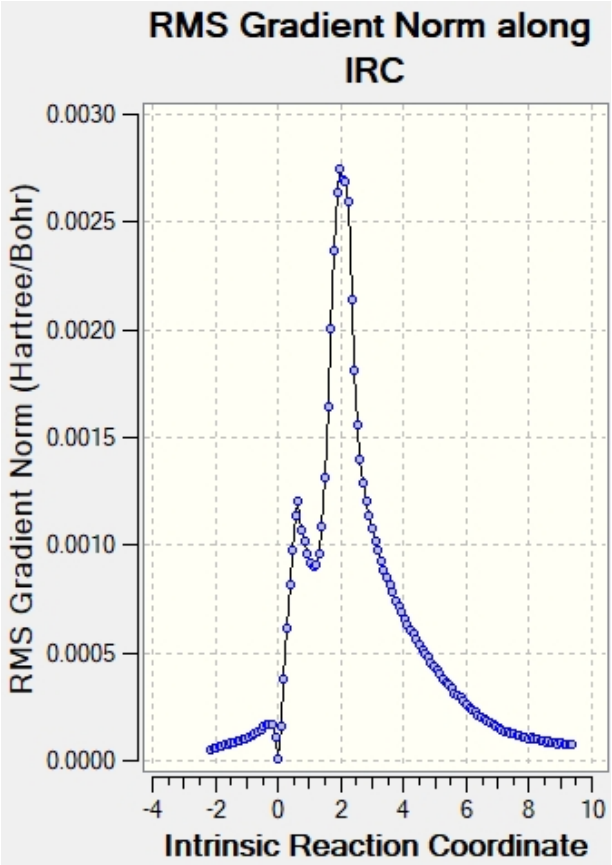
Zero-point correction=	0.490569
(Hartree/Particle)	
Thermal correction to Energy=	0.517325
Thermal correction to Enthalpy=	0.518269
Thermal correction to Gibbs Free Energy=	0.434283
Sum of electronic and zero-point Energies=	-977.637816
Sum of electronic and thermal Energies=	-977.611061
Sum of electronic and thermal Enthalpies=	-977.610116
Sum of electronic and thermal Free Energies=	-977.694102

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.734130	0.237903	1.796702
2	1	0	0.635507	1.674487	0.882838
3	1	0	-0.342217	2.184630	-0.508534
4	1	0	-1.054579	0.535651	-0.916182
5	7	0	-1.283363	1.506445	-1.303238
6	7	0	0.415143	2.583353	0.344383
7	6	0	-0.310599	3.501146	1.234075
8	1	0	-0.589344	4.406355	0.686238
9	1	0	0.309744	3.782063	2.091815
10	1	0	-1.215619	3.009888	1.596330
11	6	0	1.647486	3.176029	-0.191585
12	1	0	1.404368	4.047776	-0.806265
13	1	0	2.172396	2.437801	-0.800200
14	1	0	2.307459	3.490680	0.623785
15	6	0	1.982906	0.124938	2.550434
16	1	0	2.012231	-0.796938	3.155466
17	1	0	2.071123	0.979251	3.229630
18	1	0	2.841126	0.124553	1.875586
19	6	0	-0.383981	0.375479	2.738552
20	1	0	-0.483290	-0.508632	3.383381
21	1	0	-1.320049	0.481076	2.186885
22	1	0	-0.217962	1.264315	3.358556
23	6	0	-1.106081	1.591162	-2.750700
24	1	0	-1.829554	0.959489	-3.282691
25	1	0	-0.098999	1.263044	-3.023674
26	1	0	-1.239683	2.625296	-3.088156
27	6	0	-2.645010	1.845039	-0.883290
28	1	0	-3.391415	1.259785	-1.434608
29	1	0	-2.839734	2.912432	-1.043356
30	1	0	-2.760489	1.604073	0.176905
31	7	0	-0.675586	-0.793038	0.102978
32	6	0	0.504736	-0.954662	0.894214
33	6	0	1.714906	-1.114494	-0.013454
34	6	0	3.946042	-1.349412	-1.708888
35	6	0	2.675799	-2.101597	0.206755
36	6	0	1.880033	-0.259545	-1.106005
37	6	0	2.984848	-0.364695	-1.944852
38	6	0	3.783555	-2.221330	-0.635112
39	1	0	2.554072	-2.785105	1.043887
40	1	0	1.107568	0.476832	-1.306261
41	1	0	3.092706	0.308648	-2.791444
42	1	0	4.519037	-2.999070	-0.452057
43	1	0	4.806931	-1.441597	-2.363828
44	6	0	-1.765129	-1.439096	0.560115
45	8	0	-1.907238	-1.996884	1.662727

46	7	0	-2.874681	-1.394258	-0.327874
47	6	0	-2.648478	-1.564537	-1.751108
48	1	0	-2.737243	-2.623478	-2.046235
49	1	0	-1.646979	-1.224800	-2.013226
50	1	0	-3.391926	-0.997103	-2.328188
51	6	0	-4.074862	-2.063612	0.135182
52	1	0	-4.925656	-1.716263	-0.461532
53	1	0	-4.243550	-1.830877	1.185538
54	1	0	-4.002569	-3.158492	0.037854
55	1	0	0.427963	-1.838423	1.553290

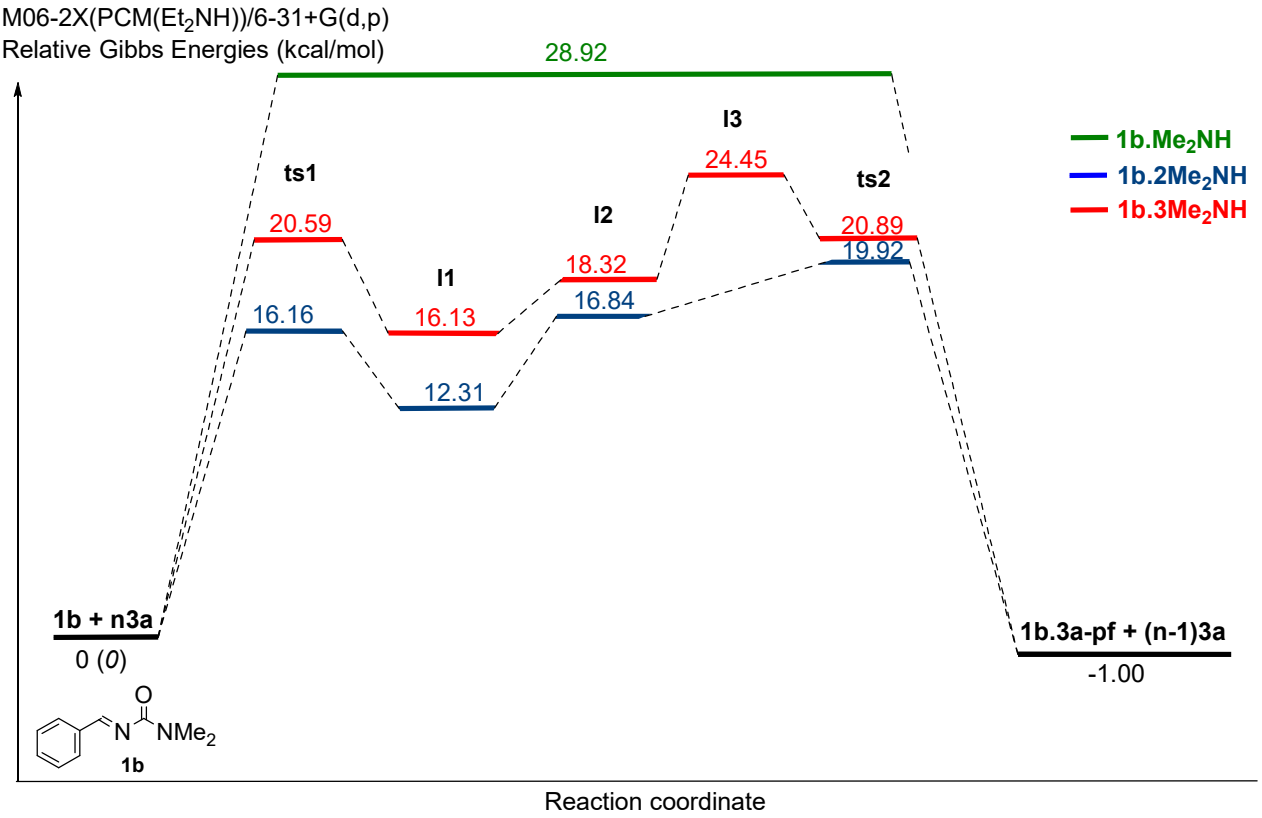
1b.3Me$_2$NH-ts2





2.2.2.-M06-2X(PCM=Diethylamine)/6-31+G(d,p) calculations

Energy profiles of the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1b** in diethylamine.



1b

Zero-point correction= (Hartree/Particle)	0.206740
Thermal correction to Energy=	0.218021
Thermal correction to Enthalpy=	0.218965
Thermal correction to Gibbs Free Energy=	0.167337
Sum of electronic and zero-point Energies=	-572.602514
Sum of electronic and thermal Energies=	-572.591233
Sum of electronic and thermal Enthalpies=	-572.590288
Sum of electronic and thermal Free Energies=	-572.641916

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.734547	-0.277593	0.000000
2	6	0	2.141552	-0.025794	0.000000
3	6	0	0.000000	0.769339	0.000000
4	7	0	2.876783	-1.156233	0.000000
5	8	0	2.650622	1.097251	0.000000
6	1	0	0.451578	1.768801	0.000000
7	6	0	-1.466205	0.699744	0.000000
8	6	0	-4.255639	0.637026	0.000000
9	6	0	-2.197793	1.892960	0.000000
10	6	0	-2.140634	-0.529780	0.000000
11	6	0	-3.529441	-0.558553	0.000000
12	6	0	-3.590936	1.862205	0.000000
13	1	0	-1.671176	2.843874	0.000000
14	1	0	-1.560829	-1.447334	0.000000
15	1	0	-4.052403	-1.509583	0.000000
16	1	0	-4.154961	2.789147	0.000000
17	1	0	-5.340893	0.610058	0.000000
18	6	0	4.325300	-0.995352	0.000000
19	1	0	4.791830	-1.979015	0.000000
20	1	0	4.650100	-0.441532	0.885334
21	1	0	4.650100	-0.441532	-0.885334
22	6	0	2.274166	-2.489317	0.000000
23	1	0	3.078356	-3.224014	0.000000
24	1	0	1.655900	-2.642485	-0.886806
25	1	0	1.655900	-2.642485	0.886806

1b.Me_2NH-ts

Zero-point correction= (Hartree/Particle)	0.300075
Thermal correction to Energy=	0.316807
Thermal correction to Enthalpy=	0.317751
Thermal correction to Gibbs Free Energy=	0.254336
Sum of electronic and zero-point Energies=	-707.582920
Sum of electronic and thermal Energies=	-707.566187
Sum of electronic and thermal Enthalpies=	-707.565243
Sum of electronic and thermal Free Energies=	-707.628658

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	-1.035696	0.383576	0.207564
2	6	0	-1.934678	-0.344433	-0.507175
3	7	0	-3.209046	-0.419989	0.036888
4	8	0	-1.667861	-0.906762	-1.585292
5	6	0	1.379704	-0.251547	-0.202809
6	6	0	3.568875	-1.927357	0.269873
7	6	0	2.547199	-0.118271	-0.959586
8	6	0	1.309372	-1.237479	0.781002
9	6	0	2.400008	-2.073399	1.016297
10	6	0	3.640916	-0.948694	-0.722046
11	1	0	2.597141	0.632601	-1.745884
12	1	0	0.387964	-1.341940	1.346357
13	1	0	2.334772	-2.843341	1.779132
14	1	0	4.543515	-0.840025	-1.315595
15	1	0	4.416731	-2.580504	0.452197
16	6	0	0.218051	0.680184	-0.450767
17	1	0	0.111053	0.843329	-1.530900
18	1	0	-0.781428	1.673970	0.560802
19	6	0	-4.100208	-1.440369	-0.484214
20	1	0	-3.903342	-1.581783	-1.544943
21	1	0	-5.136263	-1.118872	-0.345050
22	1	0	-3.961945	-2.403480	0.030380
23	6	0	-3.434895	-0.049176	1.421296
24	1	0	-2.940593	0.894051	1.648955
25	1	0	-3.063897	-0.814652	2.119660
26	1	0	-4.509881	0.071939	1.579548
27	6	0	1.308341	2.146456	1.328584
28	1	0	1.161669	3.105299	1.828755
29	1	0	2.340004	2.070110	0.969542
30	1	0	1.112205	1.335018	2.031084
31	7	0	0.356757	2.058494	0.212311
32	6	0	0.483532	3.171478	-0.735333
33	1	0	0.388412	4.114665	-0.194502
34	1	0	-0.312002	3.099175	-1.479151
35	1	0	1.457356	3.139604	-1.236131

1b.Me_2NH-pf

Zero-point correction= 0.305395
(Hartree/Particle)
Thermal correction to Energy= 0.322198
Thermal correction to Enthalpy= 0.323142
Thermal correction to Gibbs Free Energy= 0.260602
Sum of electronic and zero-point Energies= -707.631551
Sum of electronic and thermal Energies= -707.614747
Sum of electronic and thermal Enthalpies= -707.613803
Sum of electronic and thermal Free Energies= -707.676343

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.940824	-0.190411	0.085749
2	6	0	-2.194500	0.106782	-0.423594
3	7	0	-3.198666	-0.730669	-0.015751
4	8	0	-2.383869	1.069064	-1.166781

5	6	0	1.472032	-0.170886	-0.269381
6	6	0	3.906017	-1.573513	-0.238284
7	6	0	2.409940	0.003718	-1.290707
8	6	0	1.774006	-1.054840	0.773915
9	6	0	2.979366	-1.754002	0.788288
10	6	0	3.619407	-0.690333	-1.277694
11	1	0	2.186609	0.685502	-2.108145
12	1	0	1.068734	-1.200197	1.589226
13	1	0	3.195773	-2.438170	1.603002
14	1	0	4.333906	-0.545423	-2.082070
15	1	0	4.844385	-2.119001	-0.227824
16	6	0	0.185190	0.643108	-0.292945
17	1	0	0.024250	1.008032	-1.313589
18	6	0	-4.500986	-0.642306	-0.652213
19	1	0	-5.283518	-0.554208	0.108057
20	1	0	-4.698824	-1.534311	-1.258917
21	1	0	-4.519741	0.238833	-1.290056
22	6	0	-2.972260	-1.852725	0.876564
23	1	0	-2.345849	-1.555655	1.721691
24	1	0	-2.512959	-2.711057	0.366329
25	1	0	-3.935769	-2.175838	1.274724
26	6	0	0.474167	1.602954	1.954263
27	1	0	0.258473	2.518297	2.512968
28	1	0	1.520182	1.314110	2.158305
29	1	0	-0.189747	0.815114	2.320805
30	7	0	0.211199	1.844290	0.546148
31	6	0	1.086749	2.871041	0.009536
32	1	0	0.935650	3.797451	0.570951
33	1	0	0.834782	3.060638	-1.038351
34	1	0	2.157256	2.603704	0.070795
35	1	0	-0.739372	-1.156785	0.296833

1b.2Me$_2$NH-ts1

Zero-point correction= 0.398101
(Hartree/Particle)
Thermal correction to Energy= 0.420702
Thermal correction to Enthalpy= 0.421646
Thermal correction to Gibbs Free Energy= 0.344791
Sum of electronic and zero-point Energies= -842.628523
Sum of electronic and thermal Energies= -842.605922
Sum of electronic and thermal Enthalpies= -842.604977
Sum of electronic and thermal Free Energies= -842.681832

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.077917	-1.152530	-0.188831
2	6	0	-1.330643	-1.146560	-0.787340
3	7	0	-2.212954	-2.063953	-0.284541
4	8	0	-1.678397	-0.370013	-1.697258
5	6	0	2.211340	-0.401056	-0.327507
6	6	0	4.881823	-0.416699	0.505492
7	6	0	3.201504	0.193280	-1.115909
8	6	0	2.570100	-1.015605	0.877197
9	6	0	3.898469	-1.020061	1.292587
10	6	0	4.532824	0.186619	-0.702358

11	6	0	0.798079	-0.366477	-0.774335
12	7	0	-2.725096	1.619326	0.291362
13	1	0	0.626562	-0.011408	-1.794647
14	1	0	-2.824092	1.020368	-0.527658
15	1	0	2.925632	0.657670	-2.060004
16	1	0	5.295663	0.646735	-1.322747
17	1	0	5.918048	-0.423945	0.829593
18	1	0	4.171265	-1.497918	2.228645
19	1	0	1.793045	-1.488270	1.470000
20	7	0	0.344810	1.584697	-0.115901
21	1	0	-0.673498	1.570689	-0.246747
22	6	0	-3.746885	2.657129	0.281021
23	1	0	-3.550201	3.370626	1.088295
24	1	0	-4.766130	2.261019	0.422833
25	1	0	-3.714156	3.199540	-0.666797
26	6	0	0.929369	2.672331	-0.886584
27	1	0	2.016868	2.658492	-0.760986
28	1	0	0.554967	3.654516	-0.566371
29	1	0	0.693650	2.534560	-1.945664
30	6	0	-2.782279	0.806579	1.499310
31	1	0	-2.017471	0.024192	1.458572
32	1	0	-3.764443	0.329181	1.658144
33	1	0	-2.573078	1.438110	2.370060
34	6	0	0.621035	1.663760	1.310025
35	1	0	0.289483	0.733147	1.783556
36	1	0	0.103255	2.509649	1.781980
37	1	0	1.699010	1.771613	1.466501
38	6	0	-1.956436	-2.861911	0.899662
39	1	0	-0.898748	-2.822810	1.145730
40	1	0	-2.251662	-3.899987	0.713955
41	1	0	-2.541739	-2.485119	1.750894
42	6	0	-3.587729	-2.045652	-0.743780
43	1	0	-3.976998	-3.067718	-0.754506
44	1	0	-3.632271	-1.627450	-1.747470
45	1	0	-4.221126	-1.442208	-0.076599

1b.2Me$_2$NH-I1

Zero-point correction=	0.400329
(Hartree/Particle)	
Thermal correction to Energy=	0.422640
Thermal correction to Enthalpy=	0.423584
Thermal correction to Gibbs Free Energy=	0.347863
Sum of electronic and zero-point Energies=	-842.635504
Sum of electronic and thermal Energies=	-842.613193
Sum of electronic and thermal Enthalpies=	-842.612249
Sum of electronic and thermal Free Energies=	-842.687970

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.120859	1.069255	0.031665
2	6	0	1.325017	1.198956	-0.544917
3	7	0	2.133143	2.216700	-0.027257
4	8	0	1.797612	0.469309	-1.462848
5	6	0	-2.122101	0.157492	-0.264697
6	6	0	-4.880303	0.390203	0.192111

7	6	0	-3.041523	-0.408380	-1.152634
8	6	0	-2.599873	0.863418	0.843609
9	6	0	-3.969315	0.974340	1.074118
10	6	0	-4.413792	-0.296180	-0.927274
11	6	0	-0.633299	0.014662	-0.511830
12	7	0	2.598731	-1.786143	0.059368
13	1	0	-0.446863	-0.163695	-1.580768
14	1	0	2.780273	-1.263604	-0.798021
15	1	0	-2.683081	-0.927098	-2.039262
16	1	0	-5.115304	-0.734093	-1.630780
17	1	0	-5.947511	0.483121	0.369170
18	1	0	-4.327870	1.526080	1.938065
19	1	0	-1.879927	1.339119	1.502197
20	7	0	-0.151344	-1.344218	0.115398
21	1	0	0.909432	-1.381819	-0.007749
22	6	0	3.065660	-3.164075	-0.043685
23	1	0	2.740664	-3.725743	0.838911
24	1	0	4.161714	-3.236961	-0.107034
25	1	0	2.633662	-3.636245	-0.929702
26	6	0	-0.663702	-2.549550	-0.566021
27	1	0	-1.734914	-2.653845	-0.385137
28	1	0	-0.136915	-3.422529	-0.173216
29	1	0	-0.470649	-2.458713	-1.636739
30	6	0	3.211224	-1.065587	1.174535
31	1	0	2.879159	-0.023264	1.158487
32	1	0	4.310653	-1.086997	1.133122
33	1	0	2.898613	-1.522576	2.120077
34	6	0	-0.363949	-1.413773	1.576902
35	1	0	-0.033031	-0.467628	2.007537
36	1	0	0.233263	-2.239266	1.971967
37	1	0	-1.421446	-1.581204	1.789633
38	6	0	1.536553	3.264537	0.778418
39	1	0	0.837053	2.830571	1.490625
40	1	0	0.992664	3.999694	0.164593
41	1	0	2.330489	3.787223	1.320616
42	6	0	3.286713	2.622345	-0.804875
43	1	0	3.020593	3.335153	-1.601893
44	1	0	3.741210	1.746342	-1.265102
45	1	0	4.013580	3.103895	-0.143587

1b.2Me$_2$NH-I2

Zero-point correction= 0.400738
(Hartree/Particle)
Thermal correction to Energy= 0.422990
Thermal correction to Enthalpy= 0.423934
Thermal correction to Gibbs Free Energy= 0.348498
Sum of electronic and zero-point Energies= -842.628510
Sum of electronic and thermal Energies= -842.606259
Sum of electronic and thermal Enthalpies= -842.605314
Sum of electronic and thermal Free Energies= -842.680751

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.363764	0.729764	1.549580

2	1	0	0.126101	1.486303	0.838712
3	1	0	-0.618000	1.577699	-1.011105
4	7	0	-0.618775	2.429004	-0.446043
5	6	0	1.638494	1.057486	2.225410
6	1	0	1.926507	0.225869	2.873341
7	1	0	1.494034	1.956757	2.826974
8	1	0	2.415815	1.229452	1.482544
9	6	0	-0.752831	0.709755	2.525839
10	1	0	-0.512021	0.003309	3.323136
11	1	0	-1.659830	0.383176	2.021365
12	1	0	-0.880854	1.713206	2.936694
13	6	0	0.040568	3.533658	-1.134698
14	1	0	-0.494516	3.844422	-2.044030
15	1	0	1.059331	3.244855	-1.406324
16	1	0	0.097205	4.396005	-0.463315
17	6	0	-2.011037	2.722710	-0.107477
18	1	0	-2.582567	3.092011	-0.972382
19	1	0	-2.049329	3.484855	0.677809
20	1	0	-2.488261	1.808218	0.257563
21	7	0	-0.736237	-0.537280	-0.181499
22	6	0	0.359213	-0.599049	0.702943
23	6	0	1.693524	-0.712656	-0.007520
24	6	0	4.187669	-0.910023	-1.275613
25	6	0	2.704442	-1.510140	0.532492
26	6	0	1.937726	-0.028930	-1.202317
27	6	0	3.178531	-0.119386	-1.828663
28	6	0	3.945458	-1.612295	-0.096544
29	1	0	2.515867	-2.062693	1.450023
30	1	0	1.139164	0.551309	-1.653613
31	1	0	3.355827	0.416052	-2.756581
32	1	0	4.718165	-2.243841	0.331012
33	1	0	5.151869	-0.987759	-1.768511
34	6	0	-1.805205	-1.258863	0.202797
35	8	0	-1.900899	-1.979645	1.227186
36	7	0	-2.926412	-1.132830	-0.633092
37	1	0	0.277537	-1.384261	1.468343
38	6	0	-2.765813	-0.567750	-1.959001
39	1	0	-2.195956	-1.228845	-2.630122
40	1	0	-2.246092	0.389044	-1.905921
41	1	0	-3.757619	-0.403934	-2.390392
42	6	0	-3.940580	-2.167019	-0.540442
43	1	0	-3.685002	-3.049632	-1.148722
44	1	0	-4.895947	-1.769983	-0.896427
45	1	0	-4.041556	-2.480025	0.496598

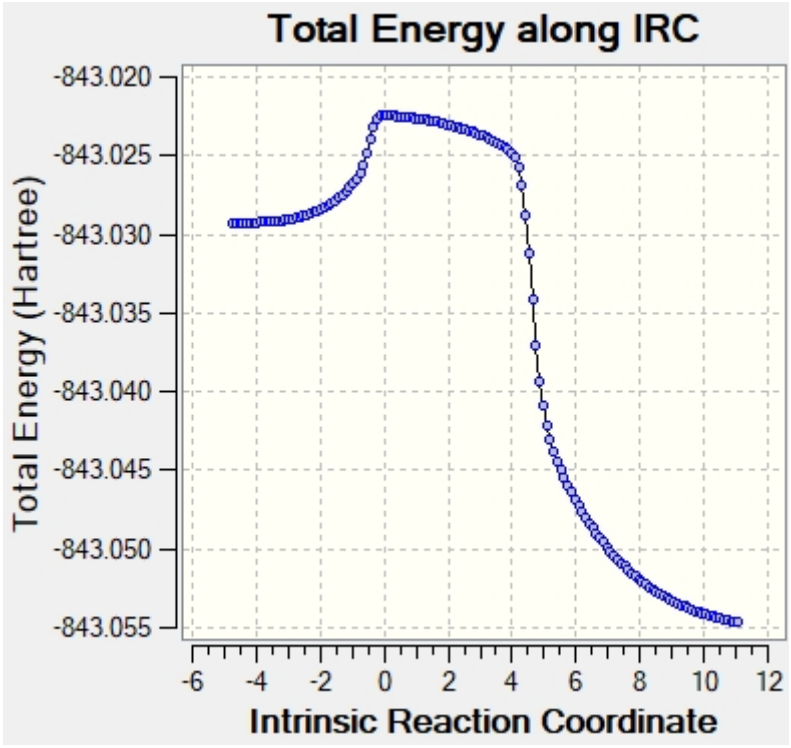
1b.2Me$_2$NH-ts2

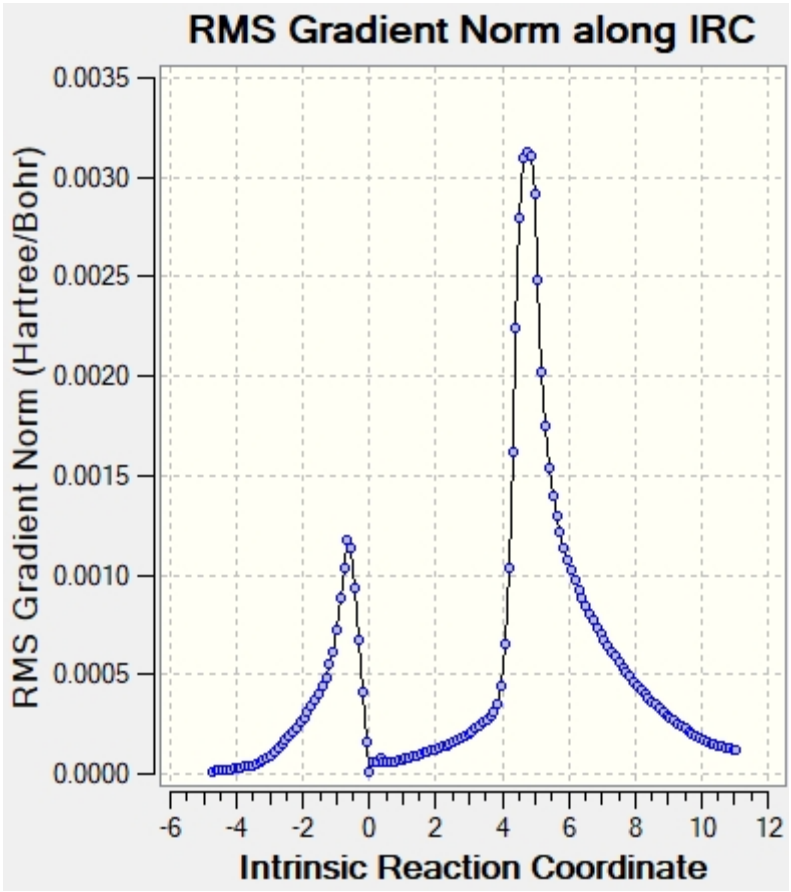
Zero-point correction=	0.397043
(Hartree/Particle)	
Thermal correction to Energy=	0.418451
Thermal correction to Enthalpy=	0.419396
Thermal correction to Gibbs Free Energy=	0.346576
Sum of electronic and zero-point Energies=	-842.625363
Sum of electronic and thermal Energies=	-842.603955
Sum of electronic and thermal Enthalpies=	-842.603011

Sum of electronic and thermal Free Energies= -842.675831

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.786843	-0.478006	-0.106436
2	6	0	1.870189	-1.119822	0.349104
3	7	0	2.985707	-1.077510	-0.518887
4	8	0	2.004018	-1.703232	1.453112
5	6	0	-1.635763	-0.716049	0.094295
6	6	0	-4.105908	-1.203841	-1.159122
7	6	0	-2.666991	-1.371525	0.773685
8	6	0	-1.849340	-0.339568	-1.234599
9	6	0	-3.076220	-0.570451	-1.855421
10	6	0	-3.893300	-1.615137	0.155843
11	1	0	-2.505275	-1.698092	1.798451
12	1	0	-1.031817	0.097551	-1.799831
13	1	0	-3.223550	-0.271284	-2.889119
14	1	0	-4.679486	-2.130752	0.699104
15	1	0	-5.059260	-1.391306	-1.643530
16	6	0	-0.318970	-0.426981	0.800308
17	6	0	4.014467	-2.079200	-0.298756
18	1	0	4.951720	-1.739083	-0.749548
19	1	0	3.749026	-3.051947	-0.744345
20	1	0	4.157089	-2.218247	0.770719
21	6	0	2.773216	-0.752089	-1.916424
22	1	0	2.288862	0.220056	-2.022512
23	1	0	2.150737	-1.498545	-2.434043
24	1	0	3.746286	-0.702516	-2.413620
25	6	0	1.854348	2.745447	-0.461465
26	1	0	2.468940	1.955710	-0.022896
27	1	0	1.792388	3.593789	0.223367
28	1	0	2.298426	3.073194	-1.405558
29	6	0	-1.643102	1.345385	2.039086
30	1	0	-1.534164	2.333452	2.494466
31	1	0	-1.939213	0.632763	2.822253
32	1	0	-2.430771	1.387147	1.285497
33	7	0	0.504923	2.200048	-0.693319
34	6	0	-0.395846	3.094850	-1.434014
35	1	0	0.003439	3.303886	-2.429714
36	1	0	-0.498868	4.032496	-0.883808
37	1	0	-1.375296	2.621021	-1.524127
38	7	0	-0.364265	0.970323	1.425969
39	6	0	0.713479	1.090106	2.421148
40	1	0	0.792387	2.132644	2.744520
41	1	0	1.657294	0.767246	1.981602
42	1	0	0.508190	0.456225	3.294012
43	1	0	-0.209790	-1.132964	1.639066
44	1	0	0.615993	1.264979	-1.122566
45	1	0	0.040556	1.797707	0.313951

1b.2Me$_2$NH-ts2





1b.3Me$_2$NH-ts1

Zero-point correction=	0.397043
(Hartree/Particle)	
Thermal correction to Energy=	0.418451
Thermal correction to Enthalpy=	0.419396
Thermal correction to Gibbs Free Energy=	0.346576
Sum of electronic and zero-point Energies=	-842.625363
Sum of electronic and thermal Energies=	-842.603955
Sum of electronic and thermal Enthalpies=	-842.603011
Sum of electronic and thermal Free Energies=	-842.675831

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.786843	-0.478006	-0.106436
2	6	0	1.870189	-1.119822	0.349104
3	7	0	2.985707	-1.077510	-0.518887
4	8	0	2.004018	-1.703232	1.453112
5	6	0	-1.635763	-0.716049	0.094295
6	6	0	-4.105908	-1.203841	-1.159122
7	6	0	-2.666991	-1.371525	0.773685
8	6	0	-1.849340	-0.339568	-1.234599
9	6	0	-3.076220	-0.570451	-1.855421
10	6	0	-3.893300	-1.615137	0.155843
11	1	0	-2.505275	-1.698092	1.798451
12	1	0	-1.031817	0.097551	-1.799831
13	1	0	-3.223550	-0.271284	-2.889119
14	1	0	-4.679486	-2.130752	0.699104
15	1	0	-5.059260	-1.391306	-1.643530
16	6	0	-0.318970	-0.426981	0.800308
17	6	0	4.014467	-2.079200	-0.298756
18	1	0	4.951720	-1.739083	-0.749548
19	1	0	3.749026	-3.051947	-0.744345
20	1	0	4.157089	-2.218247	0.770719
21	6	0	2.773216	-0.752089	-1.916424
22	1	0	2.288862	0.220056	-2.022512
23	1	0	2.150737	-1.498545	-2.434043
24	1	0	3.746286	-0.702516	-2.413620
25	6	0	1.854348	2.745447	-0.461465
26	1	0	2.468940	1.955710	-0.022896
27	1	0	1.792388	3.593789	0.223367
28	1	0	2.298426	3.073194	-1.405558
29	6	0	-1.643102	1.345385	2.039086
30	1	0	-1.534164	2.333452	2.494466
31	1	0	-1.939213	0.632763	2.822253
32	1	0	-2.430771	1.387147	1.285497
33	7	0	0.504923	2.200048	-0.693319
34	6	0	-0.395846	3.094850	-1.434014
35	1	0	0.003439	3.303886	-2.429714
36	1	0	-0.498868	4.032496	-0.883808
37	1	0	-1.375296	2.621021	-1.524127
38	7	0	-0.364265	0.970323	1.425969
39	6	0	0.713479	1.090106	2.421148
40	1	0	0.792387	2.132644	2.744520
41	1	0	1.657294	0.767246	1.981602
42	1	0	0.508190	0.456225	3.294012
43	1	0	-0.209790	-1.132964	1.639066
44	1	0	0.615993	1.264979	-1.122566
45	1	0	0.040556	1.797707	0.313951

1b.3Me$_2$NH-I1

Zero-point correction=	0.495255
(Hartree/Particle)	
Thermal correction to Energy=	0.523672
Thermal correction to Enthalpy=	0.524616
Thermal correction to Gibbs Free Energy=	0.433667
Sum of electronic and zero-point Energies=	-977.653126
Sum of electronic and thermal Energies=	-977.624708
Sum of electronic and thermal Enthalpies=	-977.623764
Sum of electronic and thermal Free Energies=	-977.714714

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.765400	1.302814	-0.033748
2	6	0	0.524768	1.511721	-0.330149
3	7	0	1.051116	2.748354	0.044577
4	8	0	1.301675	0.669435	-0.867162
5	6	0	-2.707543	-0.107548	-0.472202
6	6	0	-5.497124	-0.395825	-0.516460
7	6	0	-3.315868	-1.008242	-1.350460
8	6	0	-3.513166	0.664631	0.370641
9	6	0	-4.898214	0.518102	0.352347
10	6	0	-4.703322	-1.155654	-1.373659
11	6	0	-1.199100	0.028318	-0.439922
12	7	0	2.044801	-0.956695	1.500280
13	1	0	-0.771913	-0.304165	-1.397467
14	1	0	-2.701503	-1.589681	-2.034661
15	1	0	-5.160913	-1.855122	-2.066533
16	1	0	-6.577198	-0.505046	-0.533896
17	1	0	-5.513901	1.124597	1.009817
18	1	0	-3.036239	1.390132	1.022001
19	7	0	-0.618628	-1.056404	0.541332
20	6	0	2.555065	-2.181000	2.107223
21	1	0	1.881336	-2.508447	2.908094
22	1	0	3.558581	-2.053494	2.542114
23	1	0	2.604414	-2.972369	1.353559
24	6	0	-0.723603	-2.443758	0.046648
25	1	0	-1.764006	-2.771760	0.081297
26	1	0	-0.109152	-3.087125	0.681065
27	1	0	-0.355466	-2.482180	-0.980287
28	6	0	2.079449	0.171808	2.428822
29	1	0	1.745945	1.078696	1.915062
30	1	0	3.086224	0.346426	2.839560
31	1	0	1.403686	-0.021210	3.270237
32	6	0	-1.146214	-0.931768	1.917277
33	1	0	-1.106870	0.122383	2.195928
34	1	0	-0.510888	-1.522065	2.581158
35	1	0	-2.173754	-1.297398	1.952652
36	1	0	0.416852	-0.860350	0.634593
37	7	0	3.737736	-0.846319	-1.142774
38	6	0	5.007022	-0.641291	-1.823050
39	1	0	5.699699	-1.448438	-1.560245
40	1	0	5.452155	0.303305	-1.500034
41	1	0	4.912176	-0.624874	-2.922096

42	6	0	3.061479	-2.051301	-1.597798
43	1	0	2.083019	-2.120632	-1.111267
44	1	0	3.649671	-2.933814	-1.320051
45	1	0	2.903987	-2.078269	-2.689456
46	1	0	3.111348	-0.055522	-1.295882
47	1	0	2.630665	-0.725031	0.694885
48	6	0	0.157164	3.857659	0.316169
49	1	0	-0.710419	3.499837	0.867190
50	1	0	-0.193795	4.340220	-0.609518
51	1	0	0.687337	4.604680	0.914865
52	6	0	2.353244	3.111089	-0.477729
53	1	0	2.306234	3.449703	-1.524762
54	1	0	3.024681	2.253695	-0.423113
55	1	0	2.763008	3.923952	0.128626

1b.3Me$_2$NH-I2

Zero-point correction=	0.495618
(Hartree/Particle)	
Thermal correction to Energy=	0.523411
Thermal correction to Enthalpy=	0.524355
Thermal correction to Gibbs Free Energy=	0.436131
Sum of electronic and zero-point Energies=	-977.651737
Sum of electronic and thermal Energies=	-977.623944
Sum of electronic and thermal Enthalpies=	-977.623000
Sum of electronic and thermal Free Energies=	-977.711224

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.660951	0.095331	1.731244
2	1	0	0.845320	0.963612	1.128435
3	1	0	0.549053	2.459280	-0.375159
4	1	0	-1.011160	0.866359	-1.054831
5	7	0	-1.079400	1.823464	-1.427154
6	7	0	1.148858	2.525943	0.458966
7	6	0	0.632164	3.586171	1.322308
8	1	0	0.759310	4.586382	0.882323
9	1	0	1.159425	3.570449	2.283183
10	1	0	-0.432417	3.422709	1.509701
11	6	0	2.542743	2.757464	0.089034
12	1	0	2.692127	3.732386	-0.398167
13	1	0	2.883584	1.968923	-0.586528
14	1	0	3.167895	2.729826	0.988332
15	6	0	1.895953	-0.145671	2.509681
16	1	0	1.767245	-1.039943	3.125070
17	1	0	2.083129	0.718196	3.150709
18	1	0	2.734289	-0.283754	1.827564
19	6	0	-0.462663	0.455959	2.627949
20	1	0	-0.712014	-0.400477	3.255336
21	1	0	-1.326161	0.712645	2.015789
22	1	0	-0.159706	1.312863	3.233118
23	6	0	-1.116878	1.808829	-2.882011
24	1	0	-2.041979	1.362275	-3.284364
25	1	0	-0.266116	1.240886	-3.271116
26	1	0	-1.046308	2.832443	-3.267205

27	6	0	-2.272782	2.434420	-0.857586
28	1	0	-3.205505	1.989590	-1.243306
29	1	0	-2.290577	3.508341	-1.078101
30	1	0	-2.265890	2.305196	0.229046
31	7	0	-0.873656	-0.807888	0.051140
32	6	0	0.283705	-1.103124	0.794269
33	6	0	1.477799	-1.360639	-0.104688
34	6	0	3.677217	-1.841055	-1.775278
35	6	0	2.303713	-2.464176	0.111439
36	6	0	1.755309	-0.503660	-1.174588
37	6	0	2.851521	-0.737414	-2.000799
38	6	0	3.397730	-2.707663	-0.720681
39	1	0	2.086570	-3.141700	0.934042
40	1	0	1.094704	0.340079	-1.360947
41	1	0	3.058772	-0.063680	-2.827486
42	1	0	4.028013	-3.574164	-0.544905
43	1	0	4.527657	-2.027468	-2.423926
44	6	0	-2.017099	-1.291889	0.577747
45	8	0	-2.150392	-1.854763	1.690660
46	7	0	-3.162723	-1.083724	-0.205880
47	6	0	-3.069269	-1.016980	-1.652248
48	1	0	-3.273487	-2.000238	-2.105916
49	1	0	-2.069853	-0.704696	-1.946188
50	1	0	-3.803482	-0.304089	-2.046499
51	6	0	-4.403568	-1.662942	0.268427
52	1	0	-5.239539	-1.151789	-0.219387
53	1	0	-4.482254	-1.538512	1.346937
54	1	0	-4.473640	-2.738016	0.037865
55	1	0	0.154358	-1.933477	1.505235

1b.3Me$_2$NH-I3

Zero-point correction= 0.496880
(Hartree/Particle)
Thermal correction to Energy= 0.523524
Thermal correction to Enthalpy= 0.524468
Thermal correction to Gibbs Free Energy= 0.441570
Sum of electronic and zero-point Energies= -977.646136
Sum of electronic and thermal Energies= -977.619492
Sum of electronic and thermal Enthalpies= -977.618548
Sum of electronic and thermal Free Energies= -977.701446

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.185955	-1.114887	1.907662
2	1	0	0.589625	0.560341	1.821401
3	1	0	0.722153	1.828450	0.654200
4	1	0	-0.246038	1.350371	-0.986814
5	7	0	0.396756	2.155943	-0.991565
6	7	0	0.654762	1.627945	1.709489
7	6	0	-0.618783	2.204740	2.189949
8	1	0	-0.588990	3.291622	2.087041
9	1	0	-0.767679	1.940618	3.239340
10	1	0	-1.423856	1.783404	1.584628
11	6	0	1.834176	2.162048	2.415823
12	1	0	1.851455	3.249559	2.321801

13	1	0	2.740120	1.749435	1.970790
14	1	0	1.784980	1.888326	3.471691
15	6	0	1.023394	-2.170322	2.490407
16	1	0	0.517881	-3.147165	2.429550
17	1	0	1.210652	-1.945365	3.544489
18	1	0	1.980292	-2.251951	1.976570
19	6	0	-1.093301	-1.126619	2.634218
20	1	0	-1.589960	-2.103655	2.543337
21	1	0	-1.764895	-0.369817	2.230648
22	1	0	-0.900081	-0.917879	3.691170
23	6	0	1.388228	1.968905	-2.049369
24	1	0	0.942832	2.069060	-3.050901
25	1	0	1.836726	0.979261	-1.963546
26	1	0	2.177381	2.721987	-1.950700
27	6	0	-0.327586	3.412161	-1.171492
28	1	0	-0.854281	3.459830	-2.137025
29	1	0	0.382364	4.245086	-1.132133
30	1	0	-1.061388	3.554793	-0.374150
31	7	0	-1.022558	-0.433919	-0.083828
32	6	0	-0.047994	-1.353578	0.444480
33	6	0	1.250985	-1.236990	-0.351753
34	6	0	3.547014	-1.116004	-1.986283
35	6	0	1.231507	-1.729902	-1.662812
36	6	0	2.439520	-0.674362	0.118576
37	6	0	3.579365	-0.612958	-0.688964
38	6	0	2.361758	-1.674977	-2.472626
39	1	0	0.306761	-2.158990	-2.041732
40	1	0	2.499917	-0.306134	1.138422
41	1	0	4.493497	-0.176985	-0.295847
42	1	0	2.321258	-2.070626	-3.483155
43	1	0	4.432845	-1.076945	-2.612576
44	6	0	-2.224231	-1.000276	-0.285796
45	8	0	-2.544555	-2.201729	-0.101526
46	1	0	-0.399632	-2.395480	0.342660
47	7	0	-3.238411	-0.121131	-0.728836
48	6	0	-4.368547	-0.722667	-1.413494
49	1	0	-4.142868	-0.948034	-2.469105
50	1	0	-5.217674	-0.033143	-1.383915
51	1	0	-4.638172	-1.650435	-0.913678
52	6	0	-2.866341	1.184444	-1.224231
53	1	0	-2.257893	1.138706	-2.144598
54	1	0	-2.296450	1.721798	-0.466321
55	1	0	-3.774950	1.754284	-1.439596

