

Unexpected Reactivity of Graphene Oxide with DBU and DMF

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Electronic Supplementary Information

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1. General methods

NMR spectra were acquired using CDCl₃ as solvent, running at 300 and 75 MHz for ¹H and ¹³C, respectively. Chemical shifts (δ) are reported in ppm relative to residual solvent signals (CDCl₃, 7.26 ppm for ¹H NMR, and 77.0 ppm for ¹³C NMR). In all ¹H NMR spectra, multiplicity is indicated as follows: bs (broad singlet), s (singlet), d (doublet), t (triplet), q (quartet) or m (multiplet). Coupling constant values (in Hertz) and number of protons for each signal are also indicated.

For thin layer chromatography (TLC) Supelco silica gel plates with fluorescence indicator 254 nm were used and compounds were visualized by irradiation with UV light and/or by treatment with a solution of KMnO₄ (1.5 g), K₂CO₃ (10 g), and 10% NaOH (1.25 mL) in H₂O (200 mL) or a solution of phosphomolybdic acid (12 g), in EtOH (250 mL) followed by heating. Flash column chromatography (FCC) was performed using Merck pore 60 Å, 40-63 μm silica gel and compressed air.

FTIR essays were carried out in a Bruker IFS66v spectrometer (KBr, 99%).

Thermogravimetric analyses (TGA) were performed using a TGA Q-500 (TA Instruments) at 5 °C/min (from 25 °C to 900 °C) under nitrogen atmosphere. Elemental analyses were performed using a Leco CHNS- 932.

Photoelectron spectra (XPS) were obtained with a VG Escalab 200R spectrometer equipped with a hemispherical electron analyser and a Mg Kα (hν = 1254.6 eV) X-ray source, powered at 120 W. Binding energies were calibrated relative to the C 1s peak at 284.8 eV. High-resolution spectra envelopes were obtained by curve fitting synthetic peak components using the software "XPS peak." Symmetric Gaussian–Lorentzian curves were used to approximate the line shapes of the fitting components. Atomic ratios were computed from experimental intensity ratios and normalized by atomic sensitivity factor.

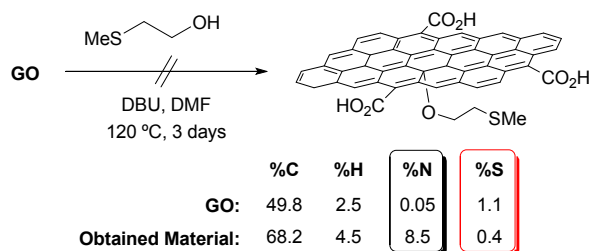
pH values were measured at open air, using a Crison pH-meter 25+ apparatus, at 25 °C.

Cyclohexane and EtOAc were supplied by *Carlo Erba* and were used without previous purification. All the other reactants were bought in *Aldrich*, *Fluka* or *Alfa Aesar*. All synthesized products are described and spectroscopic data are consistent with the references indicated next to the name of each compound.

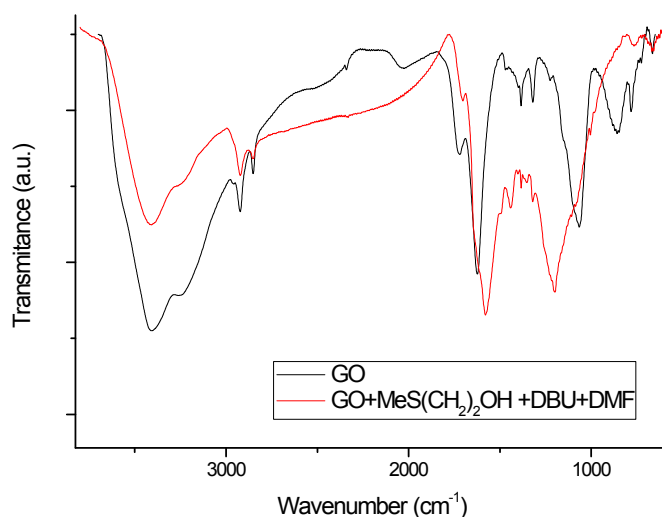
Graphene oxide (GO) was synthesized using a modified Hummers' method.¹

¹ W. S. Hummers and R. E. Offeman, *J. Am. Chem. Soc.*, 1958, **80**, 1339.

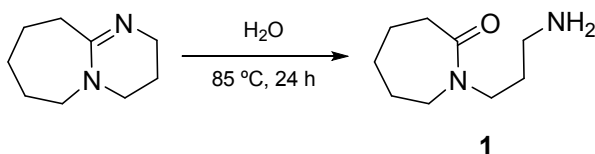
2. Attempt to anchor alcohols via epoxide ring opening



A solution of 2-(methylthio)ethanol (0.94 mL, 1 g, 10.85 mmol) in DMF (50 mL) was added to a dispersion of GO (500 mg) in DMF (50 mL), previously treated in an ultrasound bath for 30 minutes, followed by DBU (1.63 mL, 1.66 g, 10.85 mmol). The mixture was heated in a sealed tube for 3 days, after which the material was filtered and washed successively with deionized water (3 x 15 mL), MeOH (30 mL) and acetone (30 mL). The obtained material was left to stir in a vial tube at 70 °C for 3 days.



3. Synthesis of amine 1



A mixture of DBU (2.23 mL, 2.28 g, 15 mmol) and water (0.27 mL, 0.27 g, 15 mmol) was stirred at 85 °C for 24 h. Then, the mixture was extracted with CH₂Cl₂ (5 mL), dried over MgSO₄ and the organic solvent was removed under reduced pressure. The crude was purified by FCC (CHCl₃/MeOH/conc. NH₃, 9:1:1, and then CHCl₃/MeOH, 4:1) to afford compound 1. Its characterization data were in agreement with those reported in the literature.²

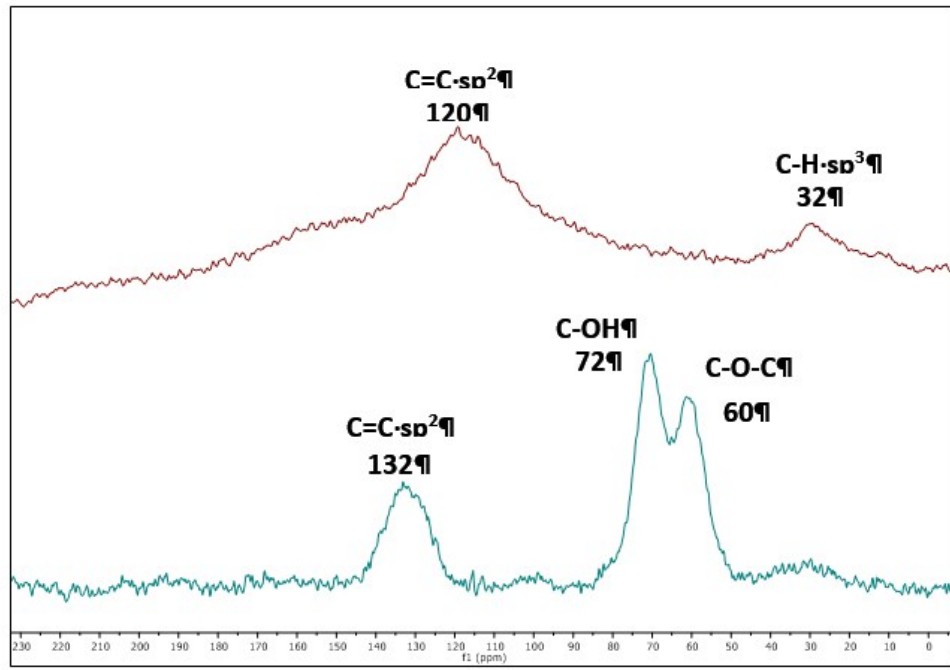
² A. Kraft, *J. Chem. Soc., Perkin Trans. 1*, 1999, 705.

4.- Characterization of Materials B-F and A'

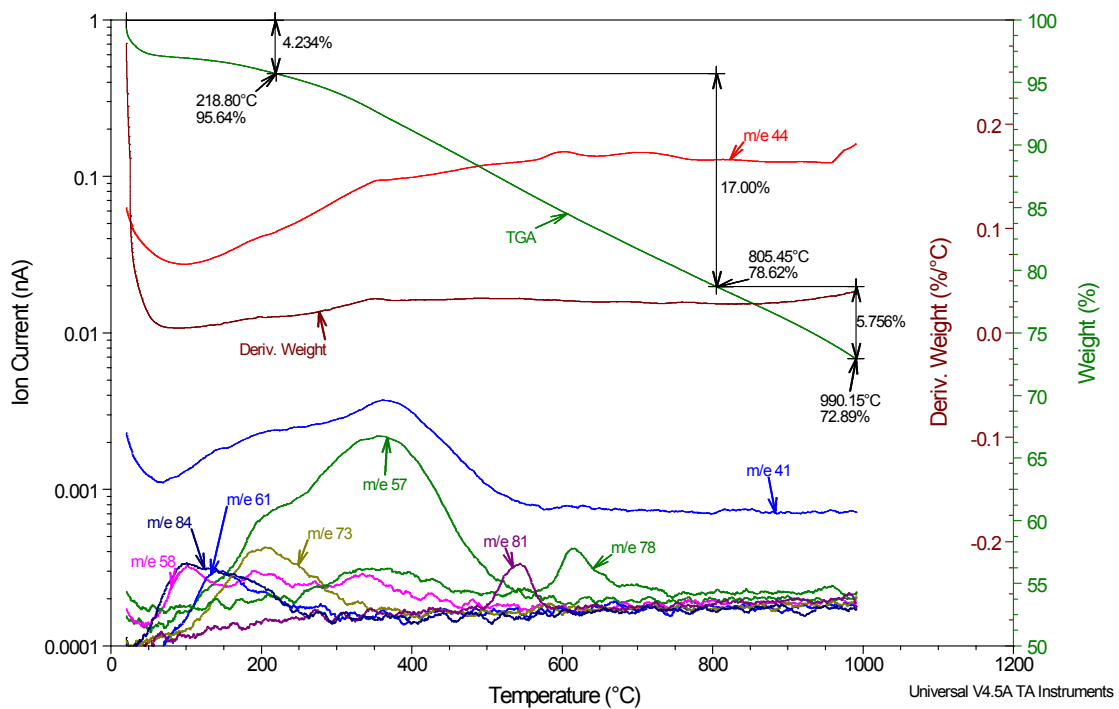
- Data of Material B (GO + DMF)

Elemental analysis: %C: 77.4, % H: 1.5; % N: 2.8, %S: 0.03.

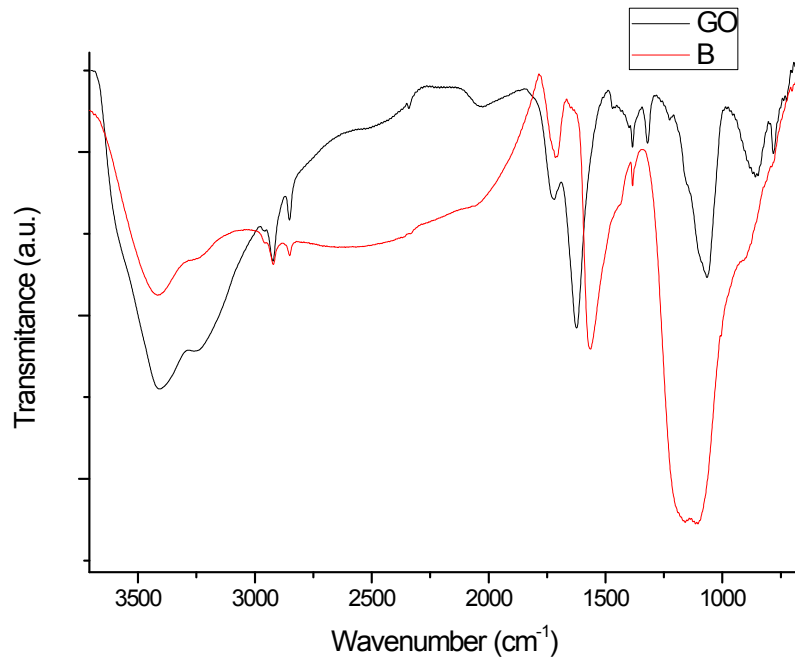
^{13}C NMR (Top, in red) and its comparison with ^{13}C NMR of GO (Bottom, green):



TGA:



FTIR:

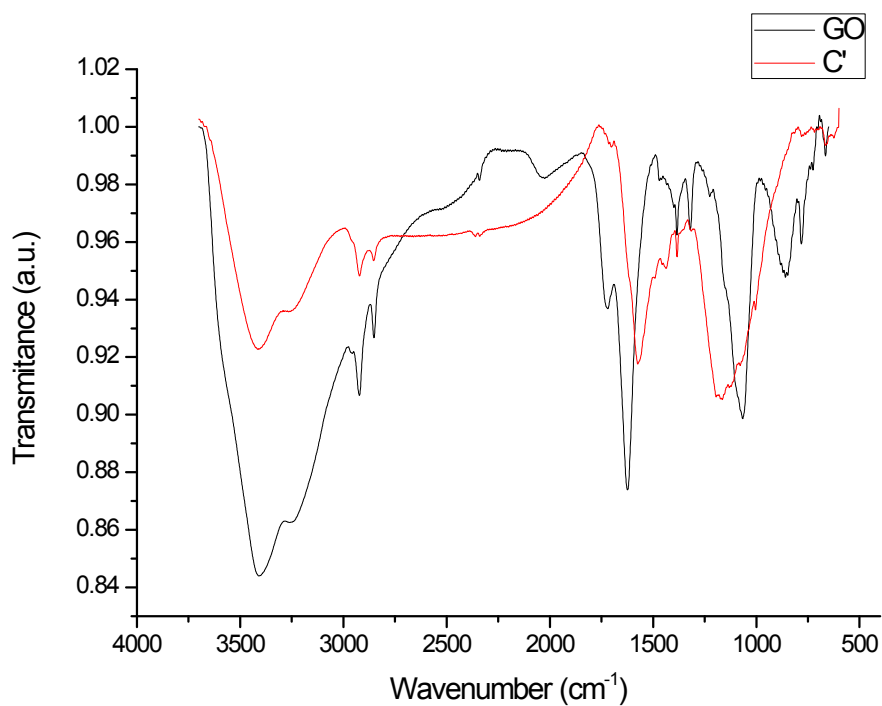
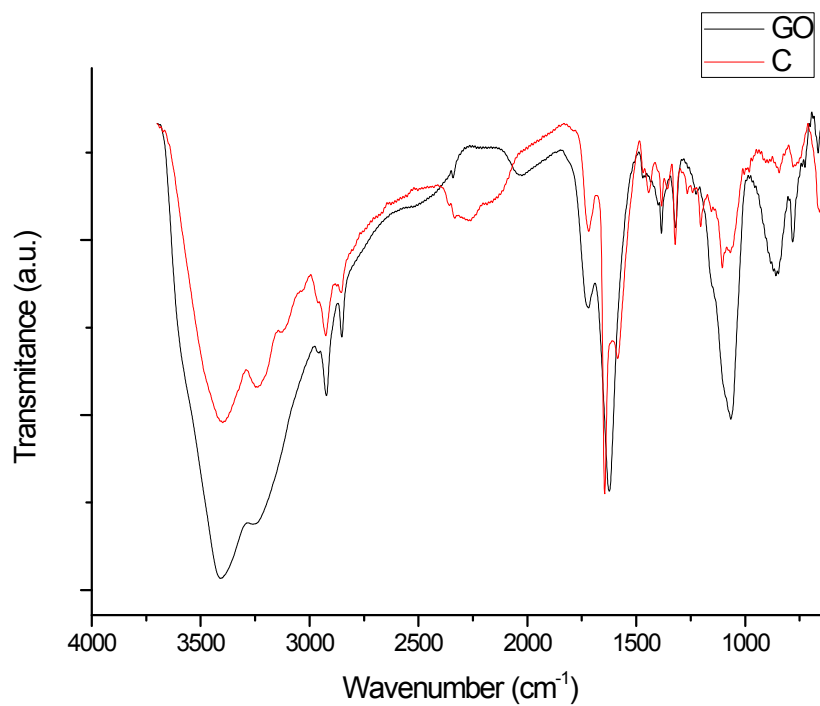


- **Data of Material C (GO + DBU in THF)**

Elemental analysis: %C: 60.2, %H: 4.5, %N: 4.5, %S: 0.1

Elemental analysis (After washing with a 2M NaOH solution, material C'): %C: 40.0; %H: 2.2; %N: 0.47; %S: 0.021.

