

Effect of ring size on the *exo/endo* selectivity of a thermal double cycloaddition of fused pyran-2-ones

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SUPPORTING INFORMATION

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1. Experimental procedures

Melting points were determined on a micro hot stage apparatus and are uncorrected. ^1H NMR spectra were recorded at 29 °C and 300 MHz using Me_4Si as an internal standard. ^{13}C NMR spectra were recorded at 75.5 MHz and are referenced against the central line of the solvent signal ($\text{DMSO}-d_6$ septet at δ 39.5 ppm). The coupling constants (J) are given in hertz. IR spectra were obtained as KBr pellets for all. The starting compounds **1A–C** were prepared according to the published procedures.¹ All other reagents and solvents were used as received from commercial suppliers. Microwave reactions were conducted in air using a focused microwave unit (Discover by CEM Corporation, Matthews, NC). The machine consists of a continuous, focused microwave power-delivery system with an operator-selectable power output from 0 to 300 W. Reactions were performed in darkness in glass vessels (capacity 10 mL) sealed with a septum. The pressure was controlled by a load cell connected to the vessel via the septum. The temperature of the contents of the vessel was monitored using a calibrated infrared temperature controller mounted under the reaction vessel. The mixtures were stirred with a Teflon-coated magnetic stirring bar in the vessel. Temperature, pressure and power profiles were recorded using commercially available software provided by the manufacturer of the microwave unit.

1.1 Conventional synthesis of the products **5** and **6**

A mixture of the starting fused pyran-2-one **1** (1 mmol), dienophile **2** (2.2 mmol) and solvent (6 mL; decalin, tetralin or toluene) was refluxed for the specified time (Table 1). Thereafter, the reaction mixture was cooled to room temperature, the volatile components were removed in vacuo, the remaining solid was treated with a minimal amount of EtOH/H₂O (1 mL) and then it was cooled in a refrigerator. The precipitated product was filtered off and washed with EtOH/H₂O.

1.2 Microwave-assisted synthesis of **5Ca**

A mixture of **5Ce** (1 mmol, 449 mg), aniline (2.4 mmol, 223 mg) and toluene (4.9 mmol, 450 mg) was irradiated in the focused microwave equipment for 1.25 h. The final temperature was set to 160 °C, the power to 250 W and the ramp time to 5 min. Thereafter, the reaction mixture was cooled to room temperature and the isolation procedure was identical to the other cases.

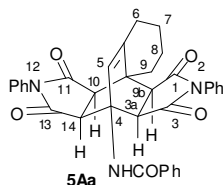
1.3 Microwave-assisted isomerisation of **5Ca** into **6Ca**

A mixture of **5Ca** (0.5 mmol, 300 mg) and toluene (1.5 mL) was irradiated in the focused microwave equipment for 3 h. The final temperature was set to 220 °C, the power to 295 W and the ramp time to 5 min. Thereafter, the reaction mixture was cooled to room temperature and the crude mixture was analyzed by ^1H NMR.

¹ Požgan, F.; Kranjc, K.; Kepe, V.; Polanc, S.; Kočevár, M. *ARKIVOC* **2007**, (viii), 97–111.

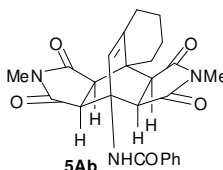
2. Analytical, physical and spectroscopic characterization data

***N*-[*rel*-(3*aR*,9*bS*,10*R*,14*S*)-2,3,3*a*,6,7,8,9,9*b*,11,12,13,14-Dodecahydro-1,3,11,13-tetraoxo-2,12-diphenyl-10*H*-4,9*a*[3',4']-endo-pyrrolo-9*aH*-benz[*e*]isoindol-4(1*H*)-yl]benzamide (5Aa)**



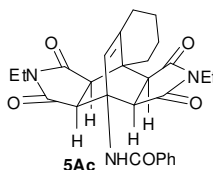
Yield: 382 mg (67%), mp 310–312 °C (MeOH). IR (KBr) ν 1769, 1707br, 1672, 1537 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ (ppm): 1.41 (m, 2H), 1.61 (m, 2H), 2.32 (m, 2H), 2.72 (m, 2H), 3.32 (d, $J = 8.1$, 2H), 4.43 (d, $J = 8.1$, 2H), 6.26 (s, 1H), 7.12 (m, 4H), 7.45 (m, 9H), 7.84 (m, 2H), 8.65 (s, 1H); ^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) δ (ppm): 21.0, 22.9, 26.4, 29.2, 41.0, 44.0, 49.1, 57.6, 123.9, 126.9, 127.6, 127.9, 128.4, 128.9, 130.9, 132.1, 135.7, 141.1, 168.0, 173.9, 175.9; MS-EI: m/z 571 (M^+ , 5%), 105 (100). Anal. Calcd for $\text{C}_{35}\text{H}_{29}\text{N}_3\text{O}_5$: C, 73.54; H, 5.11; N, 7.35. Found: C, 73.35; H, 5.14; N, 7.32.

***N*-[*rel*-(3*aR*,9*bS*,10*R*,14*S*)-2,3,3*a*,6,7,8,9,9*b*,11,12,13,14-Dodecahydro-2,12-dimethyl-1,3,11,13-tetraoxo-10*H*-4,9*a*[3',4']-endo-pyrrolo-9*aH*-benz[*e*]isoindol-4(1*H*)-yl]benzamide (5Ab)**



Yield: 276 mg (62%), mp 305–306 °C (toluene). IR (KBr) ν 1764, 1699, 1683, 1656 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ (ppm): 1.30 (m, 2H), 1.60 (m, 2H), 2.06 (m, 2H), 2.65 (m, 2H), 2.71 (s, 6H), 3.07 (d, $J = 8.0$ Hz, 2H), 4.19 (d, $J = 8.0$ Hz, 2H), 6.00 (s, 1H), 7.51 (m, 3H), 7.88 (m, 2H), 8.53 (s, 1H); ^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) δ (ppm): 20.9, 22.7, 24.2, 26.4, 28.8, 40.4, 43.8, 49.1, 57.3, 123.2, 127.6, 127.9, 130.9, 135.7, 141.0, 167.8, 174.9, 176.9; MS-EI: m/z 447 (M^+ , 3%), 105 (100). Anal. Calcd for $\text{C}_{25}\text{H}_{25}\text{N}_3\text{O}_5 \times 0.1 \text{ PhMe}$: C, 67.59; H, 5.69; N, 9.20. Found: C, 67.82; H, 5.74; N, 8.97.

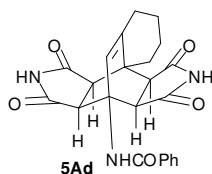
***N*-[*rel*-(3*aR*,9*bS*,10*R*,14*S*)-2,3,3*a*,6,7,8,9,9*b*,11,12,13,14-Dodecahydro-2,12-diethyl-1,3,11,13-tetraoxo-10*H*-4,9*a*[3',4']-endo-pyrrolo-9*aH*-benz[*e*]isoindol-4(1*H*)-yl]benzamide (5Ac)**



Yield: 290 mg (61%), mp 288–289 (toluene); lit.² mp 288–289 °C (toluene).

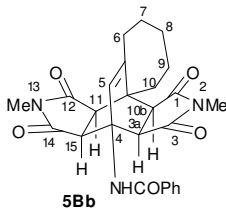
***N*-[*rel*-(3*aR*,9*bS*,10*R*,14*S*)-2,3,3*a*,6,7,8,9,9*b*,11,12,13,14-Dodecahydro-1,3,11,13-tetraoxo-10*H*-4,9*a*[3',4']-endo-pyrrolo-9*aH*-benz[*e*]isoindol-4(1*H*)-yl]benzamide (5Ad)**

² Kranjc, K.; Polanc, S.; Kočevár M. *Org. Lett.* **2003**, *5*, 2833–2836.



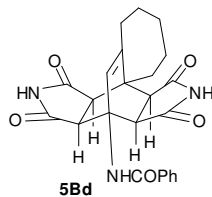
Yield: 274 mg (65%), mp 326–328 °C (EtOH). IR (KBr) ν 1769, 1716, 1644, 1532 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ (ppm): 1.35 (m, 2H), 1.57 (m, 2H), 2.16 (m, 2H), 2.58 (m, 2H), 2.96 (d, $J = 8.2$ Hz, 2H), 4.10 (d, $J = 8.2$ Hz, 2H), 6.12 (s, 1H), 7.50 (m, 3H), 7.87 (m, 2H), 8.46 (s, 1H), 11.08 (s, 2H); ^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) δ (ppm): 20.9, 22.8, 26.2, 29.2, 40.2, 44.7, 50.3, 57.1, 123.5, 127.6, 127.9, 130.8, 135.7, 140.7, 167.5, 176.2, 178.2; MS-EI: m/z 419 (M^+ , 1%), 105 (100). Anal. Calcd for $\text{C}_{23}\text{H}_{21}\text{N}_3\text{O}_5$: C, 65.86; H, 5.05; N, 10.02. Found: C, 65.75; H, 5.24; N, 9.79.