1b.3Me$_2$NH-ts2

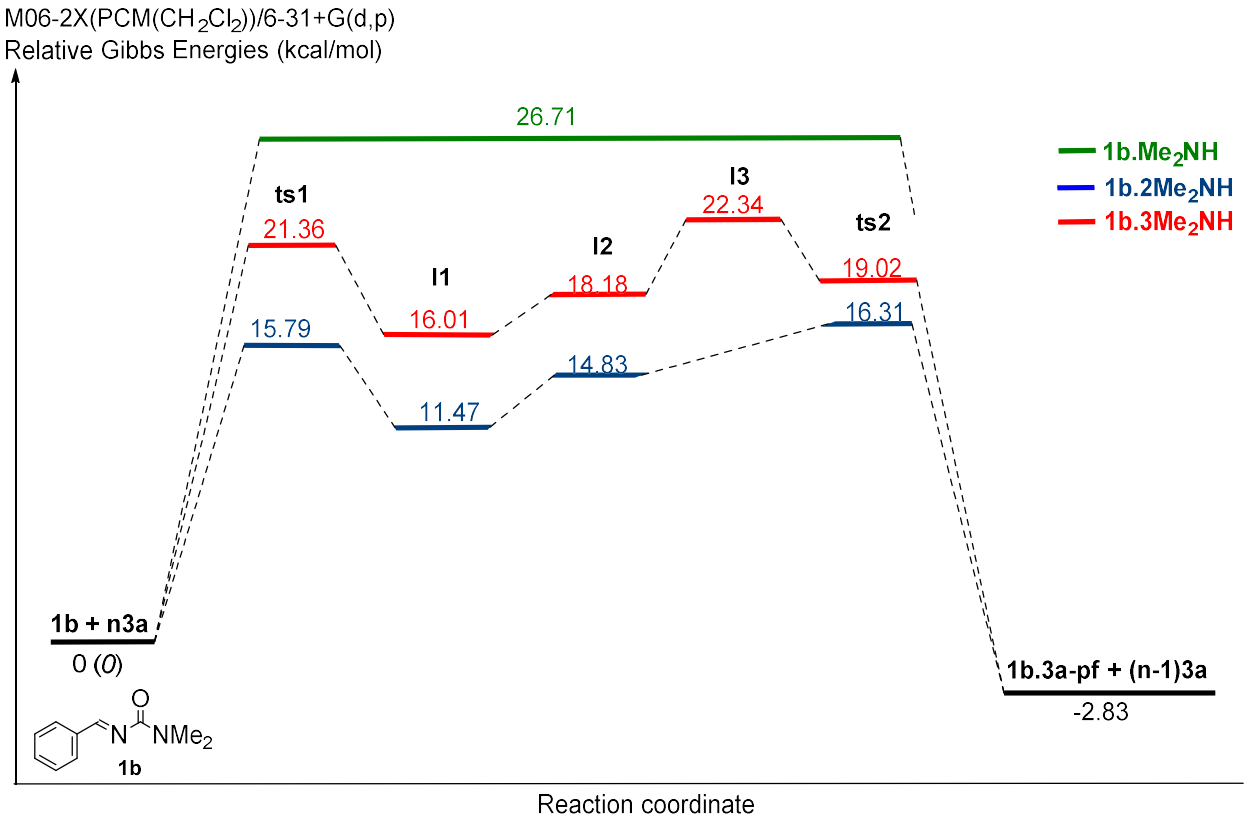
Zero-point correction= 0.490922
(Hartree/Particle)
Thermal correction to Energy= 0.517752
Thermal correction to Enthalpy= 0.518696
Thermal correction to Gibbs Free Energy= 0.434564
Sum of electronic and zero-point Energies= -977.650761
Sum of electronic and thermal Energies= -977.623931
Sum of electronic and thermal Enthalpies= -977.622987
Sum of electronic and thermal Free Energies= -977.707119

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	0.705405	0.185600	1.775951
2	1	0	0.734660	1.743499	0.872109
3	1	0	-0.297848	2.236809	-0.463161
4	1	0	-1.062135	0.595171	-0.868714
5	7	0	-1.255434	1.580035	-1.209952
6	7	0	0.517558	2.643983	0.356304
7	6	0	-0.144374	3.583106	1.275837
8	1	0	-0.424170	4.489588	0.732500
9	1	0	0.521244	3.853357	2.101860
10	1	0	-1.045111	3.117935	1.680559
11	6	0	1.730297	3.211310	-0.251249
12	1	0	1.463116	4.083341	-0.853841
13	1	0	2.203444	2.463560	-0.889704
14	1	0	2.441331	3.517591	0.522434
15	6	0	1.922859	0.042669	2.573849
16	1	0	1.901230	-0.869564	3.194663
17	1	0	2.019608	0.905818	3.239861
18	1	0	2.802546	0.001964	1.928439
19	6	0	-0.436408	0.377315	2.674188
20	1	0	-0.585502	-0.487528	3.337518
21	1	0	-1.348413	0.509878	2.088100
22	1	0	-0.263445	1.271205	3.283428
23	6	0	-1.090614	1.707654	-2.658281
24	1	0	-1.862424	1.148211	-3.201428
25	1	0	-0.110884	1.324174	-2.956035
26	1	0	-1.157354	2.760966	-2.949809
27	6	0	-2.595303	1.967300	-0.759048
28	1	0	-3.373670	1.411078	-1.295247
29	1	0	-2.750340	3.040223	-0.917326
30	1	0	-2.693683	1.740442	0.305726
31	7	0	-0.695573	-0.852603	0.083007
32	6	0	0.479299	-1.010236	0.888847
33	6	0	1.693780	-1.178938	-0.011252
34	6	0	3.929963	-1.423115	-1.697418
35	6	0	2.625175	-2.198348	0.186848
36	6	0	1.891393	-0.292796	-1.073721
37	6	0	2.998877	-0.403215	-1.908473
38	6	0	3.736220	-2.322970	-0.651478
39	1	0	2.481044	-2.901249	1.004238
40	1	0	1.145640	0.476118	-1.252653
41	1	0	3.134271	0.296481	-2.729003
42	1	0	4.450345	-3.124176	-0.485668
43	1	0	4.793691	-1.518090	-2.348360
44	6	0	-1.790789	-1.492585	0.511879
45	8	0	-1.945066	-2.112453	1.589960
46	7	0	-2.906961	-1.382908	-0.358486
47	6	0	-2.705767	-1.417866	-1.795894
48	1	0	-2.842637	-2.437917	-2.191267
49	1	0	-1.695102	-1.093766	-2.039610
50	1	0	-3.430016	-0.765830	-2.302228
51	6	0	-4.116265	-2.065586	0.056837
52	1	0	-4.957480	-1.677171	-0.527181
53	1	0	-4.299529	-1.887535	1.115410
54	1	0	-4.056467	-3.154200	-0.103347
55	1	0	0.399546	-1.891713	1.551469

2.2.3.-M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

Energy profiles for the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1b** in dichloromethane.



1b.Me_2NH-ts

Zero-point correction=	0.300053
(Hartree/Particle)	
Thermal correction to Energy=	0.316772
Thermal correction to Enthalpy=	0.317716
Thermal correction to Gibbs Free Energy=	0.254313
Sum of electronic and zero-point Energies=	-707.587524
Sum of electronic and thermal Energies=	-707.570805
Sum of electronic and thermal Enthalpies=	-707.569861
Sum of electronic and thermal Free Energies=	-707.633264

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.037548	0.383214	0.193396
2	6	0	-1.928955	-0.365285	-0.504128
3	7	0	-3.208504	-0.423206	0.025961
4	8	0	-1.649526	-0.966028	-1.561733
5	6	0	1.382797	-0.248628	-0.201127
6	6	0	3.572662	-1.921199	0.284122
7	6	0	2.555641	-0.111321	-0.949424
8	6	0	1.308232	-1.236252	0.781134
9	6	0	2.399010	-2.070704	1.022681
10	6	0	3.649421	-0.940162	-0.705469
11	1	0	2.611418	0.643758	-1.731117
12	1	0	0.385393	-1.343285	1.343683
13	1	0	2.330692	-2.840455	1.785410
14	1	0	4.556675	-0.826634	-1.290894
15	1	0	4.421147	-2.571862	0.472192
16	6	0	0.221489	0.681766	-0.457995
17	1	0	0.119792	0.840698	-1.539077
18	1	0	-0.798902	1.662441	0.546277
19	6	0	-4.089145	-1.473286	-0.454968
20	1	0	-3.893692	-1.654063	-1.509913
21	1	0	-5.127940	-1.157364	-0.327296
22	1	0	-3.940898	-2.413755	0.097038
23	6	0	-3.452151	0.013775	1.389281
24	1	0	-2.988841	0.982949	1.568737
25	1	0	-3.062694	-0.702707	2.127587
26	1	0	-4.530764	0.110898	1.535874
27	6	0	1.295232	2.157930	1.319310
28	1	0	1.139432	3.117233	1.815302
29	1	0	2.328990	2.089373	0.964729
30	1	0	1.102277	1.348348	2.024930
31	7	0	0.348366	2.060205	0.199712
32	6	0	0.473551	3.171454	-0.751021
33	1	0	0.369350	4.114539	-0.212171
34	1	0	-0.318040	3.092978	-1.498371
35	1	0	1.449914	3.145114	-1.246906

1b.Me2NH-pf

Zero-point correction=	0.305377
(Hartree/Particle)	
Thermal correction to Energy=	0.322192
Thermal correction to Enthalpy=	0.323136
Thermal correction to Gibbs Free Energy=	0.260500
Sum of electronic and zero-point Energies=	-707.635464
Sum of electronic and thermal Energies=	-707.618650
Sum of electronic and thermal Enthalpies=	-707.617705
Sum of electronic and thermal Free Energies=	-707.680342

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.942799	-0.184418	0.073584
2	6	0	-2.196657	0.107787	-0.427337
3	7	0	-3.199468	-0.724266	-0.012090
4	8	0	-2.389292	1.069921	-1.175951
5	6	0	1.471449	-0.170145	-0.270243
6	6	0	3.901954	-1.578740	-0.236813
7	6	0	2.412756	0.005925	-1.288486
8	6	0	1.767660	-1.058542	0.770972
9	6	0	2.971568	-1.760592	0.786439
10	6	0	3.620688	-0.691199	-1.274299
11	1	0	2.194335	0.691372	-2.104173
12	1	0	1.060372	-1.207425	1.583795
13	1	0	3.183171	-2.448598	1.599092
14	1	0	4.337882	-0.545214	-2.076042
15	1	0	4.838825	-2.126756	-0.225419
16	6	0	0.186371	0.646630	-0.296440
17	1	0	0.030797	1.012693	-1.317302
18	6	0	-4.503771	-0.643452	-0.647304
19	1	0	-5.285247	-0.568603	0.114956
20	1	0	-4.693513	-1.533566	-1.258958
21	1	0	-4.533171	0.241089	-1.279781
22	6	0	-2.966528	-1.849829	0.876531
23	1	0	-2.352418	-1.550643	1.729963
24	1	0	-2.491501	-2.697380	0.364109
25	1	0	-3.929550	-2.187031	1.262821
26	6	0	0.465888	1.600767	1.954972
27	1	0	0.256373	2.516492	2.515274
28	1	0	1.508187	1.302633	2.162513
29	1	0	-0.205599	0.817128	2.316629
30	7	0	0.212956	1.848810	0.544791
31	6	0	1.108226	2.865648	0.018493
32	1	0	0.961528	3.794052	0.577679
33	1	0	0.874164	3.056966	-1.033290
34	1	0	2.173990	2.585136	0.094324
35	1	0	-0.746727	-1.138143	0.338521

1b.2Me$_2$NH-ts1

Zero-point correction=	0.397899
(Hartree/Particle)	
Thermal correction to Energy=	0.420585
Thermal correction to Enthalpy=	0.421529
Thermal correction to Gibbs Free Energy=	0.344669
Sum of electronic and zero-point Energies=	-842.631230
Sum of electronic and thermal Energies=	-842.608543
Sum of electronic and thermal Enthalpies=	-842.607599
Sum of electronic and thermal Free Energies=	-842.684460

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.078184	-1.158126	-0.199785
2	6	0	-1.331886	-1.147319	-0.800479
3	7	0	-2.229706	-2.033688	-0.275618
4	8	0	-1.664975	-0.392929	-1.735088
5	6	0	2.213685	-0.411904	-0.332920
6	6	0	4.884798	-0.428325	0.497763
7	6	0	3.202132	0.189568	-1.118658
8	6	0	2.574070	-1.032237	0.868702
9	6	0	3.903025	-1.037597	1.282728
10	6	0	4.533831	0.182365	-0.706136
11	6	0	0.802061	-0.376335	-0.780668
12	7	0	-2.727659	1.598353	0.285994
13	1	0	0.629060	-0.001892	-1.793264
14	1	0	-2.816897	0.984524	-0.522937
15	1	0	2.924536	0.661525	-2.058404
16	1	0	5.295203	0.648774	-1.323532
17	1	0	5.921219	-0.435501	0.821153
18	1	0	4.177207	-1.519300	2.216352
19	1	0	1.798997	-1.506662	1.462754
20	7	0	0.356634	1.597756	-0.096676
21	1	0	-0.662827	1.589372	-0.216465
22	6	0	-3.784093	2.602049	0.265506
23	1	0	-3.609130	3.331712	1.062973
24	1	0	-4.788429	2.172972	0.415549
25	1	0	-3.772295	3.132867	-0.689336
26	6	0	0.938806	2.687434	-0.866588
27	1	0	2.027694	2.664906	-0.754876
28	1	0	0.576909	3.670640	-0.535050
29	1	0	0.690655	2.559576	-1.924064
30	6	0	-2.754401	0.802937	1.507246
31	1	0	-1.965396	0.044710	1.475321
32	1	0	-3.720033	0.296681	1.677119
33	1	0	-2.562336	1.454659	2.366755
34	6	0	0.652855	1.665292	1.325844
35	1	0	0.326824	0.732673	1.799287
36	1	0	0.146220	2.509246	1.813394
37	1	0	1.733327	1.769391	1.467278
38	6	0	-1.996038	-2.800636	0.935167
39	1	0	-0.942054	-2.761637	1.196868
40	1	0	-2.295591	-3.841203	0.773806
41	1	0	-2.591779	-2.395555	1.765076
42	6	0	-3.601750	-2.003185	-0.746966
43	1	0	-4.030725	-3.004694	-0.659727
44	1	0	-3.627236	-1.685128	-1.787510
45	1	0	-4.213482	-1.311933	-0.148473

1b.2Me$_2$NH-I1

Zero-point correction=	0.400570
(Hartree/Particle)	
Thermal correction to Energy=	0.422691
Thermal correction to Enthalpy=	0.423636
Thermal correction to Gibbs Free Energy=	0.348844
Sum of electronic and zero-point Energies=	-842.639626
Sum of electronic and thermal Energies=	-842.617504
Sum of electronic and thermal Enthalpies=	-842.616560
Sum of electronic and thermal Free Energies=	-842.691352

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.165503	1.019640	0.057753
2	6	0	1.343417	1.187927	-0.558741
3	7	0	2.162470	2.189184	-0.024216
4	8	0	1.787650	0.514041	-1.533906
5	6	0	-2.098625	0.161798	-0.258612
6	6	0	-4.854825	0.466109	0.171588
7	6	0	-3.023260	-0.347662	-1.175204
8	6	0	-2.569717	0.844463	0.867495
9	6	0	-3.938026	0.991022	1.084935
10	6	0	-4.394582	-0.198982	-0.963334
11	6	0	-0.611252	-0.020331	-0.493122
12	7	0	2.560074	-1.761065	0.052515
13	1	0	-0.423549	-0.192805	-1.562217
14	1	0	2.754658	-1.200325	-0.777965
15	1	0	-2.669677	-0.853818	-2.070963
16	1	0	-5.099599	-0.595117	-1.687694
17	1	0	-5.920915	0.585965	0.338863
18	1	0	-4.290943	1.522586	1.963698
19	1	0	-1.846882	1.271621	1.555464
20	7	0	-0.168707	-1.384329	0.129018
21	1	0	0.901414	-1.442843	0.016035
22	6	0	3.031237	-3.133293	-0.110382
23	1	0	2.696067	-3.734894	0.741136
24	1	0	4.127717	-3.198900	-0.163880
25	1	0	2.610350	-3.562516	-1.022832
26	6	0	-0.707333	-2.571126	-0.566330
27	1	0	-1.784280	-2.642058	-0.404190
28	1	0	-0.216189	-3.461583	-0.167599
29	1	0	-0.494128	-2.483776	-1.633339
30	6	0	3.150440	-1.097444	1.214904
31	1	0	2.788001	-0.066484	1.266301
32	1	0	4.249501	-1.085761	1.175781
33	1	0	2.847755	-1.624917	2.125834
34	6	0	-0.395211	-1.462142	1.588644
35	1	0	-0.048962	-0.528106	2.033024
36	1	0	0.181344	-2.303551	1.980257
37	1	0	-1.456982	-1.611956	1.792748
38	6	0	1.594537	3.173000	0.877358
39	1	0	0.959695	2.680028	1.611708
40	1	0	0.988589	3.923452	0.345371
41	1	0	2.409364	3.690474	1.392266
42	6	0	3.262810	2.668967	-0.837145
43	1	0	2.937250	3.422022	-1.572944
44	1	0	3.711875	1.834552	-1.373102

45	1	0	4.014295	3.128548	-0.188315

1b.2Me$_2$NH-I2

Zero-point correction= 0.400683
(Hartree/Particle)
Thermal correction to Energy= 0.422829
Thermal correction to Enthalpy= 0.423773
Thermal correction to Gibbs Free Energy= 0.348732
Sum of electronic and zero-point Energies= -842.634041
Sum of electronic and thermal Energies= -842.611895
Sum of electronic and thermal Enthalpies= -842.610951
Sum of electronic and thermal Free Energies= -842.685992

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.776300	-0.526738	-0.158310
2	6	0	1.839009	-1.252651	0.222667
3	7	0	2.965989	-1.125164	-0.606756
4	8	0	1.930228	-1.988752	1.240754
5	6	0	-1.651422	-0.748730	0.020106
6	6	0	-4.130891	-1.060731	-1.254420
7	6	0	-2.638252	-1.565620	0.575889
8	6	0	-1.912853	-0.101171	-1.191357
9	6	0	-3.146440	-0.248682	-1.821423
10	6	0	-3.871669	-1.725324	-0.057094
11	1	0	-2.438734	-2.085669	1.509862
12	1	0	-1.134607	0.498958	-1.651873
13	1	0	-3.337065	0.260565	-2.761298
14	1	0	-4.625606	-2.370746	0.383028
15	1	0	-5.089624	-1.182324	-1.748974
16	6	0	-0.322344	-0.576863	0.730161
17	6	0	3.956020	-2.185723	-0.549237
18	1	0	4.916029	-1.804112	-0.908652
19	1	0	3.672823	-3.048164	-1.174302
20	1	0	4.065161	-2.524908	0.478690
21	6	0	2.816707	-0.518924	-1.916356
22	1	0	2.315128	0.445239	-1.833849
23	1	0	2.235350	-1.150028	-2.606297
24	1	0	3.811259	-0.361617	-2.343203
25	6	0	1.861874	2.886956	-0.165733
26	1	0	2.419033	2.021263	0.204793
27	1	0	1.822614	3.647285	0.620844
28	1	0	2.400686	3.309098	-1.026757
29	6	0	-1.624576	1.085083	2.205097
30	1	0	-1.497019	2.008076	2.772894
31	1	0	-1.879698	0.268286	2.884925
32	1	0	-2.415444	1.211955	1.467608
33	7	0	0.503706	2.466676	-0.509960
34	6	0	-0.267308	3.522081	-1.160605
35	1	0	0.228182	3.914722	-2.060196
36	1	0	-0.405848	4.349472	-0.458283
37	1	0	-1.253147	3.140399	-1.438697
38	7	0	-0.349700	0.772080	1.521098
39	6	0	0.779953	0.817223	2.481174

40	1	0	0.878178	1.834925	2.863057
41	1	0	1.691397	0.514207	1.969368
42	1	0	0.574692	0.125836	3.301326
43	1	0	-0.227249	-1.336241	1.519246
44	1	0	0.576879	1.638883	-1.102751
45	1	0	-0.146108	1.515128	0.777732

1b.2Me$_2$NH-ts2

Zero-point correction= 0.396887
(Hartree/Particle)
Thermal correction to Energy= 0.418465
Thermal correction to Enthalpy= 0.419409
Thermal correction to Gibbs Free Energy= 0.345291
Sum of electronic and zero-point Energies= -842.632045
Sum of electronic and thermal Energies= -842.610467
Sum of electronic and thermal Enthalpies= -842.609522
Sum of electronic and thermal Free Energies= -842.683641

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.829776	-0.458805	-0.095316
2	6	0	1.900343	-1.126268	0.342653
3	7	0	3.027848	-1.065809	-0.508748
4	8	0	2.020915	-1.759479	1.426326
5	6	0	-1.589762	-0.759644	0.099506
6	6	0	-4.040033	-1.334602	-1.155837
7	6	0	-2.596580	-1.453194	0.777826
8	6	0	-1.817972	-0.384685	-1.227534
9	6	0	-3.034936	-0.659765	-1.849808
10	6	0	-3.813188	-1.740402	0.158714
11	1	0	-2.424972	-1.772346	1.803400
12	1	0	-1.019991	0.090645	-1.789198
13	1	0	-3.194152	-0.359726	-2.881424
14	1	0	-4.581234	-2.283277	0.701355
15	1	0	-4.985853	-1.555021	-1.641146
16	6	0	-0.282843	-0.427557	0.805805
17	6	0	4.023669	-2.110534	-0.344958
18	1	0	4.967705	-1.780451	-0.788525
19	1	0	3.723206	-3.051174	-0.835859
20	1	0	4.173536	-2.307096	0.714392
21	6	0	2.846901	-0.646185	-1.885328
22	1	0	2.328878	0.311785	-1.930182
23	1	0	2.268800	-1.374357	-2.476563
24	1	0	3.831304	-0.528469	-2.347450
25	6	0	1.693080	2.912127	-0.463654
26	1	0	2.368258	2.151289	-0.066619
27	1	0	1.569629	3.713810	0.266846
28	1	0	2.102408	3.322510	-1.390152
29	6	0	-1.642890	1.308510	2.041849
30	1	0	-1.559211	2.303940	2.485558
31	1	0	-1.898482	0.592119	2.835531
32	1	0	-2.444143	1.317340	1.301683
33	7	0	0.383330	2.281898	-0.715394
34	6	0	-0.600803	3.171278	-1.354117
35	1	0	-0.230762	3.524912	-2.319151
36	1	0	-0.779051	4.026153	-0.698910

37	1	0	-1.535293	2.625057	-1.495013
38	7	0	-0.362737	0.971288	1.408194
39	6	0	0.728243	1.143578	2.380417
40	1	0	0.778520	2.192857	2.685362
41	1	0	1.673677	0.849573	1.923566
42	1	0	0.558636	0.518666	3.267659
43	1	0	-0.162718	-1.120736	1.653919
44	1	0	0.542014	1.417581	-1.247011
45	1	0	-0.024929	1.794316	0.282959

1b.3Me$_2$NH-ts1

Zero-point correction= 0.491784
(Hartree/Particle)
Thermal correction to Energy= 0.519923
Thermal correction to Enthalpy= 0.520868
Thermal correction to Gibbs Free Energy= 0.431392
Sum of electronic and zero-point Energies= -977.648989
Sum of electronic and thermal Energies= -977.620849
Sum of electronic and thermal Enthalpies= -977.619905
Sum of electronic and thermal Free Energies= -977.709381

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.719265	1.333106	-0.311572
2	6	0	0.619944	1.381545	-0.689991
3	7	0	1.306339	2.481485	-0.269223
4	8	0	1.198286	0.497583	-1.351219
5	6	0	-2.825588	0.179201	-0.595296
6	6	0	-5.574561	-0.148716	-0.195268
7	6	0	-3.543675	-0.755567	-1.348208
8	6	0	-3.496905	0.959635	0.352430
9	6	0	-4.864606	0.793804	0.552554
10	6	0	-4.913229	-0.921067	-1.149935
11	6	0	-1.368371	0.311252	-0.810810
12	7	0	1.950340	-0.726584	1.610180
13	1	0	-0.955735	-0.250246	-1.653059
14	1	0	-3.024176	-1.351077	-2.095344
15	1	0	-5.463188	-1.647681	-1.739782
16	1	0	-6.641175	-0.275965	-0.037309
17	1	0	-5.380809	1.399088	1.291424
18	1	0	-2.932022	1.690725	0.922778
19	7	0	-0.774247	-1.391562	0.403958
20	6	0	2.788200	-1.675301	2.332837
21	1	0	2.195414	-2.169002	3.110952
22	1	0	3.657128	-1.200759	2.818408
23	1	0	3.155912	-2.440051	1.644077
24	6	0	-0.930506	-2.696302	-0.218073
25	1	0	-1.996886	-2.914883	-0.339955
26	1	0	-0.479808	-3.503120	0.378780
27	1	0	-0.460170	-2.687337	-1.206177
28	6	0	1.543652	0.388366	2.456828
29	1	0	0.852511	1.039239	1.912441
30	1	0	2.393087	0.993630	2.816472
31	1	0	1.015216	-0.000765	3.334414
32	6	0	-1.404514	-1.286875	1.709192

33	1	0	-1.345557	-0.247011	2.049001
34	1	0	-0.919163	-1.930993	2.456951
35	1	0	-2.460244	-1.568066	1.630954
36	1	0	0.222861	-1.167911	0.518039
37	7	0	3.800514	-0.815623	-0.949067
38	6	0	5.079485	-0.582592	-1.603277
39	1	0	5.842557	-1.231433	-1.159605
40	1	0	5.389542	0.455200	-1.451508
41	1	0	5.056473	-0.784683	-2.687620
42	6	0	3.295768	-2.159406	-1.193886
43	1	0	2.309871	-2.267665	-0.729762
44	1	0	3.971396	-2.895625	-0.743302
45	1	0	3.202793	-2.399782	-2.266664
46	1	0	3.103095	-0.155530	-1.291596
47	1	0	2.485612	-0.383296	0.811302
48	6	0	0.767041	3.484900	0.632936
49	1	0	-0.294814	3.306902	0.781429
50	1	0	0.914969	4.483482	0.209280
51	1	0	1.281155	3.439885	1.601999
52	6	0	2.736427	2.535471	-0.518410
53	1	0	3.072764	3.567480	-0.402841
54	1	0	2.955426	2.199488	-1.533324
55	1	0	3.292526	1.901254	0.187218

1b.3Me$_2$NH-I1

Zero-point correction=	0.495331
(Hartree/Particle)	
Thermal correction to Energy=	0.523588
Thermal correction to Enthalpy=	0.524532
Thermal correction to Gibbs Free Energy=	0.434364
Sum of electronic and zero-point Energies=	-977.656939
Sum of electronic and thermal Energies=	-977.628682
Sum of electronic and thermal Enthalpies=	-977.627737
Sum of electronic and thermal Free Energies=	-977.717906

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.751799	1.294228	-0.004507
2	6	0	0.532915	1.511011	-0.317616
3	7	0	1.063438	2.742639	0.070837
4	8	0	1.303061	0.683093	-0.886987
5	6	0	-2.701609	-0.100983	-0.468989
6	6	0	-5.493099	-0.364887	-0.557252
7	6	0	-3.306165	-0.963392	-1.387520
8	6	0	-3.511756	0.643595	0.394530
9	6	0	-4.897745	0.509126	0.354557
10	6	0	-4.694570	-1.098039	-1.433130
11	6	0	-1.192068	0.021364	-0.420322
12	7	0	2.023645	-0.976658	1.489243
13	1	0	-0.763681	-0.303278	-1.379567
14	1	0	-2.687801	-1.526375	-2.083332
15	1	0	-5.148782	-1.768618	-2.156080
16	1	0	-6.573660	-0.464897	-0.591312
17	1	0	-5.516301	1.093266	1.029326
18	1	0	-3.040526	1.337897	1.083127

19	7	0	-0.627704	-1.071239	0.551215
20	6	0	2.508289	-2.220431	2.080341
21	1	0	1.827677	-2.543101	2.876727
22	1	0	3.513856	-2.117695	2.516445
23	1	0	2.540316	-3.002957	1.316782
24	6	0	-0.741542	-2.452186	0.037452
25	1	0	-1.786375	-2.767168	0.050285
26	1	0	-0.148068	-3.111176	0.675294
27	1	0	-0.355737	-2.483770	-0.983059
28	6	0	2.073430	0.136163	2.436657
29	1	0	1.759890	1.056948	1.935365
30	1	0	3.080620	0.284737	2.855718
31	1	0	1.388688	-0.058297	3.269994
32	6	0	-1.165950	-0.962500	1.925297
33	1	0	-1.122883	0.086366	2.221874
34	1	0	-0.540404	-1.567108	2.585228
35	1	0	-2.195281	-1.323390	1.948440
36	1	0	0.412449	-0.886899	0.660953
37	7	0	3.755124	-0.832189	-1.136855
38	6	0	5.017138	-0.600438	-1.823861
39	1	0	5.720492	-1.404954	-1.582795
40	1	0	5.454634	0.342963	-1.487210
41	1	0	4.911899	-0.564683	-2.921308
42	6	0	3.089258	-2.037311	-1.609779
43	1	0	2.112830	-2.126708	-1.122523
44	1	0	3.686934	-2.918180	-1.348680
45	1	0	2.929825	-2.046847	-2.701297
46	1	0	3.119488	-0.046046	-1.275030
47	1	0	2.618024	-0.743100	0.691142
48	6	0	0.171562	3.844688	0.378541
49	1	0	-0.674299	3.481263	0.958728
50	1	0	-0.214437	4.329637	-0.532013
51	1	0	0.717435	4.592554	0.961270
52	6	0	2.350947	3.122682	-0.476979
53	1	0	2.275634	3.480666	-1.515965
54	1	0	3.028788	2.269124	-0.455112
55	1	0	2.771124	3.926849	0.133390

1b.3Me$_2$NH-I2

Zero-point correction=	0.496084
(Hartree/Particle)	
Thermal correction to Energy=	0.523669
Thermal correction to Enthalpy=	0.524613
Thermal correction to Gibbs Free Energy=	0.437765
Sum of electronic and zero-point Energies=	-977.656123
Sum of electronic and thermal Energies=	-977.628538
Sum of electronic and thermal Enthalpies=	-977.627594
Sum of electronic and thermal Free Energies=	-977.714442

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.638613	0.089355	-1.724314
2	1	0	-0.864233	0.955208	-1.128530
3	1	0	-0.705205	2.483283	0.362219
4	1	0	0.902114	0.942009	1.092904

5	7	0	0.904113	1.891001	1.488434
6	7	0	-1.266921	2.504028	-0.498947
7	6	0	-0.764482	3.573180	-1.361226
8	1	0	-0.953516	4.572925	-0.943482
9	1	0	-1.252739	3.517186	-2.340632
10	1	0	0.312710	3.455134	-1.505793
11	6	0	-2.686143	2.674050	-0.194977
12	1	0	-2.901772	3.647109	0.270160
13	1	0	-3.020200	1.879913	0.477643
14	1	0	-3.266867	2.604665	-1.121036
15	6	0	-1.864962	-0.209902	-2.499478
16	1	0	-1.700658	-1.105698	-3.103742
17	1	0	-2.087450	0.638263	-3.149408
18	1	0	-2.695778	-0.373145	-1.813634
19	6	0	0.466532	0.494300	-2.625648
20	1	0	0.737032	-0.349224	-3.261853
21	1	0	1.324649	0.777615	-2.017379
22	1	0	0.131553	1.343280	-3.224232
23	6	0	0.881419	1.838608	2.943320
24	1	0	1.807663	1.421092	3.373963
25	1	0	0.039645	1.226904	3.281532
26	1	0	0.752924	2.848087	3.349295
27	6	0	2.088650	2.576289	0.987866
28	1	0	3.025348	2.165065	1.400983
29	1	0	2.044314	3.641517	1.242370
30	1	0	2.131843	2.484576	-0.101681
31	7	0	0.939431	-0.756447	-0.052513
32	6	0	-0.212235	-1.089918	-0.797658
33	6	0	-1.390686	-1.415298	0.099502
34	6	0	-3.561077	-2.044299	1.758636
35	6	0	-2.110180	-2.595239	-0.091981
36	6	0	-1.762364	-0.552883	1.136359
37	6	0	-2.844720	-0.861533	1.957160
38	6	0	-3.188620	-2.913474	0.735275
39	1	0	-1.823670	-3.271695	-0.893607
40	1	0	-1.193209	0.359588	1.300764
41	1	0	-3.127307	-0.182715	2.756805
42	1	0	-3.735345	-3.838264	0.578522
43	1	0	-4.401291	-2.287074	2.401777
44	6	0	2.091274	-1.215937	-0.578470
45	8	0	2.230123	-1.805763	-1.679860
46	7	0	3.243909	-0.959692	0.182419
47	6	0	3.154581	-0.830628	1.625845
48	1	0	3.227846	-1.812634	2.121017
49	1	0	2.207786	-0.376079	1.905293
50	1	0	3.976242	-0.204523	1.990419
51	6	0	4.475567	-1.585801	-0.260978
52	1	0	5.318728	-1.078370	0.216803
53	1	0	4.569402	-1.500414	-1.341935
54	1	0	4.517792	-2.653502	0.007941
55	1	0	-0.048112	-1.910772	-1.511443

1b.3Me$_2$NH-I3

Zero-point correction= (Hartree/Particle)	0.497009
Thermal correction to Energy=	0.523677
Thermal correction to Enthalpy=	0.524622
Thermal correction to Gibbs Free Energy=	0.441660
Sum of electronic and zero-point Energies=	-977.652479
Sum of electronic and thermal Energies=	-977.625810
Sum of electronic and thermal Enthalpies=	-977.624866
Sum of electronic and thermal Free Energies=	-977.707828

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.283061	-0.060901	2.191282
2	1	0	0.738983	1.376062	1.314517
3	1	0	0.832794	1.954183	-0.301702
4	1	0	-0.310493	0.778585	-1.413286
5	7	0	0.337331	1.439662	-1.866979
6	7	0	0.831133	2.267327	0.726208
7	6	0	-0.391412	3.069976	0.945685
8	1	0	-0.341256	3.982950	0.349026
9	1	0	-0.473959	3.327453	2.003541
10	1	0	-1.248447	2.464584	0.644541
11	6	0	2.069739	2.997552	1.061867
12	1	0	2.109502	3.923280	0.485649
13	1	0	2.933706	2.381332	0.812047
14	1	0	2.078045	3.229562	2.128392
15	6	0	1.150319	-0.721948	3.173363
16	1	0	0.638538	-1.585010	3.628980
17	1	0	1.403183	-0.013715	3.967522
18	1	0	2.073276	-1.077362	2.716957
19	6	0	-0.943578	0.340105	2.893736
20	1	0	-1.447661	-0.531544	3.339175
21	1	0	-1.635084	0.819707	2.201964
22	1	0	-0.680401	1.040678	3.692167
23	6	0	1.193822	0.699693	-2.792116
24	1	0	0.634301	0.343919	-3.671160
25	1	0	1.631015	-0.160631	-2.284442
26	1	0	2.003308	1.347903	-3.144464
27	6	0	-0.390083	2.498323	-2.564119
28	1	0	-1.014154	2.110272	-3.383967
29	1	0	0.326525	3.207649	-2.990869
30	1	0	-1.034859	3.045038	-1.871486
31	7	0	-1.046529	-0.394361	0.195557
32	6	0	-0.045448	-0.977329	1.053798
33	6	0	1.199080	-1.314276	0.233279
34	6	0	3.378416	-2.064349	-1.392956
35	6	0	1.096784	-2.387090	-0.661956
36	6	0	2.411390	-0.623488	0.292213
37	6	0	3.493320	-0.992427	-0.512148
38	6	0	2.169504	-2.762166	-1.465752
39	1	0	0.153154	-2.925079	-0.724063
40	1	0	2.537974	0.195003	0.993712
41	1	0	4.426228	-0.440179	-0.443302
42	1	0	2.065703	-3.599764	-2.149156
43	1	0	4.218880	-2.355595	-2.015225
44	6	0	-2.241554	-0.992905	0.278966

45	8	0	-2.548448	-2.010723	0.957598
46	1	0	-0.411705	-1.921889	1.493524
47	7	0	-3.277204	-0.385221	-0.467169
48	6	0	-4.398732	-1.233295	-0.832608
49	1	0	-4.163799	-1.885954	-1.689932
50	1	0	-5.251609	-0.605075	-1.105131
51	1	0	-4.669538	-1.859759	0.014456
52	6	0	-2.931842	0.602911	-1.465564
53	1	0	-2.347682	0.180544	-2.301677
54	1	0	-2.347879	1.404164	-1.012288
55	1	0	-3.851879	1.033192	-1.871216

1b.3Me$_2$NH-ts2

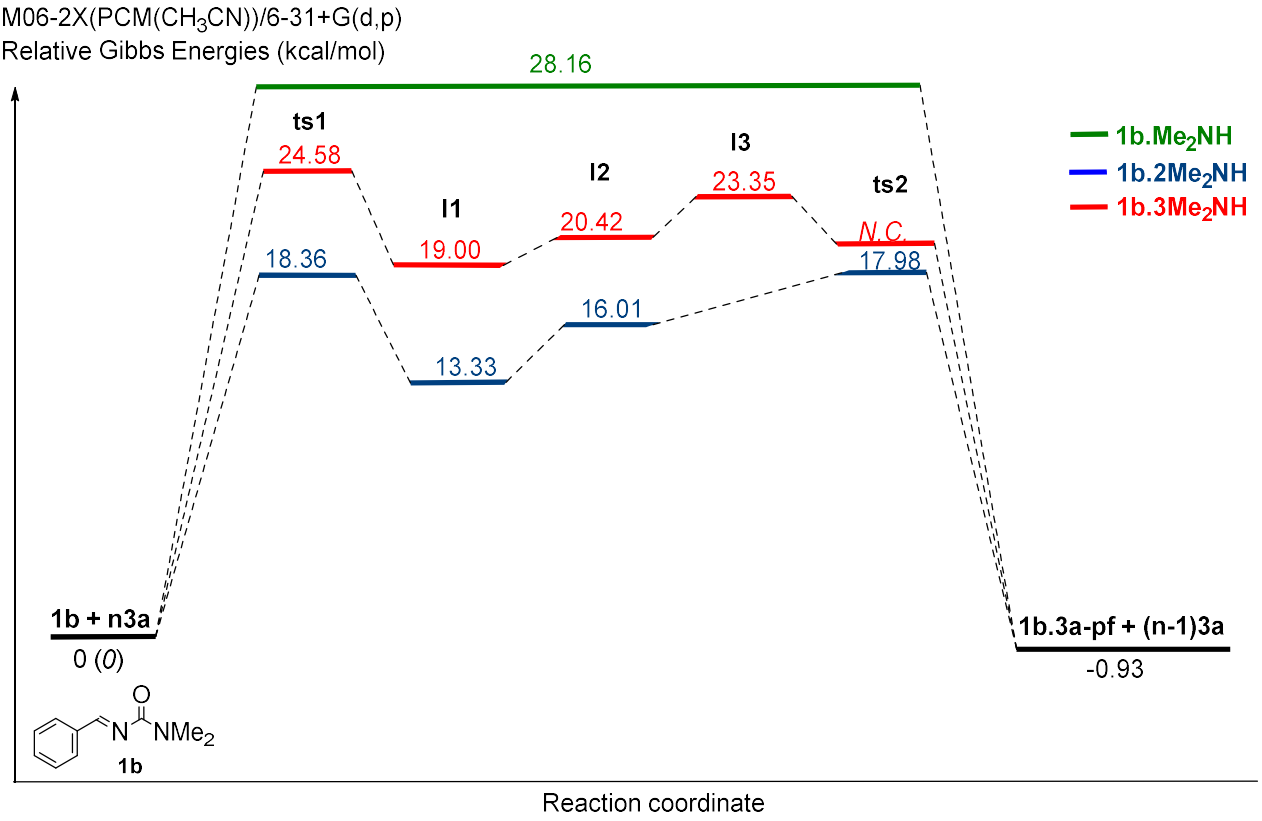
Zero-point correction=	0.491180
(Hartree/Particle)	
Thermal correction to Energy=	0.518018
Thermal correction to Enthalpy=	0.518962
Thermal correction to Gibbs Free Energy=	0.434719
Sum of electronic and zero-point Energies=	-977.656652
Sum of electronic and thermal Energies=	-977.629814
Sum of electronic and thermal Enthalpies=	-977.628870
Sum of electronic and thermal Free Energies=	-977.713113

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.684285	0.149000	1.767614
2	1	0	0.786886	1.771816	0.885965
3	1	0	-0.256622	2.261610	-0.440026
4	1	0	-1.046737	0.633284	-0.860112
5	7	0	-1.210380	1.625566	-1.180857
6	7	0	0.575878	2.669674	0.378688
7	6	0	-0.071287	3.614324	1.303851
8	1	0	-0.351397	4.519813	0.759637
9	1	0	0.604174	3.882816	2.122132
10	1	0	-0.970963	3.155361	1.718123
11	6	0	1.787788	3.227383	-0.240271
12	1	0	1.519188	4.098909	-0.842313
13	1	0	2.249274	2.475804	-0.882919
14	1	0	2.507421	3.531009	0.526227
15	6	0	1.889324	-0.011414	2.580355
16	1	0	1.846708	-0.922231	3.202927
17	1	0	1.992048	0.851839	3.244909
18	1	0	2.776098	-0.066927	1.945735
19	6	0	-0.463658	0.362518	2.650963
20	1	0	-0.631825	-0.495597	3.319766
21	1	0	-1.366900	0.508884	2.054532
22	1	0	-0.284357	1.256050	3.258284
23	6	0	-1.027304	1.776320	-2.626260
24	1	0	-1.804486	1.242393	-3.186457
25	1	0	-0.051313	1.381133	-2.920223
26	1	0	-1.070900	2.836108	-2.895585
27	6	0	-2.544562	2.041514	-0.735798
28	1	0	-3.331672	1.518630	-1.291897

29	1	0	-2.666484	3.120472	-0.876937
30	1	0	-2.659083	1.800915	0.324117
31	7	0	-0.714976	-0.876378	0.066497
32	6	0	0.455172	-1.042265	0.881065
33	6	0	1.673261	-1.218912	-0.012497
34	6	0	3.917372	-1.475906	-1.686047
35	6	0	2.579005	-2.264020	0.169743
36	6	0	1.900797	-0.312077	-1.051747
37	6	0	3.012248	-0.429182	-1.880349
38	6	0	3.694226	-2.395205	-0.662727
39	1	0	2.414088	-2.980542	0.971342
40	1	0	1.178179	0.481869	-1.215530
41	1	0	3.171624	0.288162	-2.680872
42	1	0	4.389336	-3.215261	-0.508559
43	1	0	4.784963	-1.574976	-2.331216
44	6	0	-1.818016	-1.504575	0.484465
45	8	0	-1.978537	-2.151751	1.550253
46	7	0	-2.938944	-1.357311	-0.372663
47	6	0	-2.749229	-1.327661	-1.812121
48	1	0	-2.864150	-2.333294	-2.249261
49	1	0	-1.750391	-0.967480	-2.051107
50	1	0	-3.493512	-0.673076	-2.283010
51	6	0	-4.152005	-2.048760	0.017394
52	1	0	-4.991791	-1.628755	-0.545831
53	1	0	-4.332619	-1.915387	1.082954
54	1	0	-4.103423	-3.129865	-0.192573
55	1	0	0.367100	-1.925824	1.540696

2.2.4.-M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

Energy profiles for the addition of n dimethylamine (**3a**) molecules to imine derivative **1b** in acetonitrile.