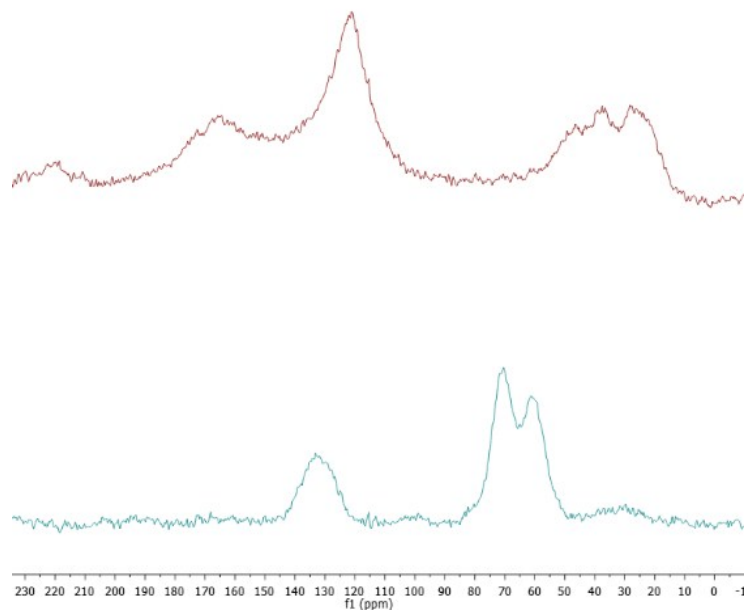
FTIR:



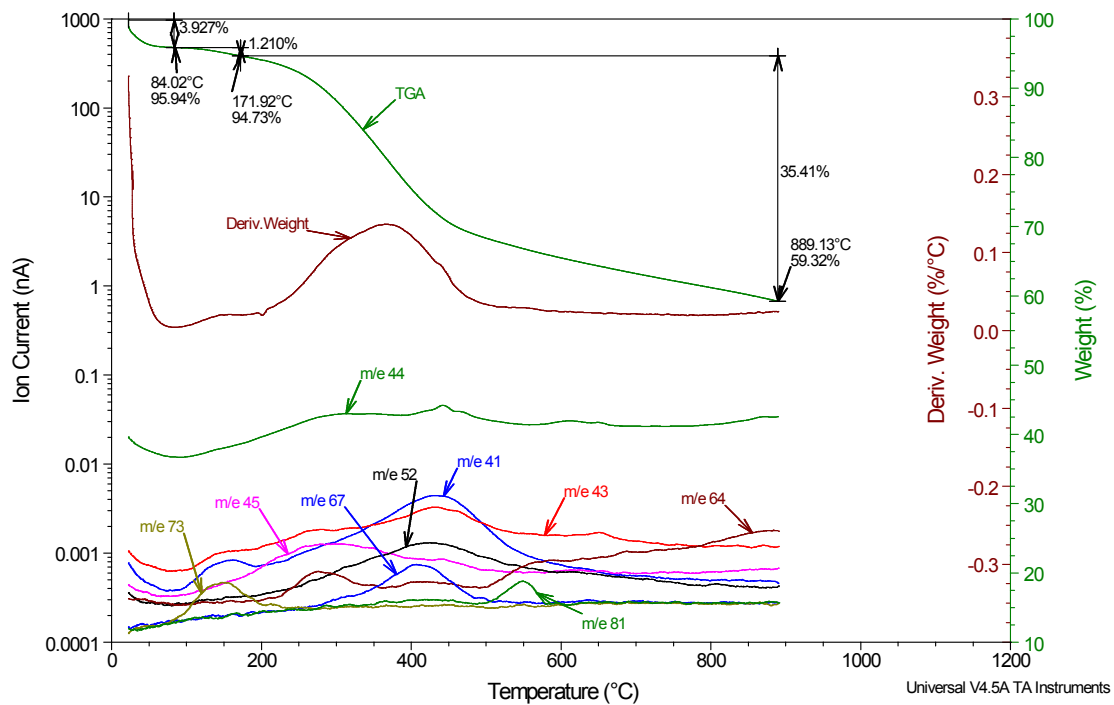
- **Data of Material D (GO + DBU in DMF)**

Elemental analysis: %C: 68.1; %H: 3.9; %N: 8.0 % S: 0.01

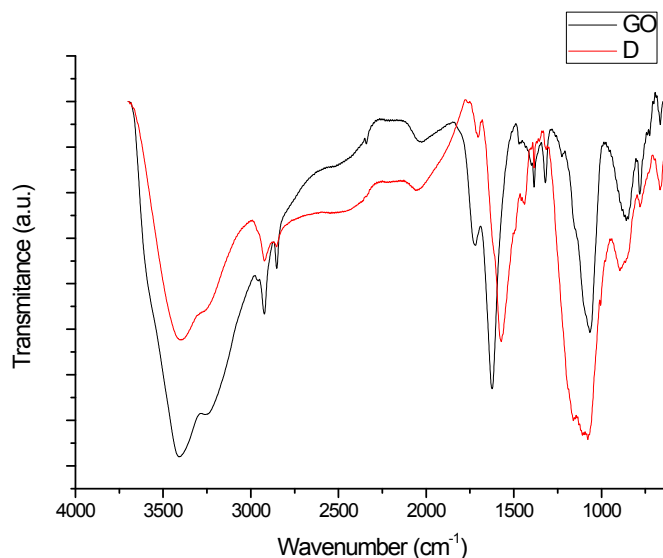
¹³C NMR (Top, in red) and its comparison with ¹³C NMR of GO (Bottom, green).



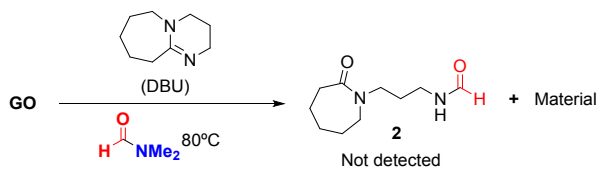
TGA:



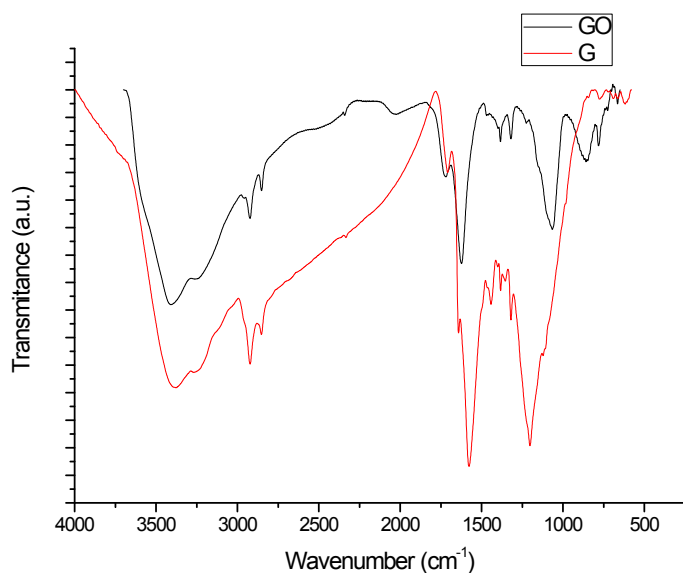
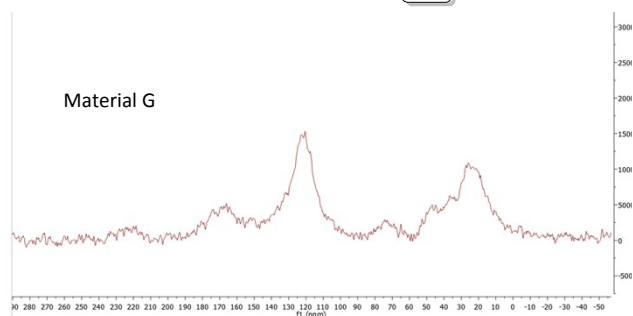
FTIR:



When we performed the reaction of GO with DBU in DMF under the same conditions used to obtain material **D** at 80 °C (4 days), we did not detect compound **2** by ^1H NMR analysis. According to the elemental analysis of the material (**G**), some nitrogen has been incorporated. This incorporation of nitrogen agrees with the fact that we do not recover an 8 % of the mass of the starting DBU in the reaction. Below is also shown the solid ^{13}C NMR and IR spectra of this material. These data agree with an incorporation of hydrolyzed DBU (**1**) at 80 °C (formation of **1** is energetically favored according to our calculations) but lower incorporation of $-\text{NMe}_2$ than when the reaction is performed at 120 °C (formation of HNMe_2 is less favored energetically).



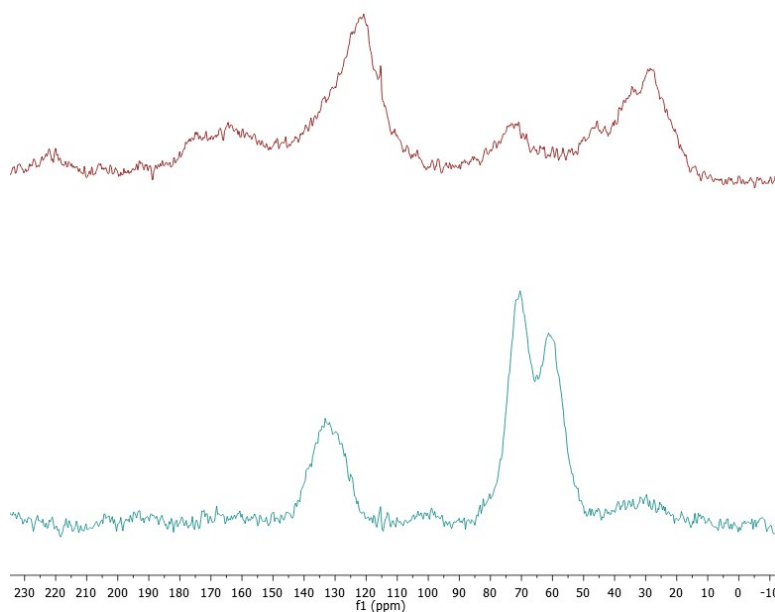
	%C	%H	%N	H/C	N/C
GO:	49.8	2.5	0.05	0.05	0.001
Obtained Material:	68.4	4.2	6.3	0.061	0.09



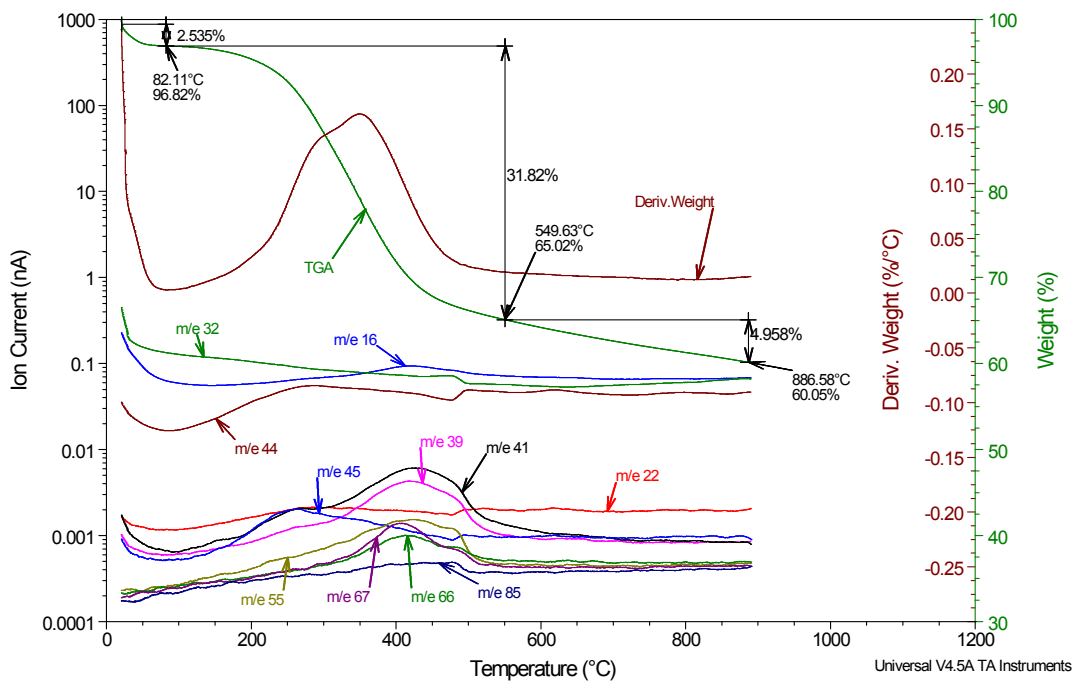
- **Data of Material E (GO + 1 + DMF)**

Elemental analysis: %C: 72.9; %H: 3.9; %N: 7.2 % S: 0.03

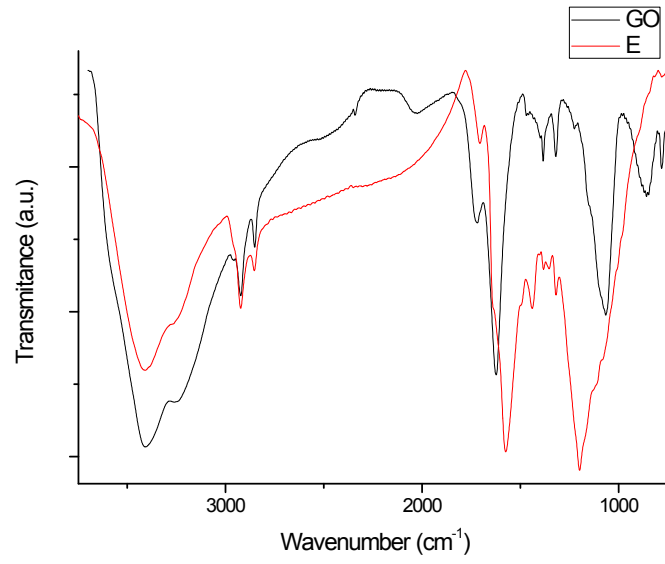
¹³C NMR (Top, in red) and its comparison with **¹³C NMR** of GO (Bottom, green)



TGA:



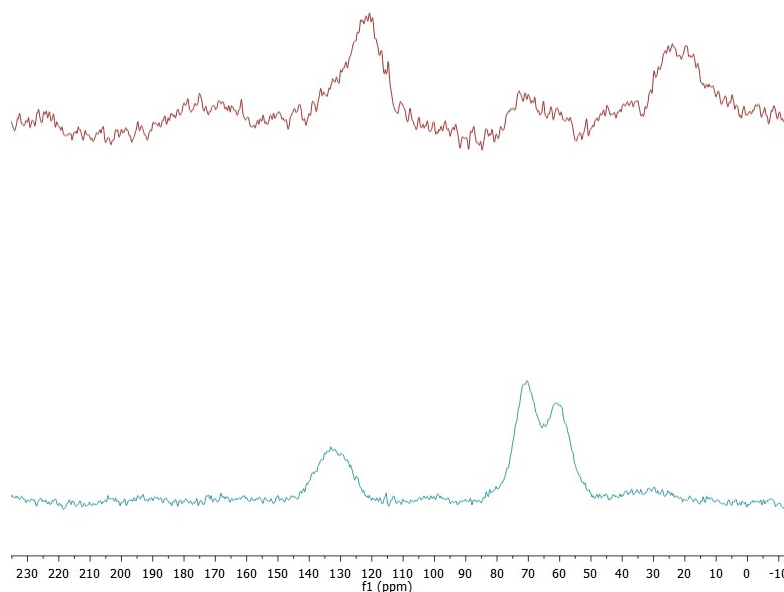
FTIR:



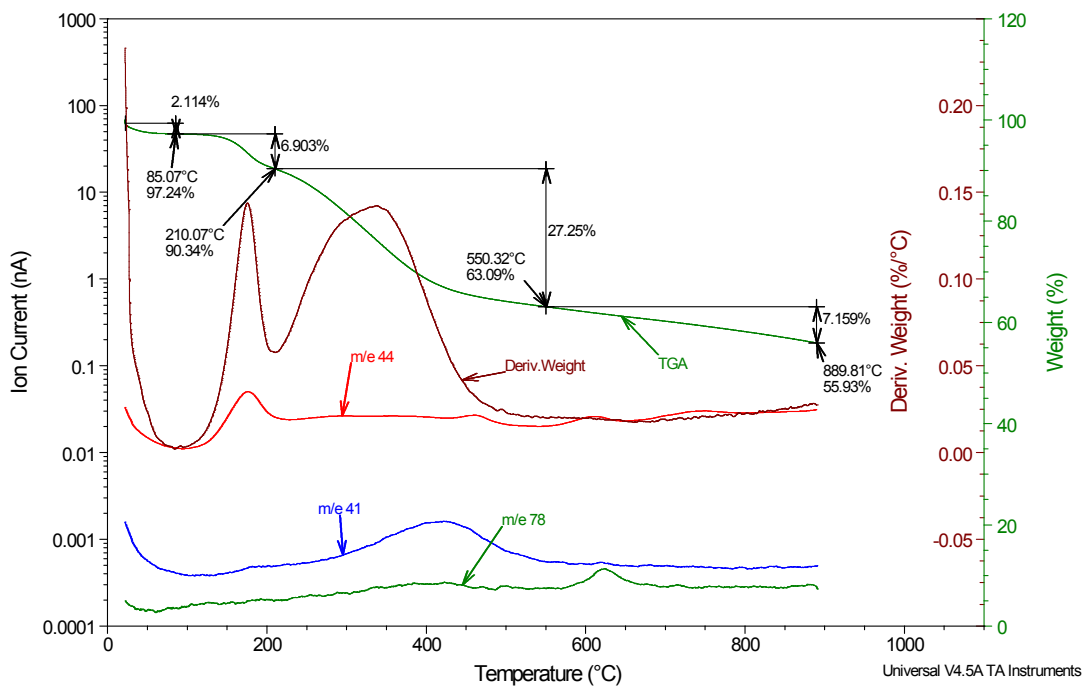
- **Data of Material F (GO + 1 in EtOH)**

Elemental analysis: %C: 65.0; %H: 2.1; %N: 5.1% S: 0.02%

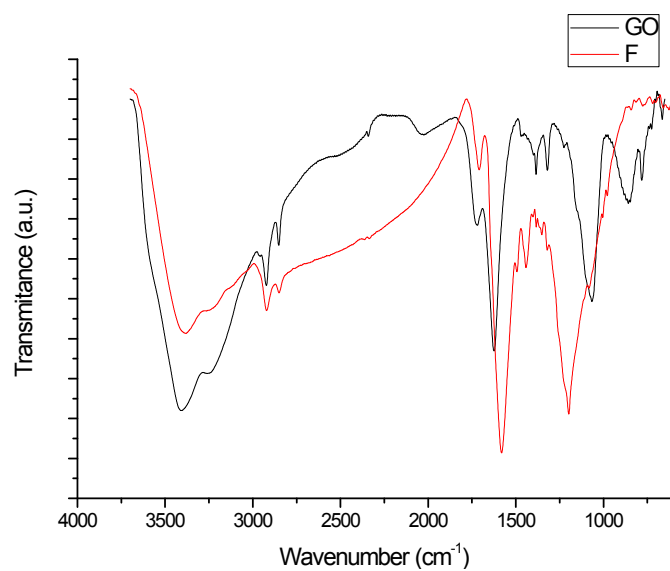
¹³C NMR (Top, in red) and its comparison with ¹³C NMR of GO (Bottom, green)



TGA:



FTIR:

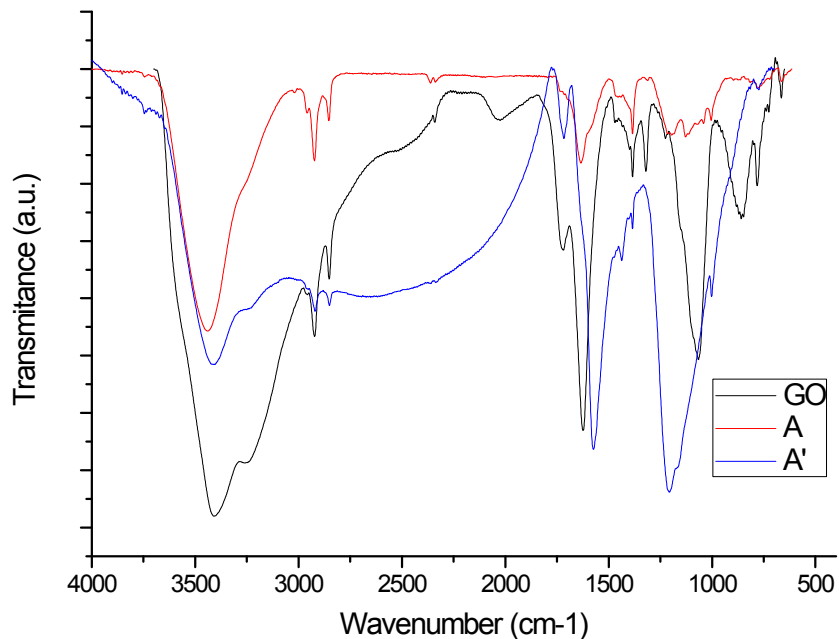


• **Data of Material A' (GO-NH (A) + DMF)**

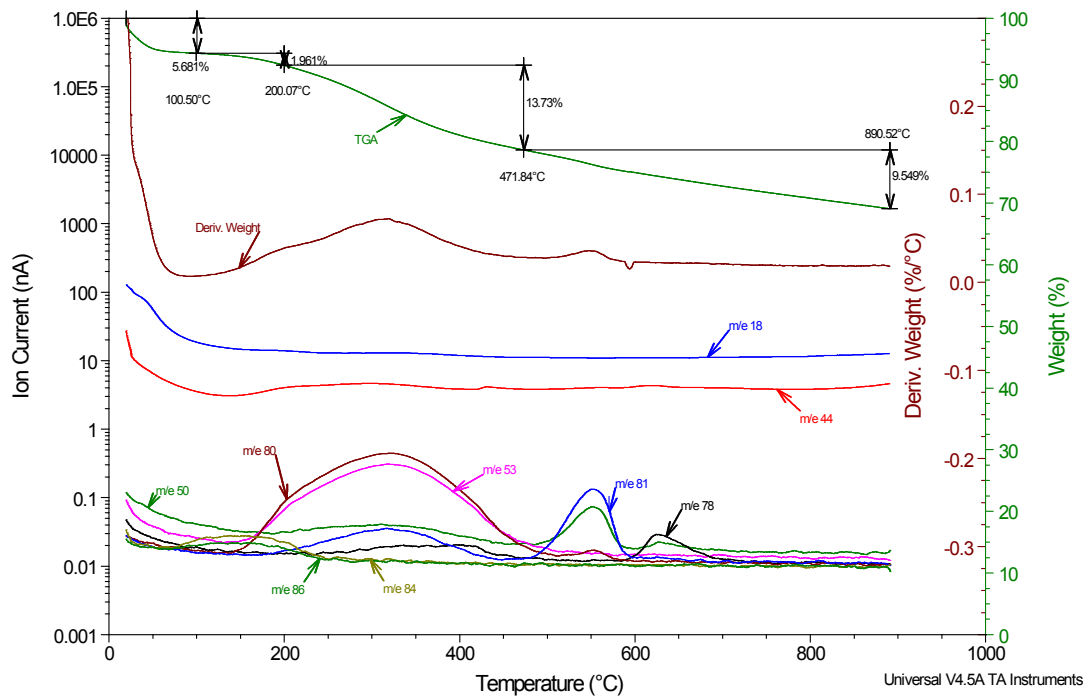
Elemental analysis of Material **A**: %C: 66.5; %H: 2.8; %N: 5.2%

Elemental analysis of Material **A'**: %C: 66.1; %H: 2.1; %N: 5.1%

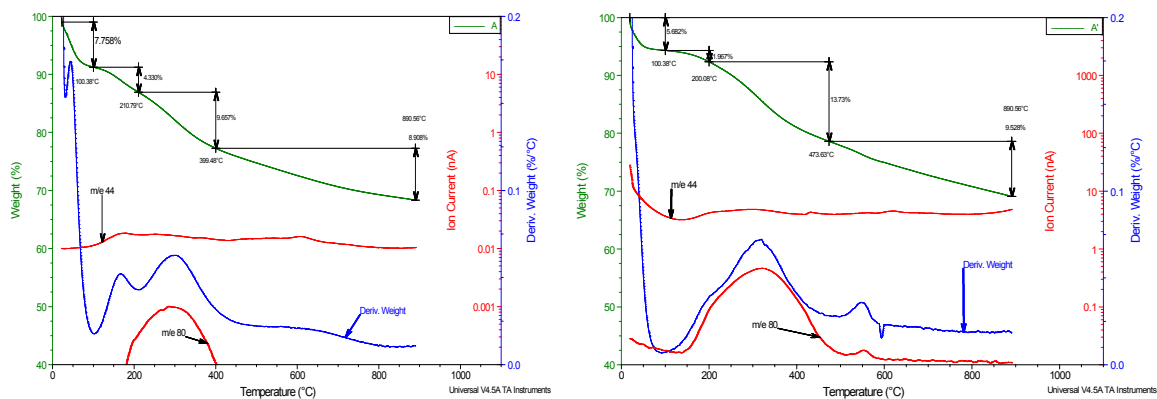
FTIR (A'):



TGA (A'):

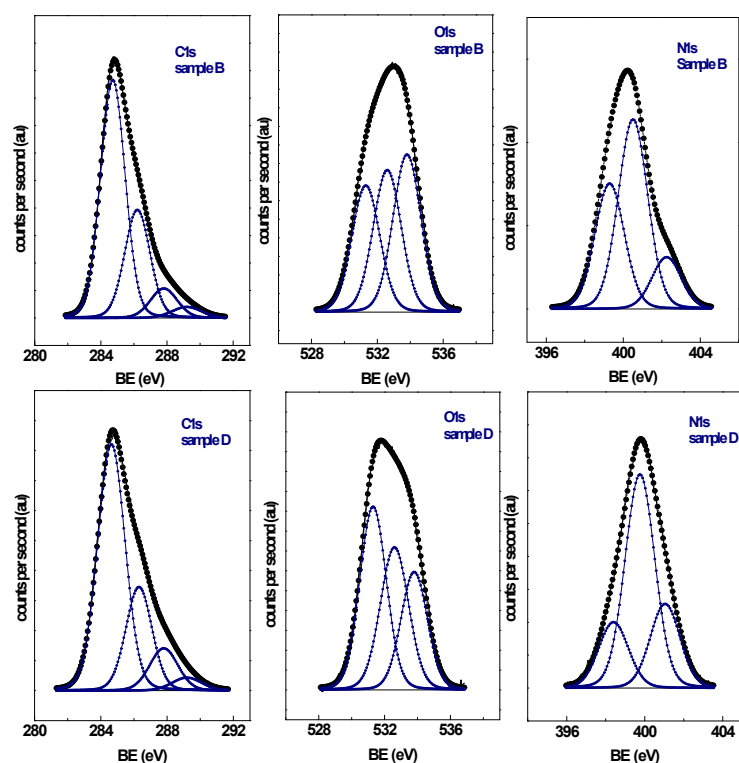


TGA plots for materials A and A':



TGA plots for materials **A** and **A'** show differences between both materials probing that the reduction method influences the material that is obtained. If we focus on the weight loss between 200 and 475°C, that seems to be the temperature range where the NMe_2 group is lost, it is slightly higher for material **A'** compared to material **A**. At this temperature range, piperazine is also removed from the material (m/e 80) and it seems logical to propose that the different profile and weight loss could be due to the NMe_2 groups that have been incorporated during DMF treatment.

- Comparison of the data of materials B-F
 - Comparison of XPS of materials B and D



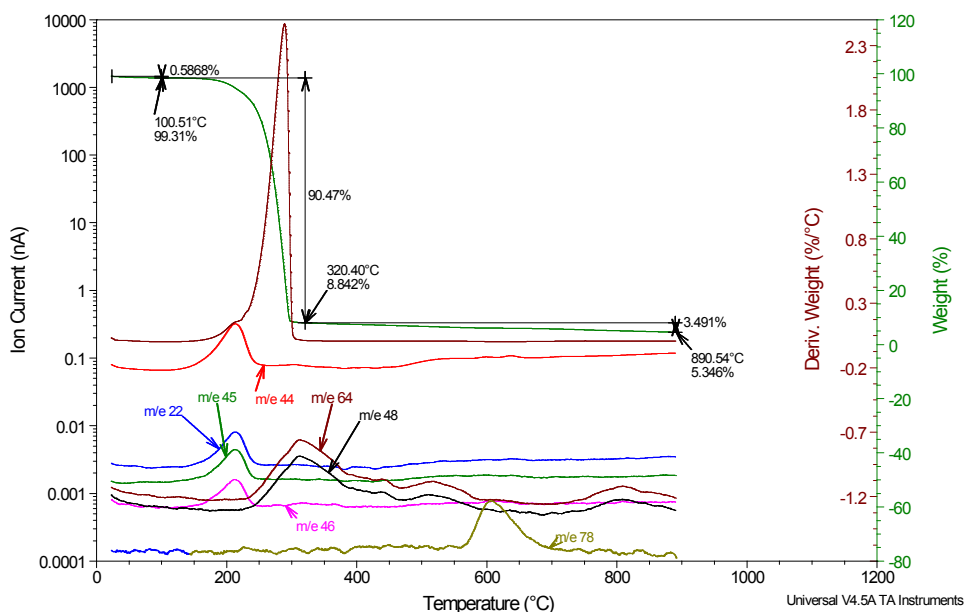
This figure shows deconvoluted XPS spectra for materials **B** and **D**. The deconvoluted C1s spectra of **B** and **D** show four components corresponding to C-C (284.6 eV), C-O/C-N (286.2 eV), C=O/N-C=O (287.8 eV) and O-C=O (289.2 eV) bonds. The O1s spectra of both samples display several component peaks representing C=O (531.3 eV), C-O (532.6 eV) and O=C-O (533.8 eV) bonds. The N1s peak can be split into three individual peaks located at 398.1 eV, 399.8 eV, and 401.8 eV.

Table S1. Binding energies (eV) of core-levels and atomic percentages of Materials B and D. In parentheses peak percentages.

	C1s	O1s	N1s	C (%at)	O (%at)	N (%at)
Material B	284.8 (60) 286.2 (28) 287.8 (8) 289.2 (4)	531.3 (30) 532.6 (33) 533.8 (37)	398.3 (34) 400.0 (52) 402.1 (14)	85.4	11.8	2.8
Material D	284.8 (61) 286.2 (24) 287.8 (11) 289.2 (4)	531.3 (40) 532.6 (34) 533.8 (26)	398.1 (18) 399.8 (59) 401.8 (23)	84.4	10.7	4.9

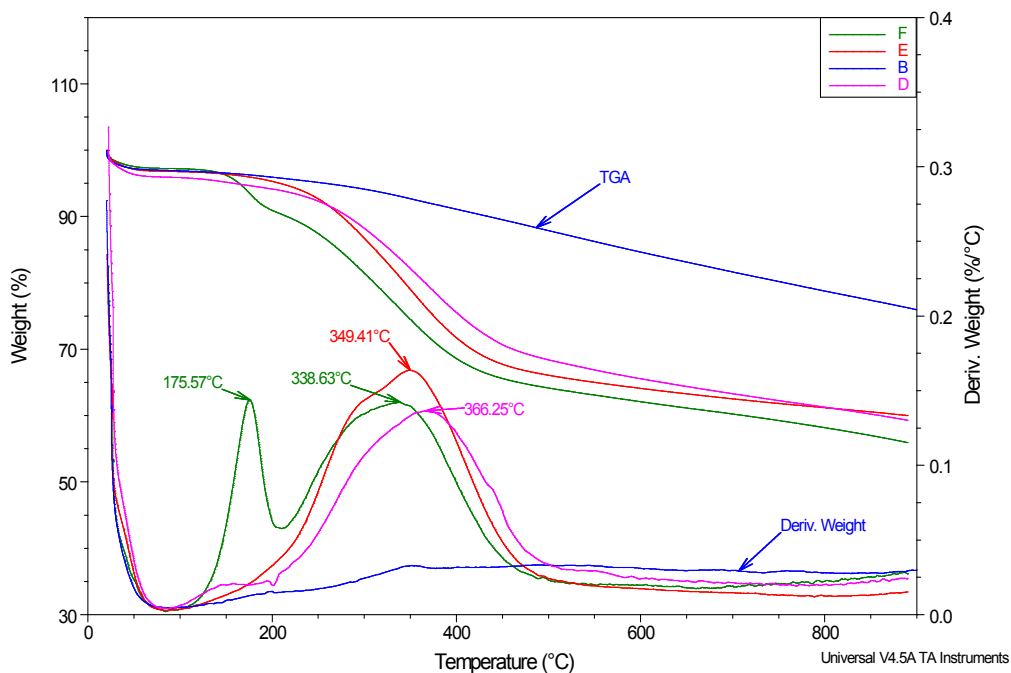
- Comparison of thermogravimetric analyses

TGA of graphene oxide:



TGA plot for graphene oxide shows a main weight loss from 150 °C to 320 °C caused by the decomposition of labile oxygen groups. This weight loss is also present in material **F** but not in materials **B**, **D** and **E**. This could be due to the lower temperature at which material **F** was prepared, and it is in agreement with the presence of oxygenated groups in material **F** observed by NMR.

TGA of materials B, D, E and F:



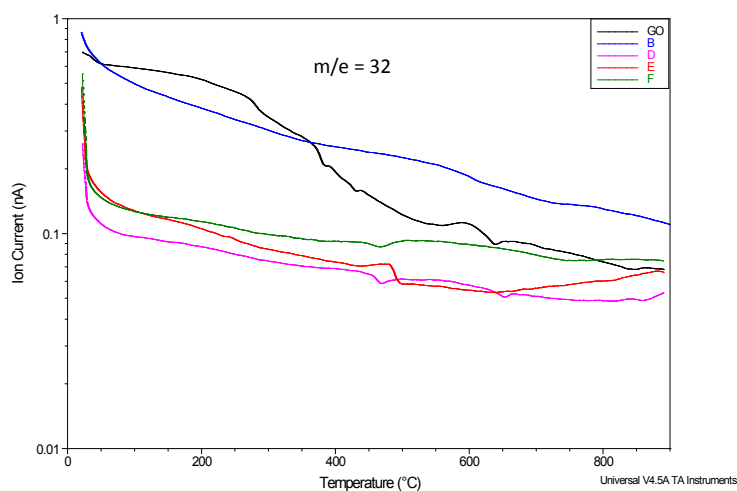
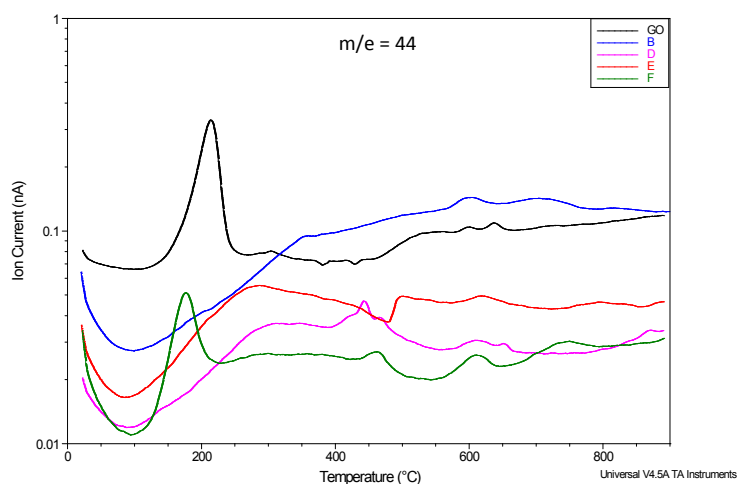
Material **B** (GO+DMF); Material **D** (GO + DBU + DMF); Material **E** (GO + **1** in DMF); Material **F** (GO + **1** in EtOH / H₂O).

We can observe that the mass loss in sample **B**, presumably due to NMe_2 groups, is quite constant. According to the mass loss in **D**, **E** and **F** (200-550 °C) their degree of functionalization should be quite similar. The maximum of the derivative displaced towards higher temperatures in the order **F**, **E** and **D** indicates that the chains anchored to the graphene are more thermally stable in **E** and **D** than in **F**. One possible explanation could be the higher degree of aromaticity in materials **E** and **D** than in **F** and the gradual loss of NMe_2 groups. The high decomposition temperature of **D** is consistent with a higher number of NMe_2 groups anchored than in **E**.

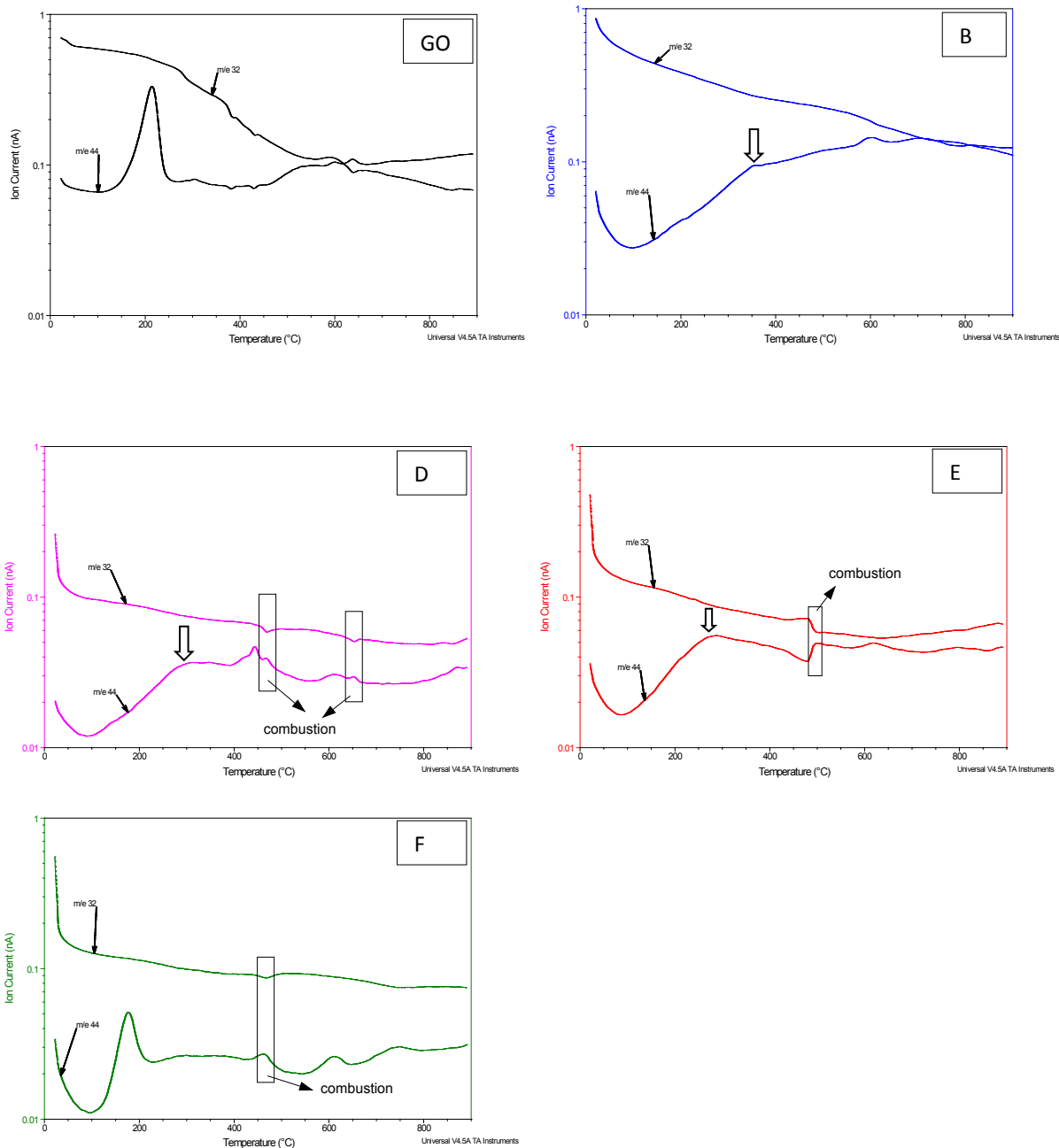
Table S2. Weight loss of materials B, D-F

Materials	% Weight loss (20-200 °C)	% Weight loss (200-550 °C)	% Weight loss at 900 °C
B	4	9.7	27
D	5.6	27.3	41
E	4.5	30.3	40
F	8.4	27.8	44

Further information regarding the functionalization was obtained using a TGA coupled to a mass spectrometer detector. The following figures show the $m/e = 44$ and 32 , respectively, detected upon heating each of GO, **B**, **D**, **E** and **F** materials.