***N*-[*rel*-(3a*R*,10b*S*,11*R*,15*S*)-2,3,3a,7,8,9,10,10b,12,13,14,15-Dodecahydro-2,13-dimethyl-1,3,12,14-tetraoxo-1*H*,11*H*-4,10a[3',4']-endo-pyrrolocyclohept[*e*]isoindol-4(6*H*)-yl]benzamide (5Bb)**



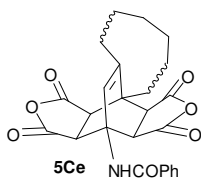
Yield: 361 mg (78%), mp 286–287 °C (toluene). IR (KBr) ν 1765, 1694, 1659, 1537 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ (ppm): 1.30 (m, 2H), 1.46 (m, 2H), 1.88 (m, 2H), 2.10 (m, 2H), 2.64 (m, 2H), 2.72 (s, 6H), 3.04 (d, $J = 8.1$, 2H), 4.22 (d, $J = 8.1$, 2H), 6.06 (s, 1H), 7.51 (m, 3H), 7.88 (m, 2H), 8.57 (s, 1H); ^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) δ (ppm): 23.9, 24.3, 26.8, 30.5, 32.7, 35.3, 44.1, 46.7, 50.4, 56.9, 124.8, 127.6, 127.9, 130.8, 135.7, 145.5, 167.7, 174.7, 176.6; MS-EI: m/z 461 (M^+ , 2%), 105 (100). Anal. Calcd for $\text{C}_{26}\text{H}_{27}\text{N}_3\text{O}_5 \times 0.5 \text{ PhMe}$: C, 69.81; H, 6.16; N, 8.28. Found: C, 69.71; H, 6.09; N, 8.25.

***N*-[*rel*-(3a*R*,10b*S*,11*R*,15*S*)-2,3,3a,7,8,9,10,10b,12,13,14,15-Dodecahydro-1,3,12,14-tetraoxo-1*H*,11*H*-4,10a[3',4']-endo-pyrrolocyclohept[*e*]isoindol-4(6*H*)-yl]benzamide (5Bd)**



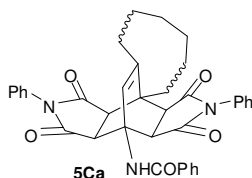
Yield: 325 mg (75%), mp 322–323 °C (toluene). IR (KBr) ν 1759, 1712, 1640, 1558 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ (ppm): 1.43 (m, 4H), 1.86 (m, 2H), 2.19 (m, 2H), 2.58 (m, 2H), 2.92 (d, $J = 8.0$ Hz, 2H), 4.15 (d, $J = 8.0$ Hz, 2H), 6.18 (s, 1H), 7.51 (m, 3H), 7.87 (m, 2H), 8.49 (s, 1H), 11.11 (s, 2H); ^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) δ (ppm): 24.0, 26.8, 30.5, 32.6, 35.6, 45.1, 46.6, 51.7, 56.7, 125.1, 127.6, 127.9, 130.8, 135.7, 145.3, 167.4, 176.1, 178.0; MS-EI: m/z 433 (M^+ , 1%), 105 (100). Anal. Calcd for $\text{C}_{24}\text{H}_{23}\text{N}_3\text{O}_5 \times \text{H}_2\text{O}$: C, 63.85; H, 5.58; N, 9.31. Found: C, 64.13; H, 5.53; N, 9.32.

***N*-[*rel*-(3a*R*,11b*S*,12*R*,16*S*)-2,3,3a,6,7,8,9,10,11,11b,13,14,15,16-Tetradecahydro-1,3,13,15-tetraoxo-4,11a[3',4']-furano-11a*H*-cyclooct[*e*]isobenzofuran-4(1*H*)-yl]benzamide (5Ce)**



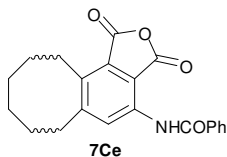
Yield: 304 mg (68%), mp 285–287 °C (EtOH). IR (KBr) ν 3418, 1852, 1785, 1655, 1537 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ (ppm): 1.43 (m, 4H), 1.54 (m, 2H), 1.91 (m, 2H), 2.33 (m, 2H), 2.66 (m, 2H), 3.59 (d, $J = 8.6$, 2H), 4.57 (d, $J = 8.6$, 2H), 6.37 (s, 1H), 7.55 (m, 3H), 7.90 (m, 2H), 8.93 (s, 1H); ^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) δ (ppm): 22.6, 25.5, 26.1, 28.0, 32.4, 32.7, 45.0, 45.4, 51.4, 55.9, 127.6, 127.8, 128.2, 131.4, 134.8, 146.1, 167.9, 169.2, 171.0; MS-ESI: m/z 450 (MH^+), 472 (MNa^+), 164 (100%). Anal. Calcd for $\text{C}_{25}\text{H}_{23}\text{NO}_7$: C, 66.81; H, 5.16; N, 3.12. Found: C, 66.90; H, 5.06; N, 3.11.

***N*-[*rel*-(3*aR*,11*bS*,12*R*,16*S*)-2,3,3*a*,6,7,8,9,10,11,11*b*,13,14,15,16-Tetradecahydro-1,3,13,15-tetraoxo-2,14-diphenyl-12*H*-4,11*a*[3',4']-endo-pyrrolocyclooct[*e*]isoindol-4(1*H*)-yl]benzamide (5Ca)**



Yield: 490 mg (82%), mp 255–257 °C (EtOH). IR (KBr) ν 3451, 1783, 1773, 1715, 1654, 1633 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ (ppm): 1.43 (m, 2H), 1.54 (m, 4H), 1.93 (m, 2H), 2.49 (m, 2H), 2.82 (m, 2H), 3.27 (d, $J = 8.1$, 2H), 4.46 (d, $J = 8.1$, 2H), 6.34 (s, 1H), 7.10 (m, 4H), 7.46 (m, 9H), 7.84 (m, 2H), 8.70 (s, 1H); ^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) δ (ppm): 23.3, 25.2, 26.8, 28.3, 33.1, 44.0, 46.4, 51.1, 57.1, 127.0, 127.4, 127.6, 127.9, 128.4, 128.9, 130.9, 132.2, 135.7, 144.4, 167.8, 173.9, 175.6 (1 signal is hidden); MS-ESI: m/z 600 (MH^+), 622 (MNa^+). Anal. Calcd for $\text{C}_{37}\text{H}_{33}\text{N}_3\text{O}_5$: C, 74.11; H, 5.55; N, 7.01. Found: C, 74.02; H, 5.54; N, 6.98.

***N*-(1,3-dioxo-1,3,6,7,8,9,10,11-octahydrocycloocta[*e*][2]benzofuran-4-yl)benzamide (7Ce)**



Yield: 310 mg (89%), mp 204–205 °C (acetone/MeOH). IR (KBr) ν 3389, 1830, 1758, 1746, 1692, 1609, 1528 cm^{-1} ; ^1H NMR (300 MHz, $\text{DMSO-}d_6$) δ (ppm): 1.35 (m, 4H), 1.71 (m, 4H), 2.95 (m, 2H), 3.18 (m, 2H), 7.63 (m, 3H), 7.98 (m, 2H), 8.33 (s, 1H), 10.22 (s, 1H); ^{13}C NMR (75.5 MHz, $\text{DMSO-}d_6$) δ (ppm): 25.0, 25.2, 25.4, 29.9, 31.7, 117.9, 127.3, 127.6, 128.4, 128.9, 132.6, 133.3, 135.4, 138.4, 153.4, 162.70, 162.74, 164.9 (1 signal is hidden); MS-ESI: m/z 350 (MH^+), 372 (MNa^+). Anal. Calcd for $\text{C}_{21}\text{H}_{19}\text{NO}_4$: C, 72.19; H, 5.48; N, 4.01. Found: C, 72.31; H, 5.60; N, 3.92.