1b.Me_2NH-ts

Zero-point correction= (Hartree/Particle)	0.299994
Thermal correction to Energy=	0.316757
Thermal correction to Enthalpy=	0.317701
Thermal correction to Gibbs Free Energy=	0.253775
Sum of electronic and zero-point Energies=	-707.590465
Sum of electronic and thermal Energies=	-707.573703
Sum of electronic and thermal Enthalpies=	-707.572758
Sum of electronic and thermal Free Energies=	-707.636685

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.040202	0.396764	0.178664
2	6	0	-1.918441	-0.380981	-0.499322
3	7	0	-3.205087	-0.424678	0.011877
4	8	0	-1.619464	-1.023167	-1.529281
5	6	0	1.381136	-0.244478	-0.198409
6	6	0	3.559386	-1.929733	0.298099
7	6	0	2.559119	-0.112958	-0.939933
8	6	0	1.296270	-1.231705	0.783766
9	6	0	2.381092	-2.072562	1.030896
10	6	0	3.646982	-0.948206	-0.690325
11	1	0	2.624498	0.643759	-1.719164
12	1	0	0.371339	-1.333743	1.343890
13	1	0	2.304821	-2.841099	1.794056
14	1	0	4.558454	-0.838319	-1.269804
15	1	0	4.403393	-2.584840	0.490688
16	6	0	0.225149	0.689983	-0.464680
17	1	0	0.130591	0.845230	-1.546950
18	1	0	-0.809149	1.669798	0.527611
19	6	0	-4.071392	-1.503080	-0.432432
20	1	0	-3.870742	-1.722402	-1.479114
21	1	0	-5.113842	-1.194010	-0.321097
22	1	0	-3.915507	-2.419463	0.156574
23	6	0	-3.473605	0.073202	1.350217
24	1	0	-3.018770	1.052443	1.492488
25	1	0	-3.092880	-0.607101	2.126192
26	1	0	-4.554800	0.170206	1.474658
27	6	0	1.285531	2.167917	1.315022
28	1	0	1.126693	3.128662	1.806914
29	1	0	2.322269	2.097819	0.969531
30	1	0	1.085211	1.360952	2.021714
31	7	0	0.348049	2.068799	0.187543
32	6	0	0.485429	3.176734	-0.765853
33	1	0	0.378948	4.121143	-0.230066
34	1	0	-0.300034	3.098805	-1.519678
35	1	0	1.465959	3.146491	-1.253065

1b.Me2NH-pf

Zero-point correction=	0.305395
(Hartree/Particle)	
Thermal correction to Energy=	0.322221
Thermal correction to Enthalpy=	0.323165
Thermal correction to Gibbs Free Energy=	0.260367
Sum of electronic and zero-point Energies=	-707.638006
Sum of electronic and thermal Energies=	-707.621179
Sum of electronic and thermal Enthalpies=	-707.620235
Sum of electronic and thermal Free Energies=	-707.683034

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.943202	-0.181903	0.060972
2	6	0	-2.197135	0.106304	-0.434331
3	7	0	-3.199660	-0.719278	-0.009664
4	8	0	-2.391530	1.064737	-1.191340
5	6	0	1.472233	-0.168662	-0.270897
6	6	0	3.900537	-1.580852	-0.235243
7	6	0	2.415851	0.008160	-1.287049
8	6	0	1.764647	-1.059432	0.769391
9	6	0	2.967690	-1.763195	0.785875
10	6	0	3.622821	-0.690865	-1.271790
11	1	0	2.200626	0.695747	-2.101775
12	1	0	1.056080	-1.210408	1.580651
13	1	0	3.176116	-2.453376	1.597436
14	1	0	4.341819	-0.544450	-2.071812
15	1	0	4.836405	-2.130541	-0.223013
16	6	0	0.187783	0.649030	-0.299723
17	1	0	0.036774	1.016914	-1.320466
18	6	0	-4.505595	-0.644982	-0.643492
19	1	0	-5.285659	-0.575055	0.120362
20	1	0	-4.691329	-1.536218	-1.254495
21	1	0	-4.541746	0.239166	-1.276063
22	6	0	-2.963512	-1.842806	0.882385
23	1	0	-2.354974	-1.539186	1.738292
24	1	0	-2.481427	-2.687357	0.372407
25	1	0	-3.926256	-2.184548	1.264670
26	6	0	0.453944	1.597070	1.956649
27	1	0	0.247044	2.512626	2.518127
28	1	0	1.492940	1.292349	2.169519
29	1	0	-0.223894	0.816183	2.312348
30	7	0	0.212368	1.850946	0.544506
31	6	0	1.122411	2.861445	0.028976
32	1	0	0.977061	3.790680	0.587077
33	1	0	0.903442	3.054631	-1.025776
34	1	0	2.184464	2.571929	0.117400
35	1	0	-0.751833	-1.122618	0.370621

1b.2Me$_2$NH-ts1

Zero-point correction=	0.397715
(Hartree/Particle)	
Thermal correction to Energy=	0.420445
Thermal correction to Enthalpy=	0.421389
Thermal correction to Gibbs Free Energy=	0.344462
Sum of electronic and zero-point Energies=	-842.633023
Sum of electronic and thermal Energies=	-842.610294
Sum of electronic and thermal Enthalpies=	-842.609349
Sum of electronic and thermal Free Energies=	-842.686277

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.077853	-1.165136	-0.202288
2	6	0	-1.333347	-1.156390	-0.802448
3	7	0	-2.234952	-2.027942	-0.262759
4	8	0	-1.661389	-0.417992	-1.751961
5	6	0	2.213119	-0.415549	-0.336877
6	6	0	4.888146	-0.430842	0.480901
7	6	0	3.196623	0.191944	-1.124557
8	6	0	2.580082	-1.039948	0.860916
9	6	0	3.911168	-1.044981	1.268372
10	6	0	4.530350	0.185083	-0.718495
11	6	0	0.800920	-0.381523	-0.780287
12	7	0	-2.729613	1.598165	0.265854
13	1	0	0.622784	0.007948	-1.786012
14	1	0	-2.817106	0.975115	-0.536036
15	1	0	2.913515	0.669158	-2.059952
16	1	0	5.287748	0.656418	-1.336969
17	1	0	5.926059	-0.437451	0.799422
18	1	0	4.190583	-1.529236	2.199081
19	1	0	1.809242	-1.516354	1.458936
20	7	0	0.360006	1.604938	-0.072443
21	1	0	-0.660253	1.602286	-0.185944
22	6	0	-3.795806	2.592169	0.236690
23	1	0	-3.627578	3.329798	1.028074
24	1	0	-4.795604	2.154415	0.390271
25	1	0	-3.788951	3.115014	-0.722614
26	6	0	0.941953	2.698212	-0.837620
27	1	0	2.031525	2.669607	-0.734149
28	1	0	0.588116	3.681009	-0.496022
29	1	0	0.686902	2.580405	-1.894680
30	6	0	-2.749208	0.814589	1.495509
31	1	0	-1.952806	0.063866	1.471462
32	1	0	-3.709744	0.300663	1.669672
33	1	0	-2.563702	1.476850	2.348191
34	6	0	0.667904	1.660281	1.348190
35	1	0	0.341965	0.726147	1.818758
36	1	0	0.170600	2.503185	1.847281
37	1	0	1.749997	1.758560	1.481461
38	6	0	-2.007970	-2.774644	0.962864
39	1	0	-0.954330	-2.739011	1.226160
40	1	0	-2.315501	-3.815282	0.819482
41	1	0	-2.602040	-2.349819	1.783606
42	6	0	-3.606804	-2.000595	-0.737235
43	1	0	-4.042911	-2.995790	-0.621461
44	1	0	-3.629699	-1.712767	-1.786642
45	1	0	-4.213600	-1.287812	-0.159770

1b.2Me$_2$NH-I1

Zero-point correction=	0.400408
(Hartree/Particle)	
Thermal correction to Energy=	0.422571
Thermal correction to Enthalpy=	0.423515
Thermal correction to Gibbs Free Energy=	0.348398
Sum of electronic and zero-point Energies=	-842.642692
Sum of electronic and thermal Energies=	-842.620530
Sum of electronic and thermal Enthalpies=	-842.619586
Sum of electronic and thermal Free Energies=	-842.694703

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.175231	1.009590	0.070789
2	6	0	1.344993	1.192362	-0.556003
3	7	0	2.165913	2.189884	-0.016882
4	8	0	1.781625	0.537761	-1.548646
5	6	0	-2.091422	0.158625	-0.254334
6	6	0	-4.849086	0.483172	0.151189
7	6	0	-3.010392	-0.318574	-1.193595
8	6	0	-2.568582	0.817239	0.883779
9	6	0	-3.937729	0.973899	1.088950
10	6	0	-4.382612	-0.159242	-0.994294
11	6	0	-0.603588	-0.033084	-0.478426
12	7	0	2.550632	-1.762850	0.030783
13	1	0	-0.412835	-0.207707	-1.546401
14	1	0	2.744169	-1.200839	-0.798787
15	1	0	-2.651533	-0.809682	-2.095583
16	1	0	-5.083132	-0.531625	-1.735381
17	1	0	-5.915730	0.610070	0.309388
18	1	0	-4.295608	1.484997	1.977746
19	1	0	-1.850866	1.216662	1.593531
20	7	0	-0.169985	-1.392876	0.148130
21	1	0	0.902128	-1.459484	0.029333
22	6	0	3.007114	-3.139329	-0.144300
23	1	0	2.676536	-3.740981	0.708581
24	1	0	4.102057	-3.213406	-0.211675
25	1	0	2.570660	-3.560214	-1.053221
26	6	0	-0.723429	-2.576429	-0.542541
27	1	0	-1.802359	-2.628355	-0.386556
28	1	0	-0.249749	-3.471629	-0.134228
29	1	0	-0.502719	-2.500437	-1.608836
30	6	0	3.158777	-1.112114	1.191688
31	1	0	2.805740	-0.078443	1.253577
32	1	0	4.257257	-1.110395	1.141161
33	1	0	2.860100	-1.642991	2.101686
34	6	0	-0.392582	-1.466412	1.609074
35	1	0	-0.039266	-0.534754	2.052366
36	1	0	0.179307	-2.311141	1.999741
37	1	0	-1.454397	-1.610227	1.816878
38	6	0	1.607470	3.151683	0.914143
39	1	0	0.997290	2.639356	1.656137
40	1	0	0.979562	3.903309	0.409681
41	1	0	2.427590	3.671313	1.417801
42	6	0	3.248214	2.694348	-0.839966
43	1	0	2.901822	3.448264	-1.565308
44	1	0	3.705782	1.872376	-1.387827
45	1	0	3.999773	3.160763	-0.196559

1b.2Me$_2$NH-I2

Zero-point correction= (Hartree/Particle)	0.400397
Thermal correction to Energy=	0.422632
Thermal correction to Enthalpy=	0.423576
Thermal correction to Gibbs Free Energy=	0.347906
Sum of electronic and zero-point Energies=	-842.637934
Sum of electronic and thermal Energies=	-842.615700
Sum of electronic and thermal Enthalpies=	-842.614755
Sum of electronic and thermal Free Energies=	-842.690425

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.791269	-0.530901	-0.147660
2	6	0	1.856656	-1.244674	0.239498
3	7	0	2.983094	-1.121423	-0.592273
4	8	0	1.955054	-1.971558	1.266444
5	6	0	-1.633750	-0.770050	0.036877
6	6	0	-4.105064	-1.141377	-1.237710
7	6	0	-2.607787	-1.595274	0.602961
8	6	0	-1.904217	-0.142786	-1.183435
9	6	0	-3.133734	-0.319668	-1.813841
10	6	0	-3.837063	-1.784822	-0.030754
11	1	0	-2.403638	-2.095869	1.546546
12	1	0	-1.137368	0.468147	-1.648725
13	1	0	-3.331693	0.175899	-2.759449
14	1	0	-4.581654	-2.435327	0.417700
15	1	0	-5.061095	-1.284989	-1.731519
16	6	0	-0.307856	-0.565021	0.744721
17	6	0	3.971457	-2.184172	-0.535311
18	1	0	4.927480	-1.808552	-0.910711
19	1	0	3.679366	-3.052360	-1.148328
20	1	0	4.094664	-2.513308	0.494406
21	6	0	2.829587	-0.523023	-1.905606
22	1	0	2.318046	0.436010	-1.827690
23	1	0	2.255015	-1.163711	-2.592782
24	1	0	3.822703	-0.359219	-2.332972
25	6	0	1.802790	2.932594	-0.217770
26	1	0	2.388358	2.074824	0.126418
27	1	0	1.750881	3.671971	0.587517
28	1	0	2.317164	3.390225	-1.075014
29	6	0	-1.622536	1.119263	2.172035
30	1	0	-1.502566	2.059507	2.712094
31	1	0	-1.868134	0.319864	2.875623
32	1	0	-2.415540	1.218541	1.432628
33	7	0	0.452122	2.481877	-0.554357
34	6	0	-0.365633	3.535952	-1.149543
35	1	0	0.099437	3.977710	-2.042177
36	1	0	-0.516436	4.329888	-0.412404
37	1	0	-1.343566	3.131651	-1.423391
38	7	0	-0.345261	0.800571	1.494120
39	6	0	0.784338	0.883880	2.451556
40	1	0	0.868192	1.911420	2.809267

41	1	0	1.700109	0.584216	1.945224
42	1	0	0.588716	0.210184	3.288765
43	1	0	-0.207681	-1.303606	1.552694
44	1	0	0.538146	1.684544	-1.184452
45	1	0	-0.151022	1.529000	0.728295

1b.2Me$_2$NH-ts2

Zero-point correction=	0.397041
(Hartree/Particle)	
Thermal correction to Energy=	0.418547
Thermal correction to Enthalpy=	0.419491
Thermal correction to Gibbs Free Energy=	0.346129
Sum of electronic and zero-point Energies=	-842.636383
Sum of electronic and thermal Energies=	-842.614878
Sum of electronic and thermal Enthalpies=	-842.613933
Sum of electronic and thermal Free Energies=	-842.687295

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.860495	-0.440535	-0.074023
2	6	0	1.914837	-1.137495	0.350186
3	7	0	3.051591	-1.066950	-0.486890
4	8	0	2.015352	-1.814162	1.412999
5	6	0	-1.556231	-0.783545	0.108605
6	6	0	-3.982606	-1.433276	-1.154285
7	6	0	-2.547821	-1.496944	0.788578
8	6	0	-1.787191	-0.422836	-1.222078
9	6	0	-2.992888	-0.735612	-1.848328
10	6	0	-3.753061	-1.821631	0.165201
11	1	0	-2.374506	-1.800175	1.818749
12	1	0	-1.001425	0.075880	-1.780738
13	1	0	-3.155913	-0.445026	-2.881975
14	1	0	-4.510291	-2.378594	0.708736
15	1	0	-4.919607	-1.682363	-1.642792
16	6	0	-0.260654	-0.414767	0.817155
17	6	0	4.007221	-2.156699	-0.385741
18	1	0	4.968208	-1.833172	-0.795929
19	1	0	3.679054	-3.049043	-0.944566
20	1	0	4.137640	-2.431744	0.658762
21	6	0	2.897067	-0.551654	-1.834503
22	1	0	2.423458	0.429824	-1.816708
23	1	0	2.289177	-1.212644	-2.472463
24	1	0	3.888026	-0.449842	-2.285661
25	6	0	1.586484	3.030587	-0.461336
26	1	0	2.299604	2.312155	-0.052193
27	1	0	1.406024	3.823718	0.266770
28	1	0	1.986609	3.464801	-1.380998
29	6	0	-1.654777	1.322024	2.010433
30	1	0	-1.588793	2.327598	2.432938
31	1	0	-1.901431	0.616697	2.816007
32	1	0	-2.450835	1.302850	1.264981
33	7	0	0.318466	2.327433	-0.730648
34	6	0	-0.712839	3.177196	-1.349274
35	1	0	-0.357783	3.585232	-2.298504

36	1	0	-0.947071	3.996214	-0.666657
37	1	0	-1.611987	2.581835	-1.518090
38	7	0	-0.364892	0.992123	1.389938
39	6	0	0.719463	1.198478	2.363755
40	1	0	0.756982	2.253678	2.647393
41	1	0	1.669887	0.907079	1.914822
42	1	0	0.549011	0.591020	3.262679
43	1	0	-0.137429	-1.088740	1.679925
44	1	0	0.523808	1.497136	-1.295153
45	1	0	-0.064874	1.791460	0.277831

1b.3Me$_2$NH-ts1

Zero-point correction=	0.492346
(Hartree/Particle)	
Thermal correction to Energy=	0.521121
Thermal correction to Enthalpy=	0.522065
Thermal correction to Gibbs Free Energy=	0.430905
Sum of electronic and zero-point Energies=	-977.649725
Sum of electronic and thermal Energies=	-977.620950
Sum of electronic and thermal Enthalpies=	-977.620006
Sum of electronic and thermal Free Energies=	-977.711166

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.393029	1.382625	-0.699268
2	6	0	0.952868	1.406066	-1.032749
3	7	0	1.518216	2.648452	-1.018792
4	8	0	1.630754	0.406031	-1.349800
5	6	0	-2.376567	0.045443	-0.404153
6	6	0	-5.153294	-0.258348	-0.236530
7	6	0	-2.970135	-1.189995	-0.678555
8	6	0	-3.184879	1.132901	-0.052036
9	6	0	-4.565748	0.979497	0.036855
10	6	0	-4.353995	-1.342182	-0.599233
11	6	0	-0.902792	0.189376	-0.489570
12	7	0	2.522880	-0.572357	1.371473
13	1	0	-0.356938	-0.711961	-0.787867
14	1	0	-2.345561	-2.035140	-0.958713
15	1	0	-4.806807	-2.304129	-0.818427
16	1	0	-6.230612	-0.375536	-0.170508
17	1	0	-5.186743	1.825363	0.315332
18	1	0	-2.714734	2.091943	0.144221
19	7	0	-0.477112	-0.273993	1.521915
20	6	0	3.349879	-1.589566	2.009464
21	1	0	3.141146	-1.609086	3.084388
22	1	0	4.428428	-1.407234	1.876592
23	1	0	3.112248	-2.571116	1.591729
24	6	0	-1.221524	-1.395295	2.082075
25	1	0	-2.279374	-1.123922	2.157833
26	1	0	-0.856962	-1.672180	3.080503
27	1	0	-1.137848	-2.262851	1.421772
28	6	0	2.895489	0.774849	1.790173
29	1	0	2.291359	1.511601	1.250761

30	1	0	3.959167	1.001128	1.612128
31	1	0	2.699516	0.891402	2.861749
32	6	0	-0.632725	0.955110	2.285078
33	1	0	-0.176234	1.780713	1.729447
34	1	0	-0.166643	0.884206	3.276317
35	1	0	-1.699014	1.168662	2.412943
36	1	0	0.528423	-0.504218	1.454641
37	7	0	2.040629	-2.561391	-1.205113
38	6	0	2.130533	-3.258715	-2.481105
39	1	0	2.547722	-4.259539	-2.325055
40	1	0	2.797914	-2.714876	-3.154463
41	1	0	1.153379	-3.377151	-2.979609
42	6	0	1.082175	-3.192963	-0.311842
43	1	0	1.002478	-2.609903	0.610858
44	1	0	1.429238	-4.198351	-0.047099
45	1	0	0.073671	-3.294726	-0.752402
46	1	0	1.761978	-1.594278	-1.368583
47	1	0	2.615264	-0.637761	0.358581
48	6	0	0.848583	3.838973	-0.524248
49	1	0	-0.212471	3.641652	-0.398800
50	1	0	0.989870	4.658405	-1.236765
51	1	0	1.279448	4.143298	0.439213
52	6	0	2.928784	2.815338	-1.312708
53	1	0	3.477509	3.100687	-0.405511
54	1	0	3.060488	3.608181	-2.056431
55	1	0	3.333669	1.882180	-1.697382

1b.3Me$_2$NH-I1

Zero-point correction=	0.495294
(Hartree/Particle)	
Thermal correction to Energy=	0.523456
Thermal correction to Enthalpy=	0.524400
Thermal correction to Gibbs Free Energy=	0.434915
Sum of electronic and zero-point Energies=	-977.659676
Sum of electronic and thermal Energies=	-977.631515
Sum of electronic and thermal Enthalpies=	-977.630571
Sum of electronic and thermal Free Energies=	-977.720055

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.737210	1.277738	0.022529
2	6	0	0.538798	1.506803	-0.315564
3	7	0	1.070403	2.734767	0.083684
4	8	0	1.300635	0.697172	-0.922216
5	6	0	-2.693944	-0.101911	-0.465130
6	6	0	-5.486994	-0.334751	-0.595429
7	6	0	-3.294981	-0.940860	-1.407553
8	6	0	-3.508322	0.633231	0.402819
9	6	0	-4.895068	0.514270	0.342100
10	6	0	-4.684116	-1.059464	-1.474434
11	6	0	-1.183570	0.006375	-0.399390
12	7	0	2.007050	-0.982331	1.475791
13	1	0	-0.751038	-0.315349	-1.357342

14	1	0	-2.673267	-1.499165	-2.104074
15	1	0	-5.135416	-1.712160	-2.215325
16	1	0	-6.567960	-0.422877	-0.645660
17	1	0	-5.516374	1.090257	1.021319
18	1	0	-3.040925	1.307660	1.113441
19	7	0	-0.636255	-1.089819	0.569818
20	6	0	2.483970	-2.235126	2.056524
21	1	0	1.806002	-2.555202	2.855677
22	1	0	3.493265	-2.142772	2.485733
23	1	0	2.502768	-3.013548	1.288566
24	6	0	-0.758595	-2.467261	0.046728
25	1	0	-1.807220	-2.769480	0.041253
26	1	0	-0.184767	-3.137138	0.690841
27	1	0	-0.356657	-2.499106	-0.967447
28	6	0	2.068178	0.123101	2.431997
29	1	0	1.760449	1.049808	1.938168
30	1	0	3.077732	0.259810	2.848740
31	1	0	1.384244	-0.073027	3.265274
32	6	0	-1.185685	-0.986423	1.940515
33	1	0	-1.138237	0.059364	2.246539
34	1	0	-0.570738	-1.600680	2.601352
35	1	0	-2.217268	-1.341120	1.953325
36	1	0	0.408841	-0.915063	0.693599
37	7	0	3.764426	-0.819770	-1.131757
38	6	0	5.030346	-0.571473	-1.806834
39	1	0	5.737906	-1.372918	-1.568246
40	1	0	5.457700	0.372188	-1.458146
41	1	0	4.932901	-0.526398	-2.904534
42	6	0	3.112385	-2.026677	-1.621203
43	1	0	2.131697	-2.128849	-1.145265
44	1	0	3.713886	-2.905065	-1.361350
45	1	0	2.965028	-2.027944	-2.714346
46	1	0	3.123978	-0.037516	-1.269409
47	1	0	2.601316	-0.748135	0.677875
48	6	0	0.177365	3.818031	0.450423
49	1	0	-0.620764	3.438909	1.086061
50	1	0	-0.278402	4.296261	-0.430926
51	1	0	0.745193	4.575971	0.997288
52	6	0	2.334228	3.141679	-0.500412
53	1	0	2.220380	3.512803	-1.531237
54	1	0	3.025176	2.298537	-0.512628
55	1	0	2.762622	3.943207	0.107205

1b.3Me$_2$NH-I2

Zero-point correction=	0.495927
(Hartree/Particle)	
Thermal correction to Energy=	0.523537
Thermal correction to Enthalpy=	0.524481
Thermal correction to Gibbs Free Energy=	0.437587
Sum of electronic and zero-point Energies=	-977.659448
Sum of electronic and thermal Energies=	-977.631838
Sum of electronic and thermal Enthalpies=	-977.630894
Sum of electronic and thermal Free Energies=	-977.717788

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.630477	0.084231	-1.720466
2	1	0	-0.871697	0.949787	-1.126798
3	1	0	-0.765650	2.482351	0.360936
4	1	0	0.875371	0.970009	1.095969
5	7	0	0.861208	1.918026	1.491440
6	7	0	-1.310733	2.486255	-0.510395
7	6	0	-0.813598	3.563565	-1.366545
8	1	0	-1.027847	4.559711	-0.952692
9	1	0	-1.284886	3.497328	-2.353324
10	1	0	0.267747	3.464822	-1.493317
11	6	0	-2.739277	2.628244	-0.234654
12	1	0	-2.982648	3.597301	0.224790
13	1	0	-3.070469	1.828637	0.432948
14	1	0	-3.299602	2.546259	-1.172020
15	6	0	-1.851209	-0.231237	-2.499766
16	1	0	-1.672456	-1.123420	-3.105097
17	1	0	-2.083845	0.614928	-3.148374
18	1	0	-2.681313	-0.407066	-1.816213
19	6	0	0.470875	0.504165	-2.619857
20	1	0	0.747319	-0.333204	-3.261723
21	1	0	1.326125	0.794218	-2.010676
22	1	0	0.127880	1.352244	-3.214672
23	6	0	0.823104	1.865143	2.946216
24	1	0	1.748314	1.456521	3.387729
25	1	0	-0.017530	1.247066	3.275489
26	1	0	0.681421	2.873670	3.349770
27	6	0	2.040210	2.621813	1.003312
28	1	0	2.979039	2.227209	1.428033
29	1	0	1.975316	3.686139	1.256480
30	1	0	2.096636	2.531226	-0.085709
31	7	0	0.957184	-0.749053	-0.051359
32	6	0	-0.194013	-1.090078	-0.798858
33	6	0	-1.366693	-1.431692	0.099876
34	6	0	-3.523200	-2.092535	1.764860
35	6	0	-2.061814	-2.627743	-0.082544
36	6	0	-1.756598	-0.568505	1.129531
37	6	0	-2.831929	-0.893173	1.953515
38	6	0	-3.133285	-2.961724	0.747812
39	1	0	-1.763439	-3.303347	-0.880538
40	1	0	-1.210224	0.359287	1.285022
41	1	0	-3.129656	-0.212819	2.746245
42	1	0	-3.661829	-3.898009	0.597378
43	1	0	-4.358864	-2.347013	2.409336
44	6	0	2.111586	-1.201297	-0.574443
45	8	0	2.254068	-1.807578	-1.668233

46	7	0	3.265936	-0.921482	0.176652
47	6	0	3.176973	-0.763175	1.617922
48	1	0	3.209071	-1.737684	2.132102
49	1	0	2.250785	-0.263035	1.887231
50	1	0	4.022703	-0.164444	1.971629
51	6	0	4.497197	-1.561262	-0.251041
52	1	0	5.340180	-1.050405	0.222653
53	1	0	4.598808	-1.493597	-1.332558
54	1	0	4.533340	-2.624457	0.035990
55	1	0	-0.022445	-1.908469	-1.513285

1b.3Me$_2$NH-I3

Zero-point correction=	0.496535
(Hartree/Particle)	
Thermal correction to Energy=	0.523416
Thermal correction to Enthalpy=	0.524361
Thermal correction to Gibbs Free Energy=	0.440470
Sum of electronic and zero-point Energies=	-977.657053
Sum of electronic and thermal Energies=	-977.630172
Sum of electronic and thermal Enthalpies=	-977.629228
Sum of electronic and thermal Free Energies=	-977.713119

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.287732	-0.011243	2.183846
2	1	0	0.776898	1.414204	1.273009
3	1	0	0.873141	1.951121	-0.351854
4	1	0	-0.315977	0.759678	-1.420853
5	7	0	0.336332	1.397000	-1.899787
6	7	0	0.886926	2.287296	0.666666
7	6	0	-0.313731	3.126292	0.874444
8	1	0	-0.243293	4.022871	0.255881
9	1	0	-0.382295	3.410300	1.926208
10	1	0	-1.188969	2.538331	0.591961
11	6	0	2.146143	2.994546	0.978157
12	1	0	2.203337	3.904421	0.379031
13	1	0	2.992888	2.351219	0.738195
14	1	0	2.165338	3.251038	2.038655
15	6	0	1.148357	-0.651140	3.185251
16	1	0	0.621893	-1.483703	3.679671
17	1	0	1.424038	0.082932	3.947498
18	1	0	2.059507	-1.044614	2.736306
19	6	0	-0.928564	0.435681	2.874978
20	1	0	-1.449493	-0.410844	3.349726
21	1	0	-1.611900	0.909120	2.170872
22	1	0	-0.648964	1.154922	3.650597
23	6	0	1.169004	0.617715	-2.814189
24	1	0	0.589593	0.231597	-3.667471
25	1	0	1.614641	-0.224433	-2.283327
26	1	0	1.972637	1.248856	-3.207947
27	6	0	-0.384174	2.446913	-2.617636
28	1	0	-1.022245	2.045760	-3.420289
29	1	0	0.337654	3.134462	-3.070039

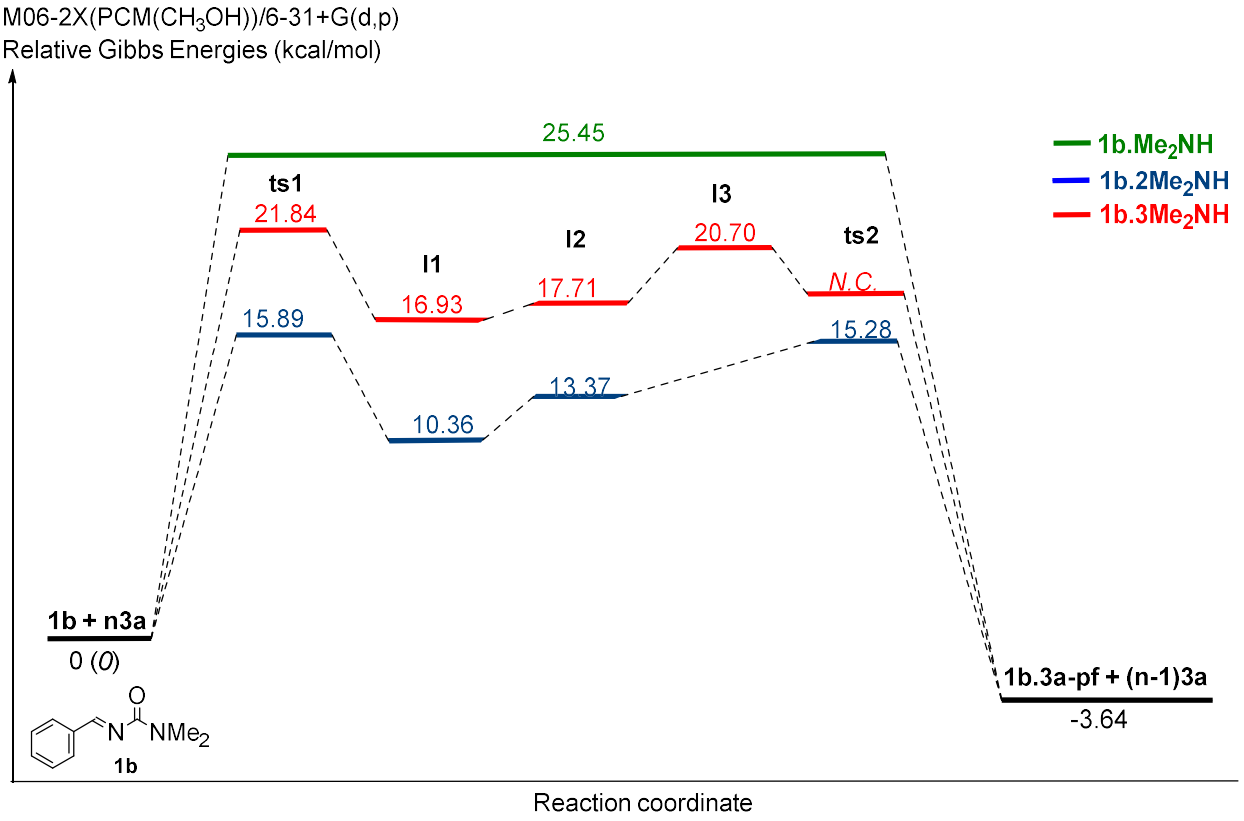
30	1	0	-1.013048	3.021317	-1.933010
31	7	0	-1.057426	-0.394202	0.209880
32	6	0	-0.054925	-0.958975	1.078651
33	6	0	1.181469	-1.329527	0.259643
34	6	0	3.346283	-2.138192	-1.358254
35	6	0	1.064167	-2.419934	-0.612246
36	6	0	2.401692	-0.651566	0.300204
37	6	0	3.476262	-1.049541	-0.500175
38	6	0	2.129544	-2.824159	-1.412027
39	1	0	0.114816	-2.949312	-0.661248
40	1	0	2.540235	0.180116	0.983257
41	1	0	4.414829	-0.505485	-0.446170
42	1	0	2.013760	-3.674534	-2.077598
43	1	0	4.180838	-2.451051	-1.977976
44	6	0	-2.256519	-0.976043	0.311378
45	8	0	-2.571912	-1.981921	1.008919
46	1	0	-0.423754	-1.888401	1.548602
47	7	0	-3.291398	-0.367941	-0.434973
48	6	0	-4.420225	-1.210025	-0.793237
49	1	0	-4.191098	-1.871126	-1.645663
50	1	0	-5.267451	-0.577048	-1.071554
51	1	0	-4.698667	-1.827260	0.058195
52	6	0	-2.942120	0.611361	-1.442045
53	1	0	-2.368706	0.177030	-2.279238
54	1	0	-2.345822	1.408423	-0.997539
55	1	0	-3.860200	1.048675	-1.844051

1b.3Me$_2$NH-ts2

No convergence reached

2.2.5.- M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

Energy profiles for the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1b** in methanol.



1b.Me_2NH-ts

```
 Zero-point correction=                           0.299996
(Hartree/Particle)
 Thermal correction to Energy=                    0.316758
 Thermal correction to Enthalpy=                  0.317703
 Thermal correction to Gibbs Free Energy=         0.253775
 Sum of electronic and zero-point Energies=           -707.590364
 Sum of electronic and thermal Energies=              -707.573602
 Sum of electronic and thermal Enthalpies=            -707.572658
 Sum of electronic and thermal Free Energies=         -707.636585

Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          7           0       -1.040067    0.396056    0.179395
      2          6           0       -1.918850   -0.380490   -0.499415
      3          7           0       -3.205247   -0.424667    0.012460
      4          8           0       -1.620626   -1.021082   -1.530493
      5          6           0        1.381278   -0.244640   -0.198462
      6          6           0        3.560138   -1.929227    0.297517
      7          6           0        2.559079   -0.112691   -0.940191
      8          6           0        1.296867   -1.232009    0.783597
      9          6           0        2.382007   -2.072524    1.030470
     10          6           0        3.647250   -0.947603   -0.690850
     11          1           0        2.624037    0.644063   -1.719425
     12          1           0        0.372009   -1.334407    1.343772
     13          1           0        2.306096   -2.841194    1.793532
     14          1           0        4.558572   -0.837417   -1.270508
     15          1           0        4.404390   -2.584080    0.489903
     16          6           0        0.224993    0.689568   -0.464339
     17          1           0        0.130085    0.844879   -1.546567
     18          1           0       -0.808796    1.669308    0.528494
     19          6           0       -4.072137   -1.501943   -0.433390
     20          1           0       -3.871831   -1.719572   -1.480490
     21          1           0       -5.114436   -1.192625   -0.321246
     22          1           0       -3.916467   -2.419399    0.154005
     23          6           0       -3.472876    0.070901    1.351805
     24          1           0       -3.017640    1.049739    1.495570
     25          1           0       -3.091947   -0.610886    2.126381
     26          1           0       -4.553979    0.168042    1.477010
     27          6           0        1.285975    2.167721    1.315007
     28          1           0        1.127112    3.128379    1.807072
     29          1           0        2.322556    2.097941    0.968983
     30          1           0        1.086270    1.360621    2.021713
     31          7           0        0.347949    2.068412    0.188007
     32          6           0        0.484468    3.176443   -0.765387
     33          1           0        0.378001    4.120815   -0.229524
     34          1           0       -0.301370    3.098298   -1.518797
     35          1           0        1.464744    3.146503   -1.253134
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1b.Me2NH-pf