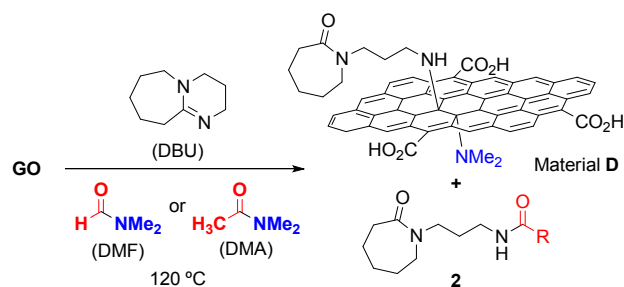
The $m/e = 44$ fragment may correspond to either NMe_2 groups or CO_2 , the latter being formed after combustion of the sample. In order to differentiate both possibilities, we also checked the $m/e = 32$ to monitor the traces of O_2 present in the chamber. The simultaneous drop of the $m/e = 32$ ion current and increase of $m/e = 44$ ion current indicates a combustion reaction generating CO_2 .



Both graphene oxide and material **F** show their main weight loss around 200 °C, which may be attributed to the removal of oxygenated groups. In materials **B**, **D** and **E** this possibility is excluded probably due to the higher temperatures employed in their preparation compared to **F**, leading to materials with less oxygenated groups. In contrast for materials **B**, **D** and **E** but not for material **F** there is a weight loss around 300 °C that corresponds to a wide peak in $m/e=44$ curves. We assigned this loss to the NMe_2 groups as there is no drop in the $m/e=32$ curve and therefore no combustion reaction.

5. Mechanistic Studies

Hydrolysis and acylation of DBU catalyzed by GO



A suspension of GO (100 mg) in DMF or DMA (5 mL) was sonicated for 30 minutes. Then DBU (0.15 mL, 153 mg, 1 mmol) was added and the reaction mixture was stirred at 120 °C during the corresponding time (2 or 4 days, see Table 2). After that time, the material was filtered through a filter plate and the solvent was removed under reduced pressure. The crude was purified by FCC (hexane/acetone, 1:4), affording **2a-b** as yellow oils.

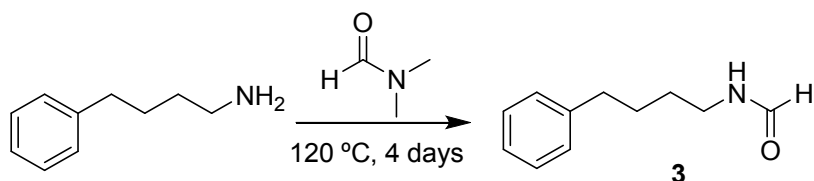
Data of *N*-((*N*'-formyl)-3-aminopropyl)azepan-2-one (**2a**, R = H):

¹H RMN (300 MHz, CDCl₃) δ 8.13 (s, 1H), 3.45 (t, *J* = 5.9 Hz, 2H), 3.34 (t, *J* = 5.4 Hz, 2H), 3.24 (q, *J* = 5.9 Hz, 2H), 2.53 (t, *J* = 5.9 Hz, 2H), 1.69 (m, 8H). **¹³C NMR** (75 MHz, CDCl₃) δ 177.0 (C=O), 161.3 (C=O), 49.6 (CH₂), 44.9 (CH₂), 37.1 (CH₂), 33.8 (CH₂), 29.8 (CH₂), 28.4 (CH₂), 27.5 (CH₂), 23.4 (CH₂). **MS** (EI): *m/z* 199 (M⁺, 5), 170 (10), 140 (64), 126 (32), 98 (100), 85 (15). **HRMS** (EI): calculated for C₁₀H₁₈N₂O₂ (M⁺): 198.1368; found: 198.1364.

Data of *N*-((*N*'-acetyl)-3-aminopropyl)azepan-2-one (**2b**, R = Me):³

¹H RMN (300 MHz, CDCl₃) δ 3.44 (t, *J* = 6.1 Hz, 2H), 3.33 (t, *J* = 5.1 Hz, 2H), 3.19 (q, *J* = 5.9 Hz, 2H), 2.54 (t, *J* = 6.1 Hz, 2H), 1.98 (s, 3H), 1.69 (m, 8H).

Transamidation of 4-phenylbutylamine



A suspension of GO (100 mg) in DMF (5 mL) was sonicated for 30 minutes. Then, 4-phenylbutylamine (0.158 mL, 149 mg, 1 mmol) and DBU (0.15 mL, 153 mg, 1 mmol) were added and the reaction mixture was stirred at 120 °C during 48 h. After that time, the material was filtered through a filter plate and the solvent was removed under reduced pressure. The crude was purified by FCC (hexane/EtOAc, 1:2 to 1:4), affording **3** as a colorless oil.

Data of *N*-(4-phenylbutyl)formamide (**3**):⁴

³ A. Guggisberg, U. Kramer, C. Heidelberger, R. Charubala, E. Stephanou, M. Hesse and H. Schmid, *Helv. Chim. Acta*, 1978, **61**, 1050.

⁴ A. K. Sharma, A. Sharma, D. Desai, S. V. Madhunapantula, S. J. Huh, G. P. Robertson and S. Amin, *J. Med.*

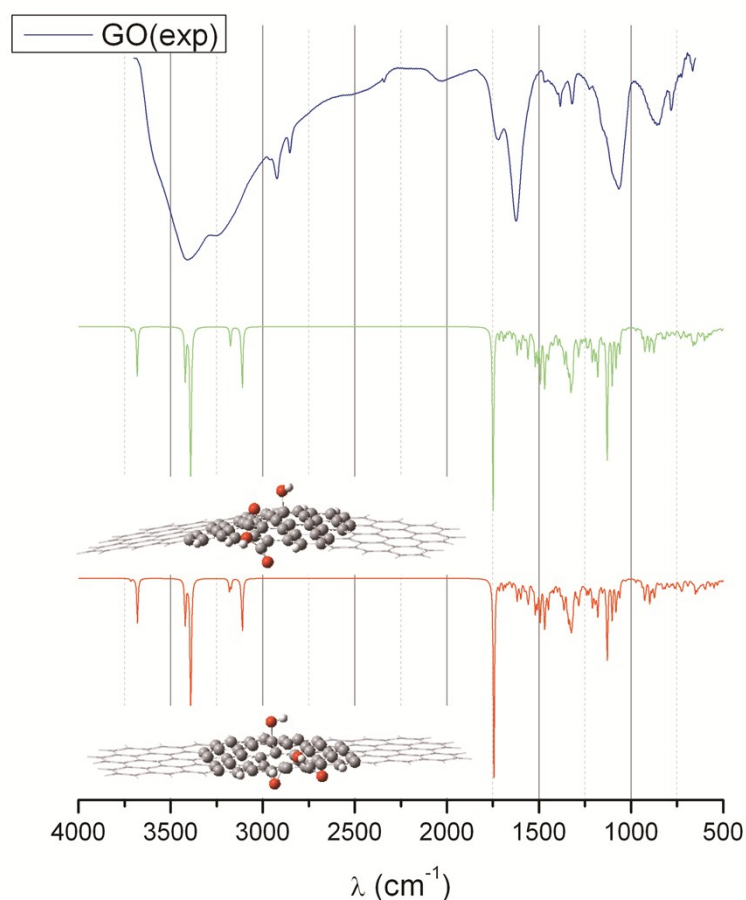
$^1\text{H NMR}$ (300 MHz, CDCl_3) δ 8.13 (s, 1H), 7.24 (m, 5H), 3.25 (m, 2H), 2.64 (t, $J = 7.1$ Hz, 2H), 1.62 (m, 4H).

6. pH measurements

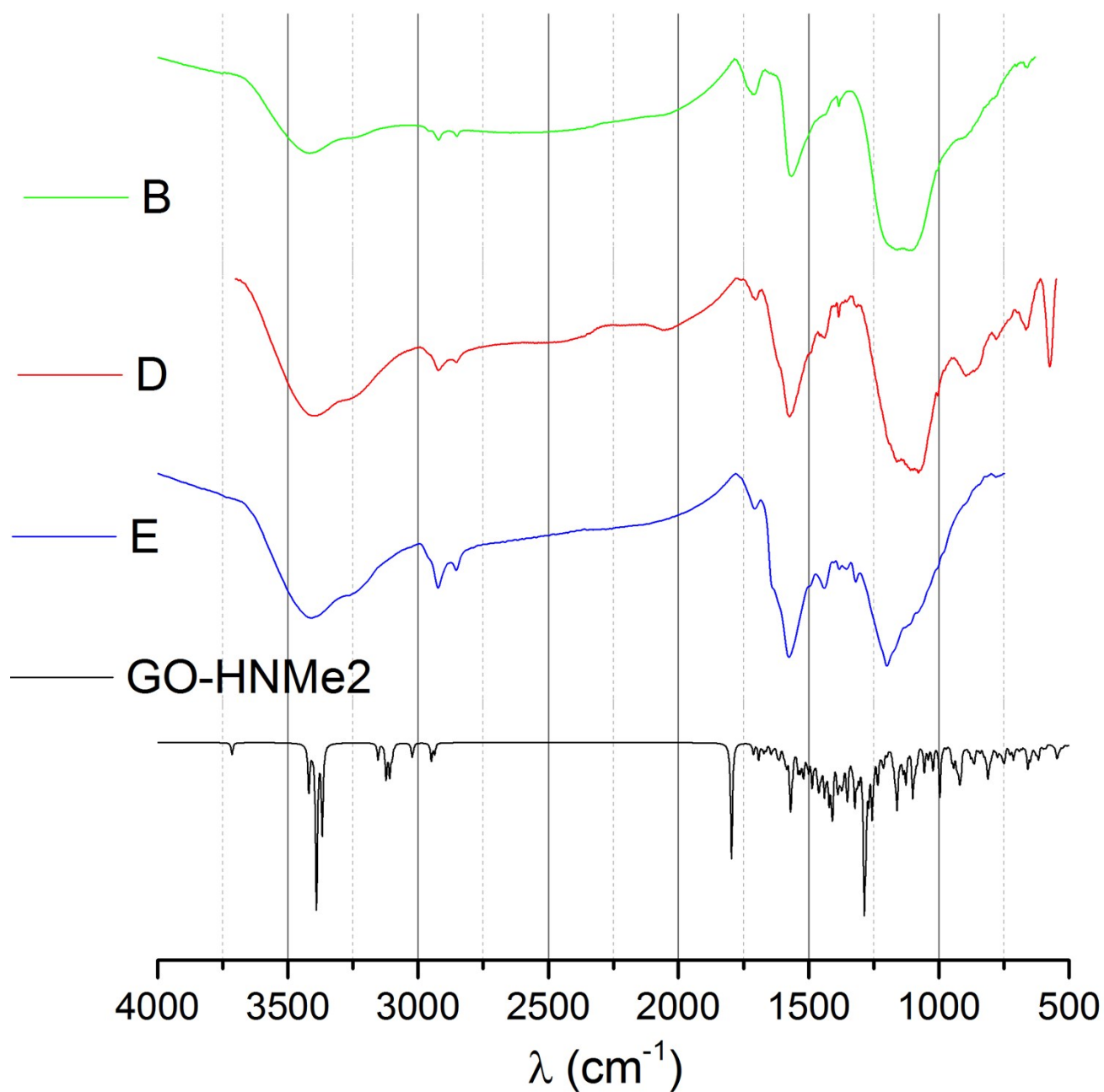
For the determination of pH, 40 mg of the corresponding material were stirred in 4 mL of deionized water during 16 h at room temperature. Then, the measurements were performed under soft stirring of the suspension.

7. Comparison between theory and experiment:

Experimental Infrared Spectrum of GO compared to two GO-models Infrared spectra achieved with ONIMO model.



Comparison between FTIR of Material B,D and E and the IR of a product of HNMe₂ insertion in the GO-model achieved with ONIOM model.



8. Cartesian Coordinates of the optimized complexes:

DMF:

Tag	X	Y	Z
C	-0.8272550	-0.6855000	-0.0002550
O	-1.9213880	-0.1576710	-0.0001350
N	0.3552680	-0.0140620	-0.0001260
H	-0.6899990	-1.7844910	-0.0002840
C	0.3173720	1.4449640	0.0001580
H	-0.2086190	1.8184080	0.8827730
H	1.3376980	1.8283560	0.0004760
H	-0.2081970	1.8187500	-0.8825630
C	1.6340810	-0.7003440	0.0002170
H	2.2236620	-0.4483490	-0.8882030
H	2.2227180	-0.4494350	0.8895870

H	1.4617730	-1.7781600	-0.0005460
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DBU

Tag	X	Y	Z
C	-2.6015760	0.7656690	0.1964770
C	-2.3804700	-0.6440990	0.7514240
C	-1.4450200	-1.4131460	-0.1780420
H	-1.9814420	-1.7135000	-1.0897110
H	-3.1931790	1.3619640	0.8975180
H	-3.1905020	0.7108170	-0.7308680
H	-3.3253500	-1.1846700	0.8596950
H	-1.9276490	-0.5705860	1.7458420
H	-1.0988420	-2.3318690	0.3069570
C	-0.3276000	0.7829830	-0.3959420
C	0.9529300	-1.2809870	-0.9018700
C	0.9669690	1.5189290	-0.6859830
C	2.0066600	-1.3462470	0.2273260
H	1.3843870	-0.7932840	-1.7793800
H	0.6868130	-2.2905650	-1.2245600
C	2.1234010	1.2522200	0.3214170
H	0.7092990	2.5766370	-0.6856030
H	1.2939370	1.2738010	-1.7014970
C	2.0467370	-0.0768610	1.0904500
H	2.9864170	-1.5324650	-0.2284100
H	1.8004070	-2.2029770	0.8782070
H	3.0797270	1.3190630	-0.2092100
H	2.1282850	2.0584390	1.0606020
H	2.8997190	-0.1398970	1.7740450
H	1.1547920	-0.0570590	1.7245360
N	-0.2803230	-0.5971830	-0.5253280
N	-1.3566780	1.4779530	-0.0674880

minA-1

Tag	Symbol X	Y	Z
C	1.9342340	1.6418440	0.1750550
C	0.7484990	2.4112370	0.7593060
C	-0.4592700	2.2470920	-0.1584700
H	-0.3375910	2.8628320	-1.0603520
H	2.7876210	1.6745840	0.8575530
H	2.2644640	2.1211370	-0.7578940
H	0.9822250	3.4725510	0.8803840
H	0.5146780	2.0093470	1.7503320
H	-1.3688800	2.5900480	0.3445700
C	0.4015360	-0.0579400	-0.4110160
C	-1.9792370	0.3968140	-0.9033670
C	0.0732380	-1.5117360	-0.6942160
C	-2.7354750	-0.3189070	0.2369480
H	-1.9136320	-0.2598640	-1.7733110
H	-2.5377330	1.2758180	-1.2338390
C	-0.9159000	-2.1750260	0.3092440
H	1.0204740	-2.0476700	-0.6746220
H	-0.3188670	-1.5865730	-1.7134400
C	-1.8279950	-1.2171940	1.0910440
H	-3.5464420	-0.9064270	-0.2089400

H	-3.2126880	0.4199520	0.8899770
H	-1.5245600	-2.9096300	-0.2290660
H	-0.3281390	-2.7408660	1.0369710
H	-2.4508810	-1.8011260	1.7761320
H	-1.2012920	-0.5822200	1.7255080
N	-0.6358730	0.8411920	-0.5354540
N	1.6143170	0.2421940	-0.0862340
O	3.2982050	-2.0535040	0.1159890
H	3.6988150	-2.0373100	-0.7585210
H	2.7998900	-1.2073580	0.1452910

TSA-12

Tag	X	Y	Z
C	-2.5051750	0.0419940	-0.7915830
C	-2.0596940	1.4961100	-0.7361130
C	-1.1315890	1.6886980	0.4562770
H	-1.6818710	1.5660410	1.3972960
H	-3.0853680	-0.1514620	-1.6974010
H	-3.1281480	-0.1965770	0.0763190
H	-2.9251220	2.1569110	-0.6419740
H	-1.5335870	1.7673800	-1.6573800
H	-0.6854200	2.6855800	0.4472520
C	-0.2699740	-0.5368500	-0.0391690
C	1.1447610	0.9677970	1.2415440
C	0.8760300	-1.5141430	-0.0197030
C	2.4994930	0.9327660	0.4727120
H	1.1432530	0.2581910	2.0738900
H	1.0000920	1.9555360	1.6791920
C	2.0054590	-1.1319980	-1.0033350
H	0.4708750	-2.4963520	-0.2477370
H	1.2620760	-1.5748800	0.9972540
C	2.4208680	0.3488340	-0.9451600
H	3.2220380	0.3649710	1.0680480
H	2.8937920	1.9506660	0.4029210
H	2.8677170	-1.7680620	-0.7765620
H	1.6975260	-1.3752380	-2.0246130
H	3.3942330	0.4712100	-1.4301630
H	1.7151390	0.9468310	-1.5291720
N	-0.0394710	0.7064560	0.4104890
N	-1.3501510	-0.8670800	-0.7848890
O	-1.4744940	-1.8670390	1.3567460
H	-1.6294430	-1.7563500	-0.2543040
H	-1.3555560	-2.5029640	2.0711510

MinA-2

Tag	X	Y	Z
C	2.5532930	0.5363650	-0.5605590
C	2.3148260	-0.9209600	-0.9442030
C	1.3127370	-1.5559450	0.0197040
H	1.7678100	-1.6657370	1.0168460
H	3.1636670	1.0400180	-1.3150910
H	3.0945300	0.5789160	0.3966380
H	3.2571580	-1.4771110	-0.9236500
H	1.9119140	-0.9638480	-1.9603750
H	1.0447510	-2.5559410	-0.3309830