3. Crystallographic data

Crystal data were collected on a Bruker Nonius KappaCCD diffractometer with Mo-K α radiation. Structures were solved by direct methods and refined by the full-matrix least-squares method (SHELXL-97). All the non-hydrogen atoms were readily located and refined anisotropically. Hydrogen atoms in NH moieties were found in the difference Fourier map and refined isotropically. All the other hydrogen atoms were placed in calculated positions. Crystallographic data for the structures of **5Ac** and **6Cc** have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC XXXX-XXXX. Copies of these data can be obtained, free of charge, on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [fax: +44 0 1223-336033 or e-mail: deposit@ccdc.cam.ac.uk].

3.1 Crystal data for **5Ac**

C₂₇H₂₉N₃O₅, $M = 475.5$, monoclinic, space group $P2_1/c$ (No. 14), $a = 7.5010(1)$ Å, $b = 14.6602(3)$ Å, $c = 21.9638(5)$ Å, $\beta = 96.394(1)^\circ$, $V = 2400.25(8)$ Å³, $Z = 4$, $T = 293(2)$ K, $D_c = 1.316$ g cm⁻³, $\mu(\text{Mo-K}\alpha) = 0.092$ mm⁻¹, $F(000) = 1008$, crystal size = $0.72 \times 0.35 \times 0.25$ mm, 9925 reflections collected, 5462 unique ($R_{\text{int}} = 0.0289$). The final $R_1 = 0.0545$, $wR_2 = 0.1370$, and for all data $R_1 = 0.0886$, $wR_2 = 0.1563$.

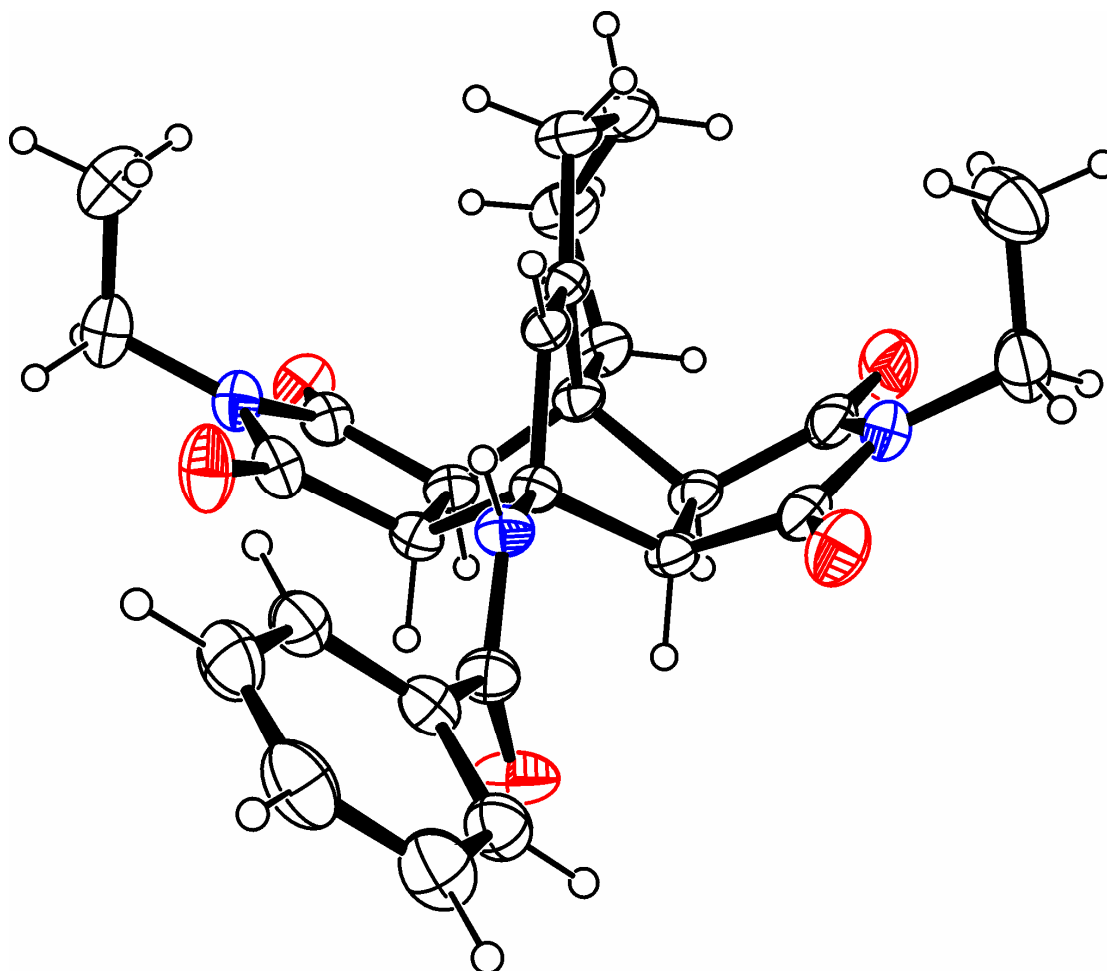


Figure 1. X-Ray crystal structure of **5Ac**. Atomic displacement parameters at 293 K are drawn at the 30% probability level.

3.2 Crystal data for 6Cc

$C_{29}H_{33}N_3O_5$, $M = 503.6$, monoclinic, space group $P21/n$ (No. 14), $a = 11.5444(2)$ Å, $b = 9.1904(2)$ Å, $c = 25.0286(5)$ Å, $\beta = 95.469(1)^\circ$, $V = 2643.39(9)$ Å³, $Z = 4$, $T = 293(2)$ K, $D_c = 1.265$ g cm⁻³, $\mu(\text{Mo-K}\alpha) = 0.087$ mm⁻¹, $F(000) = 1072$, crystal size = $0.25 \times 0.08 \times 0.08$ mm, 8548 reflections collected, 4478 unique ($R_{\text{int}} = 0.0324$). The final $R1 = 0.0492$, $wR2 = 0.1139$, and for all data $R1 = 0.0843$, $wR2 = 0.1324$.

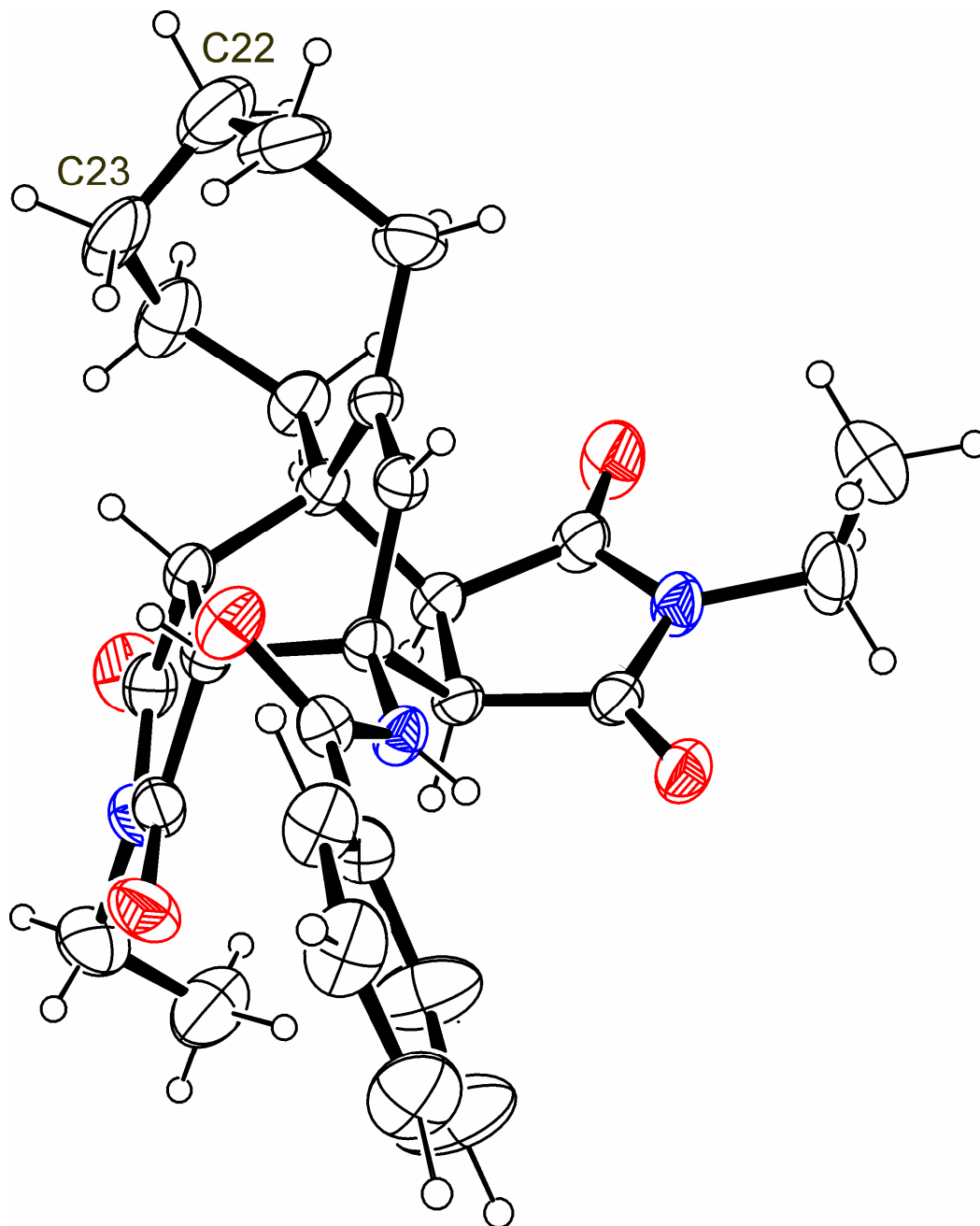


Figure 2. X-Ray crystal structure of **6Cc**. The disorder on atoms C22 and C23 is omitted for clarity. Atomic displacement parameters at 293 K are drawn at the 30% probability level.