```
 Zero-point correction=                           0.305396
(Hartree/Particle)
 Thermal correction to Energy=                    0.322222
 Thermal correction to Enthalpy=                  0.323166
 Thermal correction to Gibbs Free Energy=         0.260371
 Sum of electronic and zero-point Energies=           -707.637916
 Sum of electronic and thermal Energies=              -707.621090
 Sum of electronic and thermal Enthalpies=            -707.620145
 Sum of electronic and thermal Free Energies=         -707.682941
```

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.943202	-0.181903	0.060972
2	6	0	-2.197135	0.106304	-0.434331
3	7	0	-3.199660	-0.719278	-0.009664
4	8	0	-2.391530	1.064737	-1.191340
5	6	0	1.472233	-0.168662	-0.270897
6	6	0	3.900537	-1.580852	-0.235243
7	6	0	2.415851	0.008160	-1.287049
8	6	0	1.764647	-1.059432	0.769391
9	6	0	2.967690	-1.763195	0.785875
10	6	0	3.622821	-0.690865	-1.271790
11	1	0	2.200626	0.695747	-2.101775
12	1	0	1.056080	-1.210408	1.580651
13	1	0	3.176116	-2.453376	1.597436
14	1	0	4.341819	-0.544450	-2.071812
15	1	0	4.836405	-2.130541	-0.223013
16	6	0	0.187783	0.649030	-0.299723
17	1	0	0.036774	1.016914	-1.320466
18	6	0	-4.505595	-0.644982	-0.643492
19	1	0	-5.285659	-0.575055	0.120362
20	1	0	-4.691329	-1.536218	-1.254495
21	1	0	-4.541746	0.239166	-1.276063
22	6	0	-2.963512	-1.842806	0.882385
23	1	0	-2.354974	-1.539186	1.738292
24	1	0	-2.481427	-2.687357	0.372407
25	1	0	-3.926256	-2.184548	1.264670
26	6	0	0.453944	1.597070	1.956649
27	1	0	0.247044	2.512626	2.518127
28	1	0	1.492940	1.292349	2.169519
29	1	0	-0.223894	0.816183	2.312348
30	7	0	0.212368	1.850946	0.544506
31	6	0	1.122411	2.861445	0.028976
32	1	0	0.977061	3.790680	0.587077
33	1	0	0.903442	3.054631	-1.025776
34	1	0	2.184464	2.571929	0.117400
35	1	0	-0.751833	-1.122618	0.370621

1b.2Me$_2$NH-ts1

Zero-point correction=	0.397731
(Hartree/Particle)	
Thermal correction to Energy=	0.420454
Thermal correction to Enthalpy=	0.421398
Thermal correction to Gibbs Free Energy=	0.344499
Sum of electronic and zero-point Energies=	-842.632951
Sum of electronic and thermal Energies=	-842.610229
Sum of electronic and thermal Enthalpies=	-842.609285
Sum of electronic and thermal Free Energies=	-842.686183

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.077891	-1.164904	-0.202187
2	6	0	-1.333352	-1.156167	-0.802319
3	7	0	-2.234760	-2.028267	-0.263081
4	8	0	-1.661642	-0.417308	-1.751370
5	6	0	2.213082	-0.415362	-0.336872
6	6	0	4.888071	-0.430760	0.481029
7	6	0	3.196638	0.192134	-1.124474
8	6	0	2.579985	-1.039866	0.860875
9	6	0	3.911047	-1.044941	1.268399
10	6	0	4.530343	0.185227	-0.718351
11	6	0	0.800849	-0.381240	-0.780261
12	7	0	-2.729372	1.598295	0.266117
13	1	0	0.622766	0.007878	-1.786153
14	1	0	-2.816828	0.975528	-0.536007
15	1	0	2.913578	0.669367	-2.059874
16	1	0	5.287788	0.656555	-1.336777
17	1	0	5.925971	-0.437415	0.799593
18	1	0	4.190417	-1.529299	2.199070
19	1	0	1.809082	-1.516354	1.458747
20	7	0	0.359892	1.604624	-0.072726
21	1	0	-0.660348	1.602002	-0.186548
22	6	0	-3.795001	2.592870	0.236926
23	1	0	-3.626534	3.330294	1.028454
24	1	0	-4.795080	2.155648	0.390244
25	1	0	-3.787681	3.115860	-0.722295
26	6	0	0.942096	2.698043	-0.837500
27	1	0	2.031620	2.669536	-0.733513
28	1	0	0.587964	3.680741	-0.495931
29	1	0	0.687508	2.580334	-1.894681
30	6	0	-2.749720	0.814364	1.495511
31	1	0	-1.953683	0.063256	1.471442
32	1	0	-3.710572	0.300873	1.669255
33	1	0	-2.564114	1.476256	2.348464
34	6	0	0.667202	1.659733	1.348046
35	1	0	0.341440	0.725307	1.818175
36	1	0	0.169298	2.502286	1.847119
37	1	0	1.749196	1.758419	1.481783
38	6	0	-2.007537	-2.775438	0.962175
39	1	0	-0.953856	-2.739745	1.225319
40	1	0	-2.314909	-3.816076	0.818402
41	1	0	-2.601556	-2.351067	1.783208
42	6	0	-3.606643	-2.000786	-0.737383
43	1	0	-4.042677	-2.996071	-0.622062
44	1	0	-3.629642	-1.712422	-1.786641
45	1	0	-4.213458	-1.288336	-0.159503

1b.2Me$_2$NH-I1

Zero-point correction=	0.400417
(Hartree/Particle)	
Thermal correction to Energy=	0.422576
Thermal correction to Enthalpy=	0.423520
Thermal correction to Gibbs Free Energy=	0.348434
Sum of electronic and zero-point Energies=	-842.642582
Sum of electronic and thermal Energies=	-842.620423
Sum of electronic and thermal Enthalpies=	-842.619479
Sum of electronic and thermal Free Energies=	-842.694565

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.174946	1.009985	0.070244
2	6	0	1.345034	1.192173	-0.556135
3	7	0	2.165907	2.189837	-0.017189
4	8	0	1.781976	0.536819	-1.548103
5	6	0	-2.091675	0.158871	-0.254497
6	6	0	-4.849248	0.482611	0.152300
7	6	0	-3.010988	-0.319649	-1.192757
8	6	0	-2.568460	0.818485	0.883185
9	6	0	-3.937554	0.974743	1.088990
10	6	0	-4.383157	-0.160745	-0.992806
11	6	0	-0.603872	-0.032496	-0.479132
12	7	0	2.550918	-1.762851	0.031821
13	1	0	-0.413324	-0.206851	-1.547195
14	1	0	2.744902	-1.201109	-0.797831
15	1	0	-2.652451	-0.811389	-2.094529
16	1	0	-5.083947	-0.534114	-1.733143
17	1	0	-5.915855	0.609224	0.310978
18	1	0	-4.295133	1.486686	1.977422
19	1	0	-1.850453	1.219033	1.592001
20	7	0	-0.169919	-1.392531	0.146995
21	1	0	0.902177	-1.458709	0.028662
22	6	0	3.007638	-3.139339	-0.142367
23	1	0	2.676414	-3.740714	0.710478
24	1	0	4.102645	-3.213412	-0.208822
25	1	0	2.571972	-3.560603	-1.051494
26	6	0	-0.722533	-2.576104	-0.544247
27	1	0	-1.801435	-2.628846	-0.388343
28	1	0	-0.248255	-3.471185	-0.136338
29	1	0	-0.501802	-2.499458	-1.610494
30	6	0	3.158180	-1.111560	1.192875
31	1	0	2.804833	-0.077964	1.254160
32	1	0	4.256695	-1.109585	1.143044
33	1	0	2.859076	-1.642193	2.102885
34	6	0	-0.392897	-1.466620	1.607837
35	1	0	-0.040089	-0.534916	2.051464
36	1	0	0.179285	-2.311208	1.998407
37	1	0	-1.454713	-1.610921	1.815302
38	6	0	1.607107	3.152453	0.912767
39	1	0	0.995957	2.640830	1.654445
40	1	0	0.980045	3.904093	0.407283
41	1	0	2.427039	3.671947	1.416892
42	6	0	3.248784	2.693457	-0.839995
43	1	0	2.903048	3.447325	-1.565700
44	1	0	3.706056	1.871048	-1.387448
45	1	0	4.000369	3.159668	-0.196456

1b.2Me$_2$NH-I2

Zero-point correction=	0.400422
(Hartree/Particle)	
Thermal correction to Energy=	0.422645
Thermal correction to Enthalpy=	0.423589
Thermal correction to Gibbs Free Energy=	0.347994
Sum of electronic and zero-point Energies=	-842.637783
Sum of electronic and thermal Energies=	-842.615561
Sum of electronic and thermal Enthalpies=	-842.614617
Sum of electronic and thermal Free Energies=	-842.690211

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.790989	-0.530430	-0.147891
2	6	0	1.856133	-1.245245	0.238480
3	7	0	2.982713	-1.121001	-0.592929
4	8	0	1.953969	-1.973669	1.264258
5	6	0	-1.634186	-0.769479	0.036129
6	6	0	-4.105680	-1.138469	-1.238800
7	6	0	-2.608724	-1.594561	0.601551
8	6	0	-1.904222	-0.141245	-1.183784
9	6	0	-3.133817	-0.316979	-1.814344
10	6	0	-3.838096	-1.782933	-0.032305
11	1	0	-2.404805	-2.096083	1.544694
12	1	0	-1.136903	0.469392	-1.648682
13	1	0	-3.331439	0.179261	-2.759671
14	1	0	-4.583043	-2.433386	0.415635
15	1	0	-5.061765	-1.281183	-1.732767
16	6	0	-0.308286	-0.565720	0.744325
17	6	0	3.971326	-2.183522	-0.536981
18	1	0	4.927868	-1.806758	-0.909946
19	1	0	3.680460	-3.050330	-1.152529
20	1	0	4.092850	-2.515091	0.492146
21	6	0	2.829721	-0.520420	-1.905277
22	1	0	2.319245	0.439086	-1.825879
23	1	0	2.254409	-1.159395	-2.593401
24	1	0	3.822992	-0.356970	-2.332442
25	6	0	1.803798	2.930360	-0.214363
26	1	0	2.387459	2.071959	0.131504
27	1	0	1.751924	3.670731	0.590028
28	1	0	2.320237	3.386265	-1.071313
29	6	0	-1.622782	1.117793	2.173182
30	1	0	-1.502339	2.057235	2.714535
31	1	0	-1.869444	0.317693	2.875598
32	1	0	-2.415285	1.218590	1.433446
33	7	0	0.452893	2.481457	-0.552499
34	6	0	-0.362192	3.536156	-1.150092
35	1	0	0.105032	3.976364	-2.042387
36	1	0	-0.513029	4.331111	-0.414047
37	1	0	-1.340292	3.133128	-1.425209
38	7	0	-0.345374	0.798888	1.495618
39	6	0	0.783765	0.880310	2.453846
40	1	0	0.868564	1.907538	2.812218
41	1	0	1.699457	0.579655	1.947976
42	1	0	0.586811	0.206297	3.290486
43	1	0	-0.208190	-1.305531	1.551160
44	1	0	0.538815	1.683241	-1.181528
45	1	0	-0.150429	1.527868	0.730814

1b.2Me$_2$NH-ts2

Zero-point correction=	0.397041
(Hartree/Particle)	
Thermal correction to Energy=	0.418549
Thermal correction to Enthalpy=	0.419493
Thermal correction to Gibbs Free Energy=	0.346116
Sum of electronic and zero-point Energies=	-842.636226
Sum of electronic and thermal Energies=	-842.614719
Sum of electronic and thermal Enthalpies=	-842.613775
Sum of electronic and thermal Free Energies=	-842.687152

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.859925	-0.440509	-0.074187
2	6	0	1.914367	-1.137363	0.350169
3	7	0	3.050977	-1.067129	-0.487164
4	8	0	2.015011	-1.813482	1.413199
5	6	0	-1.556905	-0.782804	0.108388
6	6	0	-3.983680	-1.430816	-1.154674
7	6	0	-2.549055	-1.495529	0.788264
8	6	0	-1.787500	-0.422046	-1.222332
9	6	0	-2.993380	-0.733948	-1.848670
10	6	0	-3.754482	-1.819341	0.164820
11	1	0	-2.375973	-1.798990	1.818403
12	1	0	-1.001232	0.075892	-1.780977
13	1	0	-3.156078	-0.443376	-2.882375
14	1	0	-4.512124	-2.375811	0.708286
15	1	0	-4.920823	-1.679248	-1.643243
16	6	0	-0.261164	-0.414821	0.817068
17	6	0	4.006958	-2.156475	-0.385161
18	1	0	4.967906	-1.832892	-0.795417
19	1	0	3.679150	-3.049312	-0.943407
20	1	0	4.137248	-2.430736	0.659556
21	6	0	2.896192	-0.553001	-1.835164
22	1	0	2.422682	0.428554	-1.818183
23	1	0	2.288152	-1.214466	-2.472483
24	1	0	3.887083	-0.451593	-2.286584
25	6	0	1.588917	3.028355	-0.461006
26	1	0	2.301204	2.309496	-0.051167
27	1	0	1.408978	3.822197	0.266451
28	1	0	1.989658	3.461500	-1.380901
29	6	0	-1.654787	1.321787	2.011302
30	1	0	-1.588479	2.327083	2.434449
31	1	0	-1.901810	0.616123	2.816495
32	1	0	-2.450859	1.303351	1.265839
33	7	0	0.320327	2.326164	-0.730207
34	6	0	-0.709799	3.176025	-1.350639
35	1	0	-0.353794	3.582250	-2.300280
36	1	0	-0.943560	3.996351	-0.669430
37	1	0	-1.609454	2.581311	-1.519012
38	7	0	-0.365034	0.991818	1.390681
39	6	0	0.719291	1.197213	2.364689
40	1	0	0.757164	2.252254	2.648942
41	1	0	1.669662	0.905668	1.915745
42	1	0	0.548628	0.589292	3.263272
43	1	0	-0.138007	-1.089356	1.679413
44	1	0	0.525288	1.494553	-1.293056
45	1	0	-0.063905	1.791946	0.277895

1b.3Me$_2$NH-ts1

Zero-point correction= (Hartree/Particle)	0.492355
Thermal correction to Energy=	0.521126
Thermal correction to Enthalpy=	0.522070
Thermal correction to Gibbs Free Energy=	0.430924
Sum of electronic and zero-point Energies=	-977.649649
Sum of electronic and thermal Energies=	-977.620878
Sum of electronic and thermal Enthalpies=	-977.619934
Sum of electronic and thermal Free Energies=	-977.711081

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.393976	1.382964	-0.698428
2	6	0	0.951989	1.407017	-1.031436
3	7	0	1.516644	2.649752	-1.018002
4	8	0	1.630721	0.407207	-1.347291
5	6	0	-2.376974	0.044893	-0.403832
6	6	0	-5.153580	-0.259805	-0.235913
7	6	0	-2.970231	-1.190557	-0.678834
8	6	0	-3.185547	1.131908	-0.050992
9	6	0	-4.566352	0.978055	0.038050
10	6	0	-4.354029	-1.343194	-0.599362
11	6	0	-0.903247	0.189344	-0.489426
12	7	0	2.523761	-0.572494	1.371378
13	1	0	-0.357231	-0.711562	-0.788738
14	1	0	-2.345454	-2.035347	-0.959627
15	1	0	-4.806604	-2.305138	-0.819062
16	1	0	-6.230856	-0.377338	-0.169804
17	1	0	-5.187556	1.823606	0.317024
18	1	0	-2.715621	2.090989	0.145591
19	7	0	-0.476616	-0.275341	1.521068
20	6	0	3.351477	-1.589723	2.008365
21	1	0	3.142132	-1.611149	3.083143
22	1	0	4.429905	-1.405989	1.876412
23	1	0	3.115224	-2.570867	1.588907
24	6	0	-1.219965	-1.397794	2.080336
25	1	0	-2.278012	-1.127344	2.156631
26	1	0	-0.854884	-1.675353	3.078391
27	1	0	-1.135730	-2.264634	1.419171
28	6	0	2.895147	0.774583	1.791515
29	1	0	2.290829	1.511401	1.252403
30	1	0	3.958762	1.001792	1.614232
31	1	0	2.698537	0.890054	2.863101
32	6	0	-0.633113	0.952876	2.285486
33	1	0	-0.177327	1.779387	1.730639
34	1	0	-0.166886	0.881306	3.276608
35	1	0	-1.699556	1.165473	2.413654
36	1	0	0.529093	-0.504755	1.453391
37	7	0	2.041865	-2.559533	-1.206446
38	6	0	2.132477	-3.255576	-2.483040
39	1	0	2.550563	-4.256168	-2.327884
40	1	0	2.799420	-2.710494	-3.155819
41	1	0	1.155481	-3.374436	-2.981782
42	6	0	1.084176	-3.192783	-0.313640
43	1	0	1.004321	-2.610700	0.609666
44	1	0	1.432141	-4.198158	-0.050005
45	1	0	0.075582	-3.294927	-0.753959

46	1	0	1.762417	-1.592500	-1.368868
47	1	0	2.616282	-0.636696	0.358441
48	6	0	0.845853	3.840395	-0.525424
49	1	0	-0.215117	3.642399	-0.400330
50	1	0	0.986871	4.659006	-1.238951
51	1	0	1.275934	4.146350	0.437873
52	6	0	2.927321	2.817069	-1.311076
53	1	0	3.475154	3.104089	-0.403861
54	1	0	3.059213	3.608835	-2.055914
55	1	0	3.333035	1.883527	-1.693996

1b.3Me$_2$NH-I1

Zero-point correction=	0.495302
(Hartree/Particle)	
Thermal correction to Energy=	0.523462
Thermal correction to Enthalpy=	0.524406
Thermal correction to Gibbs Free Energy=	0.434916
Sum of electronic and zero-point Energies=	-977.659572
Sum of electronic and thermal Energies=	-977.631412
Sum of electronic and thermal Enthalpies=	-977.630468
Sum of electronic and thermal Free Energies=	-977.719958

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.737582	1.278316	0.021173
2	6	0	0.538758	1.506847	-0.316048
3	7	0	1.070384	2.734893	0.082913
4	8	0	1.300839	0.696539	-0.921460
5	6	0	-2.694175	-0.101856	-0.465376
6	6	0	-5.487203	-0.335794	-0.593877
7	6	0	-3.295455	-0.941655	-1.406879
8	6	0	-3.508299	0.633641	0.402499
9	6	0	-4.895034	0.514135	0.342668
10	6	0	-4.684582	-1.060826	-1.472853
11	6	0	-1.183813	0.006887	-0.400371
12	7	0	2.007518	-0.981616	1.476577
13	1	0	-0.751511	-0.315079	-1.358361
14	1	0	-2.673946	-1.500139	-2.103442
15	1	0	-5.136075	-1.714178	-2.213048
16	1	0	-6.568166	-0.424346	-0.643409
17	1	0	-5.516157	1.090426	1.021796
18	1	0	-3.040683	1.308779	1.112303
19	7	0	-0.635903	-1.089120	0.569027
20	6	0	2.484618	-2.234060	2.057811
21	1	0	1.806290	-2.554284	2.856618
22	1	0	3.493613	-2.141260	2.487647
23	1	0	2.504222	-3.012612	1.290001
24	6	0	-0.757856	-2.466725	0.046334
25	1	0	-1.806343	-2.769431	0.041444
26	1	0	-0.183369	-3.136181	0.690316
27	1	0	-0.356398	-2.498605	-0.968032
28	6	0	2.067828	0.124057	2.432527
29	1	0	1.759869	1.050523	1.938392

30	1	0	3.077174	0.261327	2.849613
31	1	0	1.383703	-0.072147	3.265641
32	6	0	-1.185004	-0.985483	1.939815
33	1	0	-1.137916	0.060456	2.245395
34	1	0	-0.569574	-1.599206	2.600706
35	1	0	-2.216437	-1.340606	1.952998
36	1	0	0.408997	-0.913954	0.692386
37	7	0	3.764087	-0.820432	-1.131750
38	6	0	5.029816	-0.572987	-1.807466
39	1	0	5.737224	-1.374487	-1.568599
40	1	0	5.457597	0.370767	-1.459553
41	1	0	4.931987	-0.528604	-2.905164
42	6	0	3.111541	-2.027476	-1.620109
43	1	0	2.131116	-2.129229	-1.143520
44	1	0	3.713060	-2.905817	-1.360094
45	1	0	2.963523	-2.029387	-2.713167
46	1	0	3.123792	-0.038091	-1.269727
47	1	0	2.601959	-0.747375	0.678812
48	6	0	0.177344	3.818645	0.448166
49	1	0	-0.621906	3.439944	1.082637
50	1	0	-0.276905	4.296899	-0.433952
51	1	0	0.744735	4.576422	0.995732
52	6	0	2.334828	3.141095	-0.500290
53	1	0	2.221883	3.512257	-1.531200
54	1	0	3.025272	2.297538	-0.511986
55	1	0	2.763253	3.942407	0.107609

1b.3Me$_2$NH-I2

Zero-point correction=	0.495935
(Hartree/Particle)	
Thermal correction to Energy=	0.523541
Thermal correction to Enthalpy=	0.524485
Thermal correction to Gibbs Free Energy=	0.437604
Sum of electronic and zero-point Energies=	-977.659329
Sum of electronic and thermal Energies=	-977.631723
Sum of electronic and thermal Enthalpies=	-977.630778
Sum of electronic and thermal Free Energies=	-977.717660

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.630845	0.084470	-1.720493
2	1	0	-0.871479	0.950036	-1.126697
3	1	0	-0.763571	2.482438	0.361040
4	1	0	0.876195	0.968967	1.096047
5	7	0	0.862733	1.917123	1.491271
6	7	0	-1.309336	2.486882	-0.509885
7	6	0	-0.812151	3.563905	-1.366329
8	1	0	-1.025437	4.560189	-0.952300
9	1	0	-1.284205	3.498019	-2.352775
10	1	0	0.269036	3.464480	-1.493913
11	6	0	-2.737543	2.629817	-0.232981
12	1	0	-2.979905	3.598969	0.226810
13	1	0	-3.068764	1.830323	0.434740

14	1	0	-3.298691	2.548375	-1.169906
15	6	0	-1.851877	-0.230407	-2.499501
16	1	0	-1.673788	-1.122837	-3.104671
17	1	0	-2.084117	0.615756	-3.148264
18	1	0	-2.681970	-0.405599	-1.815770
19	6	0	0.470542	0.503893	-2.620072
20	1	0	0.746646	-0.333661	-3.261842
21	1	0	1.325987	0.793630	-2.011018
22	1	0	0.127791	1.352054	-3.214926
23	6	0	0.825506	1.864704	2.946081
24	1	0	1.750863	1.455921	3.387126
25	1	0	-0.015077	1.246929	3.276049
26	1	0	0.684357	2.873383	3.349456
27	6	0	2.041892	2.619995	1.002221
28	1	0	2.980710	2.224853	1.426457
29	1	0	1.977880	3.684446	1.255110
30	1	0	2.097605	2.529001	-0.086803
31	7	0	0.956617	-0.749245	-0.051419
32	6	0	-0.194620	-1.090031	-0.798805
33	6	0	-1.367453	-1.431190	0.099907
34	6	0	-3.524437	-2.091052	1.764649
35	6	0	-2.063524	-2.626609	-0.083012
36	6	0	-1.756620	-0.568166	1.129969
37	6	0	-2.832192	-0.892341	1.953828
38	6	0	-3.135237	-2.960107	0.747219
39	1	0	-1.765647	-3.302129	-0.881263
40	1	0	-1.209367	0.359040	1.285890
41	1	0	-3.129311	-0.212151	2.746929
42	1	0	-3.664491	-3.895935	0.596430
43	1	0	-4.360256	-2.345168	2.409070
44	6	0	2.110907	-1.201739	-0.574648
45	8	0	2.253243	-1.807371	-1.668752
46	7	0	3.265228	-0.922833	0.176798
47	6	0	3.176272	-0.765376	1.618133
48	1	0	3.209589	-1.740129	2.131768
49	1	0	2.249465	-0.266553	1.887772
50	1	0	4.021323	-0.165816	1.972116
51	6	0	4.496423	-1.562382	-0.251343
52	1	0	5.339485	-1.051688	0.222412
53	1	0	4.597773	-1.494282	-1.332853
54	1	0	4.532624	-2.625696	0.035246
55	1	0	-0.023297	-1.908460	-1.513257

1b.3Me$_2$NH-I3

Zero-point correction=	0.496567
(Hartree/Particle)	
Thermal correction to Energy=	0.523438
Thermal correction to Enthalpy=	0.524382
Thermal correction to Gibbs Free Energy=	0.440566
Sum of electronic and zero-point Energies=	-977.656886
Sum of electronic and thermal Energies=	-977.630015
Sum of electronic and thermal Enthalpies=	-977.629071
Sum of electronic and thermal Free Energies=	-977.712887

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.286710	-0.017669	2.184340
2	1	0	0.773014	1.410810	1.277627
3	1	0	0.868664	1.952559	-0.345845
4	1	0	-0.315760	0.762375	-1.420215
5	7	0	0.336517	1.402184	-1.895854
6	7	0	0.881052	2.285945	0.673758
7	6	0	-0.321826	3.121144	0.883851
8	1	0	-0.253526	4.019990	0.268333
9	1	0	-0.391493	3.401489	1.936542
10	1	0	-1.195383	2.531725	0.599184
11	6	0	2.138349	2.995463	0.987655
12	1	0	2.193334	3.907367	0.391404
13	1	0	2.986818	2.355119	0.745801
14	1	0	2.156796	3.248711	2.048952
15	6	0	1.148257	-0.659564	3.183675
16	1	0	0.623910	-1.496163	3.673529
17	1	0	1.420571	0.071783	3.949737
18	1	0	2.061242	-1.047913	2.734005
19	6	0	-0.930719	0.424239	2.876770
20	1	0	-1.449813	-0.425128	3.348421
21	1	0	-1.614934	0.898531	2.174087
22	1	0	-0.652949	1.141468	3.654905
23	6	0	1.171516	0.627227	-2.811808
24	1	0	0.594639	0.246889	-3.669366
25	1	0	1.613992	-0.218660	-2.284255
26	1	0	1.977513	1.259447	-3.198984
27	6	0	-0.383977	2.454060	-2.610803
28	1	0	-1.021005	2.055247	-3.415442
29	1	0	0.337819	3.143649	-3.060151
30	1	0	-1.013947	3.025684	-1.924841
31	7	0	-1.056421	-0.395474	0.207874
32	6	0	-0.054113	-0.962109	1.075732
33	6	0	1.183326	-1.328799	0.256621
34	6	0	3.350201	-2.130000	-1.362200
35	6	0	1.068486	-2.417855	-0.617264
36	6	0	2.402157	-0.648409	0.298756
37	6	0	3.477746	-1.042678	-0.502067
38	6	0	2.134897	-2.818367	-1.417545
39	1	0	0.120254	-2.949127	-0.667358
40	1	0	2.538836	0.182248	0.983459
41	1	0	4.415214	-0.496847	-0.446838
42	1	0	2.021071	-3.667776	-2.084677
43	1	0	4.185566	-2.440030	-1.982249
44	6	0	-2.255211	-0.978499	0.307194
45	8	0	-2.570331	-1.985988	1.002356

46	1	0	-0.422555	-1.893327	1.542386
47	7	0	-3.289978	-0.369627	-0.438701
48	6	0	-4.418132	-1.211777	-0.798864
49	1	0	-4.188079	-1.871731	-1.651926
50	1	0	-5.265445	-0.578823	-1.076971
51	1	0	-4.696836	-1.830223	0.051603
52	6	0	-2.940805	0.611651	-1.443844
53	1	0	-2.366370	0.179275	-2.281358
54	1	0	-2.345618	1.408576	-0.997590
55	1	0	-3.858967	1.048836	-1.845817

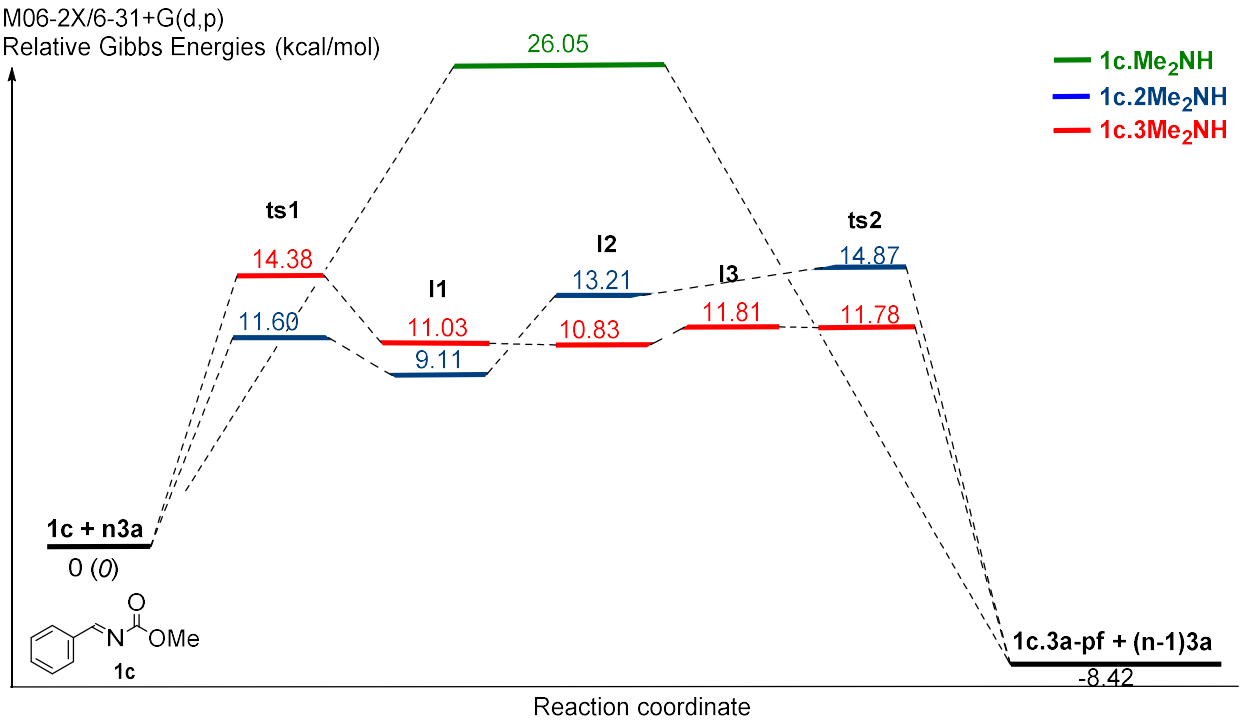
1b.3Me_2NH-ts2

Convergence not reached

2.3.-Computational data (includes IRC where appropriate) for the addition of n dimethylamine (3a) molecules (n=1-3) to imine derivative 1c in gas phase, Et_2NH, CH_2Cl_2, CH_3CN and CH_3OH

2.3.1.-M06-2X/6-31+G(d,p) calculations

Energy profiles of the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1c** in gas phase.



1c.Me_2NH-ts

Zero-point correction=	0.260079
(Hartree/Particle)	
Thermal correction to Energy=	0.275065
Thermal correction to Enthalpy=	0.276009
Thermal correction to Gibbs Free Energy=	0.216330
Sum of electronic and zero-point Energies=	-688.184226
Sum of electronic and thermal Energies=	-688.169241
Sum of electronic and thermal Enthalpies=	-688.168297
Sum of electronic and thermal Free Energies=	-688.227975

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.252150	0.273106	-0.478196
2	6	0	2.194389	-0.459724	0.152846
3	8	0	3.326104	-0.558760	-0.593703
4	8	0	2.096058	-0.990873	1.255536
5	6	0	-1.135389	-0.244049	0.183905
6	6	0	-3.461063	-1.773540	-0.061280
7	6	0	-2.196914	-0.062665	1.074088
8	6	0	-1.235803	-1.207394	-0.819168
9	6	0	-2.396531	-1.969735	-0.940305
10	6	0	-3.359744	-0.818869	0.950408
11	1	0	-2.105427	0.664618	1.878987
12	1	0	-0.390193	-1.350856	-1.485954
13	1	0	-2.468430	-2.723944	-1.718053
14	1	0	-4.178094	-0.674596	1.648947
15	1	0	-4.362402	-2.371467	-0.154979
16	6	0	0.098061	0.614424	0.314296
17	1	0	0.326521	0.757615	1.379632
18	1	0	0.999350	1.610242	-0.800822
19	6	0	-1.118343	2.170955	-1.313594
20	1	0	-0.986983	3.133136	-1.812547
21	1	0	-2.102845	2.128889	-0.836570
22	1	0	-1.040055	1.365451	-2.045079
23	7	0	-0.047748	2.015418	-0.319387
24	6	0	0.005138	3.115464	0.648637
25	1	0	0.084638	4.064524	0.114482
26	1	0	0.881345	2.985563	1.287036
27	1	0	-0.899548	3.123660	1.266542
28	6	0	4.362749	-1.327740	0.001042
29	1	0	5.184698	-1.317952	-0.714947
30	1	0	4.029888	-2.352212	0.186151
31	1	0	4.680130	-0.888035	0.950344

1c.Me_2NH-pf

Zero-point correction=	0.264790
(Hartree/Particle)	
Thermal correction to Energy=	0.280069
Thermal correction to Enthalpy=	0.281014
Thermal correction to Gibbs Free Energy=	0.221380
Sum of electronic and zero-point Energies=	-688.239500
Sum of electronic and thermal Energies=	-688.224220
Sum of electronic and thermal Enthalpies=	-688.223276
Sum of electronic and thermal Free Energies=	-688.282909

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.115534	-0.423333	0.224452
2	6	0	-2.393299	-0.346218	-0.242215
3	8	0	-3.171849	-1.266317	0.373533
4	8	0	-2.791386	0.422554	-1.089834
5	6	0	1.276541	-0.224797	-0.207483
6	6	0	3.846241	-1.344566	-0.040060
7	6	0	2.154604	-0.162579	-1.291897
8	6	0	1.706968	-0.851525	0.967634
9	6	0	2.980019	-1.410859	1.050228
10	6	0	3.430991	-0.717163	-1.212255
11	1	0	1.829944	0.318936	-2.211493
12	1	0	1.051515	-0.901667	1.834317
13	1	0	3.296653	-1.896506	1.968157
14	1	0	4.096845	-0.664619	-2.068016
15	1	0	4.837985	-1.780875	0.025080
16	6	0	-0.088155	0.440428	-0.317881
17	1	0	-0.314450	0.595081	-1.379303
18	1	0	-0.875626	-1.223457	0.789745
19	6	0	0.131516	1.819246	1.707971
20	1	0	-0.178465	2.793627	2.096567
21	1	0	1.204377	1.683549	1.932509
22	1	0	-0.441855	1.050429	2.233967
23	7	0	-0.170878	1.768591	0.289755
24	6	0	0.573449	2.764878	-0.456971
25	1	0	0.339936	3.755699	-0.056962
26	1	0	0.266713	2.741741	-1.507322
27	1	0	1.668253	2.622331	-0.404446
28	6	0	-4.530310	-1.280418	-0.062777
29	1	0	-4.586850	-1.517546	-1.127364
30	1	0	-4.996367	-0.308588	0.111686
31	1	0	-5.019232	-2.053399	0.528088

1c.2Me$_2$NH-ts1

Zero-point correction=	0.358234
(Hartree/Particle)	
Thermal correction to Energy=	0.379114
Thermal correction to Enthalpy=	0.380058
Thermal correction to Gibbs Free Energy=	0.306686
Sum of electronic and zero-point Energies=	-823.229905
Sum of electronic and thermal Energies=	-823.209025
Sum of electronic and thermal Enthalpies=	-823.208081
Sum of electronic and thermal Free Energies=	-823.281453

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.036443	1.413880	0.072409
2	6	0	1.305943	1.589002	-0.419830
3	8	0	1.945737	2.569824	0.247294
4	8	0	1.860992	0.959852	-1.316659
5	6	0	-2.126311	0.417344	-0.291080
6	6	0	-4.830559	0.083673	0.328591
7	6	0	-2.977039	-0.248430	-1.178029
8	6	0	-2.641444	0.930932	0.904160
9	6	0	-3.987331	0.759255	1.212810
10	6	0	-4.325534	-0.415840	-0.871088
11	6	0	-0.693502	0.575514	-0.625931
12	7	0	2.974399	-1.388668	0.001664
13	1	0	-0.396469	0.288721	-1.639642
14	1	0	-2.578726	-0.631113	-2.115059
15	1	0	-4.981462	-0.929584	-1.567045
16	1	0	-5.881325	-0.044766	0.569993
17	1	0	-4.383918	1.158405	2.141293
18	1	0	-1.970500	1.470501	1.565691
19	7	0	-0.061386	-1.374143	0.008796
20	6	0	3.849172	-2.530967	-0.214302
21	1	0	3.656363	-3.287477	0.553937
22	1	0	4.920275	-2.272711	-0.170414
23	1	0	3.640115	-2.978634	-1.189032
24	6	0	-0.613885	-2.519702	-0.695848
25	1	0	-1.695723	-2.561108	-0.530767
26	1	0	-0.173230	-3.468497	-0.355845
27	1	0	-0.426131	-2.413569	-1.768596
28	6	0	3.256924	-0.701175	1.254088
29	1	0	2.605501	0.173336	1.355715
30	1	0	4.305122	-0.368828	1.341227
31	1	0	3.049008	-1.374277	2.093394
32	6	0	-0.266690	-1.424074	1.447453
33	1	0	0.059856	-0.472823	1.881858
34	1	0	0.293904	-2.245999	1.914789
35	1	0	-1.332821	-1.556929	1.659412
36	6	0	3.276791	2.827590	-0.182223
37	1	0	3.298909	3.082185	-1.244306
38	1	0	3.912947	1.952454	-0.016072
39	1	0	3.623563	3.665589	0.421178
40	1	0	3.045507	-0.724016	-0.766468
41	1	0	0.950018	-1.314483	-0.173043

1c.2Me$_2$NH-I1

Zero-point correction=	0.360944
(Hartree/Particle)	
Thermal correction to Energy=	0.381605
Thermal correction to Enthalpy=	0.382549
Thermal correction to Gibbs Free Energy=	0.309535
Sum of electronic and zero-point Energies=	-823.234007
Sum of electronic and thermal Energies=	-823.213346
Sum of electronic and thermal Enthalpies=	-823.212402
Sum of electronic and thermal Free Energies=	-823.285417

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.145942	1.543512	0.037956
2	6	0	1.127202	1.772596	-0.257307
3	8	0	1.537542	3.017716	0.109031
4	8	0	1.949119	0.985062	-0.787999
5	6	0	-2.094988	0.134776	-0.279942
6	6	0	-4.848522	-0.225613	0.081699
7	6	0	-2.818837	-0.702409	-1.132339
8	6	0	-2.767452	0.814275	0.739664
9	6	0	-4.135584	0.629181	0.922824
10	6	0	-4.189516	-0.886045	-0.953416
11	6	0	-0.602431	0.315950	-0.454002
12	7	0	3.014893	-1.445895	0.163339
13	1	0	-0.304529	0.097626	-1.493717
14	1	0	-2.311938	-1.201058	-1.955969
15	1	0	-4.742865	-1.532464	-1.627753
16	1	0	-5.916454	-0.363059	0.221739
17	1	0	-4.650578	1.163052	1.715731
18	1	0	-2.199487	1.507692	1.352388
19	7	0	0.134165	-0.873438	0.302682
20	6	0	3.179606	-1.881157	-1.219675
21	1	0	2.764213	-2.889165	-1.339856
22	1	0	4.234110	-1.913799	-1.536245
23	1	0	2.641395	-1.188276	-1.872109
24	6	0	-0.126541	-2.219288	-0.239530
25	1	0	-1.147137	-2.521493	0.001128
26	1	0	0.594362	-2.911831	0.201549
27	1	0	0.011064	-2.195704	-1.322801
28	6	0	3.810718	-2.232526	1.094487
29	1	0	3.707972	-1.829384	2.105413
30	1	0	4.881358	-2.259054	0.835377
31	1	0	3.445653	-3.265935	1.102757
32	6	0	-0.056805	-0.825781	1.767124
33	1	0	0.077058	0.208250	2.088636
34	1	0	0.687886	-1.476123	2.231498
35	1	0	-1.065349	-1.167018	2.009139
36	1	0	3.262833	-0.458614	0.207659
37	1	0	1.142017	-0.690314	0.121982
38	6	0	2.897075	3.317740	-0.153450
39	1	0	3.564570	2.660195	0.413165
40	1	0	3.037965	4.351330	0.164380
41	1	0	3.127238	3.213475	-1.217016

1c.2Me$_2$NH-I2

Zero-point correction=	0.360779
(Hartree/Particle)	
Thermal correction to Energy=	0.381274
Thermal correction to Enthalpy=	0.382218