C	0.3102240	0.6227150	0.4384990
C	-1.0361630	-1.4137850	0.7481310
C	-0.9895430	1.4406510	0.4234000
C	-2.4352690	-1.0242720	0.1770250
H	-1.0012790	-1.2448960	1.8332900
H	-0.8889730	-2.4852860	0.5993350
C	-1.8705650	1.2853090	-0.8236450
H	-0.7149310	2.4964770	0.5437330
H	-1.5559240	1.1762600	1.3195960
C	-2.3607930	-0.1594760	-1.0881250
H	-3.0229120	-0.5083530	0.9438420
H	-2.9868710	-1.9412560	-0.0519370
H	-2.7367500	1.9430800	-0.6886940
H	-1.3279200	1.6547350	-1.6971860
H	-3.3502970	-0.1211730	-1.5554000
H	-1.6911590	-0.6448190	-1.7997590
N	0.0829640	-0.7565210	0.0662620
N	1.2547040	1.2158730	-0.4938370
O	0.8298170	0.6147270	1.8084250
H	1.3757750	2.1969720	-0.2666600
H	0.8667140	1.5250610	2.1207310

TsA-21

Tag	X	Y	Z
C	-2.6551630	-0.3612140	-0.5524890
C	-2.2026660	1.0297410	-0.9789350
C	-1.2231090	1.5958580	0.0470800
H	-1.7047410	1.6699310	1.0348570
H	-3.2587310	-0.8535830	-1.3180950
H	-3.2657670	-0.2786830	0.3494710
H	-3.0819470	1.6753480	-1.0668310
H	-1.7116830	0.9946490	-1.9569190
H	-0.9205060	2.6014510	-0.2539330
C	-0.2725410	-0.5950280	0.5656770
C	1.1128210	1.4042420	0.7603450
C	0.9477000	-1.5010910	0.3123880
C	2.5016370	0.8874400	0.2944710
H	1.0193510	1.3255760	1.8529440
H	1.0418180	2.4657910	0.5119910
C	1.7761820	-1.2562490	-0.9555690
H	0.5900610	-2.5365360	0.3398920
H	1.5658730	-1.4017600	1.2072950
C	2.4506530	0.1405590	-1.0445070
H	2.9469760	0.2462900	1.0604930
H	3.1733680	1.7466280	0.2021010
H	2.5487980	-2.0322670	-0.9925040
H	1.1548570	-1.4148960	-1.8449640
H	3.4703440	0.0230980	-1.4250830
H	1.9169490	0.7608820	-1.7676640
N	-0.0228290	0.7593930	0.0815730
N	-1.5074700	-1.2480790	-0.2147260
O	-0.8177490	-0.7759740	1.7920470
H	-1.5864150	-1.5505180	0.9459440
H	-1.2575960	-1.8783470	-0.9740560

Structure 1

Tag	X	Y	Z
C	2.1961160	1.0264690	-0.0648040
C	1.3458240	2.0253770	0.7015390
C	0.0188030	2.2104160	-0.0139430
H	0.1283620	2.8288510	-0.9098380
H	3.1260660	0.7864880	0.4438990
H	2.4422000	1.3874200	-1.0671610
H	1.8608820	2.9849470	0.7668680
H	1.1872570	1.6688500	1.7226840
H	-0.7163230	2.6904020	0.6339660
C	0.1111640	-0.2246610	-0.4687890
C	-2.0098880	0.9412620	-0.7796740
C	-0.6435220	-1.4784790	-0.8417690
C	-2.9054140	0.3374540	0.3245710
H	-2.1497690	0.4278750	-1.7304060
H	-2.2621950	1.9859460	-0.9557880
C	-1.6649410	-1.9493520	0.2342220
H	0.0403960	-2.2831280	-1.0952600
H	-1.1644920	-1.2524750	-1.7746120
C	-2.2684360	-0.8294690	1.0946600
H	-3.8357480	0.0188170	-0.1540870
H	-3.1794070	1.1165830	1.0402590
H	-2.4530000	-2.5013000	-0.2835750
H	-1.1726870	-2.6646080	0.8979540
H	-3.0231460	-1.2655970	1.7527440
H	-1.4950220	-0.4362600	1.7637720
N	-0.5620940	0.9120670	-0.4408610
N	1.4420870	-0.2438470	-0.2015090
C	2.1770480	-1.4488640	0.0394170
O	3.3498790	-1.4342900	0.2576820
H	1.5671240	-2.3569500	0.0311310

MinA-3

Tag	X	Y	Z
C	0.1481800	2.5951680	0.4071020
C	-1.2617000	2.6277980	-0.1937120
C	-1.5322310	1.6255730	-1.3348120
H	-0.6429220	1.5078880	-1.9545370
H	0.2115050	3.3927700	1.1541230
H	0.8678150	2.8573170	-0.3881780
H	-1.4254380	3.6329070	-0.6004270
H	-1.9995970	2.4883830	0.6030040
H	-2.3297320	2.0181150	-1.9744160
C	-1.0802240	-0.7690040	-0.9931530
C	-3.3212310	0.0959840	-0.4283240
C	-1.6404140	-2.1346190	-0.6120910
C	-3.4351630	-0.1944650	1.0865100
H	-3.7961990	-0.7083990	-0.9966370
H	-3.8743060	1.0042940	-0.6723500
C	-1.9282920	-2.3051590	0.9067680
H	-0.9044440	-2.8676230	-0.9408470
H	-2.5521660	-2.3188910	-1.1874470
C	-2.2668000	-1.0090370	1.6601040
H	-4.3875600	-0.7107500	1.2556710

H	-3.4905480	0.7501120	1.6359960
H	-2.7348010	-3.0365990	1.0270640
H	-1.0444460	-2.7431450	1.3793090
H	-2.4943290	-1.2596220	2.7012580
H	-1.3818750	-0.3653020	1.6894090
N	-1.9490460	0.2801000	-0.9182100
N	0.4598750	1.3285340	1.0723250
O	0.0957840	-0.6328840	-1.3387400
H	0.6229200	0.6120360	0.3692420
H	1.3332120	1.4137940	1.5857380
C	3.5525300	-0.3806380	1.1192200
O	3.6110940	0.7096200	1.6643760
H	3.5789570	-1.3266230	1.6920970
N	3.4492110	-0.5996770	-0.2149150
C	3.3862890	0.5182240	-1.1453840
H	4.1813970	0.4316650	-1.8936540
H	2.4174110	0.5292490	-1.6518460
H	3.5211510	1.4377900	-0.5794800
C	3.2627830	-1.9329180	-0.7617840
H	3.3212820	-2.6678840	0.0432200
H	2.2827710	-2.0069940	-1.2418750
H	4.0422770	-2.1625300	-1.4965800

TsA-32

Tag	X	Y	Z
C	-1.2101980	-2.3093880	-0.0161520
C	0.2060060	-2.3861780	0.5799130
C	1.3642050	-2.1619730	-0.4284450
H	1.0047950	-2.3213960	-1.4468810
H	-1.9277870	-2.6756310	0.7252390
H	-1.2798020	-2.9823550	-0.8786020
H	0.3165970	-3.3886730	1.0086770
H	0.2968590	-1.6796550	1.4090330
H	2.1473710	-2.9002350	-0.2402220
C	1.5916980	0.1300350	-1.2560480
C	3.1638960	-0.6305080	0.4897710
C	2.4060020	1.4167260	-1.2818290
C	2.8990830	0.3340280	1.6629990
H	4.0039060	-0.2612390	-0.1059830
H	3.4687290	-1.6061050	0.8717810
C	2.3598570	2.2763910	0.0157080
H	2.0198050	1.9877960	-2.1251170
H	3.4424610	1.1575250	-1.5218680
C	1.9973760	1.5240910	1.3054490
H	3.8745760	0.6791190	2.0269520
H	2.4353580	-0.2129570	2.4905940
H	3.3233670	2.7866220	0.1260390
H	1.6085830	3.0579190	-0.1210410
H	2.0166360	2.2358540	2.1373120
H	0.9594460	1.1904200	1.2281820
N	2.0138720	-0.8483000	-0.3990730
N	-1.6393040	-0.9714930	-0.4308310
O	0.6223490	-0.0314590	-1.9989910
H	-0.9463060	-0.5463120	-1.0595420

C	-1.9818420	0.0790470	0.7261530
H	-2.3687910	-0.5509080	1.5594800
O	-1.2110390	1.0281490	0.9286060
N	-3.4255820	0.4122850	-0.1282480
H	-2.8223960	-0.6078570	-0.7246590
C	-3.3112820	1.7046100	-0.7992540
H	-3.1327000	2.5038880	-0.0708490
H	-2.4621650	1.6902660	-1.4841110
H	-4.2220060	1.9180510	-1.3663690
C	-4.6267280	0.2947590	0.6881820
H	-4.6583420	-0.6880520	1.1650150
H	-4.6537270	1.0613470	1.4752840
H	-5.5262870	0.4017620	0.0731160

Structure 2

Tag	X	Y	Z
C	1.7894140	0.5216330	0.7964800
C	1.3028830	1.5069860	-0.2780140
C	0.4308190	0.8827480	-1.3761320
H	0.9746260	0.0675970	-1.8534470
H	0.9462520	0.1588490	1.3906490
H	2.4790590	1.0334660	1.4686890
H	2.1781460	1.9514860	-0.7636550
H	0.7642450	2.3266020	0.2124670
H	0.2229580	1.6334310	-2.1440430
C	-0.9796820	-1.0031970	-0.6900660
C	-2.0184630	1.2343080	-0.8283040
C	-2.3832330	-1.5141270	-0.3750550
C	-2.5052290	1.4909580	0.6146410
H	-2.8385050	0.8275340	-1.4269470
H	-1.7416420	2.1796260	-1.2969340
C	-2.9744080	-1.0409800	0.9843510
H	-3.0490900	-1.2241100	-1.1933710
C	-2.3946080	0.2693630	1.5377880
H	-3.5450410	1.8330190	0.5613400
H	-1.9310170	2.3113780	1.0565880
H	-4.0611370	-0.9535600	0.8835420
H	-2.7985530	-1.8222880	1.7285700
H	-2.8866370	0.4995020	2.4877600
H	-1.3399880	0.1082140	1.7813850
N	-0.8596440	0.3399170	-0.9290710
N	2.4897340	-0.6289220	0.2494540
C	3.8428090	-0.7109570	0.2104440
O	4.6159240	0.1330590	0.6236980
H	4.1857360	-1.6596720	-0.2454030
O	-0.0206420	-1.7712800	-0.7384810
H	1.9164710	-1.3621250	-0.1537900
H	-2.3105850	-2.6005540	-0.3946190

MinB-1

Tag	X	Y	Z
C	-0.5858140	2.5529280	-0.0686510
C	-1.5993420	2.3953150	1.0666680
C	-2.8336410	1.6700130	0.5393810
H	-3.4472890	2.3540210	-0.0634620

H	0.3344380	3.0125040	0.3047470
H	-0.9856340	3.2406720	-0.8284740
H	-1.8871760	3.3641490	1.4848550
H	-1.1445850	1.8096610	1.8720910
H	-3.4575500	1.3284100	1.3717940
C	-1.1631700	0.3812970	-0.7581580
C	-3.4101670	-0.5891520	-0.3715630
C	-0.8398150	-0.9387050	-1.4299050
C	-3.1419210	-1.7593110	0.6009360
H	-3.4210980	-0.9578820	-1.3993280
H	-4.4045940	-0.1716510	-0.1945650
C	-0.8088270	-2.1759060	-0.4847770
H	-1.5575700	-1.1004200	-2.2404720
C	-1.6471840	-2.0542110	0.7978010
H	-3.6609460	-2.6452520	0.2163500
H	-3.5880980	-1.5406290	1.5775780
H	-1.1245370	-3.0582770	-1.0528540
H	0.2257840	-2.3485960	-0.1792810
H	-1.5402120	-2.9778200	1.3750470
H	-1.2103610	-1.2662690	1.4196670
N	-2.4486430	0.5071130	-0.2657760
N	-0.2426940	1.2826760	-0.6989330
C	2.6302610	-0.5575040	0.1895900
O	2.4996960	-1.6916390	0.6246380
H	1.7768310	0.0600560	-0.1376340
N	3.8205080	0.0925220	0.0492910
H	0.1320910	-0.8098830	-1.9037050
C	3.8782910	1.4342990	-0.4992350
H	2.8719960	1.7538210	-0.7740810
H	4.2889690	2.1435700	0.2294150
H	4.5091690	1.4638200	-1.3953840
C	5.0634830	-0.5494290	0.4370550
H	5.5744110	0.0294570	1.2148150
H	4.8241060	-1.5395670	0.8208980
H	5.7371600	-0.6447560	-0.4220520

TsB-12

Tag	X	Y	Z
C	-0.1237040	-2.1297260	-0.9900650
C	-1.5895970	-2.4355660	-0.7001140
C	-1.8939030	-1.9918440	0.7306150
H	-1.2462090	-2.5187990	1.4397390
H	0.0536640	-2.0459030	-2.0671870
H	0.5017050	-2.9531640	-0.6244080
H	-1.7814920	-3.5018090	-0.8479000
H	-2.2406680	-1.8902630	-1.3900080
H	-2.9258610	-2.2008040	1.0174530
C	-0.4453430	-0.0657370	0.3847620
C	-2.8710610	0.2614850	0.5349140
C	-0.0822050	1.2537860	0.7530740
C	-2.7450690	1.7769840	0.2655680
H	-3.5787350	0.1141420	1.3574720
H	-3.3337240	-0.1813160	-0.3611940
C	-0.2790370	2.3101940	-0.3341030

H	-0.6294940	1.5267520	1.6535820
C	-1.7524610	2.2272000	-0.8319760
H	-2.5389150	2.3107100	1.1971000
H	-3.7572000	2.0754510	-0.0340390
H	-0.0853450	3.3029150	0.0867150
H	0.4005480	2.1696350	-1.1763930
H	-2.0826950	3.1921110	-1.2351820
H	-1.8052560	1.5161190	-1.6662960
N	-1.6568750	-0.5494460	0.8480490
N	0.3443630	-0.8888160	-0.3500380
C	1.7428220	-0.5160530	-0.8753360
O	1.8153070	0.2377730	-1.8515260
H	2.3017380	-1.4795420	-0.8580170
N	2.4780240	0.2089280	0.5667550
H	1.6315190	0.8187400	0.8600030
C	2.7858110	-0.7629800	1.6160120
H	1.8579970	-1.2089020	1.9763250
H	3.4320460	-1.5527290	1.2200090
H	3.2941550	-0.2856360	2.4589210
C	3.6143510	1.0355560	0.1525520
H	4.4845520	0.4057290	-0.0538530
H	3.3330080	1.5532590	-0.7638940
H	3.8699990	1.7566530	0.9344860

MinB-2

Tag	X	Y	Z
C	-1.7811350	-1.7191870	-0.8023560
C	-2.5160770	-2.0697610	0.5079810
C	-2.0538370	-1.1493880	1.6697560
H	-1.2502000	-1.6399190	2.2239950
H	-2.3949170	-1.0523160	-1.4159780
H	-1.5568810	-2.6005170	-1.4004400
H	-2.3246270	-3.1093830	0.7865630
H	-3.5929590	-1.9822950	0.3413330
H	-2.8647550	-0.9721120	2.3793020
C	-0.4961520	0.0745610	0.2905160
C	-2.5687470	1.1467150	0.8297420
C	0.2758750	1.1839490	0.1105960
C	-2.1048510	2.4392730	0.1075810
H	-3.0939540	1.4397420	1.7441920
H	-3.3135500	0.6598090	0.1795000
C	0.1431390	1.9479510	-1.1886450
H	0.2675730	1.8267420	0.9856450
C	-1.3798230	2.3217940	-1.2673810
H	-1.5132950	3.0527840	0.7926770
H	-3.0341960	2.9956220	-0.0619010
H	0.7604910	2.8501160	-1.1728540
H	0.4311690	1.3815630	-2.0771220
H	-1.5123560	3.2659940	-1.8076090
H	-1.8934500	1.5552190	-1.8599210
N	-1.5312890	0.1414950	1.2141340
N	-0.4946260	-1.0527420	-0.5409630
C	0.6729420	-1.5645750	-1.0976950
O	0.6844010	-2.4762070	-1.8967850
H	1.5773630	-1.0682400	-0.7152790

N	3.5150060	0.0224580	0.4141860
H	2.6803440	0.6017900	0.4608340
C	3.9260340	-0.3669380	1.7556450
H	3.0758090	-0.7979840	2.2896700
H	4.7042100	-1.1348010	1.6953600
H	4.3272990	0.4653790	2.3616020
C	4.5623980	0.7018480	-0.3352890
H	5.3885950	0.0087190	-0.5237230
H	4.1732370	1.0222410	-1.3045580
H	4.9816150	1.5855790	0.1788030

Structure 4

Tag	X	Y	Z
C	1.5733180	0.5328080	1.0064210
C	1.5697760	1.9902600	0.4946580
C	0.6420810	2.1536180	-0.7388050
H	1.2235600	2.0124920	-1.6530060
H	0.8980480	0.4284420	1.8614080
H	2.5615520	0.2102760	1.3295990
H	2.5807620	2.2995540	0.2164710
H	1.2544990	2.6466110	1.3098810
H	0.2225660	3.1610540	-0.7829600
C	-0.0536190	-0.1540230	-0.7254000
C	-1.5762090	1.4502700	0.1702110
C	-0.9408410	-1.1033140	-1.1190430
C	-2.6447090	0.3416030	0.3652500
H	-2.0856560	2.3528950	-0.1815630
H	-1.1651410	1.6866950	1.1653320
C	-1.5383410	-2.0211720	-0.0784230
H	-1.6690150	-0.7182650	-1.8253520
C	-2.2130860	-1.0405760	0.9475930
H	-3.2009500	0.1996230	-0.5654480
H	-3.3573060	0.7810220	1.0732790
H	-2.2818010	-2.6850590	-0.5268110
H	-0.8161250	-2.6567220	0.4390320
H	-3.0930310	-1.5109770	1.4008630
H	-1.5063680	-0.8596800	1.7662510
N	-0.4499000	1.1780850	-0.7749740
N	1.1445340	-0.4124930	-0.0366810
C	1.9363850	-1.5018330	-0.3498910
O	2.9372380	-1.8188540	0.2556280
H	1.5455300	-2.0421200	-1.2258340

minB-3

Tag	X	Y	Z
C	-1.9155490	0.7081000	-0.9061090
C	-1.4043440	2.1601090	-0.7798920
C	-0.1583440	2.2521980	0.1383150
H	-0.4746500	2.4520170	1.1648760
H	-1.5656660	0.2598020	-1.8409850
H	-3.0026590	0.6520090	-0.9056050
H	-2.1866050	2.8041810	-0.3700850
H	-1.1794270	2.5400390	-1.7795160
H	0.4894010	3.0785450	-0.1615100