4. Semi-empirical calculations

Tables 1–4 present the results of semi-empirical calculations (by AM1 and PM3 methods) of the energy differences between *T*- and *C*-**4C** (Table 1) and between the symmetrical (**5**) and unsymmetrical (**6**) double adducts in the series of eight- (Table 2), seven- (Table 3) and six-membered fused rings (Table 4) obtained by Gaussian 03.³

Table 1 The results of AM1 and PM3 calculations for transition states *T*-**4C** and *C*-**4C**

Compound	AM1	ΔE (kcal/mol)	PM3	ΔE (kcal/mol)
<i>C</i> - 4Cd	−0.1048158	0	−0.1231489	0
<i>T</i> - 4Cd	−0.1054868	−0.42	−0.1234081	−0.16
<i>C</i> - 4Ca	−0.0400073	0	−0.0652164	0
<i>T</i> - 4Ca	−0.0405290	−0.33	−0.0656063	−0.24
<i>C</i> - 4Ce	−0.1728959	0	−0.1871590	0
<i>T</i> - 4Ce	−0.1742149	−0.83	−0.1883689	−0.76

Table 2 The results of AM1 and PM3 calculations for symmetrical and unsymmetrical cycloadducts **5C** and **6C**

Compound	AM1	ΔE (kcal/mol)	PM3	ΔE (kcal/mol)
5Cd ^a	−0.1922094	0	−0.2309903	0
6Cd ^a	−0.2009851	−5.51	−0.2410588	−6.32
5Ca	−0.0626386	0	−0.1261276	0
6Ca	−0.0716701	−5.67	−0.1352426	−5.72
5Ce	−0.3271609	0	−0.3584418	0
6Ce ^a	−0.3340997	−4.35	−0.3682788	−6.17

^a This compound was not synthesized.

³ Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03*, Revision B.03; Gaussian, Inc., Wallingford CT, 2004.

Table 3 The results of AM1 and PM3 calculations for symmetrical and unsymmetrical cycloadducts **5B** and **6B**

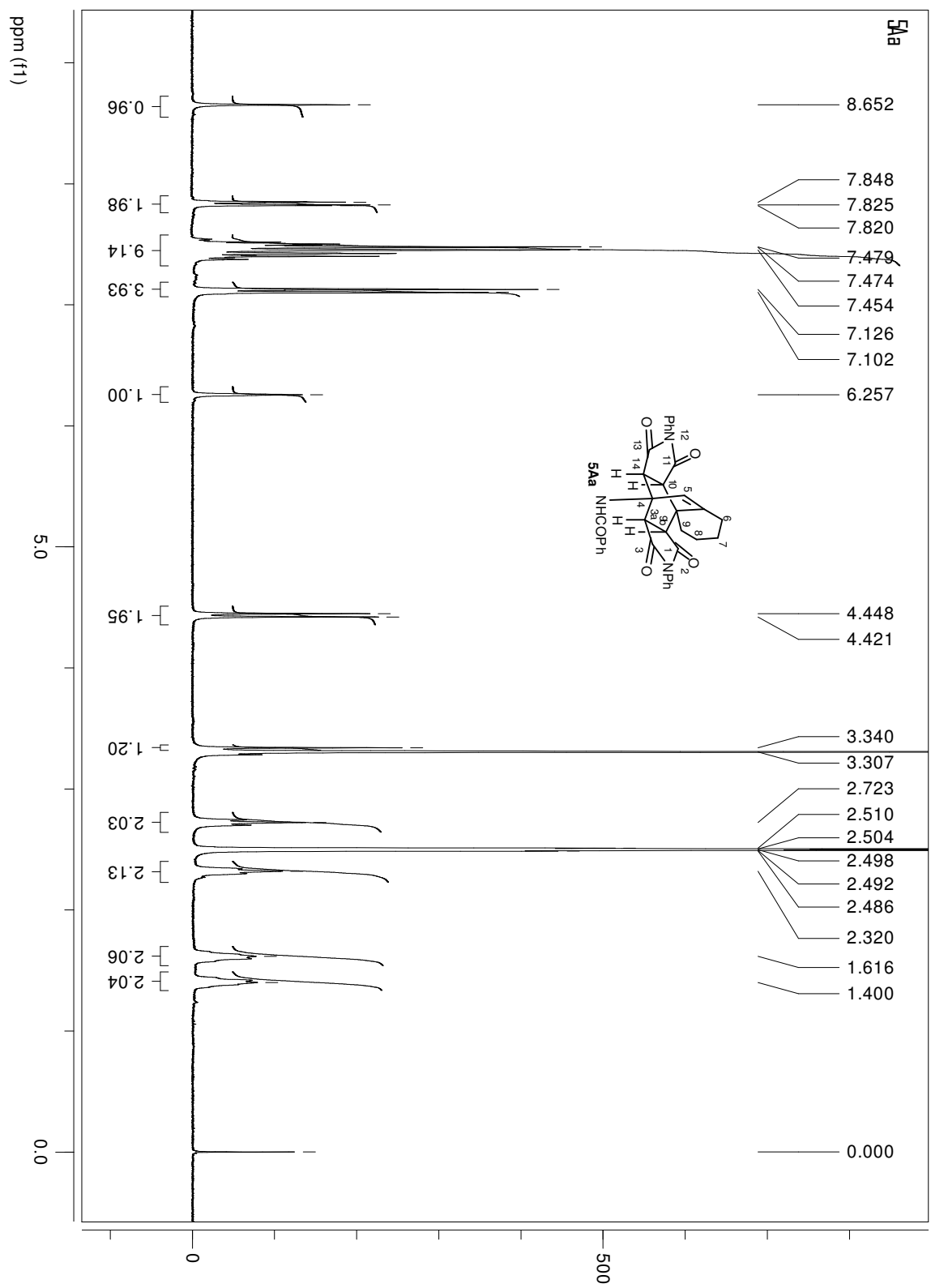
Compound	AM1	ΔE (kcal/mol)	PM3	ΔE (kcal/mol)
5Bd	-0.1958303	0	-0.2347884	0
6Bd ^a	-0.1892605	4.12	-0.2311376	2.29
5Ba ²	-0.0662200	0	-0.1190411	0
6Ba ^a	-0.0606160	3.52	-0.1151167	2.46
5Be ^a	-0.3304142	0	-0.3621360	0
6Be ^a	-0.3235702	4.29	-0.3583125	2.40