Thermal correction to Gibbs Free Energy=	0.310834
Sum of electronic and zero-point Energies=	-823.228936
Sum of electronic and thermal Energies=	-823.208441
Sum of electronic and thermal Enthalpies=	-823.207497
Sum of electronic and thermal Free Energies=	-823.278881

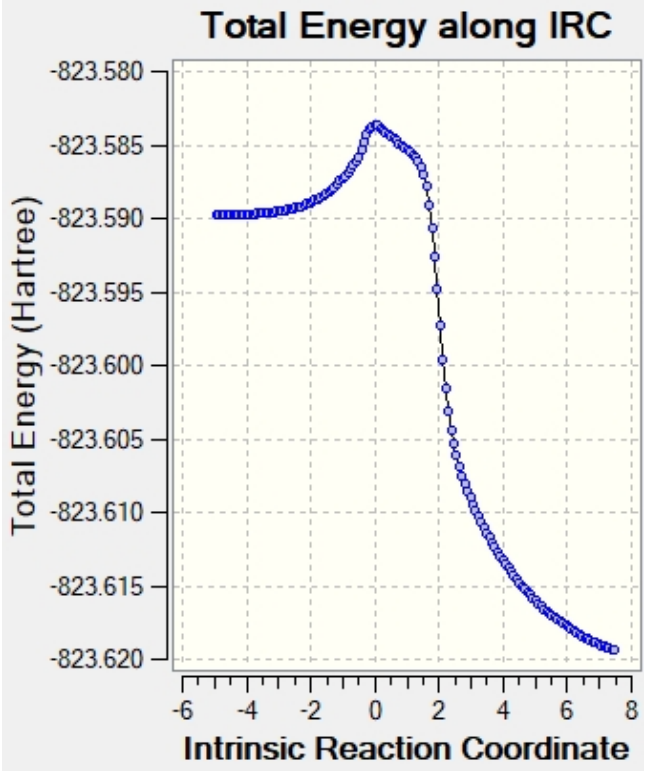
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.842653	-0.568996	-0.459861
2	6	0	1.926319	-1.332224	-0.276507
3	8	0	2.836489	-1.136699	-1.282186
4	8	0	2.186193	-2.117691	0.646097
5	6	0	-1.552879	-0.710708	-0.045047
6	6	0	-4.166872	-0.647801	-1.053358
7	6	0	-2.571353	-1.436906	0.575977
8	6	0	-1.848699	0.021725	-1.197491
9	6	0	-3.149910	0.062135	-1.692726
10	6	0	-3.872911	-1.408126	0.076985
11	1	0	-2.340747	-2.039786	1.451816
12	1	0	-1.037523	0.519277	-1.719389
13	1	0	-3.369431	0.632759	-2.590209
14	1	0	-4.653293	-1.984244	0.564698
15	1	0	-5.178786	-0.623313	-1.445787
16	6	0	-0.147163	-0.723826	0.521579
17	6	0	2.152810	2.791388	-0.164170
18	1	0	2.747638	1.937143	0.170515
19	1	0	2.156843	3.558694	0.617951
20	1	0	2.631467	3.212392	-1.060533
21	6	0	-1.197693	0.824759	2.340999
22	1	0	-0.951041	1.657035	3.004150
23	1	0	-1.468642	-0.049499	2.938679
24	1	0	-2.033847	1.097546	1.698594
25	7	0	0.784111	2.348520	-0.419100
26	6	0	-0.033616	3.380613	-1.044777
27	1	0	0.393824	3.745896	-1.990524
28	1	0	-0.126258	4.233596	-0.364320
29	1	0	-1.036212	2.990011	-1.239794
30	7	0	-0.013912	0.508859	1.516350
31	6	0	1.186729	0.337813	2.367533
32	1	0	1.398673	1.281542	2.876140
33	1	0	2.027556	0.037112	1.745987
34	1	0	0.994486	-0.450855	3.099025
35	1	0	-0.009477	-1.594900	1.181284
36	1	0	0.833683	1.496349	-0.989645
37	1	0	0.187729	1.324126	0.854512
38	6	0	4.011280	-1.925529	-1.185468
39	1	0	4.613609	-1.668031	-2.057581
40	1	0	3.769925	-2.991685	-1.193294
41	1	0	4.562143	-1.704606	-0.266452

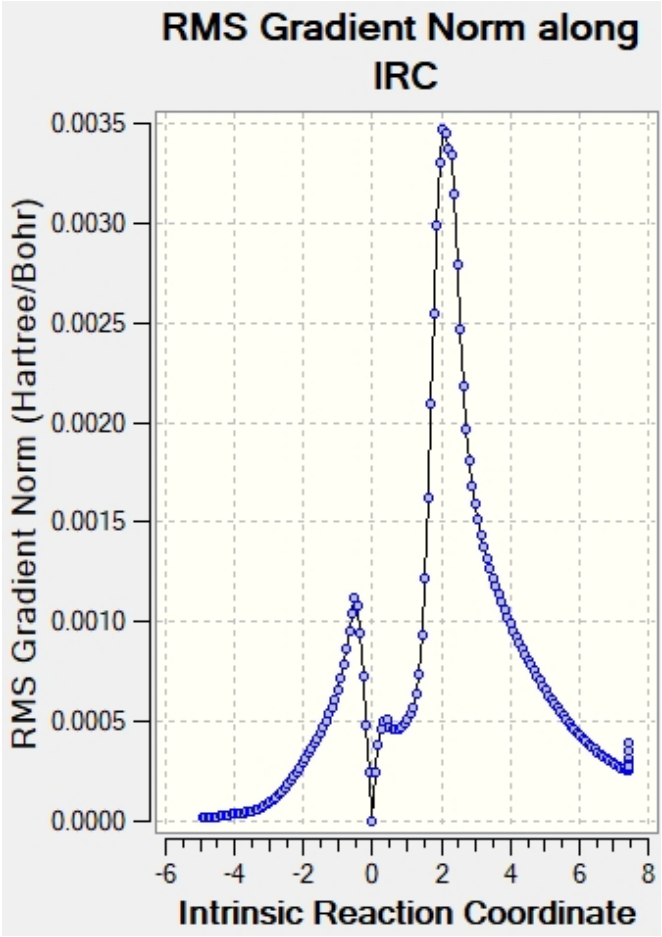
1c.2Me$_2$NH-ts2

Zero-point correction=	0.355754
(Hartree/Particle)	
Thermal correction to Energy=	0.375630
Thermal correction to Enthalpy=	0.376575
Thermal correction to Gibbs Free Energy=	0.307384
Sum of electronic and zero-point Energies=	-823.227880
Sum of electronic and thermal Energies=	-823.208004
Sum of electronic and thermal Enthalpies=	-823.207060
Sum of electronic and thermal Free Energies=	-823.276250

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.845582	-0.553984	-0.381191
2	6	0	1.907207	-1.322271	-0.129455
3	8	0	2.838526	-1.202433	-1.137353
4	8	0	2.144487	-2.050950	0.841362
5	6	0	-1.556291	-0.655150	0.037144
6	6	0	-4.157746	-0.781723	-1.013231
7	6	0	-2.592580	-1.245055	0.765769
8	6	0	-1.831409	-0.167575	-1.242587
9	6	0	-3.124243	-0.218688	-1.760806
10	6	0	-3.885254	-1.308399	0.248199
11	1	0	-2.383149	-1.668193	1.745817
12	1	0	-1.009167	0.203484	-1.846523
13	1	0	-3.321093	0.161443	-2.759094
14	1	0	-4.676632	-1.777472	0.825022
15	1	0	-5.162929	-0.831738	-1.420346
16	6	0	-0.159508	-0.553428	0.628116
17	6	0	2.228550	2.573219	-0.408721
18	1	0	2.818855	1.755503	0.010829
19	1	0	2.234351	3.424960	0.277601
20	1	0	2.675996	2.877481	-1.360446
21	6	0	-1.218955	1.219936	2.140398
22	1	0	-0.974905	2.143436	2.673921
23	1	0	-1.549850	0.471879	2.873389
24	1	0	-2.036238	1.412830	1.444204
25	7	0	0.854461	2.096874	-0.609263
26	6	0	-0.007107	3.038924	-1.327080
27	1	0	0.379775	3.236172	-2.332225
28	1	0	-0.055849	3.983074	-0.776862
29	1	0	-1.013581	2.621669	-1.405337
30	7	0	-0.024373	0.769131	1.417571
31	6	0	1.111162	0.653716	2.348944
32	1	0	1.359397	1.643661	2.745510
33	1	0	1.971280	0.231396	1.828881
34	1	0	0.859060	-0.015588	3.181410
35	1	0	-0.021841	-1.358612	1.367139
36	1	0	0.905680	1.129108	-1.030337
37	1	0	0.370952	1.632791	0.433924
38	6	0	3.984608	-2.024193	-0.988416
39	1	0	4.613011	-1.817584	-1.856189
40	1	0	3.708960	-3.082035	-0.966176
41	1	0	4.523535	-1.790622	-0.065635

1c.2Me$_2$NH-ts2





1c.3Me$_2$NH-ts1

Zero-point correction=	0.452321
(Hartree/Particle)	
Thermal correction to Energy=	0.479284
Thermal correction to Enthalpy=	0.480228
Thermal correction to Gibbs Free Energy=	0.392683
Sum of electronic and zero-point Energies=	-958.247829
Sum of electronic and thermal Energies=	-958.220865
Sum of electronic and thermal Enthalpies=	-958.219921
Sum of electronic and thermal Free Energies=	-958.307466

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.753642	1.588183	-0.310607
2	6	0	0.570707	1.804884	-0.612481
3	8	0	0.933186	3.059258	-0.284539
4	8	0	1.375414	1.012065	-1.091123
5	6	0	-2.646523	0.121793	-0.557927
6	6	0	-5.367978	-0.465369	-0.326012
7	6	0	-3.176839	-1.018961	-1.167443
8	6	0	-3.490685	0.977306	0.158357
9	6	0	-4.844672	0.680092	0.276649
10	6	0	-4.533451	-1.313524	-1.052849
11	6	0	-1.203703	0.416451	-0.680689
12	7	0	2.301512	-0.371088	1.495518
13	1	0	-0.632283	-0.213568	-1.369676
14	1	0	-2.521106	-1.674451	-1.736479
15	1	0	-4.939623	-2.199247	-1.531314
16	1	0	-6.426002	-0.691835	-0.235463
17	1	0	-5.496996	1.344669	0.834828
18	1	0	-3.063162	1.870884	0.602741
19	7	0	-0.559444	-0.950319	0.918482
20	6	0	3.099270	-1.406129	2.134152
21	1	0	2.578926	-1.782547	3.022844
22	1	0	4.095444	-1.052238	2.448353
23	1	0	3.236864	-2.235216	1.434900
24	6	0	-0.845100	-2.368131	0.775068
25	1	0	-1.929579	-2.523175	0.775045
26	1	0	-0.409012	-2.966923	1.589466
27	1	0	-0.443093	-2.734204	-0.174980
28	6	0	2.221456	0.841816	2.295565
29	1	0	1.599988	1.587918	1.789300
30	1	0	3.207941	1.289255	2.505301
31	1	0	1.749145	0.615177	3.258444
32	6	0	-1.097482	-0.379664	2.142855
33	1	0	-0.951902	0.706199	2.120084
34	1	0	-0.608578	-0.788826	3.039352
35	1	0	-2.171531	-0.586140	2.203656
36	1	0	0.462262	-0.791612	0.921872
37	7	0	3.443166	-1.015572	-1.289003
38	6	0	4.690412	-1.496689	-1.858909
39	1	0	5.022483	-2.381841	-1.304981
40	1	0	5.464069	-0.731119	-1.760737
41	1	0	4.607767	-1.778474	-2.922675
42	6	0	2.352749	-1.964012	-1.450965
43	1	0	1.430926	-1.502460	-1.087172
44	1	0	2.556068	-2.863698	-0.856981
45	1	0	2.199496	-2.279735	-2.497509

46	1	0	3.164774	-0.130194	-1.703716
47	1	0	2.709409	-0.174653	0.579909
48	6	0	2.292702	3.386723	-0.545821
49	1	0	2.513570	3.295825	-1.612357
50	1	0	2.963019	2.725845	0.012507
51	1	0	2.415605	4.417863	-0.217299

1c.3Me$_2$NH-I1

Zero-point correction=	0.456195
(Hartree/Particle)	
Thermal correction to Energy=	0.481998
Thermal correction to Enthalpy=	0.482942
Thermal correction to Gibbs Free Energy=	0.400444
Sum of electronic and zero-point Energies=	-958.257059
Sum of electronic and thermal Energies=	-958.231256
Sum of electronic and thermal Enthalpies=	-958.230312
Sum of electronic and thermal Free Energies=	-958.312809

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.355518	-1.512557	-0.300646
2	6	0	-0.796982	-1.620370	-0.939474
3	8	0	-1.187086	-2.926125	-1.070970
4	8	0	-1.550534	-0.725546	-1.397372
5	6	0	2.314669	-0.065720	-0.191342
6	6	0	5.105099	0.172261	-0.289390
7	6	0	2.912819	1.143446	-0.554705
8	6	0	3.127756	-1.165963	0.095306
9	6	0	4.514595	-1.044247	0.054141
10	6	0	4.301101	1.265997	-0.603303
11	6	0	0.804551	-0.190449	-0.124226
12	7	0	-2.393121	-0.085447	1.319759
13	1	0	0.342174	0.545702	-0.798590
14	1	0	2.288174	1.993286	-0.823018
15	1	0	4.751793	2.209127	-0.897185
16	1	0	6.186376	0.262264	-0.329598
17	1	0	5.137393	-1.905295	0.277503
18	1	0	2.646948	-2.114262	0.315395
19	7	0	0.317795	0.299224	1.279818
20	6	0	-3.117516	0.982802	1.998995
21	1	0	-2.880575	0.959908	3.068723
22	1	0	-4.209250	0.890089	1.893381
23	1	0	-2.800047	1.943753	1.584410
24	6	0	0.493007	1.742961	1.530804
25	1	0	1.556093	1.989657	1.570789
26	1	0	0.023958	1.986678	2.488138
27	1	0	-0.015843	2.291777	0.734518
28	6	0	-2.785817	-1.425017	1.754037
29	1	0	-2.217179	-2.171805	1.191740
30	1	0	-3.860669	-1.612444	1.614304
31	1	0	-2.556137	-1.543677	2.818578
32	6	0	0.852586	-0.526903	2.381951
33	1	0	0.744431	-1.574071	2.095216

34	1	0	0.273602	-0.315455	3.284782
35	1	0	1.904467	-0.284378	2.549533
36	1	0	-0.751300	0.124751	1.267417
37	7	0	-1.848673	2.162604	-0.993315
38	6	0	-3.274266	2.402530	-1.163488
39	1	0	-3.562923	3.322814	-0.641258
40	1	0	-3.844907	1.574916	-0.730109
41	1	0	-3.574724	2.503506	-2.219611
42	6	0	-1.052154	3.159969	-1.690963
43	1	0	0.011113	2.906147	-1.619623
44	1	0	-1.196574	4.142450	-1.226077
45	1	0	-1.305227	3.253082	-2.760232
46	1	0	-1.630527	1.229472	-1.350148
47	1	0	-2.509958	-0.019712	0.306130
48	6	0	-2.393656	-3.134013	-1.785192
49	1	0	-2.334780	-2.712437	-2.791939
50	1	0	-3.245670	-2.677257	-1.269860
51	1	0	-2.524668	-4.215694	-1.834788

1c.3Me$_2$NH-I2

Zero-point correction= 0.455070
(Hartree/Particle)
Thermal correction to Energy= 0.481427
Thermal correction to Enthalpy= 0.482371
Thermal correction to Gibbs Free Energy= 0.397346
Sum of electronic and zero-point Energies= -958.255404
Sum of electronic and thermal Energies= -958.229048
Sum of electronic and thermal Enthalpies= -958.228103
Sum of electronic and thermal Free Energies= -958.313129

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.449140	-0.422161	1.753682
2	1	0	0.372564	0.610672	1.449992
3	1	0	-0.327641	2.214035	0.196950
4	1	0	-1.197134	0.745688	-1.281607
5	7	0	-1.427432	1.742770	-1.389459
6	7	0	0.114147	2.264919	1.132213
7	6	0	-0.856417	2.832837	2.065671
8	1	0	-1.105361	3.878287	1.829589
9	1	0	-0.453582	2.804172	3.085237
10	1	0	-1.777967	2.245724	2.040784
11	6	0	1.331859	3.068930	1.065145
12	1	0	1.130575	4.114171	0.786741
13	1	0	2.021297	2.637254	0.334983
14	1	0	1.826956	3.070264	2.043156
15	6	0	1.691375	-0.592320	2.533117
16	1	0	1.808435	-1.646169	2.802235
17	1	0	1.627587	0.010871	3.441672
18	1	0	2.544972	-0.271219	1.936905
19	6	0	-0.743944	-0.693746	2.589457
20	1	0	-0.767019	-1.751926	2.858161
21	1	0	-1.633277	-0.457112	2.007581

22	1	0	-0.698244	-0.063226	3.480569
23	6	0	-1.230109	2.172401	-2.765078
24	1	0	-1.918260	1.678716	-3.470455
25	1	0	-0.204970	1.952977	-3.079225
26	1	0	-1.385406	3.254668	-2.844716
27	6	0	-2.806815	1.915504	-0.954005
28	1	0	-3.532665	1.479444	-1.658477
29	1	0	-3.036603	2.981809	-0.834208
30	1	0	-2.943480	1.412246	0.008214
31	7	0	-0.747306	-0.918708	-0.289570
32	6	0	0.401279	-1.273297	0.433561
33	6	0	1.675726	-0.983104	-0.333791
34	6	0	4.037775	-0.417966	-1.731219
35	6	0	2.730868	-1.895432	-0.338370
36	6	0	1.804716	0.209502	-1.052160
37	6	0	2.981151	0.494212	-1.739593
38	6	0	3.907474	-1.617656	-1.035689
39	1	0	2.628413	-2.835433	0.199393
40	1	0	0.965078	0.899195	-1.082291
41	1	0	3.070237	1.423981	-2.294623
42	1	0	4.717976	-2.340113	-1.038650
43	1	0	4.951887	-0.198792	-2.274219
44	6	0	-1.779430	-1.753751	-0.128304
45	8	0	-1.880046	-2.752882	0.595001
46	8	0	-2.845246	-1.352049	-0.896121
47	1	0	0.401306	-2.311722	0.802874
48	6	0	-3.997355	-2.173165	-0.798407
49	1	0	-4.733814	-1.733437	-1.472605
50	1	0	-4.384108	-2.190993	0.224736
51	1	0	-3.774174	-3.200025	-1.099804

1c.3Me$_2$NH-I3

Zero-point correction= 0.455044
(Hartree/Particle)
Thermal correction to Energy= 0.480921
Thermal correction to Enthalpy= 0.481865
Thermal correction to Gibbs Free Energy= 0.398925
Sum of electronic and zero-point Energies= -958.255447
Sum of electronic and thermal Energies= -958.229570
Sum of electronic and thermal Enthalpies= -958.228625
Sum of electronic and thermal Free Energies= -958.311566

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.046686	-2.094757	0.897455
2	1	0	-0.079699	-0.271904	1.744267
3	1	0	0.012883	1.392159	1.323256
4	1	0	-0.170770	1.520296	-0.519047
5	7	0	0.072483	2.354259	0.042431
6	7	0	-0.226314	0.681405	2.138374
7	6	0	-1.668571	0.855906	2.413067
8	1	0	-1.835606	1.869851	2.785215
9	1	0	-1.996870	0.130191	3.161509
10	1	0	-2.199512	0.705297	1.469396
11	6	0	0.640631	0.907289	3.305357

12	1	0	0.472773	1.916111	3.688567
13	1	0	1.682992	0.808798	2.997462
14	1	0	0.417370	0.178569	4.088159
15	6	0	0.788745	-3.297646	0.907209
16	1	0	0.430039	-4.035721	0.170125
17	1	0	0.752865	-3.758584	1.898923
18	1	0	1.826948	-3.061738	0.671647
19	6	0	-1.424746	-2.511165	1.182273
20	1	0	-1.812907	-3.191450	0.408382
21	1	0	-2.086010	-1.644854	1.223021
22	1	0	-1.443613	-3.020023	2.151330
23	6	0	1.349557	2.924010	-0.372007
24	1	0	1.302903	3.347688	-1.386001
25	1	0	2.120396	2.149748	-0.354236
26	1	0	1.639261	3.725438	0.317410
27	6	0	-1.030411	3.309600	-0.043070
28	1	0	-1.063728	3.811000	-1.021458
29	1	0	-0.922593	4.079748	0.729920
30	1	0	-1.975275	2.777788	0.094582
31	7	0	-0.887594	-0.301405	-0.465212
32	6	0	0.027561	-1.405322	-0.427042
33	6	0	1.432250	-0.850273	-0.664965
34	6	0	3.945865	0.281868	-1.242988
35	6	0	1.771719	-0.482787	-1.971879
36	6	0	2.366852	-0.624251	0.348887
37	6	0	3.616275	-0.067005	0.063855
38	6	0	3.013093	0.074844	-2.262165
39	1	0	1.040302	-0.638100	-2.761744
40	1	0	2.130751	-0.922531	1.367493
41	1	0	4.334841	0.085555	0.864496
42	1	0	3.257595	0.344688	-3.285324
43	1	0	4.918262	0.709315	-1.467466
44	6	0	-2.023957	-0.523346	-1.120077
45	8	0	-2.422117	-1.509293	-1.746005
46	8	0	-2.850296	0.593535	-1.011248
47	1	0	-0.196952	-2.148741	-1.216624
48	6	0	-4.071520	0.497494	-1.726063
49	1	0	-4.598724	1.436936	-1.548504
50	1	0	-4.671266	-0.346370	-1.373855
51	1	0	-3.890640	0.365074	-2.796551

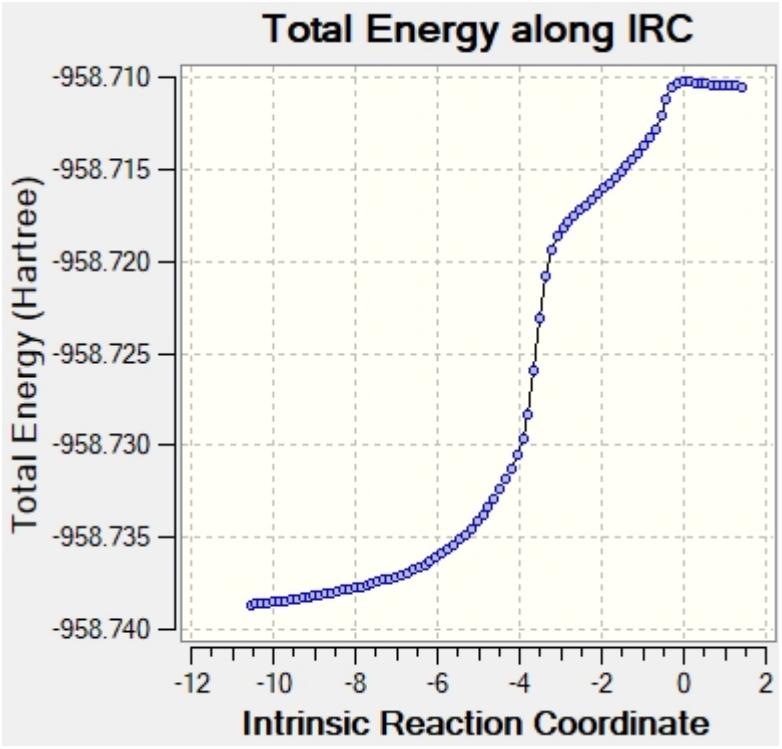
1c.3Me$_2$NH-ts2

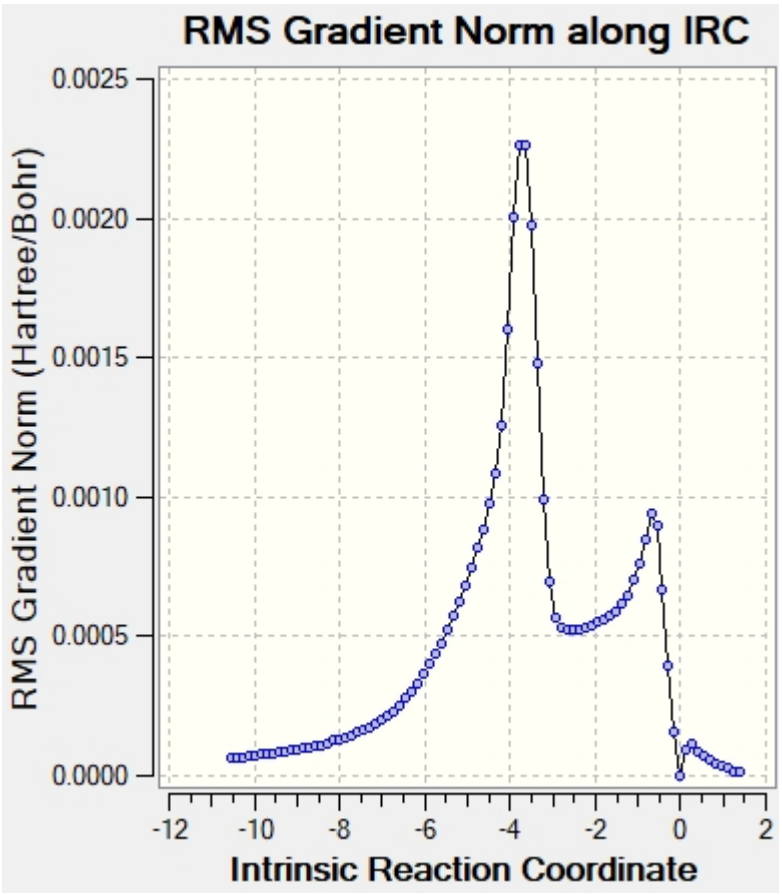
Zero-point correction= 0.452802
(Hartree/Particle)
Thermal correction to Energy= 0.477818
Thermal correction to Enthalpy= 0.478762
Thermal correction to Gibbs Free Energy= 0.398606
Sum of electronic and zero-point Energies= -958.257417
Sum of electronic and thermal Energies= -958.232401
Sum of electronic and thermal Enthalpies= -958.231457
Sum of electronic and thermal Free Energies= -958.311613

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

1	7	0	0.000837	-2.042800	0.999584
2	1	0	0.001163	-0.098114	1.749230
3	1	0	-0.002827	1.579641	1.163741
4	1	0	-0.285450	1.409699	-0.567474
5	7	0	-0.033068	2.295770	-0.073162
6	7	0	-0.158476	0.863209	2.103176
7	6	0	-1.583339	0.984485	2.463089
8	1	0	-1.780728	2.007053	2.797073
9	1	0	-1.839637	0.284716	3.264188
10	1	0	-2.169624	0.764767	1.566778
11	6	0	0.763585	1.172545	3.203044
12	1	0	0.591285	2.197423	3.541387
13	1	0	1.790574	1.084440	2.842595
14	1	0	0.611543	0.487417	4.042240
15	6	0	0.832110	-3.246480	1.049613
16	1	0	0.451136	-4.023412	0.365013
17	1	0	0.825813	-3.652372	2.065745
18	1	0	1.863734	-3.026813	0.771268
19	6	0	-1.367686	-2.432390	1.353606
20	1	0	-1.782047	-3.164325	0.643077
21	1	0	-2.023914	-1.561476	1.354448
22	1	0	-1.357169	-2.871017	2.356638
23	6	0	1.233401	2.848532	-0.546452
24	1	0	1.163930	3.179815	-1.591077
25	1	0	2.015641	2.089405	-0.473146
26	1	0	1.514931	3.710092	0.069226
27	6	0	-1.149781	3.235810	-0.179095
28	1	0	-1.209909	3.675615	-1.183409
29	1	0	-1.028502	4.048043	0.546852
30	1	0	-2.082507	2.700035	0.011990
31	7	0	-0.885430	-0.338591	-0.457141
32	6	0	0.043840	-1.428744	-0.359778
33	6	0	1.438302	-0.869733	-0.646443
34	6	0	3.926395	0.273670	-1.306842
35	6	0	1.754568	-0.553298	-1.972523
36	6	0	2.384409	-0.591444	0.343345
37	6	0	3.620774	-0.027184	0.017779
38	6	0	2.983453	0.009686	-2.303234
39	1	0	1.014654	-0.750306	-2.745054
40	1	0	2.164812	-0.849619	1.376403
41	1	0	4.348075	0.167040	0.801435
42	1	0	3.210072	0.240494	-3.340010
43	1	0	4.888807	0.705801	-1.563294
44	6	0	-2.036575	-0.617159	-1.064402
45	8	0	-2.446704	-1.655075	-1.588749
46	6	0	-4.093171	0.350848	-1.723935
47	1	0	-4.616901	1.303093	-1.619367
48	1	0	-4.686019	-0.457810	-1.287824
49	1	0	-3.931360	0.125647	-2.781866
50	1	0	-0.181025	-2.216633	-1.105336
51	8	0	-2.859211	0.506786	-1.041914

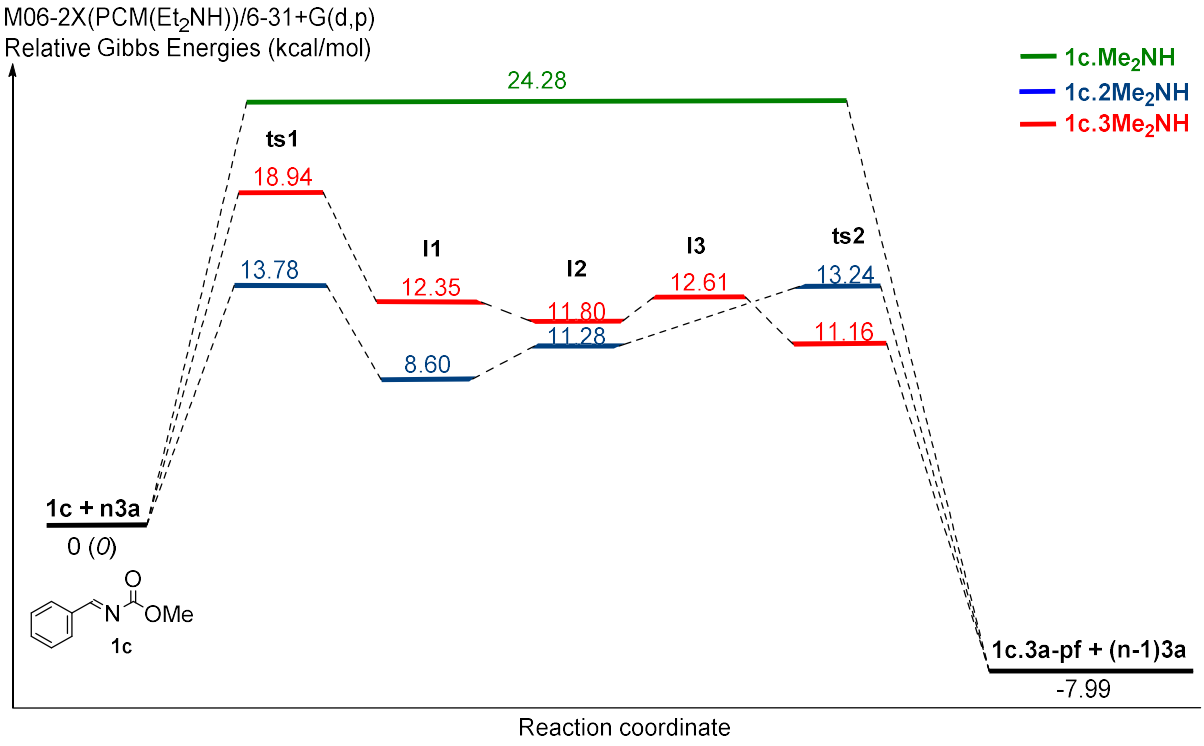
1c.3Me$_2$NH-ts2


Total Energy along IRC
Total Energy (Hartree)
-958.710
-958.715
-958.720
-958.725
-958.730
-958.735
-958.740
-12
-10
-8
-6
-4
-2
0
2
Intrinsic Reaction Coordinate


RMS Gradient Norm along IRC
RMS Gradient Norm (Hartree/Bohr)
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
-12
-10
-8
-6
-4
-2
0
2
Intrinsic Reaction Coordinate

2.3.2.-M06-2X(PCM=Diethylamine)/6-31+G(d,p) calculations

Energy profiles of the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1c** in diethylamine.



1c

Zero-point correction= (Hartree/Particle)	0.167111
Thermal correction to Energy=	0.177859
Thermal correction to Enthalpy=	0.178803
Thermal correction to Gibbs Free Energy=	0.129168
Sum of electronic and zero-point Energies=	-553.207466
Sum of electronic and thermal Energies=	-553.196718
Sum of electronic and thermal Enthalpies=	-553.195774
Sum of electronic and thermal Free Energies=	-553.245409

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.033695	-0.337077	-0.091190
2	6	0	-2.350533	0.169679	-0.107515
3	6	0	-0.118559	0.552659	0.017397
4	8	0	-3.205769	-0.810483	0.180678
5	8	0	-2.688310	1.307180	-0.362404
6	1	0	-0.376162	1.614525	0.114827
7	6	0	1.306016	0.212606	0.016070
8	6	0	4.030008	-0.374447	0.018494
9	6	0	2.246457	1.241484	0.142990
10	6	0	1.735549	-1.116323	-0.109458
11	6	0	3.093723	-1.405691	-0.108630
12	6	0	3.608220	0.948131	0.144174
13	1	0	1.906752	2.269527	0.239966
14	1	0	0.992431	-1.901254	-0.205823
15	1	0	3.429784	-2.432962	-0.205477
16	1	0	4.336445	1.746287	0.243122
17	1	0	5.090759	-0.605568	0.019677
18	6	0	-4.586632	-0.434784	0.198140
19	1	0	-5.132966	-1.341464	0.448782
20	1	0	-4.887087	-0.061374	-0.782577
21	1	0	-4.756957	0.338359	0.949667

1c.Me_2NH-ts

Zero-point correction= (Hartree/Particle)	0.260018
Thermal correction to Energy=	0.274900
Thermal correction to Enthalpy=	0.275844
Thermal correction to Gibbs Free Energy=	0.216888
Sum of electronic and zero-point Energies=	-688.196418
Sum of electronic and thermal Energies=	-688.181536
Sum of electronic and thermal Enthalpies=	-688.180592
Sum of electronic and thermal Free Energies=	-688.239549

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.255263	0.281633	0.453150
2	6	0	-2.187654	-0.470566	-0.157315

3	8	0	-3.334666	-0.528104	0.571648
4	8	0	-2.075194	-1.060739	-1.232364
5	6	0	1.142403	-0.237640	-0.181255
6	6	0	3.457515	-1.784667	0.069087
7	6	0	2.216347	-0.048002	-1.055697
8	6	0	1.227038	-1.215372	0.809697
9	6	0	2.381990	-1.987078	0.933545
10	6	0	3.373268	-0.813178	-0.928934
11	1	0	2.141812	0.696109	-1.846376
12	1	0	0.379138	-1.364842	1.471775
13	1	0	2.441016	-2.750791	1.703044
14	1	0	4.201771	-0.660424	-1.613512
15	1	0	4.354706	-2.388438	0.164920
16	6	0	-0.082870	0.630117	-0.322642
17	1	0	-0.303065	0.771296	-1.388598
18	1	0	-1.043224	1.574638	0.779665
19	6	0	1.093237	2.180477	1.322972
20	1	0	0.944408	3.139315	1.822018
21	1	0	2.086304	2.152940	0.862519
22	1	0	1.012460	1.374093	2.053368
23	7	0	0.040027	2.021254	0.310443
24	6	0	0.007810	3.124022	-0.657612
25	1	0	-0.087123	4.068771	-0.119717
26	1	0	-0.852742	2.997060	-1.317092
27	1	0	0.926906	3.138576	-1.253624
28	6	0	-4.375674	-1.315855	0.002651
29	1	0	-5.205890	-1.258915	0.705934
30	1	0	-4.054341	-2.352758	-0.120511
31	1	0	-4.677066	-0.919638	-0.970206

1c.Me_2NH-pf

Zero-point correction=	0.264501
(Hartree/Particle)	
Thermal correction to Energy=	0.279845
Thermal correction to Enthalpy=	0.280789
Thermal correction to Gibbs Free Energy=	0.220859
Sum of electronic and zero-point Energies=	-688.247328
Sum of electronic and thermal Energies=	-688.231984
Sum of electronic and thermal Enthalpies=	-688.231040
Sum of electronic and thermal Free Energies=	-688.290970

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.114455	-0.439750	0.185717
2	6	0	-2.395312	-0.345036	-0.254646
3	8	0	-3.174236	-1.264651	0.355221
4	8	0	-2.801859	0.444006	-1.086428
5	6	0	1.282097	-0.223924	-0.213268
6	6	0	3.855324	-1.333793	-0.036271
7	6	0	2.170356	-0.141099	-1.288597
8	6	0	1.702294	-0.866878	0.957070
9	6	0	2.977835	-1.421236	1.044140
10	6	0	3.449139	-0.690735	-1.203884
11	1	0	1.854244	0.353252	-2.204335
12	1	0	1.039853	-0.936537	1.816886

13	1	0	3.286778	-1.919804	1.957667
14	1	0	4.123774	-0.621462	-2.051522
15	1	0	4.848629	-1.765984	0.032812
16	6	0	-0.083860	0.437978	-0.329774
17	1	0	-0.295788	0.605188	-1.391836
18	1	0	-0.882874	-1.218344	0.784704
19	6	0	0.106975	1.785540	1.720751
20	1	0	-0.200117	2.755854	2.120994
21	1	0	1.176592	1.640836	1.951446
22	1	0	-0.473191	1.011226	2.230664
23	7	0	-0.180273	1.759269	0.296079
24	6	0	0.591837	2.760691	-0.419931
25	1	0	0.354518	3.748382	-0.015024
26	1	0	0.318980	2.750181	-1.479553
27	1	0	1.682625	2.608319	-0.336122
28	6	0	-4.542913	-1.268452	-0.057325
29	1	0	-4.617873	-1.480437	-1.125573
30	1	0	-5.006982	-0.303438	0.154651
31	1	0	-5.019940	-2.057044	0.521639

1c.2Me$_2$NH-ts1

Zero-point correction= 0.357468
(Hartree/Particle)
Thermal correction to Energy= 0.378492
Thermal correction to Enthalpy= 0.379436
Thermal correction to Gibbs Free Energy= 0.305822
Sum of electronic and zero-point Energies= -823.237465
Sum of electronic and thermal Energies= -823.216441
Sum of electronic and thermal Enthalpies= -823.215497
Sum of electronic and thermal Free Energies= -823.289111

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.044250	-1.443163	0.070686
2	6	0	-1.322187	-1.612309	-0.424677
3	8	0	-1.983411	-2.536316	0.295543
4	8	0	-1.851969	-1.027164	-1.361682
5	6	0	2.123776	-0.457176	-0.299935
6	6	0	4.827478	-0.094761	0.302859
7	6	0	2.963510	0.209254	-1.198179
8	6	0	2.648063	-0.950301	0.900810
9	6	0	3.994144	-0.765595	1.201043
10	6	0	4.312199	0.389740	-0.899452
11	6	0	0.699307	-0.634740	-0.635692
12	7	0	-2.977096	1.396760	-0.045401
13	1	0	0.381884	-0.302310	-1.627120
14	1	0	2.555440	0.586135	-2.133114
15	1	0	4.959790	0.904699	-1.602063
16	1	0	5.878235	0.045129	0.537623
17	1	0	4.397585	-1.147908	2.133511
18	1	0	1.985886	-1.478439	1.579695
19	7	0	0.080778	1.447744	0.040954
20	6	0	-3.890601	2.507965	-0.274268
21	1	0	-3.709856	3.285847	0.474913
22	1	0	-4.951595	2.216400	-0.208045

23	1	0	-3.709493	2.939287	-1.261575
24	6	0	0.694362	2.584702	-0.625138
25	1	0	1.777508	2.561020	-0.461205
26	1	0	0.312175	3.548140	-0.254814
27	1	0	0.505278	2.525879	-1.701073
28	6	0	-3.223927	0.734710	1.228991
29	1	0	-2.548103	-0.119252	1.345416
30	1	0	-4.261296	0.377620	1.340531
31	1	0	-3.020758	1.435043	2.046556
32	6	0	0.277589	1.449062	1.480187
33	1	0	-0.098558	0.506661	1.893609
34	1	0	-0.236457	2.286306	1.975051
35	1	0	1.348395	1.519719	1.701222
36	6	0	-3.326526	-2.787600	-0.114174
37	1	0	-3.351939	-3.153201	-1.142849
38	1	0	-3.925451	-1.875377	-0.043305
39	1	0	-3.706830	-3.543722	0.570383
40	1	0	-3.050160	0.713756	-0.796325
41	1	0	-0.927787	1.429304	-0.155821

1c.2Me$_2$NH-I1

Zero-point correction= 0.360377
(Hartree/Particle)
Thermal correction to Energy= 0.380827
Thermal correction to Enthalpy= 0.381771
Thermal correction to Gibbs Free Energy= 0.310070
Sum of electronic and zero-point Energies= -823.247067
Sum of electronic and thermal Energies= -823.226617
Sum of electronic and thermal Enthalpies= -823.225672
Sum of electronic and thermal Free Energies= -823.297374

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.034444	1.386562	0.233059
2	6	0	1.237678	1.679343	-0.243404
3	8	0	1.745310	2.825945	0.314813
4	8	0	1.924278	1.057326	-1.084183
5	6	0	-2.034730	0.185188	-0.227034
6	6	0	-4.822726	0.050923	0.039154
7	6	0	-2.813054	-0.439795	-1.204697
8	6	0	-2.668883	0.762703	0.877263
9	6	0	-4.053486	0.690510	1.012529
10	6	0	-4.200418	-0.509170	-1.074928
11	6	0	-0.527303	0.244509	-0.372279
12	7	0	2.862295	-1.338500	0.123204
13	1	0	-0.248770	0.116666	-1.429417
14	1	0	-2.333564	-0.862967	-2.084794
15	1	0	-4.792047	-0.990923	-1.847347
16	1	0	-5.902477	0.002395	0.142247
17	1	0	-4.535283	1.144828	1.873011
18	1	0	-2.063407	1.287725	1.609268
19	7	0	0.090584	-1.045620	0.269183
20	6	0	3.121879	-1.905848	-1.199304
21	1	0	2.698914	-2.915045	-1.254037
22	1	0	4.196118	-1.975409	-1.424087

23	1	0	2.642233	-1.273312	-1.950071
24	6	0	-0.274529	-2.301273	-0.418819
25	1	0	-1.326641	-2.530252	-0.242197
26	1	0	0.352131	-3.105750	-0.026076
27	1	0	-0.091316	-2.185272	-1.489002
28	6	0	3.537551	-2.067920	1.192417
29	1	0	3.369828	-1.564109	2.147324
30	1	0	4.621161	-2.157434	1.026017
31	1	0	3.121833	-3.078970	1.260062
32	6	0	-0.152335	-1.138003	1.726308
33	1	0	0.053493	-0.160891	2.164159
34	1	0	0.520826	-1.891469	2.140719
35	1	0	-1.190037	-1.424135	1.907120
36	1	0	3.155149	-0.363077	0.103423
37	1	0	1.150206	-0.975105	0.161849
38	6	0	3.027779	3.219100	-0.147734
39	1	0	3.776955	2.446909	0.051925
40	1	0	3.276572	4.127517	0.401642
41	1	0	3.015627	3.423215	-1.221738

1c.2Me$_2$NH-I2

Zero-point correction=	0.360638
(Hartree/Particle)	
Thermal correction to Energy=	0.381108
Thermal correction to Enthalpy=	0.382052
Thermal correction to Gibbs Free Energy=	0.310438
Sum of electronic and zero-point Energies=	-823.242893
Sum of electronic and thermal Energies=	-823.222423
Sum of electronic and thermal Enthalpies=	-823.221479
Sum of electronic and thermal Free Energies=	-823.293094

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.899001	-0.572725	-0.427938
2	6	0	1.963949	-1.344192	-0.227501
3	8	0	2.868129	-1.211249	-1.256819
4	8	0	2.228751	-2.108663	0.717912
5	6	0	-1.496292	-0.753494	0.004207
6	6	0	-4.107846	-0.870558	-1.006432
7	6	0	-2.468141	-1.529703	0.639072
8	6	0	-1.837175	-0.056253	-1.157982
9	6	0	-3.137442	-0.105344	-1.655415
10	6	0	-3.768270	-1.591382	0.137329
11	1	0	-2.204678	-2.096303	1.529295
12	1	0	-1.065347	0.494637	-1.685670
13	1	0	-3.391104	0.441431	-2.558616
14	1	0	-4.512136	-2.205574	0.635432
15	1	0	-5.118731	-0.916834	-1.399567
16	6	0	-0.093172	-0.671137	0.573786
17	6	0	1.965225	2.984265	-0.271452
18	1	0	2.635225	2.184089	0.053749
19	1	0	1.896962	3.733953	0.523606
20	1	0	2.400624	3.463316	-1.159878
21	6	0	-1.173502	0.909304	2.300882

22	1	0	-0.955640	1.787603	2.910709
23	1	0	-1.378206	0.054350	2.950254
24	1	0	-2.037896	1.103869	1.667784
25	7	0	0.639521	2.424890	-0.533842
26	6	0	-0.274865	3.404324	-1.114692
27	1	0	0.109635	3.837628	-2.048927
28	1	0	-0.430275	4.218009	-0.399564
29	1	0	-1.241967	2.935364	-1.314285
30	7	0	0.007120	0.615958	1.458980
31	6	0	1.236677	0.568591	2.285820
32	1	0	1.394405	1.548659	2.740325
33	1	0	2.080738	0.305162	1.651810
34	1	0	1.114577	-0.191362	3.060836
35	1	0	0.065696	-1.492035	1.288866
36	1	0	0.754401	1.609807	-1.141281
37	1	0	0.145194	1.407844	0.744838
38	6	0	4.041462	-2.002134	-1.145191
39	1	0	4.639255	-1.772294	-2.027976
40	1	0	3.799049	-3.067907	-1.125913
41	1	0	4.602044	-1.754699	-0.239568

1c.2Me$_2$NH-ts2

Zero-point correction= 0.356825
(Hartree/Particle)
Thermal correction to Energy= 0.376588
Thermal correction to Enthalpy= 0.377532
Thermal correction to Gibbs Free Energy= 0.308673
Sum of electronic and zero-point Energies= -823.241824
Sum of electronic and thermal Energies= -823.222061
Sum of electronic and thermal Enthalpies= -823.221117
Sum of electronic and thermal Free Energies= -823.289977

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.917831	-0.543372	-0.364043
2	6	0	1.959533	-1.323851	-0.114389
3	8	0	2.882220	-1.252339	-1.142875
4	8	0	2.206307	-2.052134	0.864432
5	6	0	-1.483407	-0.714357	0.061654
6	6	0	-4.082462	-0.994528	-0.968612
7	6	0	-2.473126	-1.379001	0.791211
8	6	0	-1.804077	-0.222527	-1.206219
9	6	0	-3.095490	-0.350817	-1.715317
10	6	0	-3.764430	-1.519298	0.283297
11	1	0	-2.229381	-1.793837	1.766749
12	1	0	-1.022876	0.226364	-1.811407
13	1	0	-3.327311	0.036539	-2.703195
14	1	0	-4.519074	-2.043461	0.861893
15	1	0	-5.086077	-1.103106	-1.368072
16	6	0	-0.091810	-0.532017	0.648230
17	6	0	2.002431	2.824997	-0.482268
18	1	0	2.685773	2.038842	-0.156309
19	1	0	1.934021	3.597506	0.287152
20	1	0	2.376243	3.269240	-1.408697

21	6	0	-1.200098	1.198641	2.136657
22	1	0	-0.998758	2.147901	2.640267
23	1	0	-1.445586	0.444403	2.896674
24	1	0	-2.055691	1.322740	1.471799
25	7	0	0.672080	2.228826	-0.691690
26	6	0	-0.315353	3.163738	-1.250475