C	-0.0908590	-0.1315720	0.5453540
C	1.4062530	0.7357680	-1.0893500
C	0.6173880	-1.2149930	0.9392080
C	2.0904490	-0.6513080	-1.2163150
H	2.1829450	1.5026090	-1.1583090
H	0.7420650	0.8688570	-1.9562810
C	0.6299800	-2.4527050	0.0767480
H	1.5931250	-0.9533810	1.3320800
C	1.2053230	-1.9361580	-1.2928620
H	2.8493670	-0.7441530	-0.4360450
H	2.6408700	-0.5883580	-2.1623210
H	1.2790270	-3.2189650	0.5066800
H	-0.3480830	-2.9121260	-0.0805870
H	1.7934640	-2.7252040	-1.7738780
H	0.3625600	-1.7298210	-1.9634460
N	0.6349580	1.0152440	0.1745030
N	-1.4548880	-0.1316970	0.2108420
C	-2.3707500	-0.8695320	0.9399180
O	-3.5450690	-0.9719570	0.6614420
H	-1.8986640	-1.3457930	1.8130980
O	3.1795530	1.0136110	1.7069700
H	2.2783350	1.1299650	1.3585950
H	3.0509500	0.8122720	2.6384330

TsB-34

Tag	X	Y	Z
C	2.4043880	-1.2234620	-0.3741160
C	1.8822170	-1.3100030	1.0790620
C	0.3606000	-1.4868260	1.2746050
H	0.1137560	-1.3368710	2.3312860
H	2.1875730	-2.1781550	-0.8700970
H	3.4963280	-1.1389180	-0.2948220
H	2.2392080	-0.4442850	1.6390680
H	2.3495640	-2.1820260	1.5536000
H	0.0804270	-2.5138660	1.0342230
C	-0.6165300	0.6928200	0.6417010
C	-1.1467850	-1.1802310	-0.7718460
C	-1.6343720	1.5461180	0.5507550
C	-2.6811160	-1.1801530	-0.7745980
H	-0.7897080	-2.2060500	-0.8653040
H	-0.7354260	-0.6278260	-1.6212180
C	-3.0632640	1.0758140	0.4318270
H	-1.4288670	2.6098180	0.4942290
C	-3.3439840	0.2033720	-0.8079910
H	-3.0407310	-1.7384830	0.0985620
H	-3.0015710	-1.7417650	-1.6591170
H	-3.3366560	0.5081770	1.3305870
H	-3.7153140	1.9521250	0.4091130
H	-4.4271260	0.0677340	-0.8925880
H	-3.0229100	0.7419590	-1.7070250
N	-0.5433760	-0.6400860	0.4648900
N	1.8763890	-0.1674440	-1.2539960
C	2.4837240	1.0116000	-1.2069940
O	3.1932610	1.5002350	-0.2802570
H	2.2360980	1.6571500	-2.0758680

O	0.7342640	1.2640920	0.9210510
H	0.7598730	2.2247750	1.0531620
H	1.4149220	0.9903170	0.1851660

MinB-4

Tag	X	Y	Z
C	-1.9742370	0.4715720	-0.8655060
C	-1.6259560	1.5031630	0.2161950
C	-0.6132300	1.0302110	1.2712090
H	-1.0219700	0.1735780	1.8094340
H	-1.0870370	0.2086490	-1.4462650
H	-2.7122480	0.8997610	-1.5456410
H	-2.5451950	1.7781380	0.7427030
H	-1.2694740	2.4160530	-0.2725250
H	-0.4813490	1.8337400	2.0072060
C	1.1649510	-0.6504740	0.7832350
C	1.4402750	1.5787990	-0.0993910
C	2.4814770	-0.9294300	0.9681960
C	2.8594060	1.1965800	-0.6078960
H	1.5130430	2.5460310	0.4123260
H	0.8154080	1.7442090	-0.9881690
C	3.2843650	-1.3626480	-0.2428720
H	2.9857320	-0.1785200	1.5650650
C	3.0820930	-0.1956370	-1.2694010
H	3.5916350	1.3432500	0.1902910
H	3.0827020	1.9629450	-1.3591400
H	4.3406840	-1.4772860	0.0140140
H	2.9664820	-2.3084510	-0.6902800
H	3.9383320	-0.1266410	-1.9498030
H	2.2104620	-0.4274220	-1.8921790
N	0.7155730	0.6320030	0.7881080
N	-2.5320120	-0.7625820	-0.3311040
C	-3.8623460	-0.9425050	-0.1356440
O	-4.7279190	-0.1278440	-0.3905880
H	-4.0889750	-1.9419230	0.2851760
O	0.2659680	-1.5966620	0.3037670
H	0.6296870	-2.4561320	0.5529480
H	-1.8780170	-1.4776720	-0.0483770

TsB-42

Tag	X	Y	Z
C	1.8833210	0.2866230	0.9784920
C	1.4065420	1.5098730	0.1789950
C	0.5302640	1.1720460	-1.0342260
H	1.0499040	0.4805910	-1.6930480
H	1.0375040	-0.2179480	1.4527320
H	2.5603420	0.6178480	1.7668130
H	2.2858950	2.0495200	-0.1867280
H	0.8778530	2.1911750	0.8550730
H	0.3296850	2.0793740	-1.6093890
C	-0.9439710	-0.7430890	-0.6913170
C	-1.8405430	1.5754870	-0.4322150
C	-1.9838280	-1.6339300	-0.2285520
C	-3.1994030	1.0503560	0.0206970

H	-1.9606890	2.1698890	-1.3461080
H	-1.4561380	2.2550950	0.3369520
C	-3.0191740	-1.3454840	0.8493660
H	-2.3829220	-2.1613480	-1.0974690
C	-3.1328620	0.1329230	1.2506430
H	-3.6975000	0.5299630	-0.8032600
H	-3.8017720	1.9391920	0.2341720
H	-4.0038750	-1.6761130	0.4977070
H	-2.8116840	-1.9417210	1.7459230
H	-4.0234510	0.2687430	1.8711720
H	-2.2806690	0.4241600	1.8771850
N	-0.7822610	0.5819880	-0.6901570
N	2.6010030	-0.6861330	0.1688440
C	3.9523400	-0.6684170	0.0383960
O	4.7023040	0.1138270	0.5899080
H	4.3145860	-1.4692890	-0.6343610
O	0.0393180	-1.5111300	-1.1255640
H	-0.6648220	-2.3224170	-0.5294260
H	2.0474610	-1.3276010	-0.3851700

GO-Isomer 1:

Tag	X	Y	Z
C	-6.0962760	0.0117860	-0.0431220
C	-4.8766450	-0.6679150	0.1111740
C	-3.6407930	0.0583040	0.2595570
C	-3.6582950	1.4805380	0.1994060
C	-4.8970130	2.1689530	0.0386080
C	-6.1113470	1.4641420	-0.0719710
C	-2.4195000	-0.6343040	0.4525100
C	-2.4357400	2.2124550	0.3212450
C	-1.2517110	1.5192870	0.5486120
C	-1.2101270	0.0934500	0.6060820
C	0.0435940	-0.6052310	0.7249460
C	1.2605610	0.0515360	0.6600540
C	1.2921650	1.5154610	0.8427820
C	-0.0207790	2.2848620	0.8259750
C	-4.8569900	-2.1291330	0.1151620
C	-3.6300390	-2.8139320	0.2549170
C	-6.0754770	-2.8507210	-0.0244840
C	-2.3997510	-2.0928910	0.4393340
C	-3.6221040	-4.2543590	0.2392490
C	-6.0661980	-4.3089970	-0.0278960
C	-1.2121220	-2.7884300	0.6034190
C	-2.3715380	-4.9252270	0.3548970
C	-4.8227320	-4.9721920	0.0996230
C	0.0445380	-2.0799820	1.0453040
C	-1.1843720	-4.2240310	0.5136730
H	-2.3549280	-6.0079520	0.2975990
H	-4.7938820	-6.0699300	0.0922280
C	1.3046900	-2.7803480	0.5929300
C	0.0569730	-4.9040340	0.5232100
C	1.2817850	-4.2201120	0.4864350
C	2.4994650	-0.6360000	0.5035580
C	3.7021230	0.0709520	0.3510990
C	2.4849400	-2.0873860	0.4354920

C	4.9465890	-0.6243520	0.1474120
C	3.7213120	-2.7892410	0.2179950
C	4.9356370	-2.0923150	0.0914490
C	2.5346890	2.2294240	0.5400030
C	3.7080280	1.5169130	0.3568920
C	4.9522730	2.2248880	0.1828480
C	6.1608170	1.5320540	0.0246090
C	6.1544930	0.0709030	-0.0004590
C	-7.3499280	-0.7093000	-0.1744570
C	-7.3300830	-2.1593170	-0.1621800
C	3.7199520	-4.2320230	0.1658410
C	2.4786540	-4.9103800	0.2948310
C	-8.5553810	-2.8923050	-0.2904130
C	-8.5326880	-4.3519760	-0.2855940
C	-7.3104200	-5.0222900	-0.1600920
H	-7.2891090	-6.1205760	-0.1592280
H	2.4672340	-5.9927060	0.2251630
C	4.9257690	-4.9334240	-0.0138630
H	4.9090850	-6.0310010	-0.0511070
C	6.1590690	-2.7955830	-0.0900840
C	6.1608490	-4.2530640	-0.1429420
C	7.4035710	-2.0860920	-0.2218650
C	7.4113270	-0.6347460	-0.1817570
C	7.4074810	2.2458450	-0.1196490
C	8.6427820	1.5391050	-0.2835950
C	8.6396980	0.0793570	-0.3165940
C	-9.8072980	-2.1882080	-0.4238900
C	-11.0386920	-2.9317020	-0.5469220
C	-9.8316010	-0.7407870	-0.4360750
C	-12.2571460	-2.2172780	-0.6746950
C	-10.9897420	-4.3935030	-0.5369330
C	-11.0881890	-0.0454320	-0.5706120
C	-12.2777880	-0.8154480	-0.6856480
C	-11.1005040	1.4451780	-0.5877210
C	-12.2884040	2.1927920	-0.7152260
C	-9.8420100	2.1593260	-0.4713570
C	-8.5974070	1.4483230	-0.3335270
C	-9.8320970	3.6143930	-0.4935020
C	-7.3641600	2.1674310	-0.2185930
C	-8.5853000	-0.0094850	-0.3133400
C	-8.5958890	4.3123890	-0.3842920
C	-7.3637580	3.6256810	-0.2486070
C	-6.1057920	4.3117310	-0.1422930
C	-4.9064080	3.6295650	-0.0060260
C	-3.6582750	4.3230810	0.0858830
C	-2.4470240	3.6806160	0.2320060
C	-1.2063480	4.4073490	0.3099820
C	0.0142280	3.7475630	0.5250250
C	1.2666800	4.3603770	0.4827090
C	2.4995200	3.6653220	0.4809150
H	1.3185670	5.4333860	0.3846700
H	-8.5997220	5.4106810	-0.4062020
H	-6.1031780	5.4097520	-0.1739820
H	-3.6938170	5.3981830	0.0102950

C	7.3983580	3.7054540	-0.0962630
C	8.6306550	4.4053570	-0.2305230
C	6.1500280	4.3834300	0.0588810
C	9.8629680	3.7192380	-0.3870570
C	11.1106450	4.4352890	-0.5189910
H	6.1439520	5.4821360	0.0701410
H	8.6275930	5.5038950	-0.2118110
H	11.0932450	5.5332430	-0.4948700
C	4.9446260	3.6891480	0.1953400
C	3.6989250	4.3580230	0.3301680
H	3.6871630	5.4414210	0.2939470
C	9.8887020	-0.6371290	-0.4873440
C	11.1384150	0.0714890	-0.6188960
C	9.8761470	-2.0847730	-0.5263770
C	12.3313540	-0.6836250	-0.7819880
C	11.1407710	1.5614950	-0.5827290
C	11.1113270	-2.8133200	-0.6969130
C	12.3217310	-2.0852440	-0.8204640
C	12.3212960	2.3203780	-0.7044460
C	9.8795420	2.2619610	-0.4178770
C	12.3033080	3.7449850	-0.6720390
H	13.2503970	4.2923930	-0.7711780
C	7.4089090	-4.9493510	-0.3199100
C	8.6226480	-4.2629030	-0.4428270
C	9.8985710	-4.9620570	-0.6188250
C	11.0749000	-4.2748260	-0.7375970
C	8.6329450	-2.8036690	-0.3966050
H	7.3982200	-6.0472760	-0.3562560
H	9.8827020	-6.0601100	-0.6520020
C	-9.8056410	-5.0668520	-0.4149250
H	-9.7812000	-6.1652160	-0.4101020
C	-11.0837300	4.3177550	-0.6281220
C	-12.2767010	3.6159380	-0.7343980
H	-13.2277730	4.1559240	-0.8359360
H	-11.0731140	5.4158940	-0.6443660
H	12.0260500	-4.8090320	-0.8684000
H	13.2651190	-2.6330360	-0.9492340
H	13.2916700	-0.1642170	-0.8826360
H	13.2870640	1.8163410	-0.8284340
H	-11.9381750	-4.9399540	-0.6323070
H	-13.1980590	-2.7764820	-0.7674770
H	-13.2438310	-0.3069760	-0.7877090
H	-13.2530780	1.6793750	-0.8034320
C	-1.2458560	5.8810080	0.0743280
O	-1.8901510	6.4462710	-0.7781030
O	-0.4861110	6.5905880	0.9526930
H	-0.5914950	7.5190180	0.6938210
O	0.1071920	-2.2039610	2.5136050
H	0.0567240	-5.9874210	0.4665870
O	0.6307310	1.9509020	2.0632580
H	-0.6199990	-1.6804750	2.8746980

GO-Isomer 2:

Tag	X	Y	Z
C	-6.1346360	0.0101600	0.0133780
C	-4.9055810	-0.6687540	0.0200790

C	-3.6653620	0.0598070	0.0525620
C	-3.6886330	1.4820340	0.0534490
C	-4.9362040	2.1701750	0.0594220
C	-6.1538490	1.4625820	0.0437770
C	-2.4301020	-0.6322210	0.0718980
C	-2.4607620	2.2130520	0.0017250
C	-1.2644950	1.5127940	-0.0848840
C	-1.2159160	0.0922650	0.0098640
C	0.0462200	-0.6004390	0.0820020
C	1.2521880	0.0488500	-0.0841820
C	1.2716050	1.4878360	-0.4264710
C	-0.0306570	2.2590590	-0.3946160
C	-4.8807220	-2.1296940	-0.0226740
C	-3.6445790	-2.8133300	0.0014110
C	-6.1036710	-2.8527690	-0.0730370
C	-2.4080790	-2.0899770	0.0896750
C	-3.6303760	-4.2532630	-0.0245130
C	-6.0892060	-4.3109100	-0.1167750
C	-1.2094560	-2.7761000	0.2065530
C	-2.3708570	-4.9173700	0.0323330
C	-4.8376130	-4.9723020	-0.0946570
C	0.0493260	-2.0296700	0.5777630
C	-1.1789760	-4.2120530	0.1524450
H	-2.3525800	-6.0005800	-0.0147510
H	-4.8081080	-6.0698210	-0.1200450
C	1.3136040	-2.7671900	0.2157490
C	0.0644990	-4.8900620	0.1851880
C	1.2920880	-4.2088700	0.1757160
C	2.5057300	-0.6319350	0.0090480
C	3.7139980	0.0708740	-0.0514400
C	2.5013980	-2.0811760	0.0912660
C	4.9741710	-0.6241820	-0.0326140
C	3.7499790	-2.7884110	0.0207860
C	4.9703210	-2.0920180	-0.0188120
C	2.5298770	2.2177140	-0.2250680
C	3.7159490	1.5155510	-0.1111450
C	4.9692410	2.2263760	-0.0801690
C	6.1885800	1.5350370	-0.0497200
C	6.1886200	0.0730790	-0.0381160
C	-7.3922860	-0.7131740	-0.0293100
C	-7.3672470	-2.1627750	-0.0753570
C	3.7504440	-4.2320190	0.0335380
C	2.4999060	-4.9054170	0.0879470
C	-8.5969690	-2.8970270	-0.1213490
C	-8.5696920	-4.3561450	-0.1704770
C	-7.3397190	-5.0246990	-0.1686440
H	-7.3170870	-6.1224470	-0.2031100
H	2.4912730	-5.9897290	0.0618190
C	4.9695390	-4.9345700	-0.0043910
H	4.9577020	-6.0329190	-0.0006890
C	6.2058600	-2.7957330	-0.0311170
C	6.2121770	-4.2543240	-0.0296920
C	7.4559690	-2.0841830	-0.0376200
C	7.4579750	-0.6319830	-0.0347580

C	7.4417320	2.2504530	-0.0442860
C	8.6888020	1.5446130	-0.0315660
C	8.6922380	0.0841280	-0.0313090
C	-9.8573360	-2.1948160	-0.1181300
C	-11.0929690	-2.9398150	-0.1627870
C	-9.8862740	-0.7479600	-0.0706320
C	-12.3194400	-2.2275920	-0.1569720
C	-11.0395770	-4.4008180	-0.2129230
C	-11.1511760	-0.0545500	-0.0670550
C	-12.3443680	-0.8263750	-0.1100820
C	-11.1675780	1.4357220	-0.0214650
C	-12.3632710	2.1816950	-0.0137820
C	-9.9051990	2.1518730	0.0135900
C	-8.6521830	1.4428440	0.0115220
C	-9.8990820	3.6066730	0.0502940
C	-7.4153220	2.1643800	0.0433020
C	-8.6360320	-0.0148040	-0.0286360
C	-8.6588570	4.3069110	0.0759560
C	-7.4181050	3.6227170	0.0701470
C	-6.1552040	4.3112960	0.0804780
C	-4.9471660	3.6314960	0.0686780
C	-3.6930000	4.3275370	0.0602080
C	-2.4741940	3.6841830	0.0166250
C	-1.2162080	4.3952520	0.0514110
C	0.0075950	3.7279730	-0.1307320
C	1.2580840	4.3469210	-0.1740600
C	2.4929950	3.6549340	-0.2166610
H	1.3131430	5.4217740	-0.0995720
H	-8.6674700	5.4052170	0.0977850
H	-6.1584080	5.4098160	0.0904630
H	-3.7296300	5.4050040	0.0573000
C	7.4266190	3.7103490	-0.0570180
C	8.6656470	4.4116610	-0.0429120
C	6.1674070	4.3864150	-0.0930100
C	9.9086260	3.7268870	-0.0252990
C	11.1623310	4.4446800	-0.0128150
H	6.1590860	5.4850980	-0.1109670
H	8.6595320	5.5103500	-0.0493990
H	11.1408830	5.5428290	-0.0129160
C	4.9553260	3.6898610	-0.1162240
C	3.6989510	4.3529850	-0.1680470
H	3.6863760	5.4370300	-0.1579190
C	9.9530060	-0.6314300	-0.0302340
C	11.2084560	0.0791640	-0.0229470
C	9.9465570	-2.0799920	-0.0381200
C	12.4130090	-0.6750990	-0.0248180
C	11.2042720	1.5698730	-0.0159170
C	11.1939700	-2.8074660	-0.0409620
C	12.4095380	-2.0774480	-0.0341170
C	12.3895050	2.3308000	-0.0040050
C	9.9312870	2.2691230	-0.0239920
C	12.3655110	3.7558770	-0.0015020
H	13.3168750	4.3047660	0.0082660
C	7.4737450	-4.9494700	-0.0439180
C	8.6931880	-4.2611270	-0.0482090