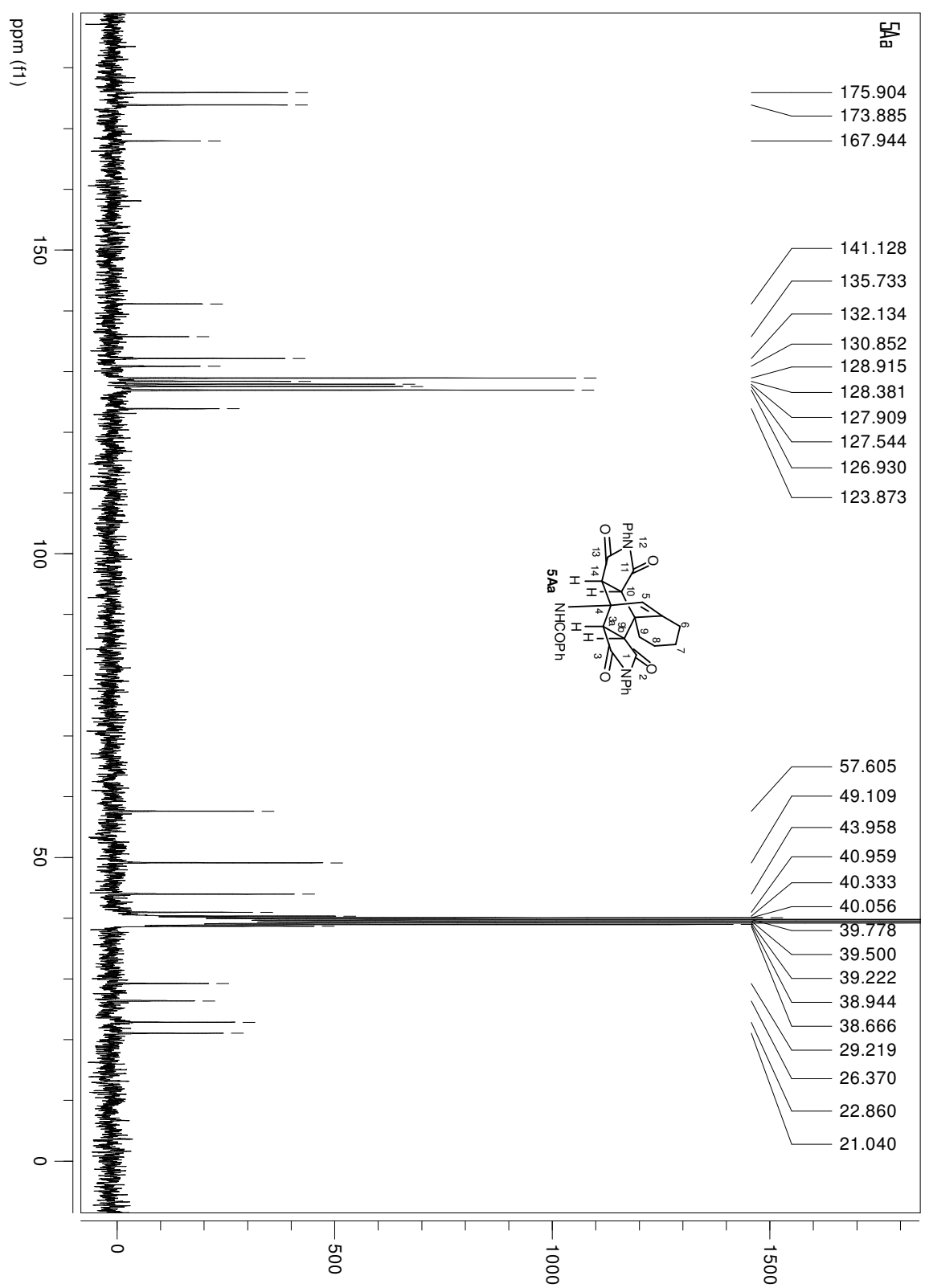
^a This compound was not synthesized.

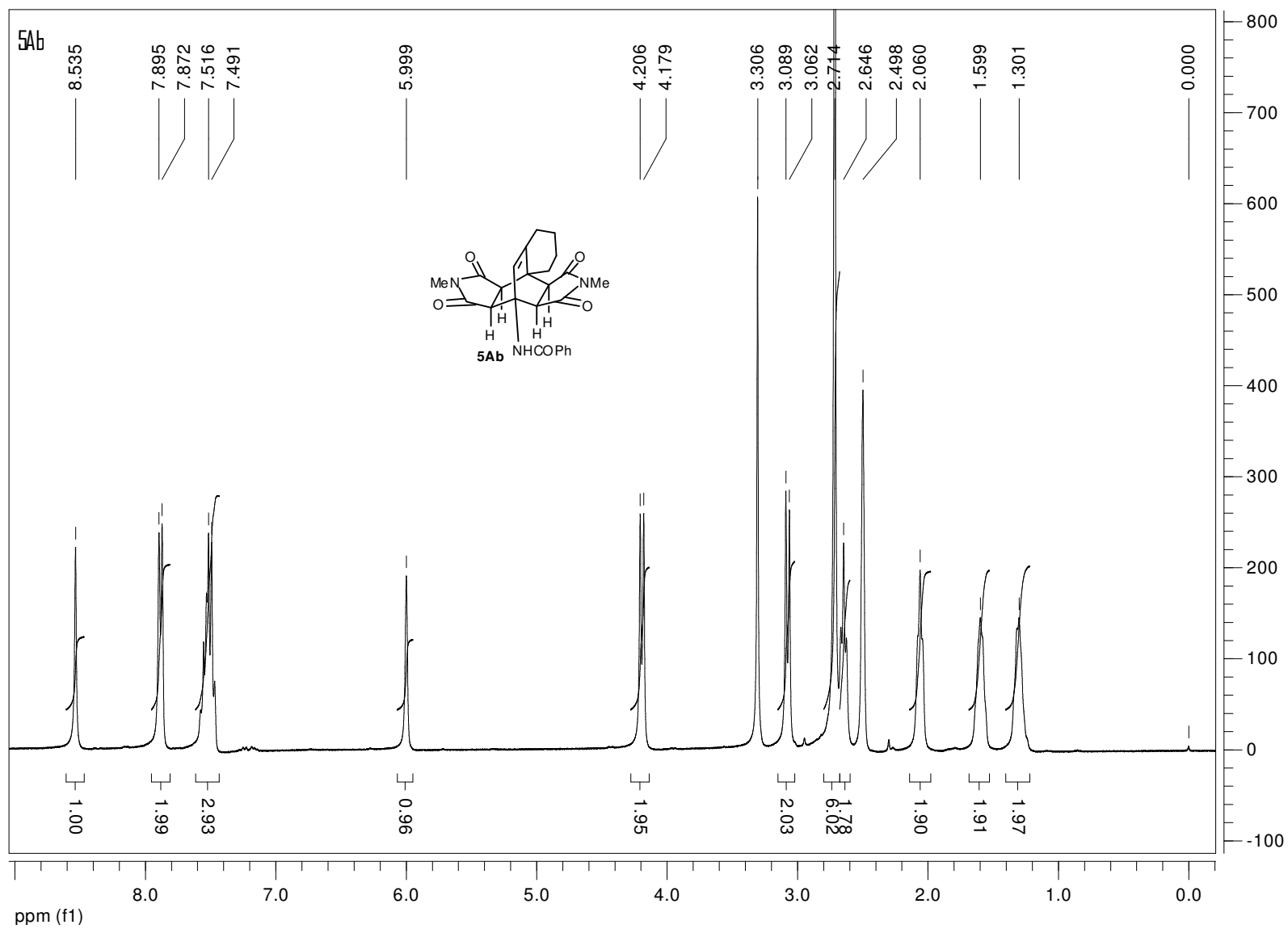
Table 4 The results of AM1 and PM3 calculations for symmetrical and unsymmetrical cycloadducts **5A** and **6A**