27	1	0	0.002041	3.523996	-2.232706
28	1	0	-0.419403	4.014465	-0.573218
29	1	0	-1.279132	2.658722	-1.339506
30	7	0	-0.006922	0.814187	1.371515
31	6	0	1.169787	0.809561	2.257519
32	1	0	1.344134	1.820960	2.636022
33	1	0	2.043734	0.469934	1.701271
34	1	0	1.010098	0.129636	3.104324
35	1	0	0.066782	-1.302543	1.419498
36	1	0	0.786096	1.373394	-1.255496
37	1	0	0.291935	1.678231	0.327445
38	6	0	4.025200	-2.079201	-0.995868
39	1	0	4.638148	-1.900180	-1.880708
40	1	0	3.746066	-3.135338	-0.945021
41	1	0	4.588890	-1.824150	-0.094215

1c.3Me$_2$NH-ts1

Zero-point correction= 0.451674
(Hartree/Particle)
Thermal correction to Energy= 0.478709
Thermal correction to Enthalpy= 0.479653
Thermal correction to Gibbs Free Energy= 0.392227
Sum of electronic and zero-point Energies= -958.254277
Sum of electronic and thermal Energies= -958.227242
Sum of electronic and thermal Enthalpies= -958.226298
Sum of electronic and thermal Free Energies= -958.313724

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.761681	1.610001	-0.364799
2	6	0	0.567860	1.817494	-0.678230
3	8	0	0.932317	3.072675	-0.360863
4	8	0	1.362518	1.018771	-1.157850
5	6	0	-2.652030	0.127638	-0.562080
6	6	0	-5.359882	-0.503028	-0.283949
7	6	0	-3.172459	-1.026832	-1.156038
8	6	0	-3.498983	0.971812	0.165804
9	6	0	-4.846180	0.653822	0.306610
10	6	0	-4.522459	-1.342280	-1.018881
11	6	0	-1.219618	0.439992	-0.717335
12	7	0	2.339414	-0.292057	1.486372
13	1	0	-0.641928	-0.216367	-1.373500
14	1	0	-2.514539	-1.677517	-1.727719
15	1	0	-4.920685	-2.238518	-1.483989
16	1	0	-6.412353	-0.746433	-0.175051
17	1	0	-5.499691	1.308753	0.874519
18	1	0	-3.084064	1.871669	0.608883
19	7	0	-0.546760	-0.960716	0.957616
20	6	0	3.240509	-1.243651	2.118902

21	1	0	2.791369	-1.624517	3.043326
22	1	0	4.220111	-0.805048	2.373532
23	1	0	3.409594	-2.085131	1.441857
24	6	0	-0.848677	-2.377190	0.835454
25	1	0	-1.935353	-2.516082	0.812665
26	1	0	-0.443945	-2.969505	1.670969
27	1	0	-0.432928	-2.767787	-0.098581
28	6	0	2.205661	0.935831	2.256233
29	1	0	1.524213	1.627606	1.750021
30	1	0	3.166959	1.450671	2.423533
31	1	0	1.775214	0.707141	3.237866
32	6	0	-1.094825	-0.364188	2.164185
33	1	0	-0.941607	0.720305	2.128051
34	1	0	-0.626809	-0.760121	3.078056
35	1	0	-2.171783	-0.559547	2.212709
36	1	0	0.473539	-0.809955	0.964053
37	7	0	3.419349	-1.093383	-1.292018
38	6	0	4.635264	-1.693429	-1.818650
39	1	0	4.942523	-2.518257	-1.165955
40	1	0	5.440916	-0.955170	-1.829557
41	1	0	4.516701	-2.099278	-2.837547
42	6	0	2.287875	-2.008064	-1.331769
43	1	0	1.386362	-1.464885	-1.037921
44	1	0	2.450709	-2.826365	-0.619492
45	1	0	2.124776	-2.455300	-2.327286
46	1	0	3.176673	-0.252779	-1.808862
47	1	0	2.692340	-0.095253	0.548821
48	6	0	2.297931	3.397343	-0.616920
49	1	0	2.522402	3.298728	-1.681342
50	1	0	2.959988	2.738815	-0.047589
51	1	0	2.420443	4.430032	-0.294971

1c.3Me$_2$NH-I1

Zero-point correction= 0.455661
(Hartree/Particle)
Thermal correction to Energy= 0.481605
Thermal correction to Enthalpy= 0.482549
Thermal correction to Gibbs Free Energy= 0.399531
Sum of electronic and zero-point Energies= -958.268099
Sum of electronic and thermal Energies= -958.242155
Sum of electronic and thermal Enthalpies= -958.241211
Sum of electronic and thermal Free Energies= -958.324229

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.354932	-1.526145	-0.296950
2	6	0	-0.786214	-1.635450	-0.953076
3	8	0	-1.165621	-2.948890	-1.093286
4	8	0	-1.535158	-0.747682	-1.430097
5	6	0	2.310926	-0.067091	-0.178591
6	6	0	5.100486	0.191205	-0.303175
7	6	0	2.896389	1.127247	-0.606808
8	6	0	3.137369	-1.140326	0.167929

9	6	0	4.523250	-1.009807	0.112312
10	6	0	4.283737	1.259442	-0.669410
11	6	0	0.801180	-0.197730	-0.105619
12	7	0	-2.396034	-0.073230	1.309791
13	1	0	0.339260	0.532378	-0.785978
14	1	0	2.263468	1.958786	-0.909639
15	1	0	4.722981	2.190845	-1.013401
16	1	0	6.180627	0.288645	-0.354483
17	1	0	5.154581	-1.850853	0.382564
18	1	0	2.674659	-2.078875	0.456061
19	7	0	0.309009	0.288080	1.285397
20	6	0	-3.094739	0.998240	2.014359
21	1	0	-2.836183	0.960571	3.077996
22	1	0	-4.188392	0.917585	1.927146
23	1	0	-2.773479	1.959420	1.604056
24	6	0	0.498710	1.733616	1.527613
25	1	0	1.563917	1.969442	1.569513
26	1	0	0.030276	1.987618	2.481632
27	1	0	0.000335	2.283153	0.725784
28	6	0	-2.800487	-1.409939	1.743948
29	1	0	-2.251894	-2.161713	1.168904
30	1	0	-3.879600	-1.580815	1.620949
31	1	0	-2.552838	-1.536738	2.802903
32	6	0	0.827744	-0.530156	2.402818
33	1	0	0.708725	-1.580913	2.137304
34	1	0	0.245897	-0.296837	3.297508
35	1	0	1.880320	-0.296662	2.576125
36	1	0	-0.765941	0.123660	1.267563
37	7	0	-1.853607	2.171919	-0.990474
38	6	0	-3.278278	2.427369	-1.151330
39	1	0	-3.548527	3.357029	-0.636796
40	1	0	-3.857596	1.614478	-0.701837
41	1	0	-3.586213	2.521991	-2.205867
42	6	0	-1.051000	3.162993	-1.692275
43	1	0	0.010553	2.902915	-1.623079
44	1	0	-1.188015	4.146101	-1.227386
45	1	0	-1.307706	3.256467	-2.760505
46	1	0	-1.643481	1.238913	-1.348925
47	1	0	-2.538040	0.004881	0.301601
48	6	0	-2.381896	-3.169317	-1.791361
49	1	0	-2.336081	-2.761753	-2.804311
50	1	0	-3.227905	-2.711745	-1.268376
51	1	0	-2.510617	-4.251545	-1.828316

1c.3Me$_2$NH-I2

Zero-point correction=	0.454983
(Hartree/Particle)	
Thermal correction to Energy=	0.481176
Thermal correction to Enthalpy=	0.482120
Thermal correction to Gibbs Free Energy=	0.397160
Sum of electronic and zero-point Energies=	-958.267290
Sum of electronic and thermal Energies=	-958.241096
Sum of electronic and thermal Enthalpies=	-958.240152
Sum of electronic and thermal Free Energies=	-958.325112

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	0.443132	-0.206226	1.743914
2	1	0	0.377064	0.791962	1.323986
3	1	0	-0.264174	2.340013	-0.007872
4	1	0	-1.268937	0.694175	-1.237212
5	7	0	-1.495631	1.669800	-1.469454
6	7	0	0.232355	2.404334	0.894228
7	6	0	-0.621125	3.089009	1.864310
8	1	0	-0.795183	4.142714	1.602248
9	1	0	-0.149737	3.059364	2.853631
10	1	0	-1.587800	2.582940	1.928564
11	6	0	1.513144	3.087129	0.720878
12	1	0	1.390145	4.138429	0.422519
13	1	0	2.106114	2.571761	-0.038870
14	1	0	2.070422	3.064949	1.663914
15	6	0	1.696004	-0.268982	2.528081
16	1	0	1.818297	-1.272991	2.943162
17	1	0	1.635754	0.459831	3.338865
18	1	0	2.541612	-0.029991	1.884318
19	6	0	-0.736632	-0.371743	2.626177
20	1	0	-0.751665	-1.389615	3.021013
21	1	0	-1.638384	-0.197540	2.040858
22	1	0	-0.670296	0.354228	3.438493
23	6	0	-1.408505	1.879206	-2.907174
24	1	0	-2.160935	1.301953	-3.469299
25	1	0	-0.416697	1.588727	-3.265993
26	1	0	-1.556788	2.940162	-3.139278
27	6	0	-2.833414	1.943791	-0.962035
28	1	0	-3.619015	1.406075	-1.516939
29	1	0	-3.046340	3.018256	-1.018271
30	1	0	-2.894518	1.633468	0.085815
31	7	0	-0.773507	-0.955014	-0.202301
32	6	0	0.387400	-1.211425	0.559322
33	6	0	1.649753	-1.037628	-0.261803
34	6	0	3.991423	-0.701568	-1.761734
35	6	0	2.698787	-1.950944	-0.149568
36	6	0	1.774946	0.040490	-1.143168
37	6	0	2.941866	0.211824	-1.883777
38	6	0	3.865410	-1.787459	-0.897757
39	1	0	2.601443	-2.798473	0.525029
40	1	0	0.943174	0.732291	-1.253031
41	1	0	3.030441	1.053263	-2.565098
42	1	0	4.671290	-2.509247	-0.806906
43	1	0	4.898024	-0.571184	-2.344701
44	6	0	-1.795995	-1.771134	0.040518
45	8	0	-1.897125	-2.706731	0.852400
46	8	0	-2.867631	-1.454389	-0.763584
47	1	0	0.390816	-2.195238	1.053975
48	6	0	-4.023398	-2.258223	-0.586019
49	1	0	-4.763354	-1.874564	-1.289512
50	1	0	-4.404481	-2.182575	0.436330
51	1	0	-3.810674	-3.308483	-0.802486

1c.3Me$_2$NH-I3

Zero-point correction=	0.455124
(Hartree/Particle)	
Thermal correction to Energy=	0.481076
Thermal correction to Enthalpy=	0.482020
Thermal correction to Gibbs Free Energy=	0.398520
Sum of electronic and zero-point Energies=	-958.267215
Sum of electronic and thermal Energies=	-958.241264
Sum of electronic and thermal Enthalpies=	-958.240320
Sum of electronic and thermal Free Energies=	-958.323819

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.038177	-2.051157	0.992379
2	1	0	-0.007381	-0.227543	1.813897
3	1	0	0.073096	1.411436	1.330025
4	1	0	-0.183771	1.524371	-0.545102
5	7	0	0.082060	2.362550	-0.008476
6	7	0	-0.140719	0.742789	2.168865
7	6	0	-1.572387	0.932142	2.490895
8	1	0	-1.722864	1.959381	2.830037
9	1	0	-1.870217	0.236343	3.278389
10	1	0	-2.139266	0.746989	1.575863
11	6	0	0.765225	1.018851	3.299159
12	1	0	0.605603	2.042757	3.641671
13	1	0	1.797436	0.907048	2.964549
14	1	0	0.563483	0.324021	4.116535
15	6	0	0.803318	-3.248920	1.042771
16	1	0	0.434368	-4.023079	0.348770
17	1	0	0.788709	-3.661700	2.055550
18	1	0	1.835532	-3.019462	0.777085
19	6	0	-1.405009	-2.451860	1.340801
20	1	0	-1.807963	-3.186638	0.625371
21	1	0	-2.067487	-1.585877	1.344428
22	1	0	-1.396602	-2.898146	2.339794
23	6	0	1.331565	2.932839	-0.499149
24	1	0	1.224253	3.359814	-1.507412
25	1	0	2.101224	2.157600	-0.528439
26	1	0	1.662883	3.731682	0.173702
27	6	0	-1.027094	3.313246	-0.046301
28	1	0	-1.121349	3.798355	-1.029196
29	1	0	-0.877245	4.095219	0.706727
30	1	0	-1.959877	2.782706	0.160895
31	7	0	-0.927801	-0.334381	-0.432815
32	6	0	-0.001677	-1.430286	-0.363272
33	6	0	1.393182	-0.883686	-0.671283
34	6	0	3.886630	0.220542	-1.376632
35	6	0	1.697021	-0.588650	-2.005204
36	6	0	2.353235	-0.601300	0.303603
37	6	0	3.592502	-0.057321	-0.043949
38	6	0	2.928705	-0.044082	-2.358484
39	1	0	0.948753	-0.789147	-2.769028
40	1	0	2.147470	-0.841748	1.343443
41	1	0	4.328973	0.141846	0.729518
42	1	0	3.144966	0.170994	-3.400793
43	1	0	4.850563	0.638466	-1.650375
44	6	0	-2.046279	-0.561968	-1.102030
45	8	0	-2.440074	-1.563675	-1.723182

46	8	0	-2.869717	0.557908	-1.045146
47	1	0	-0.240053	-2.213570	-1.109426
48	6	0	-4.079124	0.461830	-1.779847
49	1	0	-4.594394	1.412901	-1.634678
50	1	0	-4.702394	-0.360080	-1.416585
51	1	0	-3.884548	0.304326	-2.844740

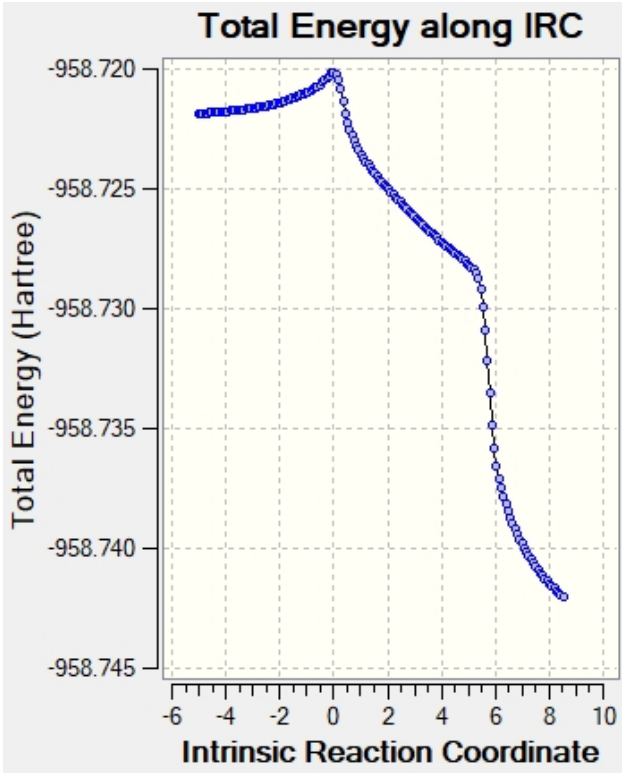
1c.3Me$_2$NH-ts2

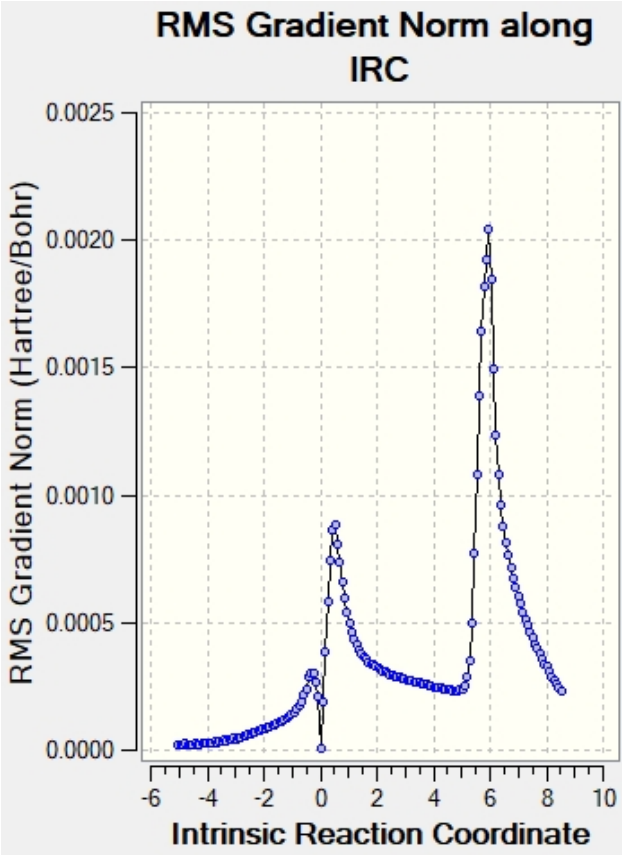
Zero-point correction=	0.450803
(Hartree/Particle)	
Thermal correction to Energy=	0.476384
Thermal correction to Enthalpy=	0.477328
Thermal correction to Gibbs Free Energy=	0.393990
Sum of electronic and zero-point Energies=	-958.269312
Sum of electronic and thermal Energies=	-958.243731
Sum of electronic and thermal Enthalpies=	-958.242787
Sum of electronic and thermal Free Energies=	-958.326125

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.549684	-0.162503	1.827520
2	1	0	-0.014405	1.442575	1.172172
3	1	0	-1.051419	1.970944	-0.214470
4	1	0	-1.274008	0.429711	-1.133518
5	7	0	-1.665867	1.388719	-1.287399
6	7	0	-0.504087	2.317701	0.839643
7	6	0	-1.539271	2.663905	1.827074
8	1	0	-2.107311	3.530167	1.477263
9	1	0	-1.087567	2.901557	2.795838
10	1	0	-2.216513	1.816300	1.947906
11	6	0	0.465140	3.404353	0.636692
12	1	0	-0.048639	4.282351	0.235983
13	1	0	1.230521	3.082974	-0.072289
14	1	0	0.947920	3.674787	1.581129
15	6	0	1.795292	-0.134366	2.592776
16	1	0	2.088900	-1.141390	2.936993
17	1	0	1.658187	0.500387	3.473235
18	1	0	2.607757	0.276357	1.990225
19	6	0	-0.545493	-0.574617	2.708519
20	1	0	-0.366267	-1.574082	3.136666
21	1	0	-1.479201	-0.608699	2.144238
22	1	0	-0.645079	0.146962	3.525946
23	6	0	-1.307073	1.923904	-2.601638
24	1	0	-1.756492	1.333875	-3.408897
25	1	0	-0.221149	1.909536	-2.724301
26	1	0	-1.656725	2.957510	-2.687831
27	6	0	-3.115340	1.338848	-1.073276
28	1	0	-3.616798	0.788388	-1.877226
29	1	0	-3.519519	2.355734	-1.027635
30	1	0	-3.318032	0.821860	-0.132643
31	7	0	-0.563184	-0.962180	-0.146367
32	6	0	0.622072	-1.092941	0.653254
33	6	0	1.850595	-0.760899	-0.177365
34	6	0	4.117653	-0.096222	-1.697617
35	6	0	2.972995	-1.588611	-0.177408

36	6	0	1.872693	0.396985	-0.959614
37	6	0	2.995137	0.735439	-1.709715
38	6	0	4.100706	-1.261935	-0.934586
39	1	0	2.965496	-2.496909	0.420465
40	1	0	0.983682	1.020301	-0.989171
41	1	0	2.994450	1.639685	-2.312476
42	1	0	4.965029	-1.919234	-0.927763
43	1	0	4.993383	0.159958	-2.285894
44	6	0	-1.423132	-1.965383	-0.074408
45	8	0	-1.403891	-3.012401	0.594730
46	6	0	-3.508670	-2.727868	-0.917183
47	1	0	-4.278605	-2.378294	-1.607566
48	1	0	-3.938279	-2.871564	0.078347
49	1	0	-3.106744	-3.684137	-1.263500
50	1	0	0.735184	-2.119137	1.050051
51	8	0	-2.509034	-1.723124	-0.908239

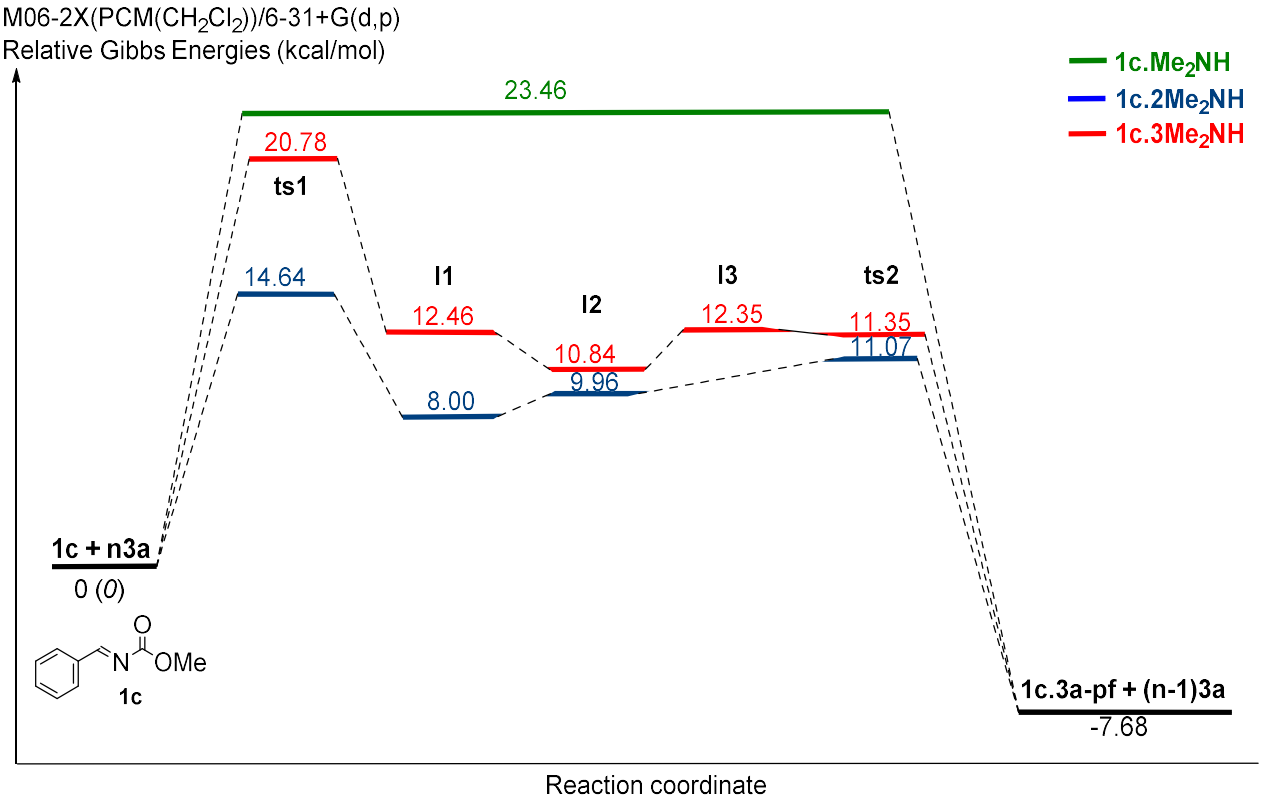
1c.3Me$_2$NH-ts2





2.3.3.-M06-2X(PCM=Dichloromethane)/6-31+G(d,p) calculations

Energy profiles for the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1c** in dichloromethane.



1c.Me_2NH-ts

Zero-point correction=	0.259862
(Hartree/Particle)	
Thermal correction to Energy=	0.274764
Thermal correction to Enthalpy=	0.275708
Thermal correction to Gibbs Free Energy=	0.216637
Sum of electronic and zero-point Energies=	-688.200960
Sum of electronic and thermal Energies=	-688.186058
Sum of electronic and thermal Enthalpies=	-688.185113
Sum of electronic and thermal Free Energies=	-688.244185

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.256867	0.285011	0.444780
2	6	0	-2.185577	-0.475083	-0.157650
3	8	0	-3.337075	-0.520066	0.564303
4	8	0	-2.066614	-1.086058	-1.222112
5	6	0	1.143517	-0.235650	-0.181326
6	6	0	3.456453	-1.786656	0.072654
7	6	0	2.216882	-0.051720	-1.058117
8	6	0	1.228482	-1.208812	0.814608
9	6	0	2.382045	-1.982669	0.940329
10	6	0	3.372408	-0.819110	-0.929488
11	1	0	2.144403	0.691415	-1.849664
12	1	0	0.383774	-1.353153	1.481889
13	1	0	2.441438	-2.741518	1.714587
14	1	0	4.200737	-0.669544	-1.614915
15	1	0	4.353001	-2.391040	0.170452
16	6	0	-0.079005	0.635548	-0.326240
17	1	0	-0.297218	0.776042	-1.392373
18	1	0	-1.059687	1.565574	0.769746
19	6	0	1.081909	2.181752	1.327444
20	1	0	0.930289	3.141568	1.823283
21	1	0	2.079186	2.152806	0.876166
22	1	0	0.993311	1.377433	2.059369
23	7	0	0.037407	2.023872	0.305542
24	6	0	0.018057	3.127309	-0.662886
25	1	0	-0.080971	4.070868	-0.124081
26	1	0	-0.835611	3.003274	-1.331635
27	1	0	0.943514	3.141548	-1.248784
28	6	0	-4.380968	-1.311553	0.002752
29	1	0	-5.214210	-1.237332	0.700444
30	1	0	-4.066358	-2.352683	-0.099396
31	1	0	-4.675078	-0.928589	-0.977352

1c.Me_2NH-pf

Zero-point correction=	0.264486
(Hartree/Particle)	
Thermal correction to Energy=	0.279776
Thermal correction to Enthalpy=	0.280721
Thermal correction to Gibbs Free Energy=	0.221099
Sum of electronic and zero-point Energies=	-688.250434
Sum of electronic and thermal Energies=	-688.235144
Sum of electronic and thermal Enthalpies=	-688.234200
Sum of electronic and thermal Free Energies=	-688.293822

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.115505	-0.438064	0.181625
2	6	0	-2.395695	-0.345159	-0.255791
3	8	0	-3.175298	-1.259063	0.358356
4	8	0	-2.803236	0.441359	-1.092506
5	6	0	1.282440	-0.223812	-0.211916
6	6	0	3.853896	-1.337018	-0.031949
7	6	0	2.169316	-0.148448	-1.289207
8	6	0	1.702327	-0.861091	0.961780
9	6	0	2.977387	-1.417014	1.050153
10	6	0	3.447480	-0.699821	-1.202988
11	1	0	1.853392	0.341571	-2.207321
12	1	0	1.041325	-0.926440	1.822884
13	1	0	3.286388	-1.911166	1.966012
14	1	0	4.121103	-0.636254	-2.051843
15	1	0	4.846555	-1.770485	0.038497
16	6	0	-0.082999	0.438521	-0.332726
17	1	0	-0.291473	0.601644	-1.395970
18	1	0	-0.888542	-1.200774	0.802964
19	6	0	0.096701	1.790685	1.716538
20	1	0	-0.203953	2.764877	2.111998
21	1	0	1.163485	1.638221	1.953457
22	1	0	-0.491910	1.022314	2.225587
23	7	0	-0.181038	1.763264	0.288689
24	6	0	0.609778	2.756141	-0.421255
25	1	0	0.375246	3.747490	-0.023937
26	1	0	0.354512	2.742387	-1.485201
27	1	0	1.697388	2.594643	-0.320048
28	6	0	-4.545280	-1.268776	-0.053081
29	1	0	-4.620749	-1.496731	-1.117929
30	1	0	-5.009719	-0.301699	0.147556
31	1	0	-5.021083	-2.049599	0.536951

1c.2Me$_2$NH-ts1

Zero-point correction= (Hartree/Particle)	0.357197
Thermal correction to Energy=	0.378279
Thermal correction to Enthalpy=	0.379223
Thermal correction to Gibbs Free Energy=	0.305542
Sum of electronic and zero-point Energies=	-823.240383
Sum of electronic and thermal Energies=	-823.219301
Sum of electronic and thermal Enthalpies=	-823.218357
Sum of electronic and thermal Free Energies=	-823.292037

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.045754	-1.456226	0.069733
2	6	0	-1.326595	-1.619027	-0.427978
3	8	0	-1.995630	-2.527909	0.301881
4	8	0	-1.846982	-1.039503	-1.372499
5	6	0	2.126436	-0.476429	-0.298068
6	6	0	4.825426	-0.093045	0.311781
7	6	0	2.964907	0.190093	-1.198013
8	6	0	2.649141	-0.956868	0.908967
9	6	0	3.993102	-0.762370	1.212484
10	6	0	4.311411	0.380778	-0.895610
11	6	0	0.707055	-0.664091	-0.641293
12	7	0	-2.986377	1.397650	-0.043999
13	1	0	0.389256	-0.323541	-1.629244
14	1	0	2.556992	0.560525	-2.135492
15	1	0	4.957956	0.896475	-1.598523
16	1	0	5.874294	0.055464	0.549506
17	1	0	4.395326	-1.134267	2.149616
18	1	0	1.988856	-1.480321	1.593224
19	7	0	0.086661	1.474194	0.024550
20	6	0	-3.935838	2.482702	-0.256610
21	1	0	-3.759580	3.268360	0.485323
22	1	0	-4.986049	2.161376	-0.164485
23	1	0	-3.789257	2.914057	-1.249510
24	6	0	0.701986	2.601511	-0.656276
25	1	0	1.787330	2.566834	-0.508131
26	1	0	0.337454	3.572066	-0.285957
27	1	0	0.498138	2.539274	-1.729216
28	6	0	-3.187198	0.738445	1.240516
29	1	0	-2.485427	-0.095476	1.349001
30	1	0	-4.211254	0.353483	1.377253
31	1	0	-2.985583	1.450547	2.048101
32	6	0	0.301277	1.485897	1.461000
33	1	0	-0.076330	0.550580	1.889115
34	1	0	-0.197999	2.331174	1.957974
35	1	0	1.375504	1.549507	1.667909
36	6	0	-3.344845	-2.768751	-0.100290
37	1	0	-3.376802	-3.150880	-1.122580
38	1	0	-3.930386	-1.847489	-0.040884
39	1	0	-3.732481	-3.509022	0.596894
40	1	0	-3.065238	0.708158	-0.788280
41	1	0	-0.923118	1.460017	-0.162321

1c.2Me$_2$NH-I1

Zero-point correction=	0.455339
(Hartree/Particle)	
Thermal correction to Energy=	0.481316
Thermal correction to Enthalpy=	0.482260
Thermal correction to Gibbs Free Energy=	0.399260
Sum of electronic and zero-point Energies=	-958.273217
Sum of electronic and thermal Energies=	-958.247241
Sum of electronic and thermal Enthalpies=	-958.246296
Sum of electronic and thermal Free Energies=	-958.329296

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.363202	-1.525031	-0.321867
2	6	0	-0.781512	-1.634893	-0.971220
3	8	0	-1.156027	-2.951464	-1.113994
4	8	0	-1.534988	-0.749685	-1.444248
5	6	0	2.317407	-0.063786	-0.183349
6	6	0	5.108074	0.198643	-0.288129
7	6	0	2.904162	1.121994	-0.633451
8	6	0	3.143663	-1.125523	0.198365
9	6	0	4.529926	-0.993362	0.152096
10	6	0	4.291936	1.256012	-0.686425
11	6	0	0.807053	-0.193945	-0.122042
12	7	0	-2.392188	-0.081875	1.313508
13	1	0	0.352197	0.533323	-0.810191
14	1	0	2.272490	1.946365	-0.957429
15	1	0	4.731795	2.181123	-1.046011
16	1	0	6.188367	0.297927	-0.331022
17	1	0	5.160674	-1.825202	0.450620
18	1	0	2.683972	-2.057488	0.511528
19	7	0	0.301078	0.293401	1.258003
20	6	0	-3.060038	0.983080	2.058578
21	1	0	-2.738957	0.945112	3.104920
22	1	0	-4.155595	0.892129	2.032202
23	1	0	-2.769727	1.947545	1.633238
24	6	0	0.500957	1.738376	1.499926
25	1	0	1.567531	1.963869	1.558935
26	1	0	0.019403	1.998381	2.445319
27	1	0	0.021702	2.291819	0.689833
28	6	0	-2.765981	-1.422376	1.764043
29	1	0	-2.245222	-2.169197	1.157435
30	1	0	-3.848890	-1.598698	1.698393
31	1	0	-2.459856	-1.550638	2.807201
32	6	0	0.796890	-0.523087	2.387788
33	1	0	0.678902	-1.574956	2.127038
34	1	0	0.197675	-0.283286	3.269058
35	1	0	1.846354	-0.292365	2.581365
36	1	0	-0.777528	0.133379	1.233000
37	7	0	-1.878614	2.176489	-0.977211
38	6	0	-3.305936	2.427101	-1.123836
39	1	0	-3.569405	3.366163	-0.623522
40	1	0	-3.879672	1.623810	-0.650464
41	1	0	-3.628036	2.502349	-2.175768
42	6	0	-1.087111	3.161992	-1.700125
43	1	0	-0.023893	2.907173	-1.639785
44	1	0	-1.222469	4.149691	-1.245077
45	1	0	-1.356966	3.241980	-2.766234

46	1	0	-1.668357	1.240675	-1.327044
47	1	0	-2.585973	-0.000323	0.315256
48	6	0	-2.386191	-3.177830	-1.787760
49	1	0	-2.360030	-2.778234	-2.804600
50	1	0	-3.221752	-2.718305	-1.250555
51	1	0	-2.514757	-4.260196	-1.815474

1c.2Me$_2$NH-I2

Zero-point correction= 0.455033
(Hartree/Particle)
Thermal correction to Energy= 0.481264
Thermal correction to Enthalpy= 0.482208
Thermal correction to Gibbs Free Energy= 0.395702
Sum of electronic and zero-point Energies= -958.272543
Sum of electronic and thermal Energies= -958.246312
Sum of electronic and thermal Enthalpies= -958.245368
Sum of electronic and thermal Free Energies= -958.331874

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.460134	-0.109687	1.741120
2	1	0	0.394838	0.870632	1.275440
3	1	0	-0.255812	2.369210	-0.103477
4	1	0	-1.336740	0.669416	-1.186345
5	7	0	-1.577378	1.627818	-1.468589
6	7	0	0.268896	2.459773	0.778963
7	6	0	-0.542763	3.206639	1.740593
8	1	0	-0.704180	4.249464	1.431759
9	1	0	-0.041666	3.214467	2.715151
10	1	0	-1.516258	2.723980	1.857962
11	6	0	1.557157	3.110062	0.541303
12	1	0	1.443311	4.147871	0.196435
13	1	0	2.122604	2.549928	-0.207454
14	1	0	2.136719	3.122188	1.470593
15	6	0	1.720260	-0.135613	2.518456
16	1	0	1.852171	-1.123104	2.968122
17	1	0	1.660114	0.621289	3.302412
18	1	0	2.559103	0.086509	1.860124
19	6	0	-0.710805	-0.231670	2.641825
20	1	0	-0.703252	-1.219017	3.108495
21	1	0	-1.620014	-0.109557	2.055023
22	1	0	-0.648942	0.548109	3.402684
23	6	0	-1.543909	1.744563	-2.919284
24	1	0	-2.311923	1.128170	-3.415774
25	1	0	-0.563239	1.438786	-3.295381
26	1	0	-1.710368	2.787166	-3.213403
27	6	0	-2.896803	1.933979	-0.932044
28	1	0	-3.701685	1.368650	-1.429682
29	1	0	-3.111146	3.003548	-1.043525
30	1	0	-2.923895	1.686929	0.133819
31	7	0	-0.771656	-0.965739	-0.150332
32	6	0	0.400102	-1.172716	0.615428
33	6	0	1.651851	-1.041196	-0.229871
34	6	0	3.969266	-0.795326	-1.783809

35	6	0	2.704900	-1.944260	-0.077182
36	6	0	1.760806	-0.018827	-1.177765
37	6	0	2.916058	0.107874	-1.945753
38	6	0	3.859656	-1.825625	-0.851715
39	1	0	2.620562	-2.747622	0.650931
40	1	0	0.926768	0.665404	-1.316184
41	1	0	2.993684	0.906636	-2.677745
42	1	0	4.668765	-2.538746	-0.728118
43	1	0	4.866306	-0.700487	-2.387987
44	6	0	-1.775200	-1.794732	0.113707
45	8	0	-1.858644	-2.717569	0.944831
46	8	0	-2.854628	-1.519540	-0.697471
47	1	0	0.413361	-2.130028	1.158718
48	6	0	-3.998361	-2.337287	-0.500806
49	1	0	-4.750183	-1.970347	-1.200380
50	1	0	-4.371288	-2.256310	0.523874
51	1	0	-3.774788	-3.386607	-0.711599

1c.2Me$_2$NH-ts2

Zero-point correction=	0.356423
(Hartree/Particle)	
Thermal correction to Energy=	0.376387
Thermal correction to Enthalpy=	0.377331
Thermal correction to Gibbs Free Energy=	0.307500
Sum of electronic and zero-point Energies=	-823.248800
Sum of electronic and thermal Energies=	-823.228837
Sum of electronic and thermal Enthalpies=	-823.227892
Sum of electronic and thermal Free Energies=	-823.297723

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.947550	-0.543773	-0.362334
2	6	0	1.985281	-1.323394	-0.107915
3	8	0	2.906663	-1.269957	-1.140268
4	8	0	2.235193	-2.047321	0.877177
5	6	0	-1.451763	-0.744372	0.073133
6	6	0	-4.047025	-1.105042	-0.940281
7	6	0	-2.419259	-1.427747	0.815178
8	6	0	-1.792584	-0.270401	-1.196495
9	6	0	-3.082466	-0.439561	-1.697767
10	6	0	-3.708984	-1.608190	0.315543
11	1	0	-2.160179	-1.822228	1.795180
12	1	0	-1.029824	0.202705	-1.806745
13	1	0	-3.331265	-0.064104	-2.685989
14	1	0	-4.446745	-2.144791	0.904401
15	1	0	-5.049529	-1.243502	-1.333208
16	6	0	-0.062831	-0.522491	0.652174
17	6	0	1.895528	2.937242	-0.522586
18	1	0	2.619701	2.176001	-0.227074
19	1	0	1.801752	3.682201	0.270474
20	1	0	2.232736	3.426027	-1.440337
21	6	0	-1.191995	1.216935	2.105117
22	1	0	-1.004640	2.181581	2.583364
23	1	0	-1.415888	0.475358	2.883595

24	1	0	-2.054391	1.309953	1.444153
25	7	0	0.589186	2.287132	-0.728763
26	6	0	-0.457483	3.204280	-1.206971
27	1	0	-0.177060	3.650191	-2.164812
28	1	0	-0.594511	3.995625	-0.467173
29	1	0	-1.393809	2.654323	-1.318818
30	7	0	0.003166	0.837860	1.338809
31	6	0	1.187796	0.881281	2.213415
32	1	0	1.344572	1.905437	2.562490
33	1	0	2.063250	0.547199	1.655913
34	1	0	1.047794	0.222640	3.080220
35	1	0	0.106659	-1.271836	1.441887
36	1	0	0.720500	1.482702	-1.352133
37	1	0	0.259386	1.686972	0.286333
38	6	0	4.057439	-2.084624	-0.981269
39	1	0	4.665986	-1.918460	-1.871426
40	1	0	3.788294	-3.142139	-0.909096
41	1	0	4.623111	-1.805656	-0.088104

1c.3Me$_2$NH-ts1

Zero-point correction= 0.451611
(Hartree/Particle)
Thermal correction to Energy= 0.478616
Thermal correction to Enthalpy= 0.479561
Thermal correction to Gibbs Free Energy= 0.392359
Sum of electronic and zero-point Energies= -958.256779
Sum of electronic and thermal Energies= -958.229774
Sum of electronic and thermal Enthalpies= -958.228829
Sum of electronic and thermal Free Energies= -958.316031

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.767315	1.624985	-0.373453
2	6	0	0.566988	1.829071	-0.682165
3	8	0	0.932040	3.081254	-0.357602
4	8	0	1.358619	1.029517	-1.162273
5	6	0	-2.656560	0.139603	-0.569374
6	6	0	-5.357328	-0.514316	-0.276621
7	6	0	-3.170120	-1.019529	-1.161147
8	6	0	-3.506577	0.975451	0.165320
9	6	0	-4.850341	0.646316	0.313016
10	6	0	-4.516712	-1.346275	-1.016717
11	6	0	-1.229155	0.461450	-0.734639
12	7	0	2.350945	-0.290686	1.486948
13	1	0	-0.646233	-0.200663	-1.379349
14	1	0	-2.509371	-1.665501	-1.734738
15	1	0	-4.909572	-2.246314	-1.478893
16	1	0	-6.406882	-0.767116	-0.161518
17	1	0	-5.505863	1.294148	0.886604
18	1	0	-3.098404	1.876730	0.611620
19	7	0	-0.543686	-0.979497	0.965916
20	6	0	3.277554	-1.221764	2.113711
21	1	0	2.846379	-1.605880	3.045144

22	1	0	4.251123	-0.762750	2.355377
23	1	0	3.455180	-2.063964	1.439749
24	6	0	-0.849852	-2.394861	0.842611
25	1	0	-1.936789	-2.528267	0.798734
26	1	0	-0.466428	-2.988455	1.687601
27	1	0	-0.419296	-2.790641	-0.082398
28	6	0	2.198790	0.935484	2.256164
29	1	0	1.502963	1.614430	1.751961
30	1	0	3.151063	1.468221	2.418670
31	1	0	1.776047	0.700012	3.239482
32	6	0	-1.100174	-0.381565	2.167442
33	1	0	-0.942338	0.702508	2.135386
34	1	0	-0.645622	-0.779526	3.087562
35	1	0	-2.178824	-0.571221	2.204539
36	1	0	0.475805	-0.830823	0.977248
37	7	0	3.419513	-1.098856	-1.303912
38	6	0	4.625892	-1.719760	-1.830427
39	1	0	4.933553	-2.532946	-1.163536
40	1	0	5.436707	-0.988012	-1.866358
41	1	0	4.492698	-2.145971	-2.838900
42	6	0	2.280710	-2.006377	-1.317429
43	1	0	1.384663	-1.453157	-1.025597
44	1	0	2.444162	-2.812798	-0.592120
45	1	0	2.107117	-2.470060	-2.303413
46	1	0	3.180148	-0.268960	-1.839311
47	1	0	2.690477	-0.088452	0.545731
48	6	0	2.301103	3.406116	-0.604663
49	1	0	2.529727	3.313627	-1.668500
50	1	0	2.957883	2.743281	-0.034829
51	1	0	2.423148	4.436465	-0.275947

1c.3Me$_2$NH-I1

Zero-point correction=	0.455339
(Hartree/Particle)	
Thermal correction to Energy=	0.481316
Thermal correction to Enthalpy=	0.482260
Thermal correction to Gibbs Free Energy=	0.399260
Sum of electronic and zero-point Energies=	-958.273217
Sum of electronic and thermal Energies=	-958.247241
Sum of electronic and thermal Enthalpies=	-958.246296
Sum of electronic and thermal Free Energies=	-958.329296

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.363202	-1.525031	-0.321867
2	6	0	-0.781512	-1.634893	-0.971220
3	8	0	-1.156027	-2.951464	-1.113994
4	8	0	-1.534988	-0.749685	-1.444248
5	6	0	2.317407	-0.063786	-0.183349
6	6	0	5.108074	0.198643	-0.288129
7	6	0	2.904162	1.121994	-0.633451
8	6	0	3.143663	-1.125523	0.198365
9	6	0	4.529926	-0.993362	0.152096

10	6	0	4.291936	1.256012	-0.686425
11	6	0	0.807053	-0.193945	-0.122042
12	7	0	-2.392188	-0.081875	1.313508
13	1	0	0.352197	0.533323	-0.810191
14	1	0	2.272490	1.946365	-0.957429
15	1	0	4.731795	2.181123	-1.046011
16	1	0	6.188367	0.297927	-0.331022
17	1	0	5.160674	-1.825202	0.450620
18	1	0	2.683972	-2.057488	0.511528
19	7	0	0.301078	0.293401	1.258003
20	6	0	-3.060038	0.983080	2.058578
21	1	0	-2.738957	0.945112	3.104920