C	9.9820710	-4.9588210	-0.0543440
C	11.1635010	-4.2697770	-0.0505550
C	8.6978220	-2.8009640	-0.0420290
H	7.4693340	-6.0480760	-0.0455510
H	9.9719670	-6.0574370	-0.0606910
C	-9.8479400	-5.0720850	-0.2171320
H	-9.8212810	-6.1697650	-0.2549930
C	-11.1589660	4.3079420	0.0557530
C	-12.3554640	3.6044750	0.0253550
H	-13.3126760	4.1431420	0.0299020
H	-11.1520980	5.4058840	0.0839620
H	12.1238320	-4.8035900	-0.0540630
H	13.3622910	-2.6241850	-0.0361260
H	13.3780120	-0.1546330	-0.0198440
H	13.3640310	1.8283850	0.0032870
H	-11.9913950	-4.9486330	-0.2475390
H	-13.2636580	-2.7879530	-0.1904690
H	-13.3169460	-0.3200780	-0.1079680
H	-13.3311720	1.6673640	-0.0389800
C	-1.2488710	5.8667480	0.2867090
O	-2.0158690	6.6547380	-0.2181580
O	-0.3206080	6.2919050	1.1875620
H	-0.4472140	7.2510530	1.2520320
O	0.1049690	-1.9920740	2.0530680
H	0.0649950	-5.9746280	0.1588930
O	0.5722120	1.8586940	-1.6444220
H	-0.7049660	-1.5625340	2.3567490

Hydrogen bond Interaction of HNMe2 with GO

Isomer1

Tag	X	Y	Z
C	6.0468440	0.1964190	-0.1743300
C	4.8353500	0.8583850	0.0670470
C	3.6012680	0.1323870	0.2188690
C	3.6186590	-1.3109030	0.0874960
C	4.8687500	-1.9787290	-0.1771170
C	6.0662090	-1.2594680	-0.2969640
C	2.3958540	0.8135350	0.4507610
C	2.4579420	-2.0567600	0.2266120
C	1.2184690	-1.3745420	0.6141150
C	1.1664220	0.1015600	0.5571330
C	-0.0590190	0.7371760	0.6847680
C	-1.3052740	0.0370810	0.5196990
C	-1.3253260	-1.3756050	0.3623020
C	-0.0759280	-2.1376770	0.5572970
C	4.8108490	2.3269760	0.1636280
C	3.5939890	2.9966410	0.3739310
C	6.0257070	3.0566740	0.0355480
C	2.3639030	2.2661430	0.5214860
C	3.5766460	4.4384700	0.4656760
C	6.0142320	4.5117510	0.1349450
C	1.1734480	2.9289940	0.7418420
C	2.3285700	5.0895650	0.6543460
C	4.7758870	5.1639970	0.3492120

C	-0.0857680	2.1815400	1.1181020
C	1.1344540	4.3766280	0.7659710
H	2.3080740	6.1733870	0.6822270
H	4.7507530	6.2595450	0.4223900
C	-1.3455990	2.9078460	0.7178840
C	-0.0996270	5.0376160	0.8356290
C	-1.3324170	4.3434140	0.7392050
C	-2.5228950	0.7562340	0.4114860
C	-3.7328660	0.0627420	0.1557290
C	-2.5206900	2.2103720	0.4937580
C	-4.9758800	0.7776120	0.0336380
C	-3.7578150	2.9240140	0.3391090
C	-4.9744440	2.2342790	0.1356020
C	-2.5012960	-2.0631850	0.0899730
C	-3.7307280	-1.3505240	0.0006250
C	-4.9499190	-2.0550630	-0.2363870
C	-6.1714770	-1.3594890	-0.3227080
C	-6.1796660	0.0890330	-0.1907900
C	7.2932690	0.9303630	-0.3081130
C	7.2727310	2.3777520	-0.1947070
C	-3.7683710	4.3611990	0.4235610
C	-2.5285160	5.0375350	0.6098870
C	8.4924230	3.1221690	-0.3195570
C	8.4695000	4.5777940	-0.2101040
C	7.2532520	5.2348330	0.0097490
H	7.2331040	6.3303930	0.0887230
H	-2.5276120	6.1216070	0.6362530
C	-4.9786950	5.0703260	0.3149890
H	-4.9664310	6.1663490	0.3845290
C	-6.2002750	2.9459700	0.0246250
C	-6.2108030	4.4011120	0.1211860
C	-7.4415230	2.2471250	-0.1840700
C	-7.4404280	0.8008380	-0.2981590
C	-7.4102770	-2.0670640	-0.5495600
C	-8.6511990	-1.3573700	-0.6392790
C	-8.6616660	0.0955860	-0.5133480
O	0.5859340	-1.9093420	1.8301650
C	9.7374650	2.4342190	-0.5547820
C	10.9624060	3.1895620	-0.6768200
C	9.7622170	0.9908770	-0.6712420
C	12.1745810	2.4916090	-0.9085360
C	10.9136600	4.6465180	-0.5593040
C	11.0134480	0.3135860	-0.9101090
C	12.1957560	1.0941160	-1.0215460
C	11.0285580	-1.1715780	-1.0341030
C	12.2106780	-1.9003320	-1.2702330
C	9.7779840	-1.8991860	-0.9091290
C	8.5397580	-1.2075640	-0.6664470
C	9.7743780	-3.3519320	-1.0314760
C	7.3151480	-1.9410700	-0.5436300
C	8.5238550	0.2474900	-0.5462690
C	8.5534590	-4.0644560	-0.9111460
C	7.3202910	-3.3954990	-0.6691890
C	6.0840400	-4.0999860	-0.5441180
C	4.8779000	-3.4358320	-0.3012380

C	3.6527910	-4.1424760	-0.1832020
C	2.4414650	-3.4931260	0.0598130
C	1.2123370	-4.2144080	0.0976920
C	-0.0383920	-3.5693060	0.1545400
C	-1.2432990	-4.2045150	-0.0845320
C	-2.4863900	-3.5144080	-0.1001240
H	-1.2522280	-5.2611150	-0.3250770
H	8.5591560	-5.1589810	-1.0065210
H	6.0860310	-5.1945680	-0.6414030
H	3.6647250	-5.2123200	-0.3392860
C	-7.3862180	-3.5190520	-0.6883310
C	-8.6047100	-4.2096380	-0.9015370
C	-6.1199570	-4.1962200	-0.6082600
C	-9.8490300	-3.5220490	-0.9858800
C	-11.0866380	-4.2303430	-1.1998480
H	-6.1034610	-5.2884040	-0.7240250
H	-8.5920330	-5.3031000	-1.0053450
H	-11.0591240	-5.3240270	-1.2965030
C	-4.9335790	-3.5136990	-0.3949890
C	-3.6664750	-4.1845130	-0.3308970
H	-3.6495370	-5.2587270	-0.4764280
C	-9.9156160	0.8171360	-0.6110300
C	-11.1584630	0.1163170	-0.8234310
C	-9.9130110	2.2603740	-0.4949560
C	-12.3565940	0.8766430	-0.9090820
C	-11.1481490	-1.3691980	-0.9492020
C	-11.1526280	2.9940800	-0.5914620
C	-12.3572170	2.2742860	-0.7967520
C	-12.3216110	-2.1213680	-1.1580340
C	-9.8817970	-2.0730110	-0.8570080
C	-12.2876450	-3.5388510	-1.2811810
H	-13.2279390	-4.0828660	-1.4434770
C	-7.4639660	5.1041280	0.0162710
C	-8.6733870	4.4268330	-0.1785000
C	-9.9545490	5.1313150	-0.2827890
C	-11.1256650	4.4521270	-0.4765510
C	-8.6747010	2.9704860	-0.2857300
H	-7.4600920	6.1999780	0.0933130
H	-9.9470200	6.2268340	-0.2000690
C	9.7353460	5.3048000	-0.3394500
H	9.7101730	6.3999130	-0.2546960
C	11.0232220	-4.0363620	-1.2746160
C	12.2049440	-3.3205240	-1.3889210
H	13.1529010	-3.8437360	-1.5736060
H	11.0149700	-5.1308360	-1.3663400
H	-12.0801080	4.9910940	-0.5527230
H	-13.3042970	2.8259380	-0.8699830
H	-13.3124950	0.3639630	-1.0690660
H	-13.2918930	-1.6161040	-1.2303800
H	11.8570410	5.2015160	-0.6549800
H	13.1100570	3.0597960	-1.0016190
H	13.1568950	0.5983930	-1.2019760
H	13.1682760	-1.3755370	-1.3684520
C	1.2365000	-5.7252860	0.0185970

O	1.6019010	-6.3242820	-0.9644060
O	0.8194720	-6.3452570	1.1201920
H	0.6840530	-5.7039430	1.9004170
O	-0.1805990	2.1764290	2.5911860
H	0.5611910	1.6478390	2.9138540
H	-0.1156150	6.1216340	0.8674050
N	0.5607450	-4.7540540	3.2943120
H	0.6409430	-3.7873080	2.9816160
C	-0.7438610	-4.9440830	3.9393620
H	-1.5360730	-4.6418230	3.2524770
H	-0.8827580	-6.0023080	4.1757320
H	-0.8459110	-4.3672960	4.8691480
C	1.6877550	-5.0666330	4.1809630
H	1.6767630	-6.1325380	4.4227810
H	2.6256510	-4.8448890	3.6687330
H	1.6591650	-4.4995690	5.1219540

Isomer 2

Tag	X	Y	Z
C	-6.0981510	-0.0058550	-0.1814840
C	-4.8779790	-0.6771970	-0.0292760
C	-3.6451910	0.0409570	0.1964640
C	-3.6723010	1.4907130	0.2127980
C	-4.9376050	2.1633260	0.0554960
C	-6.1326130	1.4523550	-0.1245960
C	-2.4399310	-0.6546220	0.3616120
C	-2.5105000	2.2335540	0.3912180
C	-1.2624720	1.5198510	0.6910270
C	-1.2113470	0.0497900	0.5299490
C	0.0098050	-0.5965810	0.6174400
C	1.2562680	0.1104450	0.4863850
C	1.2772340	1.5309140	0.3990980
C	0.0363690	2.2926000	0.6681450
C	-4.8437880	-2.1447030	-0.1018480
C	-3.6223470	-2.8254490	0.0443800
C	-6.0513570	-2.8671530	-0.3180840
C	-2.4023280	-2.1065670	0.2896380
C	-3.5986860	-4.2675160	-0.0198830
C	-6.0283110	-4.3236290	-0.3925670
C	-1.2165950	-2.7834450	0.4708450
C	-2.3523490	-4.9300040	0.1421390
C	-4.7865390	-4.9862010	-0.2401470
C	0.0251530	-2.0688510	0.9612560
C	-1.1723630	-4.2227450	0.3690510
H	-2.3249130	-6.0122050	0.0707750
H	-4.7510370	-6.0829080	-0.2895600
C	1.3003780	-2.7643890	0.5348790
C	0.0585460	-4.8930340	0.4488400
C	1.2934280	-4.2002400	0.4675490
C	2.4763970	-0.6037660	0.3400470
C	3.6858670	0.0975610	0.1085140
C	2.4794980	-2.0602400	0.3643470
C	4.9321370	-0.6108930	-0.0322980
C	3.7210100	-2.7669690	0.2038370
C	4.9377460	-2.0690050	0.0327680
C	2.4523650	2.2208940	0.1245230

C	3.6804560	1.5135900	-0.0067220
C	4.8963640	2.2263100	-0.2392060
C	6.1199480	1.5373260	-0.3454700
C	6.1336550	0.0868190	-0.2412780
C	-7.3401750	-0.7298820	-0.3921980
C	-7.3060640	-2.1790050	-0.4618770
C	3.7363300	-4.2065830	0.2326610
C	2.4916760	-4.8910470	0.3476190
C	-8.5189380	-2.9152350	-0.6731690
C	-8.4815770	-4.3725490	-0.7488020
C	-7.2585200	-5.0389890	-0.6109850
H	-7.2264060	-6.1356900	-0.6662410
H	2.4890780	-5.9750400	0.3120450
C	4.9497470	-4.9088560	0.1236060
H	4.9390570	-6.0066570	0.1548830
C	6.1668590	-2.7736500	-0.0894890
C	6.1828300	-4.2306400	-0.0308840
C	7.4058760	-2.0652070	-0.2763360
C	7.3978350	-0.6170170	-0.3617190
C	7.3544610	2.2543540	-0.5626710
C	8.5988590	1.5521740	-0.6650420
C	8.6161290	0.0975670	-0.5631870
O	-0.6101710	1.9726150	1.9214910
C	-9.7728280	-2.2166640	-0.8088280
C	-10.9910160	-2.9634480	-1.0187320
C	-9.8129650	-0.7711480	-0.7334390
C	-12.2126400	-2.2550490	-1.1451440
C	-10.9265590	-4.4225360	-1.0934380
C	-11.0740900	-0.0828870	-0.8650410
C	-12.2494420	-0.8554410	-1.0691140
C	-11.1062270	1.4049540	-0.7847500
C	-12.2999340	2.1438870	-0.8989500
C	-9.8611100	2.1239710	-0.5817030
C	-8.6121900	1.4213410	-0.4538850
C	-9.8736940	3.5796760	-0.5057780
C	-7.3920930	2.1458910	-0.2567260
C	-8.5802390	-0.0362370	-0.5265190
C	-8.6572710	4.2839180	-0.3129240
C	-7.4127950	3.6037790	-0.1880610
C	-6.1793140	4.2981030	-0.0007250
C	-4.9612210	3.6204810	0.1161010
C	-3.7410330	4.3251360	0.2727830
C	-2.5040440	3.6829910	0.3686630
C	-1.2663120	4.4137890	0.4198900
C	-0.0050610	3.7528770	0.3665840
C	1.1899390	4.3647040	0.0569140
C	2.4312690	3.6719340	-0.0250380
H	1.2131900	5.4264430	-0.1380530
H	-8.6753730	5.3811580	-0.2599660
H	-6.1911400	5.3957910	0.0457620
H	-3.7845710	5.4015490	0.2640540
C	7.3228110	3.7082500	-0.6767990
C	8.5376750	4.4078970	-0.8813210
C	6.0535200	4.3778510	-0.5787280

C	9.7852950	3.7279490	-0.9778060
C	11.0194100	4.4454570	-1.1813010
H	6.0318860	5.4719480	-0.6731630
H	8.5197920	5.5028220	-0.9670560
H	10.9865050	5.5403190	-1.2613140
C	4.8720690	3.6862310	-0.3686760
C	3.6015540	4.3498110	-0.2707470
H	3.5790750	5.4274430	-0.3879580
C	9.8737070	-0.6161640	-0.6715010
C	11.1133680	0.0941520	-0.8704140
C	9.8782090	-2.0612170	-0.5802630
C	12.3156140	-0.6587270	-0.9652810
C	11.0956870	1.5812990	-0.9737370
C	11.1216240	-2.7870900	-0.6862390
C	12.3232250	-2.0578940	-0.8757940
C	12.2652830	2.3424110	-1.1711410
C	9.8256400	2.2772280	-0.8713250
C	12.2238750	3.7613890	-1.2731310
H	13.1613290	4.3126080	-1.4273090
C	7.4394650	-4.9257430	-0.1407730
C	8.6475080	-4.2390550	-0.3113030
C	9.9324060	-4.9353090	-0.4225860
C	11.1011970	-4.2470070	-0.5978820
C	8.6427040	-2.7810060	-0.3884280
H	7.4396660	-6.0231150	-0.0899390
H	9.9297770	-6.0322420	-0.3610950
C	-9.7402350	-5.0908140	-0.9664200
H	-9.7031430	-6.1873460	-1.0236390
C	-11.1338380	4.2749500	-0.6315060
C	-12.3104850	3.5668690	-0.8219790
H	-13.2668300	4.0987270	-0.9166960
H	-11.1384660	5.3717460	-0.5730990
H	12.0584850	-4.7800290	-0.6799300
H	13.2732320	-2.6035000	-0.9557230
H	13.2692150	-0.1385910	-1.1145440
H	13.2381290	1.8432800	-1.2510160
H	-11.8649160	-4.9706680	-1.2552670
H	-13.1431280	-2.8165910	-1.3046550
H	-13.2176570	-0.3513310	-1.1720840
H	-13.2537720	1.6252710	-1.0512660
C	-1.3122170	5.8992600	0.4487190
O	-2.1244130	6.6163860	-0.0969750
O	-0.3287350	6.4509810	1.2141910
H	-0.4705490	7.4075390	1.1539490
O	-0.0403030	-2.2173490	2.4015190
H	0.3323240	-1.4209050	2.8691450
H	0.0709520	-5.9766590	0.4033460
N	0.6252600	-0.0355330	3.9857110
H	0.3095890	0.7468020	3.4160770
C	-0.3188290	-0.2405080	5.0856600
H	-1.3234990	-0.3678840	4.6792050
H	-0.0574010	-1.1546730	5.6259620
H	-0.3306270	0.5919990	5.8056560
C	1.9962250	0.1961680	4.4382880
H	2.3733000	-0.7014600	4.9366750