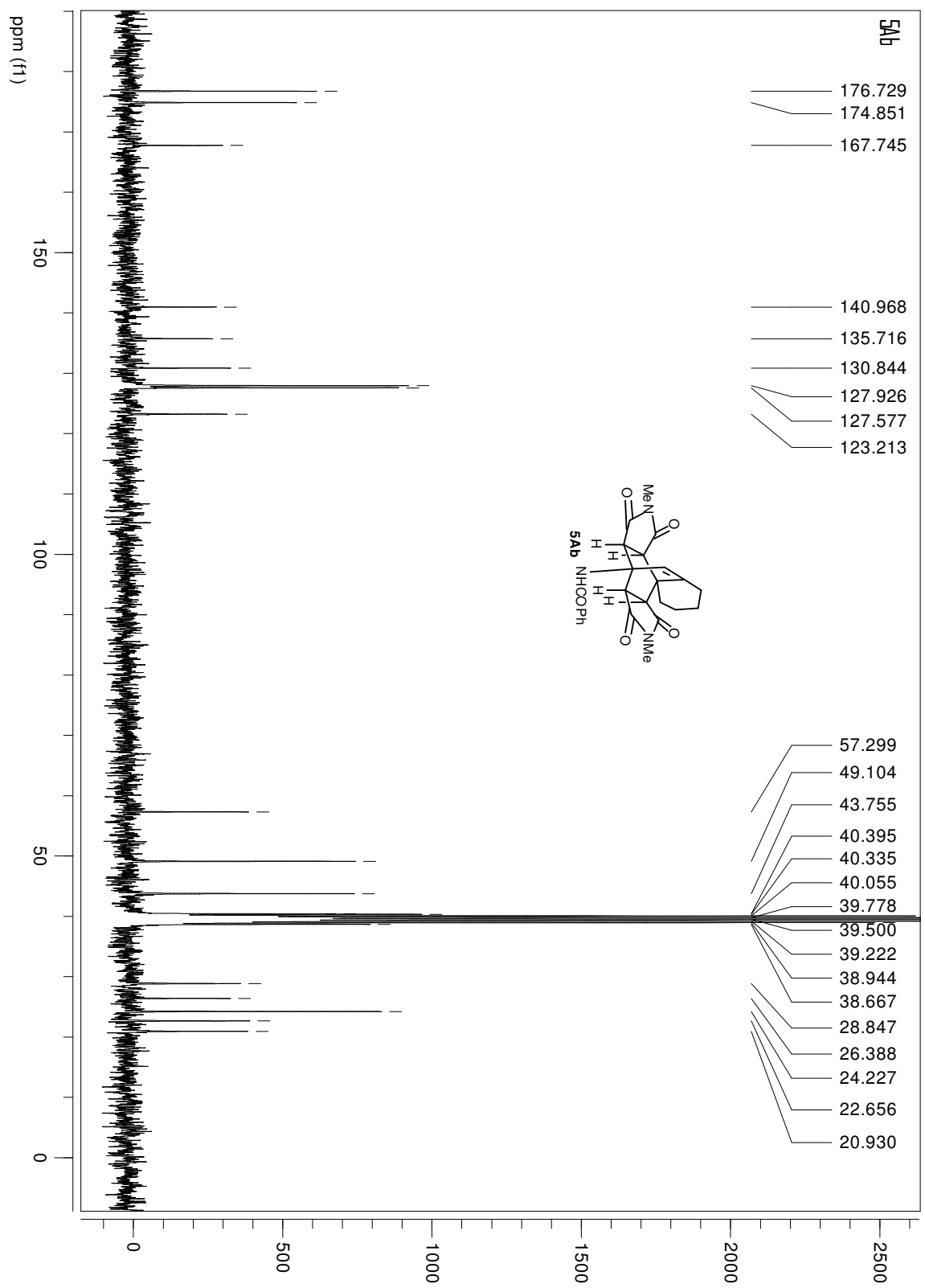
Compound	AM1	ΔE (kcal/mol)	PM3	ΔE (kcal/mol)
5Ad	-0.1945112	0	-0.2375499	0
6Ad ^a	-0.1858723	5.42	-0.2302593	4.57
5Aa	-0.0649757	0	-0.1218625	0
6Aa ^a	-0.0571902	4.89	-0.1141734	4.82
5Ae ^a	-0.3284924	0	-0.3647146	0
6Ae ^a	-0.3199644	5.35	-0.3575456	4.50

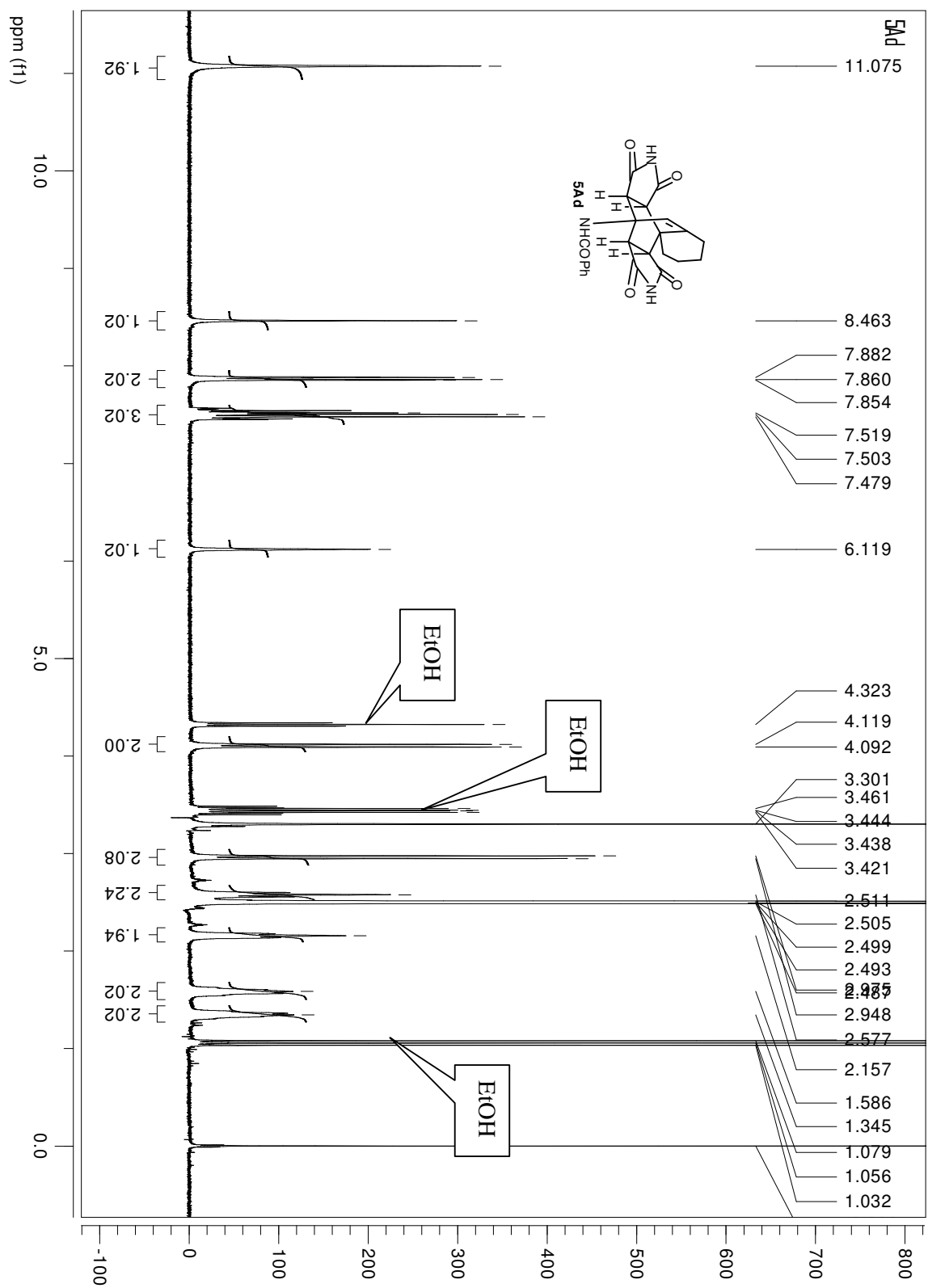
^a This compound was not synthesized.