22	1	0	-4.155595	0.892129	2.032202
23	1	0	-2.769727	1.947545	1.633238
24	6	0	0.500957	1.738376	1.499926
25	1	0	1.567531	1.963869	1.558935
26	1	0	0.019403	1.998381	2.445319
27	1	0	0.021702	2.291819	0.689833
28	6	0	-2.765981	-1.422376	1.764043
29	1	0	-2.245222	-2.169197	1.157435
30	1	0	-3.848890	-1.598698	1.698393
31	1	0	-2.459856	-1.550638	2.807201
32	6	0	0.796890	-0.523087	2.387788
33	1	0	0.678902	-1.574956	2.127038
34	1	0	0.197675	-0.283286	3.269058
35	1	0	1.846354	-0.292365	2.581365
36	1	0	-0.777528	0.133379	1.233000
37	7	0	-1.878614	2.176489	-0.977211
38	6	0	-3.305936	2.427101	-1.123836
39	1	0	-3.569405	3.366163	-0.623522
40	1	0	-3.879672	1.623810	-0.650464
41	1	0	-3.628036	2.502349	-2.175768
42	6	0	-1.087111	3.161992	-1.700125
43	1	0	-0.023893	2.907173	-1.639785
44	1	0	-1.222469	4.149691	-1.245077
45	1	0	-1.356966	3.241980	-2.766234
46	1	0	-1.668357	1.240675	-1.327044
47	1	0	-2.585973	-0.000323	0.315256
48	6	0	-2.386191	-3.177830	-1.787760
49	1	0	-2.360030	-2.778234	-2.804600
50	1	0	-3.221752	-2.718305	-1.250555
51	1	0	-2.514757	-4.260196	-1.815474

1c.3Me$_2$NH-I2

Zero-point correction=	0.455033
(Hartree/Particle)	
Thermal correction to Energy=	0.481264
Thermal correction to Enthalpy=	0.482208
Thermal correction to Gibbs Free Energy=	0.395702
Sum of electronic and zero-point Energies=	-958.272543
Sum of electronic and thermal Energies=	-958.246312
Sum of electronic and thermal Enthalpies=	-958.245368
Sum of electronic and thermal Free Energies=	-958.331874

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.460134	-0.109687	1.741120
2	1	0	0.394838	0.870632	1.275440
3	1	0	-0.255812	2.369210	-0.103477
4	1	0	-1.336740	0.669416	-1.186345
5	7	0	-1.577378	1.627818	-1.468589
6	7	0	0.268896	2.459773	0.778963
7	6	0	-0.542763	3.206639	1.740593
8	1	0	-0.704180	4.249464	1.431759
9	1	0	-0.041666	3.214467	2.715151
10	1	0	-1.516258	2.723980	1.857962
11	6	0	1.557157	3.110062	0.541303
12	1	0	1.443311	4.147871	0.196435
13	1	0	2.122604	2.549928	-0.207454
14	1	0	2.136719	3.122188	1.470593
15	6	0	1.720260	-0.135613	2.518456
16	1	0	1.852171	-1.123104	2.968122
17	1	0	1.660114	0.621289	3.302412
18	1	0	2.559103	0.086509	1.860124
19	6	0	-0.710805	-0.231670	2.641825
20	1	0	-0.703252	-1.219017	3.108495
21	1	0	-1.620014	-0.109557	2.055023
22	1	0	-0.648942	0.548109	3.402684
23	6	0	-1.543909	1.744563	-2.919284
24	1	0	-2.311923	1.128170	-3.415774
25	1	0	-0.563239	1.438786	-3.295381
26	1	0	-1.710368	2.787166	-3.213403
27	6	0	-2.896803	1.933979	-0.932044
28	1	0	-3.701685	1.368650	-1.429682
29	1	0	-3.111146	3.003548	-1.043525
30	1	0	-2.923895	1.686929	0.133819
31	7	0	-0.771656	-0.965739	-0.150332
32	6	0	0.400102	-1.172716	0.615428
33	6	0	1.651851	-1.041196	-0.229871
34	6	0	3.969266	-0.795326	-1.783809
35	6	0	2.704900	-1.944260	-0.077182
36	6	0	1.760806	-0.018827	-1.177765
37	6	0	2.916058	0.107874	-1.945753
38	6	0	3.859656	-1.825625	-0.851715
39	1	0	2.620562	-2.747622	0.650931
40	1	0	0.926768	0.665404	-1.316184
41	1	0	2.993684	0.906636	-2.677745
42	1	0	4.668765	-2.538746	-0.728118
43	1	0	4.866306	-0.700487	-2.387987
44	6	0	-1.775200	-1.794732	0.113707

45	8	0	-1.858644	-2.717569	0.944831
46	8	0	-2.854628	-1.519540	-0.697471
47	1	0	0.413361	-2.130028	1.158718
48	6	0	-3.998361	-2.337287	-0.500806
49	1	0	-4.750183	-1.970347	-1.200380
50	1	0	-4.371288	-2.256310	0.523874
51	1	0	-3.774788	-3.386607	-0.711599

1c.3Me$_2$NH-I3

Zero-point correction=	0.455053
(Hartree/Particle)	
Thermal correction to Energy=	0.481042
Thermal correction to Enthalpy=	0.481986
Thermal correction to Gibbs Free Energy=	0.397849
Sum of electronic and zero-point Energies=	-958.272273
Sum of electronic and thermal Energies=	-958.246284
Sum of electronic and thermal Enthalpies=	-958.245340
Sum of electronic and thermal Free Energies=	-958.329478

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.044147	-1.940603	1.159930
2	1	0	0.024147	-0.124033	1.860034
3	1	0	0.026175	1.491490	1.297712
4	1	0	-0.393147	1.524234	-0.567810
5	7	0	-0.075881	2.391635	-0.111851
6	7	0	-0.146696	0.861490	2.163925
7	6	0	-1.581610	1.003740	2.497988
8	1	0	-1.772866	2.035421	2.800066
9	1	0	-1.838462	0.326655	3.315120
10	1	0	-2.152809	0.758085	1.600651
11	6	0	0.757023	1.233764	3.270166
12	1	0	0.561460	2.268378	3.556285
13	1	0	1.790468	1.140836	2.934636
14	1	0	0.584219	0.577457	4.124800
15	6	0	0.956134	-3.074032	1.334128
16	1	0	0.650084	-3.929139	0.707810
17	1	0	0.940948	-3.393206	2.379827
18	1	0	1.978877	-2.807007	1.068812
19	6	0	-1.297389	-2.387903	1.546685
20	1	0	-1.628762	-3.243612	0.935448
21	1	0	-2.018613	-1.580161	1.424169
22	1	0	-1.279194	-2.695023	2.596445
23	6	0	1.134455	2.895303	-0.752348
24	1	0	0.939023	3.274546	-1.766933
25	1	0	1.876632	2.095770	-0.815249
26	1	0	1.553619	3.715727	-0.159432
27	6	0	-1.158143	3.372044	-0.118071
28	1	0	-1.346866	3.775838	-1.124175
29	1	0	-0.907402	4.209301	0.542651
30	1	0	-2.078120	2.903218	0.239568
31	7	0	-0.921868	-0.405994	-0.409892
32	6	0	0.048006	-1.455318	-0.249112

33	6	0	1.417579	-0.892841	-0.630468
34	6	0	3.854137	0.239277	-1.475451
35	6	0	1.707296	-0.745817	-1.991380
36	6	0	2.364142	-0.454236	0.298801
37	6	0	3.574950	0.104624	-0.117272
38	6	0	2.911062	-0.186720	-2.413870
39	1	0	0.971545	-1.073171	-2.723085
40	1	0	2.172102	-0.578489	1.360982
41	1	0	4.298770	0.432577	0.623405
42	1	0	3.116425	-0.085658	-3.475472
43	1	0	4.795508	0.670148	-1.802351
44	6	0	-2.005338	-0.711204	-1.099805
45	8	0	-2.346053	-1.763046	-1.676040
46	8	0	-2.865318	0.380128	-1.143886
47	1	0	-0.169634	-2.315286	-0.912027
48	6	0	-4.051570	0.198873	-1.900296
49	1	0	-4.593737	1.143834	-1.839044
50	1	0	-4.666315	-0.607795	-1.490935
51	1	0	-3.825423	-0.030613	-2.945439

1c.3Me$_2$NH-ts2

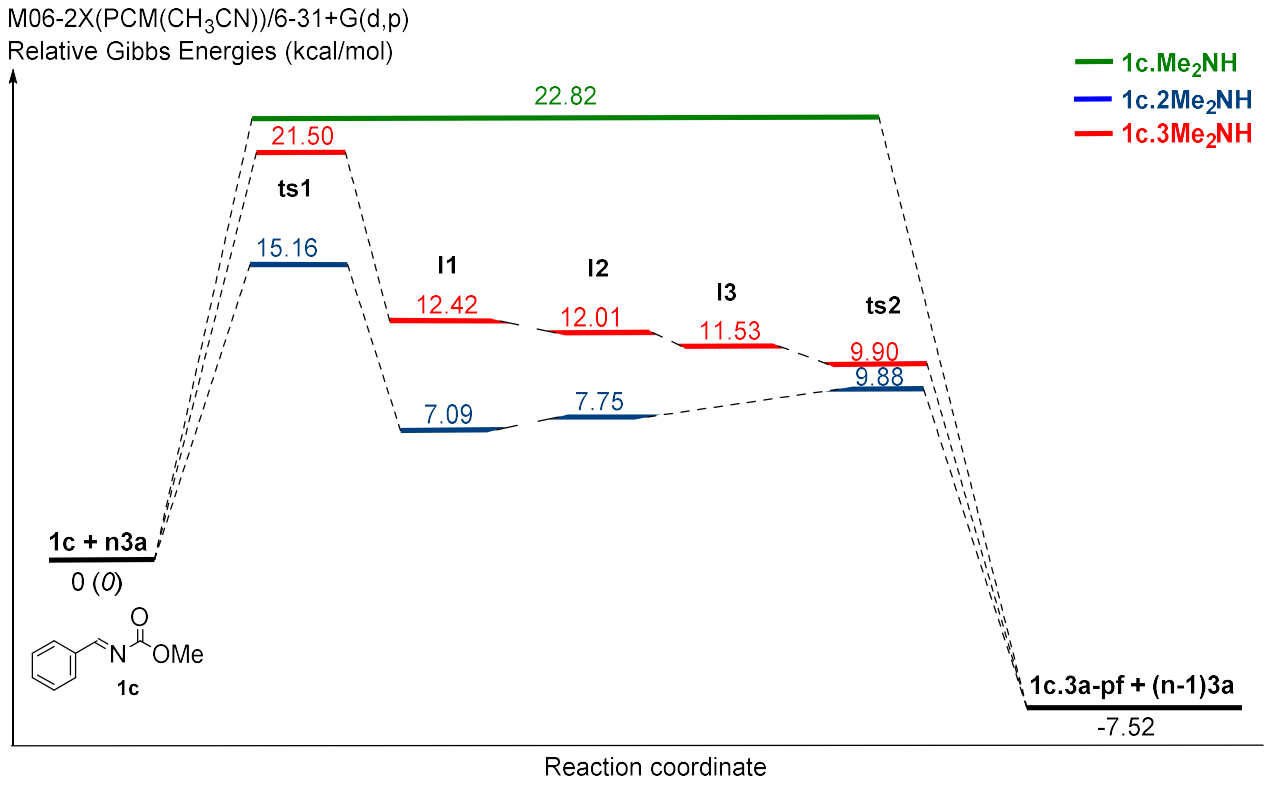
Zero-point correction=	0.450917
(Hartree/Particle)	
Thermal correction to Energy=	0.476350
Thermal correction to Enthalpy=	0.477294
Thermal correction to Gibbs Free Energy=	0.395097
Sum of electronic and zero-point Energies=	-958.275246
Sum of electronic and thermal Energies=	-958.249813
Sum of electronic and thermal Enthalpies=	-958.248869
Sum of electronic and thermal Free Energies=	-958.331066

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.543323	-0.019272	1.805427
2	1	0	0.041788	1.600609	1.056617
3	1	0	-1.055174	2.001766	-0.308827
4	1	0	-1.327345	0.367966	-1.066168
5	7	0	-1.744284	1.308196	-1.257229
6	7	0	-0.425141	2.455320	0.658148
7	6	0	-1.376132	2.980508	1.652244
8	1	0	-1.909270	3.835541	1.228642
9	1	0	-0.852608	3.298932	2.559183
10	1	0	-2.096879	2.201912	1.908661
11	6	0	0.577849	3.456119	0.262004
12	1	0	0.076471	4.304031	-0.211331
13	1	0	1.278086	3.013193	-0.448176
14	1	0	1.134379	3.812305	1.134443
15	6	0	1.776784	0.057664	2.586525
16	1	0	2.039633	-0.914876	3.038747
17	1	0	1.642323	0.784469	3.392594
18	1	0	2.608831	0.384579	1.960179
19	6	0	-0.575011	-0.319073	2.701086
20	1	0	-0.434869	-1.284791	3.214881

21	1	0	-1.504470	-0.362994	2.129621
22	1	0	-0.657073	0.469154	3.455842
23	6	0	-1.516568	1.739996	-2.637623
24	1	0	-2.013843	1.072657	-3.351186
25	1	0	-0.445096	1.745735	-2.852979
26	1	0	-1.906948	2.752758	-2.775180
27	6	0	-3.167521	1.255254	-0.907394
28	1	0	-3.728037	0.637551	-1.618053
29	1	0	-3.586636	2.266636	-0.900439
30	1	0	-3.272525	0.810274	0.085111
31	7	0	-0.567369	-1.002815	-0.081785
32	6	0	0.618354	-1.055089	0.726863
33	6	0	1.845246	-0.795612	-0.133070
34	6	0	4.101944	-0.251706	-1.713908
35	6	0	2.985940	-1.592737	-0.038665
36	6	0	1.842893	0.267880	-1.040107
37	6	0	2.960796	0.547124	-1.820923
38	6	0	4.109085	-1.325923	-0.825957
39	1	0	2.997942	-2.427728	0.658145
40	1	0	0.939071	0.862088	-1.140792
41	1	0	2.942258	1.379917	-2.518552
42	1	0	4.988552	-1.957852	-0.744883
43	1	0	4.974704	-0.040834	-2.324277
44	6	0	-1.402516	-2.019298	0.028562
45	8	0	-1.358452	-3.047838	0.730654
46	6	0	-3.480045	-2.849778	-0.782717
47	1	0	-4.260016	-2.531028	-1.476330
48	1	0	-3.902084	-2.971155	0.218835
49	1	0	-3.067604	-3.809332	-1.107453
50	1	0	0.735643	-2.040257	1.216999
51	8	0	-2.495484	-1.830060	-0.809070

2.3.4.-M06-2X(PCM=Acetonitrile)/6-31+G(d,p) calculations

Energy profiles for the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1c** in acetonitrile.



1c.Me_2NH-ts

Zero-point correction=	0.259713
(Hartree/Particle)	
Thermal correction to Energy=	0.274659
Thermal correction to Enthalpy=	0.275603
Thermal correction to Gibbs Free Energy=	0.216214
Sum of electronic and zero-point Energies=	-688.203738
Sum of electronic and thermal Energies=	-688.188792
Sum of electronic and thermal Enthalpies=	-688.187848
Sum of electronic and thermal Free Energies=	-688.247236

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.258905	0.288718	0.438473
2	6	0	-2.184580	-0.478416	-0.157420
3	8	0	-3.339182	-0.514467	0.559280
4	8	0	-2.060354	-1.105304	-1.213190
5	6	0	1.143194	-0.234606	-0.181888
6	6	0	3.455634	-1.786554	0.076317
7	6	0	2.211619	-0.062620	-1.067326
8	6	0	1.233388	-1.195831	0.825628
9	6	0	2.386452	-1.970237	0.953472
10	6	0	3.366713	-0.830715	-0.936695
11	1	0	2.136569	0.673011	-1.865426
12	1	0	0.394194	-1.330319	1.501932
13	1	0	2.450093	-2.718768	1.737356
14	1	0	4.191342	-0.689619	-1.628286
15	1	0	4.352170	-2.390579	0.176277
16	6	0	-0.077369	0.639006	-0.329601
17	1	0	-0.293740	0.779001	-1.396039
18	1	0	-1.070759	1.563392	0.759816
19	6	0	1.072301	2.181292	1.331217
20	1	0	0.921035	3.143301	1.822611
21	1	0	2.073417	2.146619	0.888865
22	1	0	0.973345	1.380147	2.065393
23	7	0	0.035985	2.026162	0.300438
24	6	0	0.030573	3.129400	-0.668837
25	1	0	-0.070429	4.072765	-0.130313
26	1	0	-0.816743	3.008796	-1.346103
27	1	0	0.961999	3.140872	-1.245116
28	6	0	-4.384375	-1.309358	0.003087
29	1	0	-5.220714	-1.221446	0.695220
30	1	0	-4.074689	-2.353476	-0.081763
31	1	0	-4.671663	-0.937874	-0.983253

1c.Me_2NH-pf

Zero-point correction=	0.264499
(Hartree/Particle)	
Thermal correction to Energy=	0.279744
Thermal correction to Enthalpy=	0.280688
Thermal correction to Gibbs Free Energy=	0.221296
Sum of electronic and zero-point Energies=	-688.252384
Sum of electronic and thermal Energies=	-688.237139
Sum of electronic and thermal Enthalpies=	-688.236195
Sum of electronic and thermal Free Energies=	-688.295586

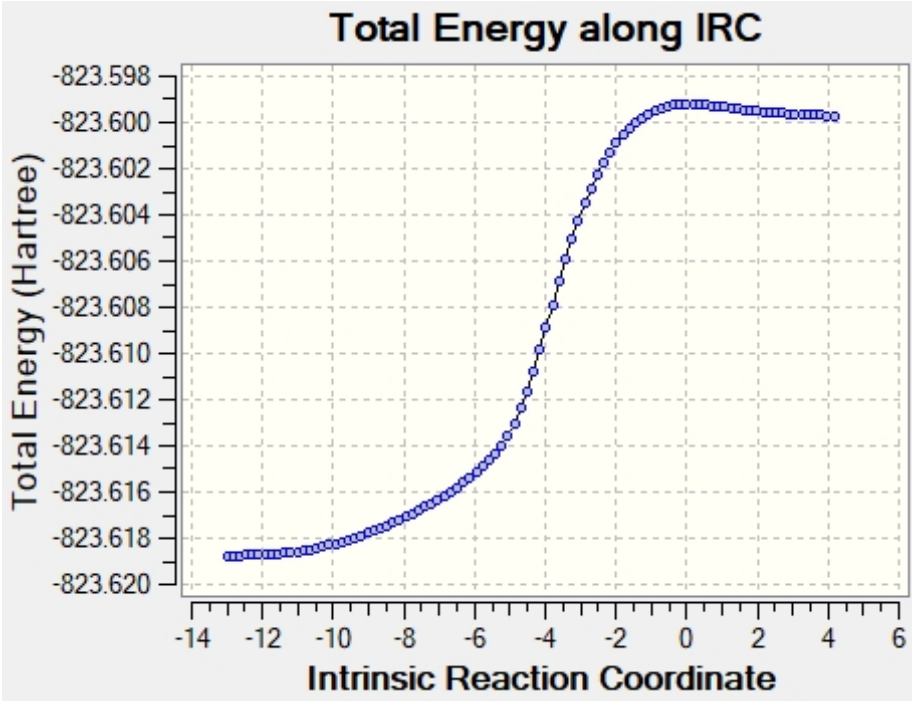
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.116787	-0.433680	0.185011
2	6	0	-2.395325	-0.346554	-0.255290
3	8	0	-3.176372	-1.253275	0.365078
4	8	0	-2.801444	0.432118	-1.101988
5	6	0	1.281832	-0.223537	-0.209175
6	6	0	3.850699	-1.342477	-0.029519
7	6	0	2.165445	-0.157989	-1.289968
8	6	0	1.703187	-0.853839	0.967824
9	6	0	2.977234	-1.412538	1.055941
10	6	0	3.442477	-0.712314	-1.203914
11	1	0	1.848216	0.326580	-2.210508
12	1	0	1.044891	-0.912512	1.831359
13	1	0	3.287576	-1.901298	1.974204
14	1	0	4.113489	-0.656462	-2.055345
15	1	0	4.842343	-1.778263	0.040932
16	6	0	-0.082951	0.439700	-0.332484
17	1	0	-0.290730	0.596847	-1.396640
18	1	0	-0.893635	-1.182168	0.825149
19	6	0	0.094294	1.801637	1.711066
20	1	0	-0.200596	2.779808	2.100871
21	1	0	1.159577	1.644189	1.950164
22	1	0	-0.499119	1.039215	2.223351
23	7	0	-0.180388	1.768891	0.281822
24	6	0	0.621281	2.753528	-0.429191
25	1	0	0.390521	3.748516	-0.038947
26	1	0	0.374271	2.734643	-1.495050
27	1	0	1.706823	2.585703	-0.319317
28	6	0	-4.546137	-1.269811	-0.048925
29	1	0	-4.619245	-1.514731	-1.110120
30	1	0	-5.011451	-0.300336	0.137108
31	1	0	-5.022397	-2.041790	0.552050

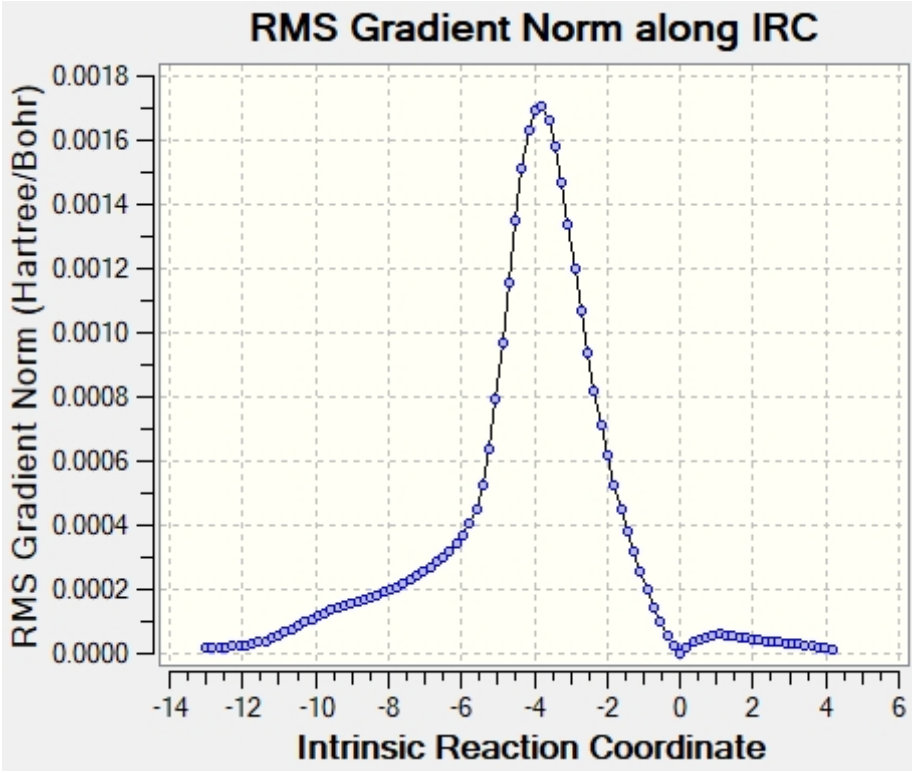
1c.2Me$_2$NH-ts1

Zero-point correction=	0.357043
(Hartree/Particle)	
Thermal correction to Energy=	0.378174
Thermal correction to Enthalpy=	0.379119
Thermal correction to Gibbs Free Energy=	0.305380
Sum of electronic and zero-point Energies=	-823.242166
Sum of electronic and thermal Energies=	-823.221034
Sum of electronic and thermal Enthalpies=	-823.220090
Sum of electronic and thermal Free Energies=	-823.293829

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.048932	-1.462168	0.069846
2	6	0	-1.330888	-1.620877	-0.430613
3	8	0	-2.005152	-2.521111	0.303635
4	8	0	-1.844852	-1.043449	-1.379269
5	6	0	2.127746	-0.489994	-0.294783
6	6	0	4.822789	-0.093637	0.323637
7	6	0	2.967815	0.173129	-1.196128
8	6	0	2.646666	-0.959477	0.918548
9	6	0	3.988795	-0.758894	1.226120
10	6	0	4.312454	0.370153	-0.889343
11	6	0	0.711808	-0.682813	-0.644705
12	7	0	-2.992883	1.399210	-0.036626
13	1	0	0.396790	-0.340978	-1.632818
14	1	0	2.562295	0.536825	-2.137218
15	1	0	4.960155	0.883597	-1.592756
16	1	0	5.870032	0.060322	0.564909
17	1	0	4.388120	-1.121809	2.167958
18	1	0	1.986109	-1.477459	1.606728
19	7	0	0.091433	1.491607	0.004325
20	6	0	-3.977489	2.457182	-0.229169
21	1	0	-3.806427	3.248781	0.507524
22	1	0	-5.015410	2.106029	-0.112376
23	1	0	-3.865624	2.890177	-1.225836
24	6	0	0.700569	2.609064	-0.698294
25	1	0	1.788067	2.570299	-0.567290
26	1	0	0.347845	3.585891	-0.332626
27	1	0	0.480031	2.536504	-1.767216
28	6	0	-3.147337	0.739622	1.254599
29	1	0	-2.418458	-0.072140	1.352510
30	1	0	-4.156070	0.324618	1.413820
31	1	0	-2.950557	1.461261	2.054768
32	6	0	0.328010	1.520694	1.437139
33	1	0	-0.042160	0.590863	1.883523
34	1	0	-0.162658	2.371824	1.933009
35	1	0	1.405380	1.586762	1.626387
36	6	0	-3.357740	-2.755248	-0.095103
37	1	0	-3.393008	-3.145739	-1.114009
38	1	0	-3.935599	-1.829036	-0.041497
39	1	0	-3.749768	-3.487086	0.608242
40	1	0	-3.075275	0.705003	-0.776136
41	1	0	-0.920286	1.477990	-0.168766

1c.2Me$_2$NH-ts1





1c.2Me$_2$NH-I1

Zero-point correction=	0.455218
(Hartree/Particle)	
Thermal correction to Energy=	0.481192
Thermal correction to Enthalpy=	0.482137
Thermal correction to Gibbs Free Energy=	0.399179
Sum of electronic and zero-point Energies=	-958.276546
Sum of electronic and thermal Energies=	-958.250572
Sum of electronic and thermal Enthalpies=	-958.249627
Sum of electronic and thermal Free Energies=	-958.332585

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.364949	-1.526930	-0.316910
2	6	0	-0.774860	-1.638927	-0.974305
3	8	0	-1.146770	-2.957520	-1.115545
4	8	0	-1.524409	-0.756635	-1.457951
5	6	0	2.317469	-0.061457	-0.179484
6	6	0	5.107429	0.207338	-0.299144
7	6	0	2.899176	1.117212	-0.654375
8	6	0	3.148761	-1.112255	0.222137
9	6	0	4.534542	-0.977044	0.168269
10	6	0	4.286509	1.254209	-0.715090
11	6	0	0.807402	-0.193840	-0.113623
12	7	0	-2.390884	-0.080201	1.309224
13	1	0	0.351061	0.531648	-0.802495
14	1	0	2.264112	1.934337	-0.989587
15	1	0	4.721972	2.174060	-1.092836
16	1	0	6.187238	0.309218	-0.347153
17	1	0	5.168977	-1.799851	0.483528
18	1	0	2.696105	-2.038955	0.560493
19	7	0	0.301550	0.291587	1.263895
20	6	0	-3.056286	0.983046	2.060250
21	1	0	-2.734677	0.939266	3.105880
22	1	0	-4.151756	0.893690	2.032750
23	1	0	-2.764267	1.948833	1.639367
24	6	0	0.501834	1.737863	1.501567
25	1	0	1.568549	1.963948	1.554587
26	1	0	0.025340	1.999269	2.448823
27	1	0	0.019223	2.289378	0.692216
28	6	0	-2.768869	-1.421427	1.754909
29	1	0	-2.256408	-2.167374	1.140248
30	1	0	-3.852901	-1.591566	1.694530
31	1	0	-2.456461	-1.557097	2.795091
32	6	0	0.799424	-0.520366	2.396487
33	1	0	0.681438	-1.573552	2.141753
34	1	0	0.201997	-0.276761	3.277569
35	1	0	1.848954	-0.288415	2.587685
36	1	0	-0.778588	0.131433	1.238799
37	7	0	-1.889453	2.174966	-0.975432
38	6	0	-3.317824	2.422186	-1.119044
39	1	0	-3.581991	3.360011	-0.617086
40	1	0	-3.889362	1.617704	-0.645018
41	1	0	-3.642099	2.498609	-2.170305
42	6	0	-1.101169	3.165318	-1.695544
43	1	0	-0.037209	2.914030	-1.636072
44	1	0	-1.239440	4.150788	-1.236901
45	1	0	-1.372291	3.248386	-2.761172

46	1	0	-1.675675	1.240995	-1.327039
47	1	0	-2.589431	0.007131	0.312690
48	6	0	-2.378785	-3.189407	-1.785804
49	1	0	-2.352998	-2.801860	-2.807331
50	1	0	-3.212411	-2.723051	-1.252010
51	1	0	-2.509245	-4.271664	-1.801710

1c.2Me$_2$NH-I2

Zero-point correction= 0.455204
(Hartree/Particle)
Thermal correction to Energy= 0.481359
Thermal correction to Enthalpy= 0.482303
Thermal correction to Gibbs Free Energy= 0.397841
Sum of electronic and zero-point Energies= -958.275870
Sum of electronic and thermal Energies= -958.249716
Sum of electronic and thermal Enthalpies= -958.248772
Sum of electronic and thermal Free Energies= -958.333233

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.463953	-0.054326	1.745956
2	1	0	0.407832	0.915498	1.256879
3	1	0	-0.228797	2.399467	-0.156059
4	1	0	-1.349410	0.677071	-1.142657
5	7	0	-1.578714	1.610619	-1.505958
6	7	0	0.293398	2.495713	0.725669
7	6	0	-0.509925	3.274119	1.670508
8	1	0	-0.660935	4.310164	1.335367
9	1	0	-0.006360	3.300711	2.643040
10	1	0	-1.487669	2.804022	1.802087
11	6	0	1.591639	3.124508	0.479873
12	1	0	1.491884	4.155801	0.112572
13	1	0	2.153770	2.541857	-0.254055
14	1	0	2.165834	3.148503	1.411957
15	6	0	1.725672	-0.076121	2.522484
16	1	0	1.850341	-1.056924	2.988250
17	1	0	1.672323	0.694192	3.293236
18	1	0	2.564734	0.128556	1.858769
19	6	0	-0.707691	-0.140413	2.650361
20	1	0	-0.709176	-1.115247	3.142809
21	1	0	-1.615893	-0.021284	2.061110
22	1	0	-0.635924	0.657191	3.391085
23	6	0	-1.539803	1.589314	-2.961450
24	1	0	-2.308107	0.930395	-3.400227
25	1	0	-0.558508	1.247866	-3.304019
26	1	0	-1.703081	2.599211	-3.354008
27	6	0	-2.898190	1.977980	-1.008525
28	1	0	-3.705592	1.371620	-1.451679
29	1	0	-3.104805	3.031681	-1.228743
30	1	0	-2.932680	1.842627	0.077027
31	7	0	-0.781362	-0.960411	-0.113369
32	6	0	0.395227	-1.146550	0.654296
33	6	0	1.641691	-1.048281	-0.203254
34	6	0	3.944209	-0.874708	-1.789071

35	6	0	2.679743	-1.967755	-0.045594
36	6	0	1.758793	-0.044452	-1.170248
37	6	0	2.906794	0.046386	-1.954339
38	6	0	3.826901	-1.885294	-0.836407
39	1	0	2.590486	-2.754630	0.699628
40	1	0	0.937903	0.655327	-1.310767
41	1	0	2.991344	0.831474	-2.700123
42	1	0	4.624561	-2.610332	-0.708257
43	1	0	4.835424	-0.807922	-2.405362
44	6	0	-1.779136	-1.789725	0.165916
45	8	0	-1.855737	-2.702798	1.009727
46	8	0	-2.862554	-1.533827	-0.647043
47	1	0	0.407353	-2.088121	1.223888
48	6	0	-4.004087	-2.352201	-0.435610
49	1	0	-4.761270	-1.992501	-1.132949
50	1	0	-4.370549	-2.262506	0.590434
51	1	0	-3.780644	-3.402777	-0.640423

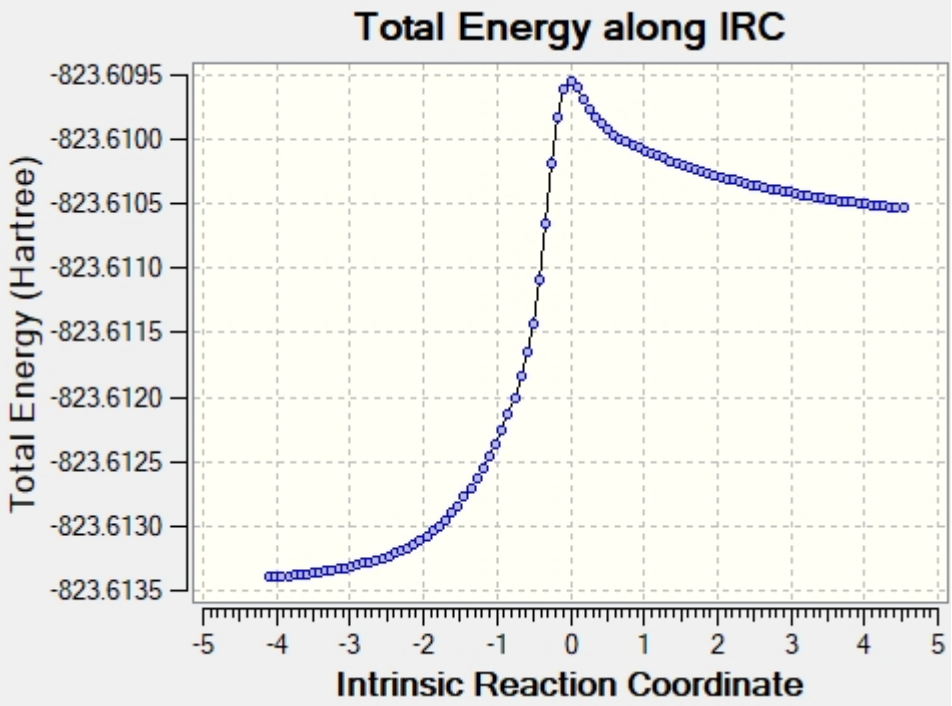
1c.2Me$_2$NH-ts2

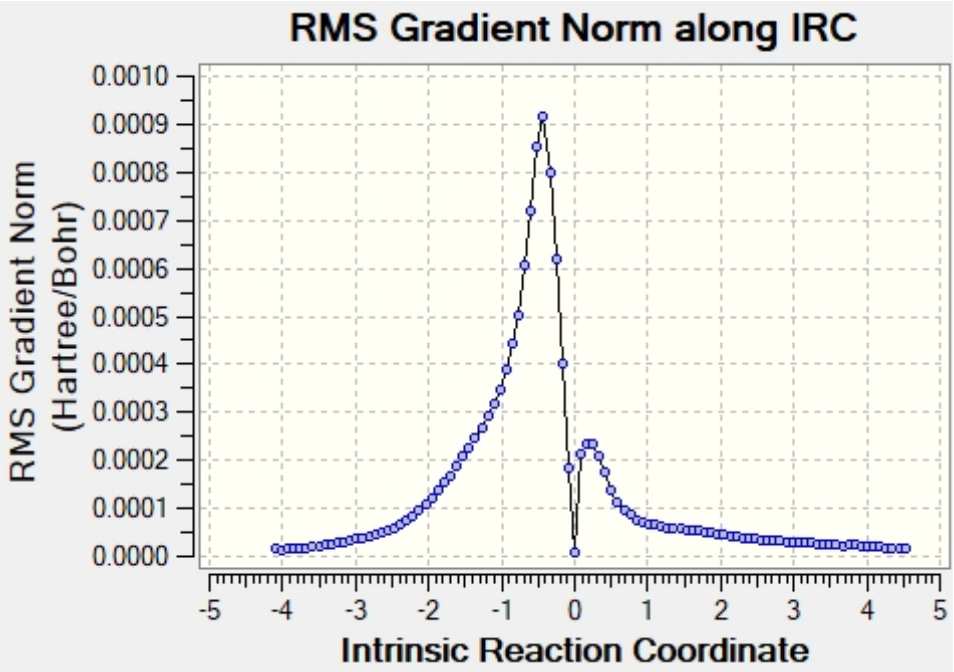
Zero-point correction=	0.356324
(Hartree/Particle)	
Thermal correction to Energy=	0.376316
Thermal correction to Enthalpy=	0.377261
Thermal correction to Gibbs Free Energy=	0.307306
Sum of electronic and zero-point Energies=	-823.253221
Sum of electronic and thermal Energies=	-823.233229
Sum of electronic and thermal Enthalpies=	-823.232285
Sum of electronic and thermal Free Energies=	-823.302240

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.956933	-0.551317	-0.369120
2	6	0	1.994508	-1.328274	-0.113277
3	8	0	2.914864	-1.280102	-1.147401
4	8	0	2.247185	-2.051311	0.873811
5	6	0	-1.441035	-0.758454	0.073652
6	6	0	-4.036825	-1.146184	-0.926977
7	6	0	-2.389611	-1.474141	0.809401
8	6	0	-1.801181	-0.261947	-1.182296
9	6	0	-3.091543	-0.444877	-1.677099
10	6	0	-3.679764	-1.669006	0.315427
11	1	0	-2.116328	-1.880295	1.780744
12	1	0	-1.055509	0.245328	-1.786192
13	1	0	-3.356665	-0.049498	-2.653173
14	1	0	-4.403094	-2.230045	0.899368
15	1	0	-5.039985	-1.294014	-1.314739
16	6	0	-0.052531	-0.524145	0.647813
17	6	0	1.855130	2.985353	-0.524103
18	1	0	2.594653	2.228729	-0.255994
19	1	0	1.758965	3.707395	0.289364
20	1	0	2.174125	3.503985	-1.431930
21	6	0	-1.186066	1.210992	2.094862
22	1	0	-1.004260	2.178655	2.568203
23	1	0	-1.396952	0.468400	2.875594

24	1	0	-2.052614	1.294420	1.438204
25	7	0	0.555354	2.322059	-0.732752
26	6	0	-0.509022	3.243124	-1.164195
27	1	0	-0.244362	3.730958	-2.105852
28	1	0	-0.648954	4.001605	-0.391421
29	1	0	-1.438933	2.685264	-1.289275
30	7	0	0.008618	0.839906	1.321615
31	6	0	1.198828	0.901526	2.188373
32	1	0	1.343992	1.928731	2.532295
33	1	0	2.074913	0.577866	1.625708
34	1	0	1.071331	0.244833	3.058393
35	1	0	0.120555	-1.265964	1.443954
36	1	0	0.686393	1.551555	-1.394743
37	1	0	0.243810	1.685495	0.278826
38	6	0	4.074309	-2.082086	-0.982769
39	1	0	4.680804	-1.916700	-1.874276
40	1	0	3.816484	-3.141848	-0.902727
41	1	0	4.637726	-1.789384	-0.092669

1c.2Me$_2$NH-ts2





1c.3Me$_2$NH-ts1

Zero-point correction=	0.451420
(Hartree/Particle)	
Thermal correction to Energy=	0.478488
Thermal correction to Enthalpy=	0.479432
Thermal correction to Gibbs Free Energy=	0.391824
Sum of electronic and zero-point Energies=	-958.258518
Sum of electronic and thermal Energies=	-958.231450
Sum of electronic and thermal Enthalpies=	-958.230506
Sum of electronic and thermal Free Energies=	-958.318115

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.770145	1.634849	-0.380024
2	6	0	0.567589	1.836817	-0.684374
3	8	0	0.932285	3.087132	-0.355140
4	8	0	1.357918	1.036741	-1.163779
5	6	0	-2.657819	0.146842	-0.575096
6	6	0	-5.354060	-0.521919	-0.275586
7	6	0	-3.165243	-1.017745	-1.162011
8	6	0	-3.511446	0.979847	0.159147
9	6	0	-4.853064	0.643624	0.309971
10	6	0	-4.509721	-1.351721	-1.014178
11	6	0	-1.233574	0.474787	-0.745246
12	7	0	2.361382	-0.292872	1.488138
13	1	0	-0.645763	-0.192898	-1.379139
14	1	0	-2.501190	-1.662531	-1.733004
15	1	0	-4.897861	-2.256149	-1.471647
16	1	0	-6.401787	-0.780753	-0.157502
17	1	0	-5.511253	1.288799	0.883427
18	1	0	-3.108593	1.883836	0.604736
19	7	0	-0.542286	-0.989791	0.979666
20	6	0	3.309532	-1.206258	2.109190
21	1	0	2.895243	-1.590786	3.047963
22	1	0	4.278672	-0.731010	2.336894
23	1	0	3.491745	-2.050321	1.438731
24	6	0	-0.851673	-2.404881	0.861278
25	1	0	-1.938355	-2.534465	0.799443
26	1	0	-0.486317	-2.995184	1.716775
27	1	0	-0.407730	-2.808735	-0.053752
28	6	0	2.196995	0.933338	2.254804
29	1	0	1.489768	1.601460	1.751925
30	1	0	3.142627	1.479555	2.410868
31	1	0	1.781924	0.694988	3.240667
32	6	0	-1.106968	-0.385633	2.173978
33	1	0	-0.945533	0.697944	2.140751
34	1	0	-0.664196	-0.781469	3.100966
35	1	0	-2.186857	-0.570726	2.201410
36	1	0	0.476830	-0.843807	0.995681
37	7	0	3.413136	-1.104936	-1.317014
38	6	0	4.611051	-1.738412	-1.849250
39	1	0	4.922235	-2.544620	-1.175606
40	1	0	5.424602	-1.010880	-1.903994
41	1	0	4.464174	-2.176409	-2.850579
42	6	0	2.270458	-2.008356	-1.307498
43	1	0	1.379001	-1.449472	-1.012274
44	1	0	2.439053	-2.806908	-0.574815
45	1	0	2.084992	-2.482621	-2.286117

46	1	0	3.172111	-0.282552	-1.863026
47	1	0	2.687295	-0.088387	0.542701
48	6	0	2.303374	3.412795	-0.596233
49	1	0	2.534968	3.323609	-1.659549
50	1	0	2.957045	2.748060	-0.025418
51	1	0	2.424330	4.441938	-0.263879

1c.3Me$_2$NH-I1

Zero-point correction= (Hartree/Particle)	0.455218
Thermal correction to Energy=	0.481192
Thermal correction to Enthalpy=	0.482137
Thermal correction to Gibbs Free Energy=	0.399179
Sum of electronic and zero-point Energies=	-958.276546
Sum of electronic and thermal Energies=	-958.250572
Sum of electronic and thermal Enthalpies=	-958.249627
Sum of electronic and thermal Free Energies=	-958.332585

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.364949	-1.526930	-0.316910
2	6	0	-0.774860	-1.638927	-0.974305
3	8	0	-1.146770	-2.957520	-1.115545
4	8	0	-1.524409	-0.756635	-1.457951
5	6	0	2.317469	-0.061457	-0.179484
6	6	0	5.107429	0.207338	-0.299144
7	6	0	2.899176	1.117212	-0.654375
8	6	0	3.148761	-1.112255	0.222137
9	6	0	4.534542	-0.977044	0.168269
10	6	0	4.286509	1.254209	-0.715090
11	6	0	0.807402	-0.193840	-0.113623
12	7	0	-2.390884	-0.080201	1.309224
13	1	0	0.351061	0.531648	-0.802495
14	1	0	2.264112	1.934337	-0.989587
15	1	0	4.721972	2.174060	-1.092836
16	1	0	6.187238	0.309218	-0.347153
17	1	0	5.168977	-1.799851	0.483528
18	1	0	2.696105	-2.038955	0.560493
19	7	0	0.301550	0.291587	1.263895
20	6	0	-3.056286	0.983046	2.060250
21	1	0	-2.734677	0.939266	3.105880
22	1	0	-4.151756	0.893690	2.032750
23	1	0	-2.764267	1.948833	1.639367
24	6	0	0.501834	1.737863	1.501567
25	1	0	1.568549	1.963948	1.554587
26	1	0	0.025340	1.999269	2.448823
27	1	0	0.019223	2.289378	0.692216
28	6	0	-2.768869	-1.421427	1.754909
29	1	0	-2.256408	-2.167374	1.140248
30	1	0	-3.852901	-1.591566	1.694530
31	1	0	-2.456461	-1.557097	2.795091
32	6	0	0.799424	-0.520366	2.396487
33	1	0	0.681438	-1.573552	2.141753

34	1	0	0.201997	-0.276761	3.277569
35	1	0	1.848954	-0.288415	2.587685
36	1	0	-0.778588	0.131433	1.238799
37	7	0	-1.889453	2.174966	-0.975432
38	6	0	-3.317824	2.422186	-1.119044
39	1	0	-3.581991	3.360011	-0.617086
40	1	0	-3.889362	1.617704	-0.645018
41	1	0	-3.642099	2.498609	-2.170305
42	6	0	-1.101169	3.165318	-1.695544
43	1	0	-0.037209	2.914030	-1.636072
44	1	0	-1.239440	4.150788	-1.236901
45	1	0	-1.372291	3.248386	-2.761172
46	1	0	-1.675675	1.240995	-1.327039
47	1	0	-2.589431	0.007131	0.312690
48	6	0	-2.378785	-3.189407	-1.785804
49	1	0	-2.352998	-2.801860	-2.807331
50	1	0	-3.212411	-2.723051	-1.252010
51	1	0	-2.509245	-4.271664	-1.801710

1c.3Me$_2$NH-I2

Zero-point correction= 0.455204
(Hartree/Particle)
Thermal correction to Energy= 0.481359
Thermal correction to Enthalpy= 0.482303
Thermal correction to Gibbs Free Energy= 0.397841
Sum of electronic and zero-point Energies= -958.275870
Sum of electronic and thermal Energies= -958.249716
Sum of electronic and thermal Enthalpies= -958.248772
Sum of electronic and thermal Free Energies= -958.333233

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.463953	-0.054326	1.745956
2	1	0	0.407832	0.915498	1.256879
3	1	0	-0.228797	2.399467	-0.156059
4	1	0	-1.349410	0.677071	-1.142657
5	7	0	-1.578714	1.610619	-1.505958
6	7	0	0.293398	2.495713	0.725669
7	6	0	-0.509925	3.274119	1.670508
8	1	0	-0.660935	4.310164	1.335367
9	1	0	-0.006360	3.300711	2.643040
10	1	0	-1.487669	2.804022	1.802087
11	6	0	1.591639	3.124508	0.479873
12	1	0	1.491884	4.155801	0.112572
13	1	0	2.153770	2.541857	-0.254055
14	1	0	2.165834	3.148503	1.411957
15	6	0	1.725672	-0.076121	2.522484
16	1	0	1.850341	-1.056924	2.988250
17	1	0	1.672323	0.694192	3.293236
18	1	0	2.564734	0.128556	1.858769
19	6	0	-0.707691	-0.140413	2.650361
20	1	0	-0.709176	-1.115247	3.142809
21	1	0	-1.615893	-0.021284	2.061110
22	1	0	-0.635924	0.657191	3.391085

23	6	0	-1.539803	1.589314	-2.961450
24	1	0	-2.308107	0.930395	-3.400227
25	1	0	-0.558508	1.247866	-3.304019
26	1	0	-1.703081	2.599211	-3.354008
27	6	0	-2.898190	1.977980	-1.008525
28	1	0	-3.705592	1.371620	-1.451679
29	1	0	-3.104805	3.031681	-1.228743
30	1	0	-2.932680	1.842627	0.077027
31	7	0	-0.781362	-0.960411	-0.113369
32	6	0	0.395227	-1.146550	0.654296
33	6	0	1.641691	-1.048281	-0.203254
34	6	0	3.944209	-0.874708	-1.789071
35	6	0	2.679743	-1.967755	-0.045594
36	6	0	1.758793	-0.044452	-1.170248
37	6	0	2.906794	0.046386	-1.954339
38	6	0	3.826901	-1.885294	-0.836407
39	1	0	2.590486	-2.754630	0.699628
40	1	0	0.937903	0.655327	-1.310767
41	1	0	2.991344	0.831474	-2.700123
42	1	0	4.624561	-2.610332	-0.708257
43	1	0	4.835424	-0.807922	-2.405362
44	6	0	-1.779136	-1.789725	0.165916
45	8	0	-1.855737	-2.702798	1.009727
46	8	0	-2.862554	-1.533827	-0.647043
47	1	0	0.407353	-2.088121	1.223888
48	6	0	-4.004087	-2.352201	-0.435610
49	1	0	-4.761270	-1.992501	-1.132949
50	1	0	-4.370549	-2.262506	0.590434
51	1	0	-3.780644	-3.402777	-0.640423

1c.3Me$_2$NH-I3

Zero-point correction= 0.454848
(Hartree/Particle)
Thermal correction to Energy= 0.481026
Thermal correction to Enthalpy= 0.481971
Thermal correction to Gibbs Free Energy= 0.396711
Sum of electronic and zero-point Energies= -958.275853
Sum of electronic and thermal Energies= -958.249675
Sum of electronic and thermal Enthalpies= -958.248730
Sum of electronic and thermal Free Energies= -958.333990

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.026242	-1.698606	1.432736
2	1	0	0.051447	0.165017	1.871658
3	1	0	0.105165	1.684824	1.085292
4	1	0	-0.385168	1.479083	-0.772592