H	2.6365760	0.3975490	3.5775000
H	2.0836550	1.0378830	5.1428930
Isomer 3			
Tag	X	Y	Z
C	-6.0402860	-0.3956960	-0.0657040
C	-4.8198910	-1.0577860	0.1243540
C	-3.5890190	-0.3286850	0.3091100
C	-3.6186180	1.1200100	0.2600980
C	-4.8812380	1.7843600	0.0573710
C	-6.0746640	1.0636440	-0.0925010
C	-2.3795420	-1.0137550	0.5011410
C	-2.4606740	1.8703990	0.4264790
C	-1.2179380	1.1726890	0.7756690
C	-1.1549800	-0.2991770	0.6436390
C	0.0723490	-0.9340990	0.7557510
C	1.3143440	-0.2217340	0.6293630
C	1.3271100	1.1972390	0.5275860
C	0.0770340	1.9529720	0.7649230
C	-4.7843270	-2.5285730	0.1369920
C	-3.5622670	-3.1995430	0.3146410
C	-5.9930160	-3.2612780	-0.0310820
C	-2.3393910	-2.4677350	0.5056070
C	-3.5356050	-4.6436320	0.3326110
C	-5.9693540	-4.7195050	-0.0165450
C	-1.1472950	-3.1327660	0.7092140
C	-2.2853230	-5.2948760	0.5067830
C	-4.7266420	-5.3722050	0.1668610
C	0.1025450	-2.3943900	1.1320270
C	-1.1003210	-4.5788750	0.6714020
H	-2.2569470	-6.3787750	0.4850630
H	-4.6920860	-6.4698020	0.1810320
C	1.3702350	-3.0989950	0.7167990
C	0.1362840	-5.2373120	0.7353650
C	1.3657650	-4.5345690	0.6849040
C	2.5368290	-0.9318550	0.4981300
C	3.7445570	-0.2269950	0.2687540
C	2.5427340	-2.3880780	0.5279370
C	4.9919430	-0.9310130	0.1274050
C	3.7849940	-3.0911220	0.3582290
C	4.9990850	-2.3898970	0.1842950
C	2.5024900	1.8920960	0.2719140
C	3.7352110	1.1896190	0.1570240
C	4.9506390	1.9070990	-0.0587950
C	6.1765740	1.2217810	-0.1631660
C	6.1926150	-0.2297150	-0.0729940
C	-7.2819100	-1.1313370	-0.2338430
C	-7.2476310	-2.5822940	-0.2140390
C	3.8036260	-4.5305040	0.3957330
C	2.5662340	-5.2192270	0.5464820
C	-8.4612680	-3.3291700	-0.3777160
C	-8.4243310	-4.7883170	-0.3613040
C	-7.2012330	-5.4456250	-0.1853320
H	-7.1702160	-6.5436800	-0.1726880
H	2.5701480	-6.3036140	0.5357350

C	5.0184730	-5.2296890	0.2748090
H	5.0113430	-6.3273830	0.3097620
C	6.2296970	-3.0912840	0.0581040
C	6.2482240	-4.5484250	0.1107430
C	7.4676120	-2.3796210	-0.1238800
C	7.4580480	-0.9307210	-0.1965050
C	7.4115590	1.9426980	-0.3666250
C	8.6571240	1.2432270	-0.4722850
C	8.6758490	-0.2125880	-0.3870200
O	-0.5936840	1.6495560	2.0023150
C	-9.7147680	-2.6398840	-0.5570200
C	-10.9335670	-3.3977130	-0.7186840
C	-9.7543130	-1.1924300	-0.5743620
C	-12.1546810	-2.6980790	-0.8907130
C	-10.8699240	-4.8586320	-0.6994660
C	-11.0147160	-0.5133260	-0.7514540
C	-12.1905670	-1.2964920	-0.9056500
C	-11.0459460	0.9766290	-0.7677160
C	-12.2385060	1.7075380	-0.9341020
C	-9.8009780	1.7066370	-0.6061970
C	-8.5528330	1.0126750	-0.4303010
C	-9.8132150	3.1643480	-0.6217560
C	-7.3333880	1.7479960	-0.2720850
C	-8.5214700	-0.4467120	-0.4123710
C	-8.5975930	3.8789320	-0.4654810
C	-7.3546330	3.2074710	-0.2907260
C	-6.1227450	3.9120680	-0.1317620
C	-4.9066590	3.2429730	0.0392150
C	-3.6882620	3.9547970	0.1819600
C	-2.4565320	3.3167060	0.3435590
C	-1.2256700	4.0531730	0.3907610
C	0.0323800	3.4050090	0.4273450
C	1.2387550	4.0324180	0.1758530
C	2.4801600	3.3453250	0.1282480
H	1.2583070	5.0965320	-0.0076060
H	-8.6155520	4.9772850	-0.4794590
H	-6.1353020	5.0106320	-0.1471920
H	-3.7275070	5.0297860	0.1120460
C	7.3792280	3.3979790	-0.4642680
C	8.5944640	4.1012000	-0.6547360
C	6.1091390	4.0648880	-0.3670530
C	9.8430020	3.4237310	-0.7543540
C	11.0772300	4.1447650	-0.9443460
H	6.0865840	5.1598670	-0.4499610
H	8.5757800	5.1970290	-0.7274460
H	11.0436100	5.2405030	-1.0107350
C	4.9260570	3.3695420	-0.1746400
C	3.6555660	4.0293940	-0.0878900
H	3.6317470	5.1079820	-0.1955670
C	9.9346030	-0.9236670	-0.4996300
C	11.1740090	-0.2098790	-0.6871610
C	9.9404460	-2.3695760	-0.4237900
C	12.3772310	-0.9603000	-0.7880850
C	11.1551040	1.2784330	-0.7723060
C	11.1849660	-3.0928650	-0.5348480

C	12.3860540	-2.3604160	-0.7143050
C	12.3247800	2.0428800	-0.9559930
C	9.8841000	1.9718340	-0.6656010
C	12.2826180	3.4629710	-1.0403110
H	13.2201690	4.0168230	-1.1840470
C	7.5059630	-5.2409580	-0.0071690
C	8.7124540	-4.5513060	-0.1751250
C	9.9983520	-5.2449430	-0.2924970
C	11.1663250	-4.5536580	-0.4608870
C	8.7055740	-3.0925980	-0.2405300
H	7.5080650	-6.3385960	0.0376990
H	9.9970550	-6.3423850	-0.2406960
C	-9.6837860	-5.5180150	-0.5309930
H	-9.6474670	-6.6160090	-0.5181530
C	-11.0721750	3.8507930	-0.7972740
C	-12.2482860	3.1324750	-0.9481560
H	-13.2038270	3.6575920	-1.0810230
H	-11.0763130	4.9490250	-0.8082050
H	12.1243770	-5.0846190	-0.5471710
H	13.3368210	-2.9041120	-0.7981650
H	13.3306320	-0.4375840	-0.9292980
H	13.2983010	1.5455070	-1.0384080
H	-11.8086460	-5.4155010	-0.8251620
H	-13.0854980	-3.2681730	-1.0137210
H	-13.1583550	-0.7993890	-1.0412010
H	-13.1920670	1.1808070	-1.0572820
C	-1.2720440	5.5524900	0.3041490
O	-1.9990330	6.1720550	-0.4563620
O	-0.4478130	6.1572160	1.1577860
H	-0.5447530	7.1632350	1.0359570
O	0.1793530	-2.4517400	2.6034110
H	-0.5242720	-1.8814600	2.9403810
H	0.1568930	-6.3218360	0.7254950
N	-0.8848940	8.7805410	0.6729330
H	-1.5770050	8.5051430	-0.0207600
C	-1.5343630	9.5249730	1.7554810
H	-2.3578850	8.9335140	2.1596150
H	-0.8150570	9.6990840	2.5597410
H	-1.9270170	10.4990780	1.4303670
C	0.1985670	9.5228430	0.0233820
H	1.0059120	9.6911210	0.7408050
H	0.5958540	8.9341930	-0.8056680
H	-0.1233280	10.5000470	-0.3642390

Insertion of HNMe₂ on GO:

TS:

Tag	X	Y	Z
C	6.0111680	0.1146420	-0.0920980
C	4.7826400	0.7789910	0.1010910
C	3.5715460	0.0373190	0.3247460
C	3.6300300	-1.3759760	0.3779190
C	4.8182440	-2.0445730	0.0597020
C	6.0363480	-1.3246230	-0.1466960
C	2.3330630	0.7171020	0.4502180

C	2.4269830	-2.1684020	0.8673420
C	1.1246460	-1.4254250	0.6401750
C	1.0984370	-0.0439880	0.5487310
C	-0.1612800	0.6628460	0.6248030
C	-1.3876930	-0.0280990	0.5056390
C	-1.4030590	-1.4534010	0.4795740
C	-0.1500600	-2.1976340	0.8934130
C	4.7362810	2.2295350	0.0738860
C	3.4973440	2.8895780	0.2202640
C	5.9435270	2.9730220	-0.0955850
C	2.2815270	2.1483330	0.4095000
C	3.4693860	4.3306240	0.1920280
C	5.9127770	4.4303900	-0.1070100
C	1.0661310	2.8341900	0.5783170
C	2.2148270	4.9837380	0.3211090
C	4.6558360	5.0717330	0.0336920
C	-0.1694450	2.1101210	1.0256080
C	1.0287090	4.2688520	0.4994420
H	2.1835050	6.0673600	0.2615020
H	4.6055430	6.1693130	0.0194600
C	-1.4273690	2.8178920	0.6010310
C	-0.1970450	4.9622000	0.5514390
C	-1.4145170	4.2562100	0.5325130
C	-2.6157640	0.6781920	0.3877660
C	-3.8285310	-0.0288980	0.1995260
C	-2.6088110	2.1234740	0.4037600
C	-5.0681790	0.6719450	0.0527470
C	-3.8461150	2.8245620	0.2223790
C	-5.0646630	2.1318290	0.0708210
C	-2.5733760	-2.1464620	0.2664960
C	-3.8186830	-1.4462910	0.1279430
C	-5.0301000	-2.1618030	-0.0591080
C	-6.2618960	-1.4761510	-0.1695110
C	-6.2741470	-0.0268530	-0.1182190
C	7.2435560	0.8529310	-0.2780170
C	7.2033500	2.3014900	-0.2608590
C	-3.8576010	4.2644000	0.2290850
C	-2.6153350	4.9442620	0.3672990
C	8.4153740	3.0516660	-0.4265250
C	8.3736140	4.5085810	-0.4162260
C	7.1415970	5.1623230	-0.2622740
H	7.1047450	6.2602850	-0.2613200
H	-2.6088420	6.0302940	0.3184460
C	-5.0659290	4.9746470	0.0920720
H	-5.0494370	6.0738740	0.1007170
C	-6.2903050	2.8381240	-0.0644560
C	-6.3025560	4.2976910	-0.0498080
C	-7.5348250	2.1280100	-0.2175360
C	-7.5341180	0.6781390	-0.2498070
C	-7.4987360	-2.1971780	-0.3407440
C	-8.7435860	-1.4948860	-0.4534480
C	-8.7565580	-0.0393530	-0.4092410
C	9.6716300	2.3621860	-0.6088390
C	10.8878770	3.1209170	-0.7654440
C	9.7116850	0.9154680	-0.6472020

C	12.1104680	2.4194310	-0.9487880
C	10.8219570	4.5806030	-0.7367170
C	10.9640370	0.2342250	-0.8483640
C	12.1443420	1.0207700	-0.9898940
C	10.9841470	-1.2542110	-0.9124300
C	12.1695850	-1.9917140	-1.1171140
C	9.7357510	-1.9808830	-0.7700440
C	8.4960470	-1.2823180	-0.5487400
C	9.7267360	-3.4317120	-0.8520220
C	7.2688910	-2.0141650	-0.3990170
C	8.4770870	0.1675650	-0.4847840
C	8.4886940	-4.1406470	-0.7279130
C	7.2698160	-3.4716960	-0.5065530
C	5.9998390	-4.1611180	-0.4155510
C	4.8257700	-3.5005080	-0.1488640
C	3.5447350	-4.1687890	-0.1706410
C	2.3882800	-3.5752520	0.2410290
C	1.1332160	-4.2510530	0.1859640
C	-0.1079960	-3.6155560	0.3322840
C	-1.3050540	-4.2613740	0.0781160
C	-2.5610480	-3.6036970	0.1196180
H	-1.3030200	-5.2947900	-0.2473510
H	8.4968470	-5.2360850	-0.8107150
H	5.9875440	-5.2468410	-0.5816860
H	3.5144180	-5.1575250	-0.6047430
C	-7.4716140	-3.6548800	-0.4000640
C	-8.6879430	-4.3560470	-0.5579830
C	-6.1955050	-4.3235690	-0.3016030
C	-9.9392570	-3.6758570	-0.6633170
C	-11.1757580	-4.3965050	-0.8206740
H	-6.1791070	-5.4202690	-0.3611770
H	-8.6757840	-5.4536380	-0.6021750
H	-11.1473750	-5.4939160	-0.8570280
C	-5.0131430	-3.6310390	-0.1423940
C	-3.7341920	-4.2881730	-0.0751600
H	-3.7095340	-5.3648530	-0.2002920
C	-10.0123160	0.6758990	-0.5306480
C	-11.2561910	-0.0373830	-0.6863950
C	-10.0098090	2.1237320	-0.4961340
C	-12.4566950	0.7175710	-0.7981250
C	-11.2440450	-1.5273250	-0.7289340
C	-11.2506330	2.8504870	-0.6169490
C	-12.4575340	2.1190690	-0.7647210
C	-12.4189880	-2.2923650	-0.8796080
C	-9.9755070	-2.2232350	-0.6148140
C	-12.3816160	-3.7130380	-0.9240260
H	-13.3216970	-4.2684450	-1.0429850
C	-7.5565540	4.9951880	-0.1784700
C	-8.7681420	4.3067870	-0.3191940
C	-10.0514700	5.0033770	-0.4461210
C	-11.2239600	4.3127430	-0.5851110
C	-8.7687610	2.8459700	-0.3437520
H	-7.5524120	6.0937480	-0.1631240
H	-10.0446260	6.1017720	-0.4256470

C	9.6329670	5.2394850	-0.5749310
H	9.5965070	6.3374160	-0.5612450
C	10.9693700	-4.1215390	-1.0655910
C	12.1588510	-3.4100830	-1.1908010
H	13.1050590	-3.9439650	-1.3522390
H	10.9628560	-5.2181370	-1.1277610
H	-12.1801090	4.8460840	-0.6786830
H	-13.4062300	2.6653180	-0.8558350
H	-13.4142580	0.1963050	-0.9158090
H	-13.3916090	-1.7937780	-0.9666190
H	11.7600980	5.1402650	-0.8551330
H	13.0414190	2.9908530	-1.0652240
H	13.1101190	0.5233720	-1.1394200
H	13.1281110	-1.4707270	-1.2264150
C	1.1440590	-5.7459640	-0.0165120
O	1.6043190	-6.3194520	-0.9651990
O	0.5969300	-6.4566630	1.0054280
H	0.2535970	-5.8461950	1.6718610
O	-0.2311680	2.1448780	2.5156560
H	0.6048740	1.7888940	2.8426400
H	-0.2025520	6.0447460	0.5245790
O	-0.2901210	-2.3466840	2.3423690
H	1.1073054	-2.5008592	2.7963498
N	2.5070900	-2.3892690	2.4095370
C	3.5197960	-3.3387900	2.8889230
H	3.3918740	-4.3121600	2.4228180
H	4.5500520	-2.9972470	2.7170320
H	3.3791760	-3.4545350	3.9660590
C	2.5952100	-1.1523270	3.2039090
H	1.7715970	-0.4851040	2.9620990
H	2.4963840	-1.4282060	4.2562140
H	3.5461280	-0.6184940	3.0774320

Product:

Tag	X	Y	Z
C	6.0111680	0.1146420	-0.0920980
C	4.7826400	0.7789910	0.1010910
C	3.5715460	0.0373190	0.3247460
C	3.6300300	-1.3759760	0.3779190
C	4.8182440	-2.0445730	0.0597020
C	6.0363480	-1.3246230	-0.1466960
C	2.3330630	0.7171020	0.4502180
C	2.4269830	-2.1684020	0.8673420
C	1.1246460	-1.4254250	0.6401750
C	1.0984370	-0.0439880	0.5487310
C	-0.1612800	0.6628460	0.6248030
C	-1.3876930	-0.0280990	0.5056390
C	-1.4030590	-1.4534010	0.4795740
C	-0.1500600	-2.1976340	0.8934130
C	4.7362810	2.2295350	0.0738860
C	3.4973440	2.8895780	0.2202640
C	5.9435270	2.9730220	-0.0955850
C	2.2815270	2.1483330	0.4095000
C	3.4693860	4.3306240	0.1920280
C	5.9127770	4.4303900	-0.1070100
C	1.0661310	2.8341900	0.5783170

C	2.2148270	4.9837380	0.3211090
C	4.6558360	5.0717330	0.0336920
C	-0.1694450	2.1101210	1.0256080
C	1.0287090	4.2688520	0.4994420
H	2.1835050	6.0673600	0.2615020
H	4.6055430	6.1693130	0.0194600
C	-1.4273690	2.8178920	0.6010310
C	-0.1970450	4.9622000	0.5514390
C	-1.4145170	4.2562100	0.5325130
C	-2.6157640	0.6781920	0.3877660
C	-3.8285310	-0.0288980	0.1995260
C	-2.6088110	2.1234740	0.4037600
C	-5.0681790	0.6719450	0.0527470
C	-3.8461150	2.8245620	0.2223790
C	-5.0646630	2.1318290	0.0708210
C	-2.5733760	-2.1464620	0.2664960
C	-3.8186830	-1.4462910	0.1279430
C	-5.0301000	-2.1618030	-0.0591080
C	-6.2618960	-1.4761510	-0.1695110
C	-6.2741470	-0.0268530	-0.1182190
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C	7.2033500	2.3014900	-0.2608590
C	-3.8576010	4.2644000	0.2290850
C	-2.6153350	4.9442620	0.3672990
C	8.4153740	3.0516660	-0.4265250
C	8.3736140	4.5085810	-0.4162260
C	7.1415970	5.1623230	-0.2622740
H	7.1047450	6.2602850	-0.2613200
H	-2.6088420	6.0302940	0.3184460
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H	-5.0494370	6.0738740	0.1007170
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C	-6.3025560	4.2976910	-0.0498080
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C	-8.7565580	-0.0393530	-0.4092410
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C	9.7116850	0.9154680	-0.6472020
C	12.1104680	2.4194310	-0.9487880
C	10.8219570	4.5806030	-0.7367170
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C	12.1695850	-1.9917140	-1.1171140
C	9.7357510	-1.9808830	-0.7700440
C	8.4960470	-1.2823180	-0.5487400
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H	-8.6757840	-5.4536380	-0.6021750
H	-11.1473750	-5.4939160	-0.8570280
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H	-3.7095340	-5.3648530	-0.2002920
C	-10.0123160	0.6758990	-0.5306480
C	-11.2561910	-0.0373830	-0.6863950
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H	-10.0446260	6.1017720	-0.4256470
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C	12.1588510	-3.4100830	-1.1908010
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H	-12.1801090	4.8460840	-0.6786830
H	-13.4062300	2.6653180	-0.8558350
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C	1.1440590	-5.7459640	-0.0165120
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O	0.5969300	-6.4566630	1.0054280
H	0.2535970	-5.8461950	1.6718610
O	-0.2311680	2.1448780	2.5156560
H	0.6048740	1.7888940	2.8426400
H	-0.2025520	6.0447460	0.5245790
O	-0.2901210	-2.3466840	2.3423690
H	0.6041590	-2.6062570	2.6462270
N	2.5070900	-2.3892690	2.4095370
C	3.5197960	-3.3387900	2.8889230
H	3.3918740	-4.3121600	2.4228180
H	4.5500520	-2.9972470	2.7170320
H	3.3791760	-3.4545350	3.9660590
C	2.5952100	-1.1523270	3.2039090
H	1.7715970	-0.4851040	2.9620990
H	2.4963840	-1.4282060	4.2562140
H	3.5461280	-0.6184940	3.0774320