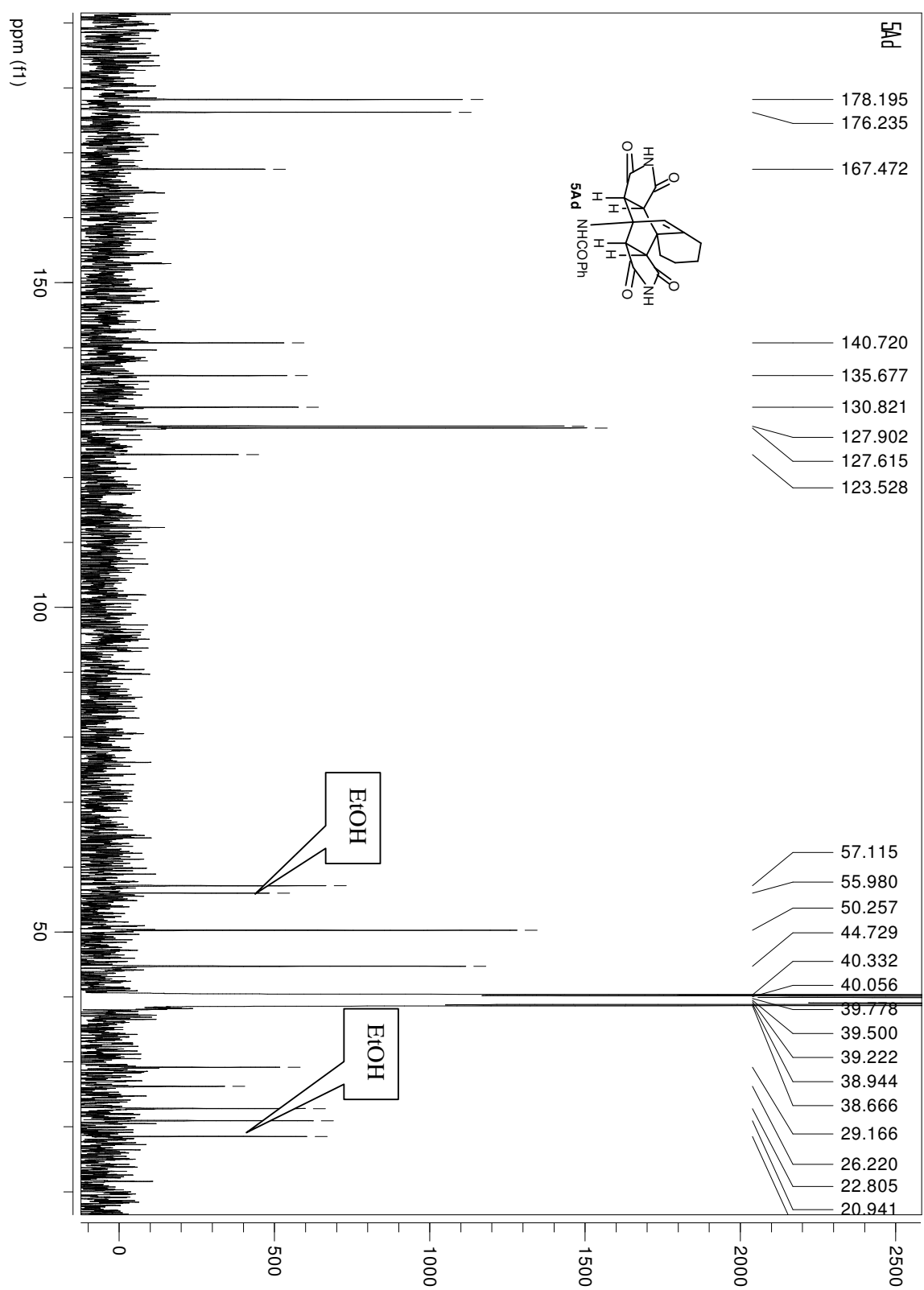


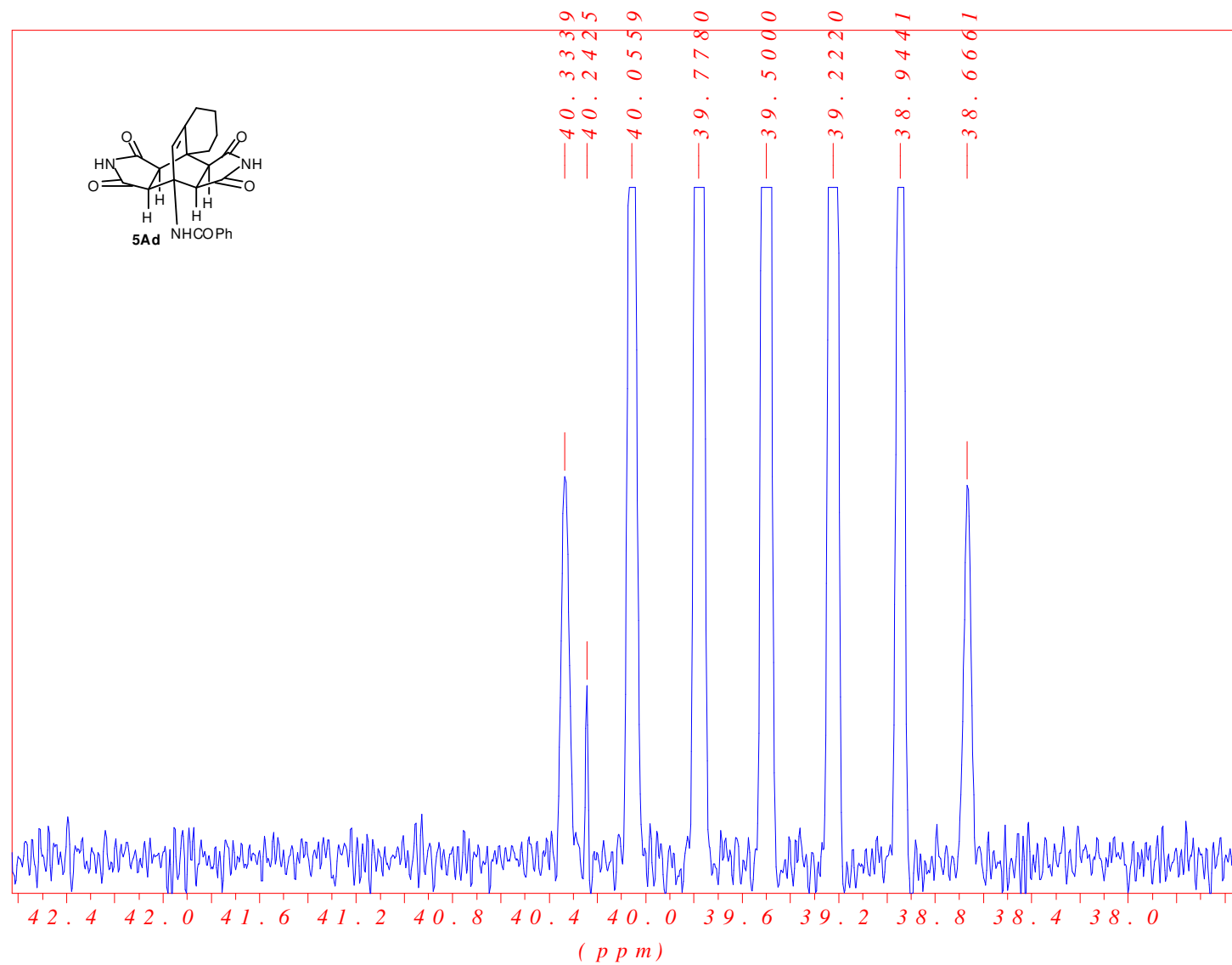


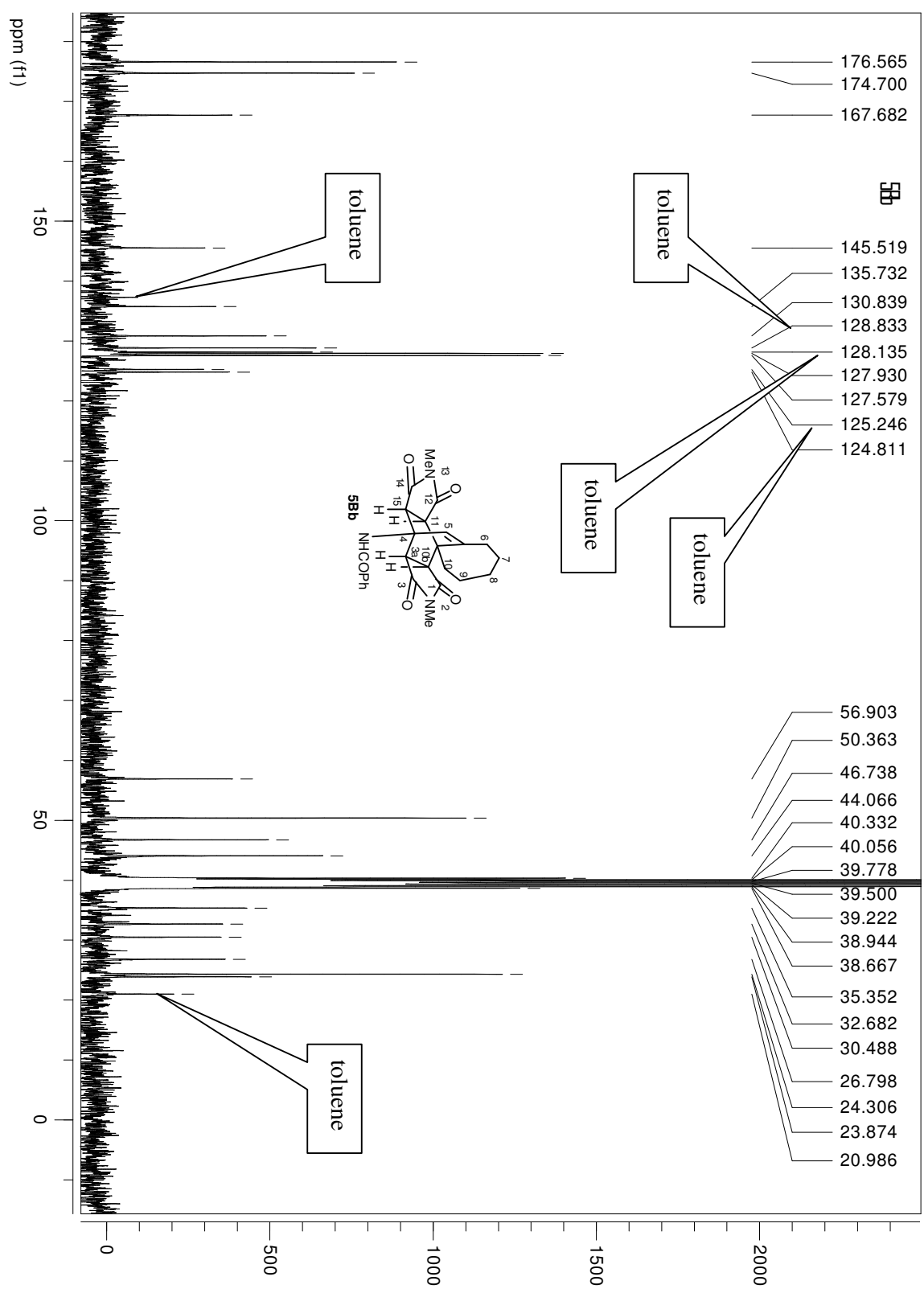