5	7	0	0.003400	2.376389	-0.450582
6	7	0	-0.079706	1.192364	2.030700
7	6	0	-1.504234	1.430979	2.354827
8	1	0	-1.657019	2.499650	2.516607
9	1	0	-1.773058	0.878315	3.256869
10	1	0	-2.096917	1.086502	1.505277
11	6	0	0.850656	1.685257	3.066648

12	1	0	0.692790	2.755758	3.205428
13	1	0	1.876162	1.510546	2.739574
14	1	0	0.666616	1.161566	4.005982
15	6	0	0.848258	-2.814543	1.803029
16	1	0	0.508616	-3.754775	1.336097
17	1	0	0.828611	-2.944395	2.888250
18	1	0	1.877563	-2.633018	1.494816
19	6	0	-1.381294	-2.029142	1.885265
20	1	0	-1.742360	-2.964016	1.425892
21	1	0	-2.075146	-1.229992	1.625572
22	1	0	-1.370589	-2.153299	2.971858
23	6	0	1.221725	2.694074	-1.188583
24	1	0	1.015357	2.951025	-2.238805
25	1	0	1.898252	1.836653	-1.163928
26	1	0	1.724104	3.548705	-0.722764
27	6	0	-1.001075	3.430048	-0.565455
28	1	0	-1.219325	3.685160	-1.613344
29	1	0	-0.647263	4.335853	-0.061390
30	1	0	-1.930846	3.108701	-0.089310
31	7	0	-0.946842	-0.429705	-0.389229
32	6	0	-0.005784	-1.461278	-0.037429
33	6	0	1.381158	-1.017539	-0.502722
34	6	0	3.855438	-0.136930	-1.523342
35	6	0	1.673193	-1.119029	-1.867529
36	6	0	2.347962	-0.463238	0.340169
37	6	0	3.576763	-0.028815	-0.162664
38	6	0	2.894625	-0.684481	-2.377228
39	1	0	0.925775	-1.541310	-2.536144
40	1	0	2.159916	-0.395235	1.407863
41	1	0	4.314092	0.392858	0.514257
42	1	0	3.099636	-0.775801	-3.439777
43	1	0	4.809774	0.199948	-1.916057
44	6	0	-2.048894	-0.833372	-0.992191
45	8	0	-2.430878	-1.972505	-1.332707
46	8	0	-2.877673	0.248756	-1.261611
47	1	0	-0.245489	-2.417654	-0.542103
48	6	0	-4.098980	-0.054896	-1.917408
49	1	0	-4.610301	0.899095	-2.053865
50	1	0	-4.719440	-0.723312	-1.313766
51	1	0	-3.923925	-0.522137	-2.890618

1c.3Me$_2$NH-ts2

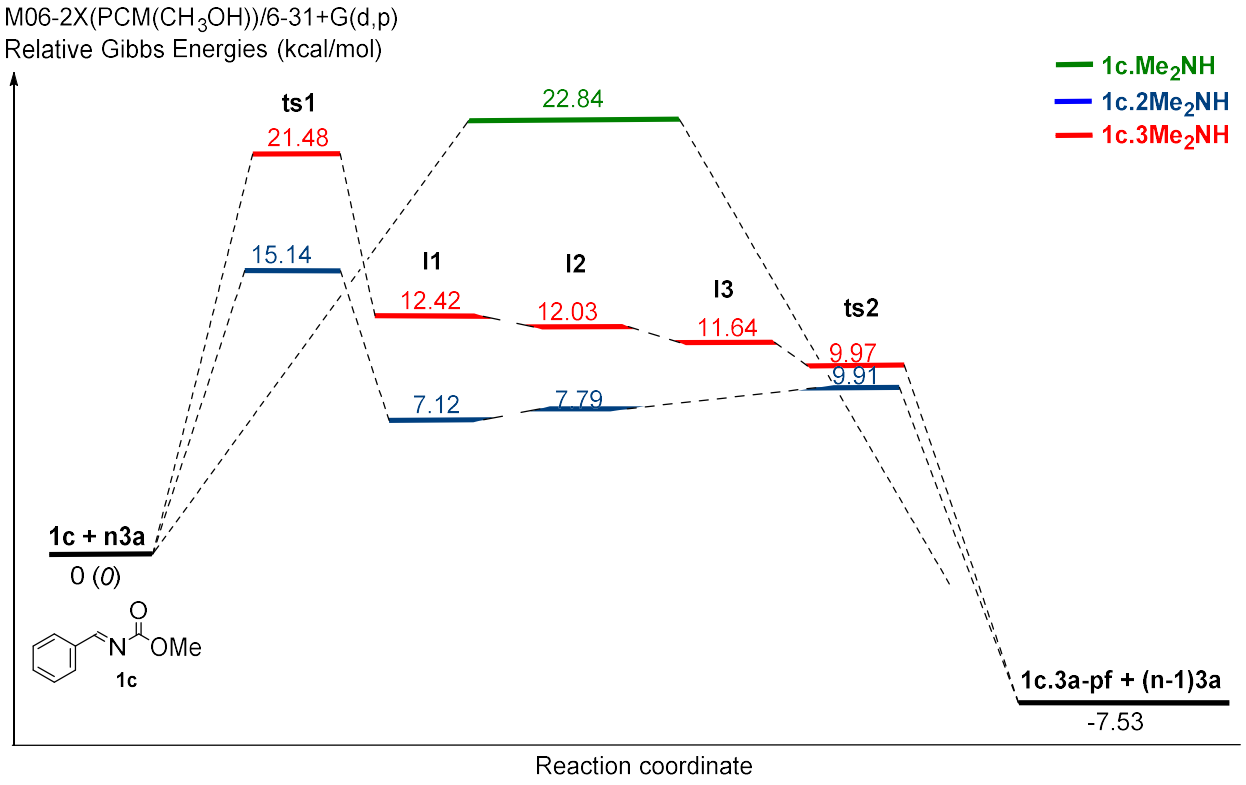
Zero-point correction= 0.450298
(Hartree/Particle)
Thermal correction to Energy= 0.476030
Thermal correction to Enthalpy= 0.476974
Thermal correction to Gibbs Free Energy= 0.393536
Sum of electronic and zero-point Energies= -958.279832
Sum of electronic and thermal Energies= -958.254100
Sum of electronic and thermal Enthalpies= -958.253156
Sum of electronic and thermal Free Energies= -958.336594

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

1	7	0	0.523225	0.007536	1.786669
2	1	0	0.056838	1.665357	1.029653
3	1	0	-1.054813	2.018658	-0.331528
4	1	0	-1.333702	0.357977	-1.037351
5	7	0	-1.751245	1.294481	-1.242401
6	7	0	-0.408828	2.507734	0.613340
7	6	0	-1.345430	3.072973	1.599666
8	1	0	-1.881364	3.912165	1.149279
9	1	0	-0.809223	3.424029	2.486730
10	1	0	-2.065228	2.307261	1.894896
11	6	0	0.592865	3.489149	0.167358
12	1	0	0.088061	4.315348	-0.338991
13	1	0	1.286827	3.014820	-0.528700
14	1	0	1.155395	3.882028	1.019777
15	6	0	1.742510	0.095039	2.588679
16	1	0	1.988688	-0.867610	3.070924
17	1	0	1.599501	0.843980	3.372413
18	1	0	2.588672	0.398998	1.969808
19	6	0	-0.613709	-0.259770	2.668126
20	1	0	-0.494961	-1.216382	3.204868
21	1	0	-1.534326	-0.301450	2.082398
22	1	0	-0.697277	0.544376	3.405396
23	6	0	-1.541069	1.691469	-2.636678
24	1	0	-2.049270	1.007159	-3.326203
25	1	0	-0.472501	1.691561	-2.865833
26	1	0	-1.932315	2.700769	-2.793343
27	6	0	-3.170552	1.253572	-0.873634
28	1	0	-3.739947	0.616107	-1.559334
29	1	0	-3.588046	2.265066	-0.891767
30	1	0	-3.264932	0.840912	0.133828
31	7	0	-0.561723	-1.031135	-0.087856
32	6	0	0.614698	-1.053677	0.737395
33	6	0	1.849166	-0.809277	-0.115998
34	6	0	4.120580	-0.290364	-1.683428
35	6	0	2.988396	-1.605472	0.001604
36	6	0	1.855348	0.240705	-1.038943
37	6	0	2.980753	0.507352	-1.813565
38	6	0	4.119258	-1.350971	-0.779057
39	1	0	2.994774	-2.427892	0.713463
40	1	0	0.953993	0.836014	-1.155680
41	1	0	2.969196	1.330690	-2.522361
42	1	0	4.998372	-1.980617	-0.678458
43	1	0	4.999627	-0.088133	-2.287659
44	6	0	-1.399090	-2.041614	0.042414
45	8	0	-1.360807	-3.055140	0.769560
46	6	0	-3.477293	-2.885864	-0.760618
47	1	0	-4.252736	-2.577921	-1.463781
48	1	0	-3.904524	-2.981647	0.241429
49	1	0	-3.070055	-3.854897	-1.063404
50	1	0	0.732722	-2.025999	1.253367
51	8	0	-2.486198	-1.872428	-0.806064

2.3.5.- M06-2X(PCM=Methanol)/6-31+G(d,p) calculations

Energy profiles for the addition of n dimethylamine (**3a**) molecules (n=1-3) to imine derivative **1c** in methanol.



1c.Me_2NH-ts

Zero-point correction=	0.259718 (Hartree/Particle)
Thermal correction to Energy=	0.274662
Thermal correction to Enthalpy=	0.275606
Thermal correction to Gibbs Free Energy=	0.216233
Sum of electronic and zero-point Energies=	-688.203644
Sum of electronic and thermal Energies=	-688.188700
Sum of electronic and thermal Enthalpies=	-688.187756
Sum of electronic and thermal Free Energies=	-688.247129

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.258811	0.288555	0.438719
2	6	0	-2.184605	-0.478296	-0.157430
3	8	0	-3.339093	-0.514684	0.559465
4	8	0	-2.060578	-1.104575	-1.213543
5	6	0	1.143223	-0.234636	-0.181861
6	6	0	3.455663	-1.786583	0.076159
7	6	0	2.211908	-0.062075	-1.066866
8	6	0	1.233140	-1.196449	0.825097
9	6	0	2.386213	-1.970851	0.952850
10	6	0	3.367007	-0.830161	-0.936323
11	1	0	2.137022	0.673951	-1.864625
12	1	0	0.393687	-1.331404	1.500983
13	1	0	2.449633	-2.719878	1.736280
14	1	0	4.191832	-0.688648	-1.627597
15	1	0	4.352192	-2.390636	0.176026
16	6	0	-0.077414	0.638888	-0.329460
17	1	0	-0.293864	0.778908	-1.395883
18	1	0	-1.070353	1.563397	0.760258
19	6	0	1.072711	2.181338	1.331048
20	1	0	0.921405	3.143242	1.822643
21	1	0	2.073660	2.146956	0.888297
22	1	0	0.974240	1.380048	2.065129
23	7	0	0.036030	2.026072	0.300664
24	6	0	0.029982	3.129333	-0.668568
25	1	0	-0.070939	4.072691	-0.130009
26	1	0	-0.817625	3.008581	-1.345449
27	1	0	0.961137	3.140952	-1.245286
28	6	0	-4.384251	-1.309429	0.003063
29	1	0	-5.220469	-1.222033	0.695416
30	1	0	-4.074391	-2.353441	-0.082458
31	1	0	-4.671801	-0.937485	-0.983035

1c.Me_2NH-tpf

Zero-point correction=	0.264498 (Hartree/Particle)
Thermal correction to Energy=	0.279745
Thermal correction to Enthalpy=	0.280689
Thermal correction to Gibbs Free Energy=	0.221291
Sum of electronic and zero-point Energies=	-688.252317
Sum of electronic and thermal Energies=	-688.237071
Sum of electronic and thermal Enthalpies=	-688.236126
Sum of electronic and thermal Free Energies=	-688.295525

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.116741	-0.433841	0.184841
2	6	0	-2.395350	-0.346471	-0.255306
3	8	0	-3.176319	-1.253519	0.364777
4	8	0	-2.801560	0.432569	-1.101552
5	6	0	1.281855	-0.223549	-0.209292
6	6	0	3.850815	-1.342281	-0.029596
7	6	0	2.165611	-0.157615	-1.289938
8	6	0	1.703131	-0.854135	0.967582
9	6	0	2.977214	-1.412733	1.055722
10	6	0	3.442684	-0.711831	-1.203864
11	1	0	1.848451	0.327177	-2.210385
12	1	0	1.044720	-0.913076	1.831015
13	1	0	3.287487	-1.901713	1.973893
14	1	0	4.113811	-0.655675	-2.055184
15	1	0	4.842496	-1.777981	0.040865
16	6	0	-0.082948	0.439665	-0.332519
17	1	0	-0.290736	0.597049	-1.396644
18	1	0	-0.893433	-1.182906	0.824234
19	6	0	0.094329	1.801196	1.711276
20	1	0	-0.200745	2.779229	2.101293
21	1	0	1.159651	1.643883	1.950335
22	1	0	-0.498960	1.038571	2.223407
23	7	0	-0.180406	1.768684	0.282070
24	6	0	0.620938	2.753612	-0.428844
25	1	0	0.390044	3.748469	-0.038340
26	1	0	0.373699	2.734938	-1.494650
27	1	0	1.706546	2.585984	-0.319220
28	6	0	-4.546102	-1.269798	-0.049107
29	1	0	-4.619315	-1.514071	-1.110445
30	1	0	-5.011386	-0.300416	0.137501
31	1	0	-5.022330	-2.042123	0.551456

1c.2Me$_2$NH-ts1

Zero-point correction=	0.357046 (Hartree/Particle)
Thermal correction to Energy=	0.378177
Thermal correction to Enthalpy=	0.379121
Thermal correction to Gibbs Free Energy=	0.305379
Sum of electronic and zero-point Energies=	-823.242108
Sum of electronic and thermal Energies=	-823.220977
Sum of electronic and thermal Enthalpies=	-823.220032
Sum of electronic and thermal Free Energies=	-823.293774

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.048855	-1.461887	0.069911
2	6	0	-1.330764	-1.620710	-0.430449
3	8	0	-2.004856	-2.521272	0.303610
4	8	0	-1.844941	-1.043198	-1.378964
5	6	0	2.127650	-0.489452	-0.294894
6	6	0	4.822918	-0.093804	0.323025
7	6	0	2.967683	0.173623	-1.196298
8	6	0	2.646734	-0.959288	0.918219
9	6	0	3.988967	-0.759043	1.225551
10	6	0	4.312431	0.370296	-0.889766
11	6	0	0.711555	-0.681987	-0.644476
12	7	0	-2.992674	1.398959	-0.036933
13	1	0	0.396394	-0.340116	-1.632536
14	1	0	2.562064	0.537516	-2.137271
15	1	0	4.960107	0.883681	-1.593246
16	1	0	5.870251	0.059867	0.564096
17	1	0	4.388414	-1.122246	2.167229
18	1	0	1.986168	-1.477333	1.606341
19	7	0	0.091272	1.491078	0.005331
20	6	0	-3.976009	2.457874	-0.230603
21	1	0	-3.804969	3.249351	0.506231
22	1	0	-5.014420	2.107778	-0.114927
23	1	0	-3.862639	2.890716	-1.227168
24	6	0	0.700755	2.608711	-0.696717
25	1	0	1.788173	2.570008	-0.565100
26	1	0	0.347727	3.585413	-0.331032
27	1	0	0.480791	2.536361	-1.765775
28	6	0	-3.149036	0.739608	1.254161
29	1	0	-2.421251	-0.073056	1.352706
30	1	0	-4.158414	0.325828	1.412536
31	1	0	-2.952076	1.461029	2.054487
32	6	0	0.327406	1.519630	1.438242
33	1	0	-0.043268	0.589776	1.884154
34	1	0	-0.163181	2.370771	1.934162
35	1	0	1.404724	1.585287	1.627905
36	6	0	-3.357311	-2.755670	-0.095286
37	1	0	-3.392443	-3.145685	-1.114381
38	1	0	-3.935509	-1.829682	-0.041302
39	1	0	-3.749134	-3.487955	0.607718
40	1	0	-3.074748	0.704806	-0.776521
41	1	0	-0.920459	1.477862	-0.167881

1c.2Me$_2$NH-I1

Zero-point correction=	0.455224 (Hartree/Particle)
Thermal correction to Energy=	0.481198
Thermal correction to Enthalpy=	0.482142
Thermal correction to Gibbs Free Energy=	0.399188
Sum of electronic and zero-point Energies=	-958.276427
Sum of electronic and thermal Energies=	-958.250454
Sum of electronic and thermal Enthalpies=	-958.249510
Sum of electronic and thermal Free Energies=	-958.332463

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.364945	-1.526874	-0.317237
2	6	0	-0.775109	-1.638869	-0.974215
3	8	0	-1.146960	-2.957431	-1.115560
4	8	0	-1.524985	-0.756525	-1.457283
5	6	0	2.317482	-0.061534	-0.179673
6	6	0	5.107476	0.207036	-0.298531
7	6	0	2.899413	1.117391	-0.653642
8	6	0	3.148551	-1.112723	0.221343
9	6	0	4.534356	-0.977619	0.167883
10	6	0	4.286768	1.254282	-0.713947
11	6	0	0.807402	-0.193852	-0.114100
12	7	0	-2.390961	-0.080143	1.309398
13	1	0	0.351151	0.531682	-0.802994
14	1	0	2.264498	1.934773	-0.988525
15	1	0	4.722424	2.174318	-1.091028
16	1	0	6.187308	0.308824	-0.346261
17	1	0	5.168629	-1.800754	0.482613
18	1	0	2.695593	-2.039618	0.558747
19	7	0	0.301461	0.291722	1.263464
20	6	0	-3.056333	0.983116	2.060365
21	1	0	-2.734494	0.939530	3.105948
22	1	0	-4.151809	0.893673	2.033149
23	1	0	-2.764498	1.948880	1.639286
24	6	0	0.501810	1.737940	1.501276
25	1	0	1.568530	1.963907	1.554723
26	1	0	0.024954	1.999382	2.448351
27	1	0	0.019532	2.289540	0.691785
28	6	0	-2.768581	-1.421379	1.755334
29	1	0	-2.255896	-2.167313	1.140842
30	1	0	-3.852572	-1.591837	1.695012
31	1	0	-2.456150	-1.556766	2.795553
32	6	0	0.799070	-0.520395	2.396033
33	1	0	0.681105	-1.573537	2.141075
34	1	0	0.201418	-0.276913	3.277015
35	1	0	1.848567	-0.288507	2.587503
36	1	0	-0.778627	0.131630	1.238327
37	7	0	-1.889048	2.175068	-0.975561
38	6	0	-3.317389	2.422418	-1.119161
39	1	0	-3.581472	3.360315	-0.617281
40	1	0	-3.888979	1.618012	-0.645070
41	1	0	-3.641684	2.498755	-2.170419
42	6	0	-1.100704	3.165199	-1.695902
43	1	0	-0.036765	2.913795	-1.636450
44	1	0	-1.238851	4.150782	-1.237452
45	1	0	-1.371851	3.248073	-2.761535
46	1	0	-1.675421	1.241013	-1.327068
47	1	0	-2.589503	0.006952	0.312837
48	6	0	-2.379028	-3.189240	-1.785687
49	1	0	-2.353457	-2.801309	-2.807073

50	1	0	-3.212649	-2.723160	-1.251627
51	1	0	-2.509343	-4.271513	-1.801938

1c.2Me$_2$NH-I2

Zero-point correction=	0.455204 (Hartree/Particle)
Thermal correction to Energy=	0.481354
Thermal correction to Enthalpy=	0.482298
Thermal correction to Gibbs Free Energy=	0.397855
Sum of electronic and zero-point Energies=	-958.275749
Sum of electronic and thermal Energies=	-958.249599
Sum of electronic and thermal Enthalpies=	-958.248655
Sum of electronic and thermal Free Energies=	-958.333097

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.463658	-0.056383	1.745734
2	1	0	0.408683	0.914107	1.257635
3	1	0	-0.227640	2.398356	-0.155266
4	1	0	-1.351471	0.678516	-1.138749
5	7	0	-1.579720	1.612398	-1.502024
6	7	0	0.295228	2.493861	0.726205
7	6	0	-0.507763	3.271415	1.672000
8	1	0	-0.658600	4.307865	1.338025
9	1	0	-0.004155	3.296824	2.644554
10	1	0	-1.485623	2.801379	1.803051
11	6	0	1.593401	3.122750	0.480450
12	1	0	1.493587	4.155050	0.115945
13	1	0	2.154260	2.541806	-0.255778
14	1	0	2.168923	3.144151	1.411787
15	6	0	1.724730	-0.079894	2.523176
16	1	0	1.848070	-1.061046	2.988588
17	1	0	1.671670	0.690130	3.294258
18	1	0	2.564486	0.124227	1.860168
19	6	0	-0.708697	-0.142673	2.649155
20	1	0	-0.711594	-1.118235	3.140155
21	1	0	-1.616351	-0.021887	2.059375
22	1	0	-0.636742	0.653813	3.391092
23	6	0	-1.539221	1.590966	-2.957488
24	1	0	-2.307645	0.932654	-3.396945
25	1	0	-0.557907	1.248538	-3.299001
26	1	0	-1.701180	2.600973	-3.350327
27	6	0	-2.899594	1.980528	-1.006231
28	1	0	-3.706733	1.374561	-1.450384
29	1	0	-3.105385	3.034349	-1.226682
30	1	0	-2.935452	1.845200	0.079275
31	7	0	-0.781231	-0.960639	-0.114998
32	6	0	0.395017	-1.147628	0.652801
33	6	0	1.641790	-1.048454	-0.204197
34	6	0	3.944752	-0.872413	-1.789007
35	6	0	2.680583	-1.967021	-0.046298
36	6	0	1.758314	-0.044400	-1.170994
37	6	0	2.906507	0.047691	-1.954619
38	6	0	3.827994	-1.883295	-0.836600
39	1	0	2.591712	-2.754207	0.698645

40	1	0	0.936458	0.654202	-1.311591
41	1	0	2.990588	0.832916	-2.700319
42	1	0	4.626245	-2.607666	-0.708334
43	1	0	4.836160	-0.804723	-2.404928
44	6	0	-1.779749	-1.789185	0.164076
45	8	0	-1.857218	-2.702249	1.007762
46	8	0	-2.862911	-1.532187	-0.648903
47	1	0	0.406915	-2.089680	1.221636
48	6	0	-4.004857	-2.350089	-0.438005
49	1	0	-4.761564	-1.990168	-1.135754
50	1	0	-4.371811	-2.260207	0.587855
51	1	0	-3.781665	-3.400754	-0.642598

1c.2Me$_2$NH-ts2

Zero-point correction=	0.356322 (Hartree/Particle)
Thermal correction to Energy=	0.376315
Thermal correction to Enthalpy=	0.377259
Thermal correction to Gibbs Free Energy=	0.307298
Sum of electronic and zero-point Energies=	-823.253073
Sum of electronic and thermal Energies=	-823.233080
Sum of electronic and thermal Enthalpies=	-823.232135
Sum of electronic and thermal Free Energies=	-823.302097

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.957110	-0.550793	-0.368622
2	6	0	1.994750	-1.327750	-0.112856
3	8	0	2.915174	-1.279199	-1.146889
4	8	0	2.247382	-2.050896	0.874096
5	6	0	-1.440841	-0.758315	0.073904
6	6	0	-4.036406	-1.146433	-0.927209
7	6	0	-2.390183	-1.472118	0.810516
8	6	0	-1.800104	-0.264029	-1.183160
9	6	0	-3.090351	-0.447165	-1.678223
10	6	0	-3.680217	-1.667113	0.316358
11	1	0	-2.117518	-1.876770	1.782658
12	1	0	-1.053691	0.241359	-1.787731
13	1	0	-3.354738	-0.053658	-2.655254
14	1	0	-4.404124	-2.226702	0.900976
15	1	0	-5.039456	-1.294463	-1.315182
16	6	0	-0.052385	-0.523884	0.648210
17	6	0	1.854203	2.985678	-0.524506
18	1	0	2.594300	2.229587	-0.256501
19	1	0	1.757570	3.707629	0.288997
20	1	0	2.172771	3.504574	-1.432325
21	6	0	-1.186070	1.211088	2.095523
22	1	0	-1.004403	2.178824	2.568797
23	1	0	-1.396707	0.468548	2.876393
24	1	0	-2.052800	1.294270	1.439070
25	7	0	0.554967	2.321365	-0.733177
26	6	0	-0.509864	3.241001	-1.166478
27	1	0	-0.245511	3.726975	-2.109185
28	1	0	-0.650157	4.001037	-0.395303
29	1	0	-1.439481	2.682366	-1.290323

30	7	0	0.008525	0.840228	1.322116
31	6	0	1.198817	0.901970	2.188688
32	1	0	1.343649	1.929086	2.533042
33	1	0	2.074940	0.578829	1.625791
34	1	0	1.071771	0.244857	3.058471
35	1	0	0.120775	-1.265734	1.444308
36	1	0	0.686974	1.549709	-1.393717
37	1	0	0.243429	1.685881	0.278410
38	6	0	4.074209	-2.081826	-0.982687
39	1	0	4.680910	-1.916032	-1.873986
40	1	0	3.815867	-3.141528	-0.903497
41	1	0	4.637625	-1.790109	-0.092266

1c.3Me$_2$NH-ts1

Zero-point correction=	0.451427 (Hartree/Particle)
Thermal correction to Energy=	0.478492
Thermal correction to Enthalpy=	0.479436
Thermal correction to Gibbs Free Energy=	0.391846
Sum of electronic and zero-point Energies=	-958.258458
Sum of electronic and thermal Energies=	-958.231393
Sum of electronic and thermal Enthalpies=	-958.230449
Sum of electronic and thermal Free Energies=	-958.318039

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.770139	1.634672	-0.379662
2	6	0	0.567534	1.836707	-0.683993
3	8	0	0.932146	3.087158	-0.355107
4	8	0	1.358000	1.036547	-1.163119
5	6	0	-2.657821	0.146697	-0.574945
6	6	0	-5.354170	-0.521759	-0.275685
7	6	0	-3.165384	-1.017697	-1.162105
8	6	0	-3.511371	0.979686	0.159388
9	6	0	-4.853039	0.643606	0.310095
10	6	0	-4.509911	-1.351526	-1.014397
11	6	0	-1.233491	0.474538	-0.744916
12	7	0	2.361086	-0.293034	1.488107
13	1	0	-0.645784	-0.192897	-1.379183
14	1	0	-2.501403	-1.662446	-1.733227
15	1	0	-4.898157	-2.255800	-1.472084
16	1	0	-6.401941	-0.780464	-0.157712
17	1	0	-5.511172	1.288786	0.883610
18	1	0	-3.108392	1.883574	0.605071
19	7	0	-0.542284	-0.989603	0.979116
20	6	0	3.308354	-1.207250	2.109265
21	1	0	2.893370	-1.591929	3.047674
22	1	0	4.277678	-0.732692	2.337633
23	1	0	3.490392	-2.051125	1.438526
24	6	0	-0.851663	-2.404673	0.860481
25	1	0	-1.938367	-2.534325	0.799270
26	1	0	-0.485717	-2.995171	1.715585
27	1	0	-0.408211	-2.808230	-0.054923
28	6	0	2.197229	0.933065	2.255050

29	1	0	1.490643	1.601814	1.752105
30	1	0	3.143180	1.478593	2.411611
31	1	0	1.781657	0.694724	3.240705
32	6	0	-1.106621	-0.385706	2.173734
33	1	0	-0.945172	0.697872	2.140667
34	1	0	-0.663511	-0.781765	3.100461
35	1	0	-2.186496	-0.570818	2.201467
36	1	0	0.476844	-0.843607	0.994978
37	7	0	3.413440	-1.104529	-1.316734
38	6	0	4.611561	-1.737490	-1.849074
39	1	0	4.922739	-2.544039	-1.175833
40	1	0	5.425011	-1.009799	-1.903202
41	1	0	4.464985	-2.174942	-2.850692
42	6	0	2.270900	-2.008107	-1.308009
43	1	0	1.379330	-1.449507	-1.012591
44	1	0	2.439480	-2.807095	-0.575795
45	1	0	2.085646	-2.481795	-2.286953
46	1	0	3.172407	-0.281778	-1.862174
47	1	0	2.687550	-0.088481	0.542876
48	6	0	2.303180	3.412819	-0.596321
49	1	0	2.534848	3.323091	-1.659579
50	1	0	2.956923	2.748450	-0.025154
51	1	0	2.424023	4.442156	-0.264509

1c.3Me$_2$NH-I1

Zero-point correction=	0.455224 (Hartree/Particle)
Thermal correction to Energy=	0.481198
Thermal correction to Enthalpy=	0.482142
Thermal correction to Gibbs Free Energy=	0.399188
Sum of electronic and zero-point Energies=	-958.276427
Sum of electronic and thermal Energies=	-958.250454
Sum of electronic and thermal Enthalpies=	-958.249510
Sum of electronic and thermal Free Energies=	-958.332463

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.364945	-1.526874	-0.317237
2	6	0	-0.775109	-1.638869	-0.974215
3	8	0	-1.146960	-2.957431	-1.115560
4	8	0	-1.524985	-0.756525	-1.457283
5	6	0	2.317482	-0.061534	-0.179673
6	6	0	5.107476	0.207036	-0.298531
7	6	0	2.899413	1.117391	-0.653642
8	6	0	3.148551	-1.112723	0.221343
9	6	0	4.534356	-0.977619	0.167883
10	6	0	4.286768	1.254282	-0.713947
11	6	0	0.807402	-0.193852	-0.114100
12	7	0	-2.390961	-0.080143	1.309398
13	1	0	0.351151	0.531682	-0.802994
14	1	0	2.264498	1.934773	-0.988525
15	1	0	4.722424	2.174318	-1.091028
16	1	0	6.187308	0.308824	-0.346261
17	1	0	5.168629	-1.800754	0.482613

18	1	0	2.695593	-2.039618	0.558747
19	7	0	0.301461	0.291722	1.263464
20	6	0	-3.056333	0.983116	2.060365
21	1	0	-2.734494	0.939530	3.105948
22	1	0	-4.151809	0.893673	2.033149
23	1	0	-2.764498	1.948880	1.639286
24	6	0	0.501810	1.737940	1.501276
25	1	0	1.568530	1.963907	1.554723
26	1	0	0.024954	1.999382	2.448351
27	1	0	0.019532	2.289540	0.691785
28	6	0	-2.768581	-1.421379	1.755334
29	1	0	-2.255896	-2.167313	1.140842
30	1	0	-3.852572	-1.591837	1.695012
31	1	0	-2.456150	-1.556766	2.795553
32	6	0	0.799070	-0.520395	2.396033
33	1	0	0.681105	-1.573537	2.141075
34	1	0	0.201418	-0.276913	3.277015
35	1	0	1.848567	-0.288507	2.587503
36	1	0	-0.778627	0.131630	1.238327
37	7	0	-1.889048	2.175068	-0.975561
38	6	0	-3.317389	2.422418	-1.119161
39	1	0	-3.581472	3.360315	-0.617281
40	1	0	-3.888979	1.618012	-0.645070
41	1	0	-3.641684	2.498755	-2.170419
42	6	0	-1.100704	3.165199	-1.695902
43	1	0	-0.036765	2.913795	-1.636450
44	1	0	-1.238851	4.150782	-1.237452
45	1	0	-1.371851	3.248073	-2.761535
46	1	0	-1.675421	1.241013	-1.327068
47	1	0	-2.589503	0.006952	0.312837
48	6	0	-2.379028	-3.189240	-1.785687
49	1	0	-2.353457	-2.801309	-2.807073
50	1	0	-3.212649	-2.723160	-1.251627
51	1	0	-2.509343	-4.271513	-1.801938

1c.3Me$_2$NH-I2

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Zero-point correction=                           0.455204 (Hartree/Particle)
Thermal correction to Energy=                    0.481354
Thermal correction to Enthalpy=                  0.482298
Thermal correction to Gibbs Free Energy=         0.397855
Sum of electronic and zero-point Energies=           -958.275749
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Sum of electronic and thermal Energies= -958.249599
Sum of electronic and thermal Enthalpies= -958.248655
Sum of electronic and thermal Free Energies= -958.333097

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.463658	-0.056383	1.745734
2	1	0	0.408683	0.914107	1.257635
3	1	0	-0.227640	2.398356	-0.155266
4	1	0	-1.351471	0.678516	-1.138749
5	7	0	-1.579720	1.612398	-1.502024
6	7	0	0.295228	2.493861	0.726205
7	6	0	-0.507763	3.271415	1.672000
8	1	0	-0.658600	4.307865	1.338025
9	1	0	-0.004155	3.296824	2.644554
10	1	0	-1.485623	2.801379	1.803051
11	6	0	1.593401	3.122750	0.480450
12	1	0	1.493587	4.155050	0.115945
13	1	0	2.154260	2.541806	-0.255778
14	1	0	2.168923	3.144151	1.411787
15	6	0	1.724730	-0.079894	2.523176
16	1	0	1.848070	-1.061046	2.988588
17	1	0	1.671670	0.690130	3.294258
18	1	0	2.564486	0.124227	1.860168
19	6	0	-0.708697	-0.142673	2.649155
20	1	0	-0.711594	-1.118235	3.140155
21	1	0	-1.616351	-0.021887	2.059375
22	1	0	-0.636742	0.653813	3.391092
23	6	0	-1.539221	1.590966	-2.957488
24	1	0	-2.307645	0.932654	-3.396945
25	1	0	-0.557907	1.248538	-3.299001
26	1	0	-1.701180	2.600973	-3.350327
27	6	0	-2.899594	1.980528	-1.006231
28	1	0	-3.706733	1.374561	-1.450384
29	1	0	-3.105385	3.034349	-1.226682
30	1	0	-2.935452	1.845200	0.079275
31	7	0	-0.781231	-0.960639	-0.114998
32	6	0	0.395017	-1.147628	0.652801
33	6	0	1.641790	-1.048454	-0.204197
34	6	0	3.944752	-0.872413	-1.789007
35	6	0	2.680583	-1.967021	-0.046298
36	6	0	1.758314	-0.044400	-1.170994
37	6	0	2.906507	0.047691	-1.954619
38	6	0	3.827994	-1.883295	-0.836600
39	1	0	2.591712	-2.754207	0.698645
40	1	0	0.936458	0.654202	-1.311591
41	1	0	2.990588	0.832916	-2.700319
42	1	0	4.626245	-2.607666	-0.708334
43	1	0	4.836160	-0.804723	-2.404928
44	6	0	-1.779749	-1.789185	0.164076
45	8	0	-1.857218	-2.702249	1.007762
46	8	0	-2.862911	-1.532187	-0.648903
47	1	0	0.406915	-2.089680	1.221636
48	6	0	-4.004857	-2.350089	-0.438005
49	1	0	-4.761564	-1.990168	-1.135754
50	1	0	-4.371811	-2.260207	0.587855
51	1	0	-3.781665	-3.400754	-0.642598

1c.3Me$_2$NH-I3

Zero-point correction=	0.454907 (Hartree/Particle)
Thermal correction to Energy=	0.481071
Thermal correction to Enthalpy=	0.482015
Thermal correction to Gibbs Free Energy=	0.396872
Sum of electronic and zero-point Energies=	-958.275673
Sum of electronic and thermal Energies=	-958.249509
Sum of electronic and thermal Enthalpies=	-958.248565
Sum of electronic and thermal Free Energies=	-958.333708

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.028957	-1.703883	1.425393
2	1	0	0.046313	0.158418	1.871055
3	1	0	0.104035	1.681317	1.091268
4	1	0	-0.380983	1.481676	-0.768414
5	7	0	0.007199	2.378026	-0.443157
6	7	0	-0.085015	1.185152	2.033844
7	6	0	-1.510827	1.423031	2.352921
8	1	0	-1.663769	2.491061	2.518773
9	1	0	-1.783704	0.866612	3.251432
10	1	0	-2.100048	1.082504	1.499345
11	6	0	0.841163	1.672782	3.075984
12	1	0	0.682927	2.742586	3.219529
13	1	0	1.867977	1.499451	2.752294
14	1	0	0.653165	1.144413	4.011919
15	6	0	0.844665	-2.821433	1.792875
16	1	0	0.506194	-3.759592	1.320952
17	1	0	0.822385	-2.956100	2.877467
18	1	0	1.874714	-2.638504	1.488009
19	6	0	-1.385057	-2.036407	1.873450
20	1	0	-1.745426	-2.968651	1.408303
21	1	0	-2.078208	-1.235704	1.616605
22	1	0	-1.376572	-2.166159	2.959415
23	6	0	1.226902	2.697454	-1.178126
24	1	0	1.022458	2.956724	-2.228159
25	1	0	1.903468	1.840058	-1.154180
26	1	0	1.728321	3.551109	-0.709480
27	6	0	-0.996788	3.432235	-0.557369
28	1	0	-1.212472	3.690385	-1.605043
29	1	0	-0.643961	4.336504	-0.049850
30	1	0	-1.927809	3.109734	-0.084476
31	7	0	-0.945449	-0.427229	-0.393421
32	6	0	-0.005332	-1.460386	-0.043835
33	6	0	1.382724	-1.015259	-0.504375
34	6	0	3.859903	-0.132524	-1.516096
35	6	0	1.677907	-1.112150	-1.868832
36	6	0	2.347775	-0.464239	0.342672
37	6	0	3.578051	-0.028883	-0.155721
38	6	0	2.900774	-0.676506	-2.374142
39	1	0	0.931845	-1.531696	-2.540654
40	1	0	2.157195	-0.399841	1.410138
41	1	0	4.314071	0.389958	0.524373
42	1	0	3.108228	-0.764198	-3.436520
43	1	0	4.815392	0.205053	-1.905382
44	6	0	-2.048114	-0.828971	-0.996722

45	8	0	-2.430958	-1.967092	-1.339268
46	8	0	-2.876364	0.254261	-1.263374
47	1	0	-0.244225	-2.414672	-0.552838
48	6	0	-4.098094	-0.047396	-1.919273
49	1	0	-4.608643	0.907231	-2.054175
50	1	0	-4.718934	-0.716196	-1.316427
51	1	0	-3.923723	-0.513381	-2.893208

1c.3Me$_2$NH-ts2

Zero-point correction=	0.450323	(Hartree/Particle)
Thermal correction to Energy=	0.476042	
Thermal correction to Enthalpy=	0.476986	
Thermal correction to Gibbs Free Energy=	0.393624	
Sum of electronic and zero-point Energies=	-958.279669	
Sum of electronic and thermal Energies=	-958.253950	
Sum of electronic and thermal Enthalpies=	-958.253006	
Sum of electronic and thermal Free Energies=	-958.336368	

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.523989	0.006435	1.787552
2	1	0	0.057284	1.663187	1.030615
3	1	0	-1.053950	2.018422	-0.330488
4	1	0	-1.333740	0.358686	-1.037889
5	7	0	-1.750917	1.295473	-1.242483
6	7	0	-0.408057	2.506113	0.614742
7	6	0	-1.344631	3.070853	1.601368
8	1	0	-1.880451	3.910423	1.151535
9	1	0	-0.808422	3.421281	2.488683
10	1	0	-2.064504	2.305013	1.896079
11	6	0	0.594014	3.487540	0.169657
12	1	0	0.089583	4.314360	-0.336069
13	1	0	1.287887	3.013509	-0.526689
14	1	0	1.156605	3.879542	1.022439
15	6	0	1.743908	0.093196	2.588673
16	1	0	1.990477	-0.869882	3.069849
17	1	0	1.601521	0.841404	3.373231
18	1	0	2.589591	0.397711	1.969416
19	6	0	-0.612268	-0.261683	2.669665
20	1	0	-0.492969	-1.218679	3.205589
21	1	0	-1.533278	-0.303152	2.084538
22	1	0	-0.695452	0.541927	3.407572
23	6	0	-1.540503	1.693318	-2.636448
24	1	0	-2.048916	1.009706	-3.326508
25	1	0	-0.471917	1.693069	-2.865548
26	1	0	-1.931296	2.702904	-2.792478
27	6	0	-3.170222	1.254878	-0.873773
28	1	0	-3.739889	0.618081	-1.559871
29	1	0	-3.587349	2.266551	-0.891246
30	1	0	-3.264759	0.841537	0.133396
31	7	0	-0.562474	-1.029920	-0.087259
32	6	0	0.614434	-1.053899	0.737191
33	6	0	1.848559	-0.809259	-0.116640

34	6	0	4.119287	-0.289885	-1.684944
35	6	0	2.987852	-1.605471	0.000218
36	6	0	1.854341	0.240947	-1.039313
37	6	0	2.979393	0.507829	-1.814358
38	6	0	4.118351	-1.350752	-0.780886
39	1	0	2.994521	-2.428159	0.711763
40	1	0	0.952849	0.836117	-1.155624
41	1	0	2.967476	1.331288	-2.523016
42	1	0	4.997487	-1.980469	-0.680923
43	1	0	4.998039	-0.087522	-2.289561
44	6	0	-1.399713	-2.040693	0.041939
45	8	0	-1.361019	-3.055182	0.767615
46	6	0	-3.477987	-2.884134	-0.761449
47	1	0	-4.253869	-2.575359	-1.463774
48	1	0	-3.904689	-2.981657	0.240655
49	1	0	-3.070540	-3.852544	-1.065920
50	1	0	0.732226	-2.026744	1.252199
51	8	0	-2.487260	-1.870313	-0.805769