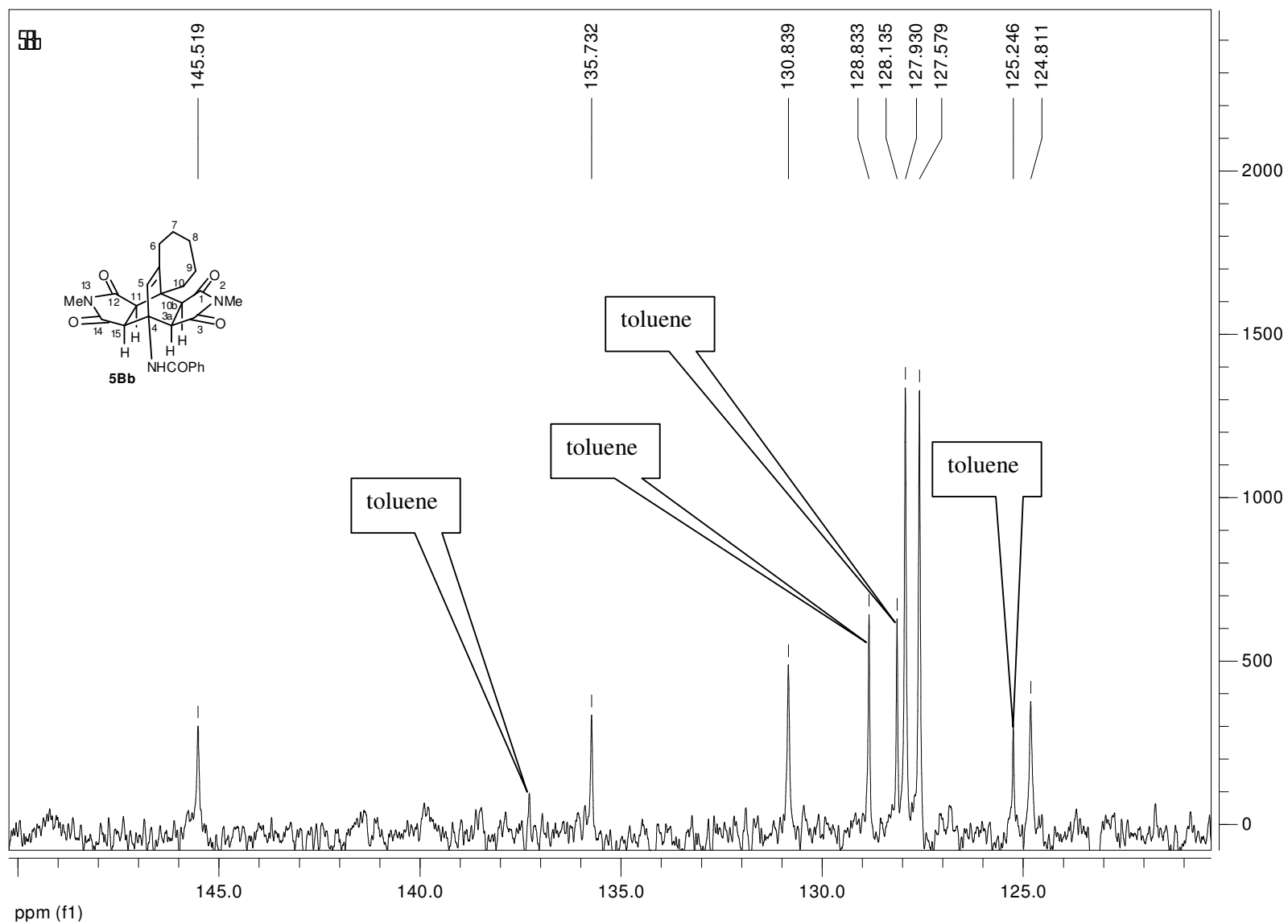


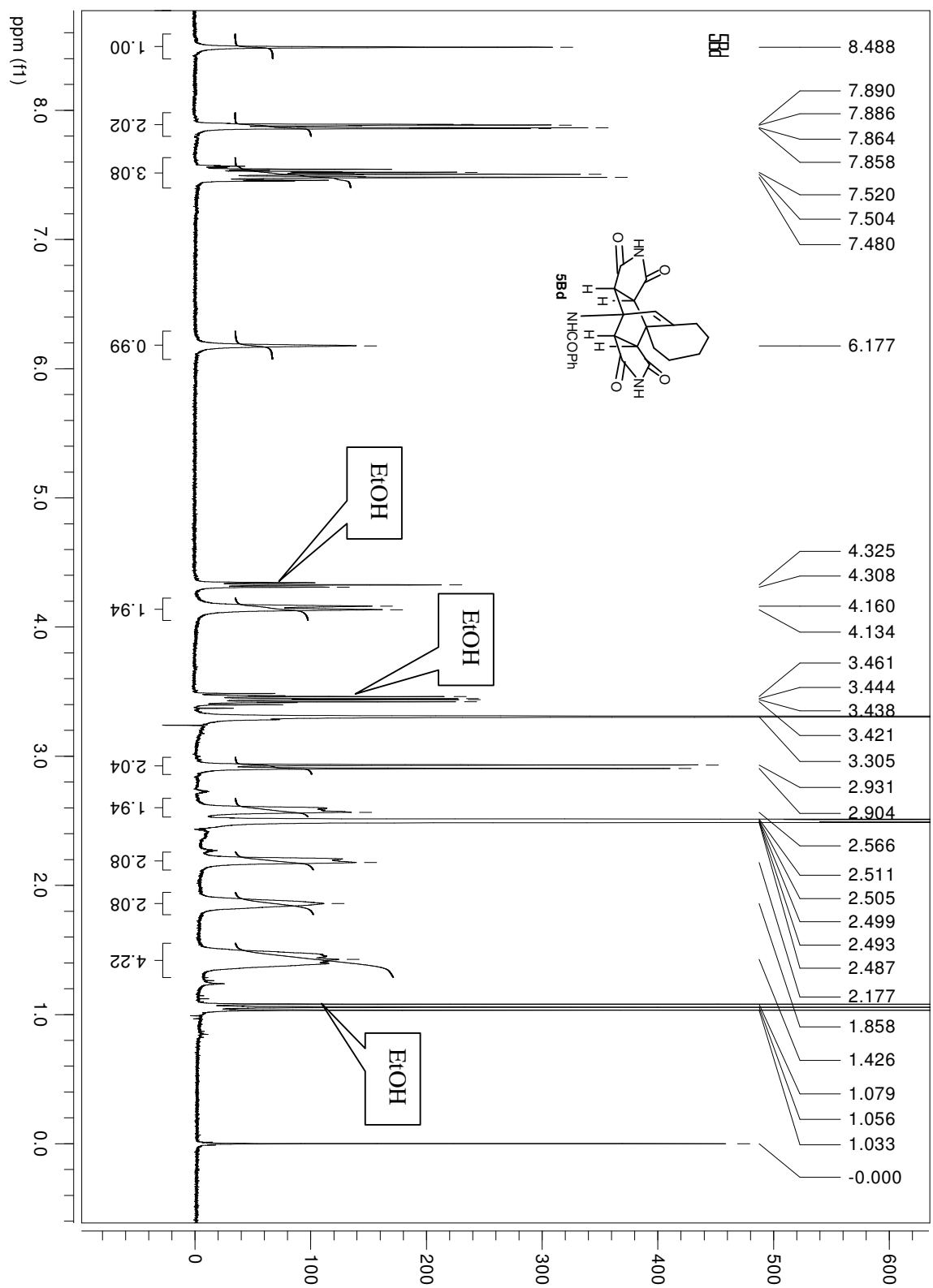


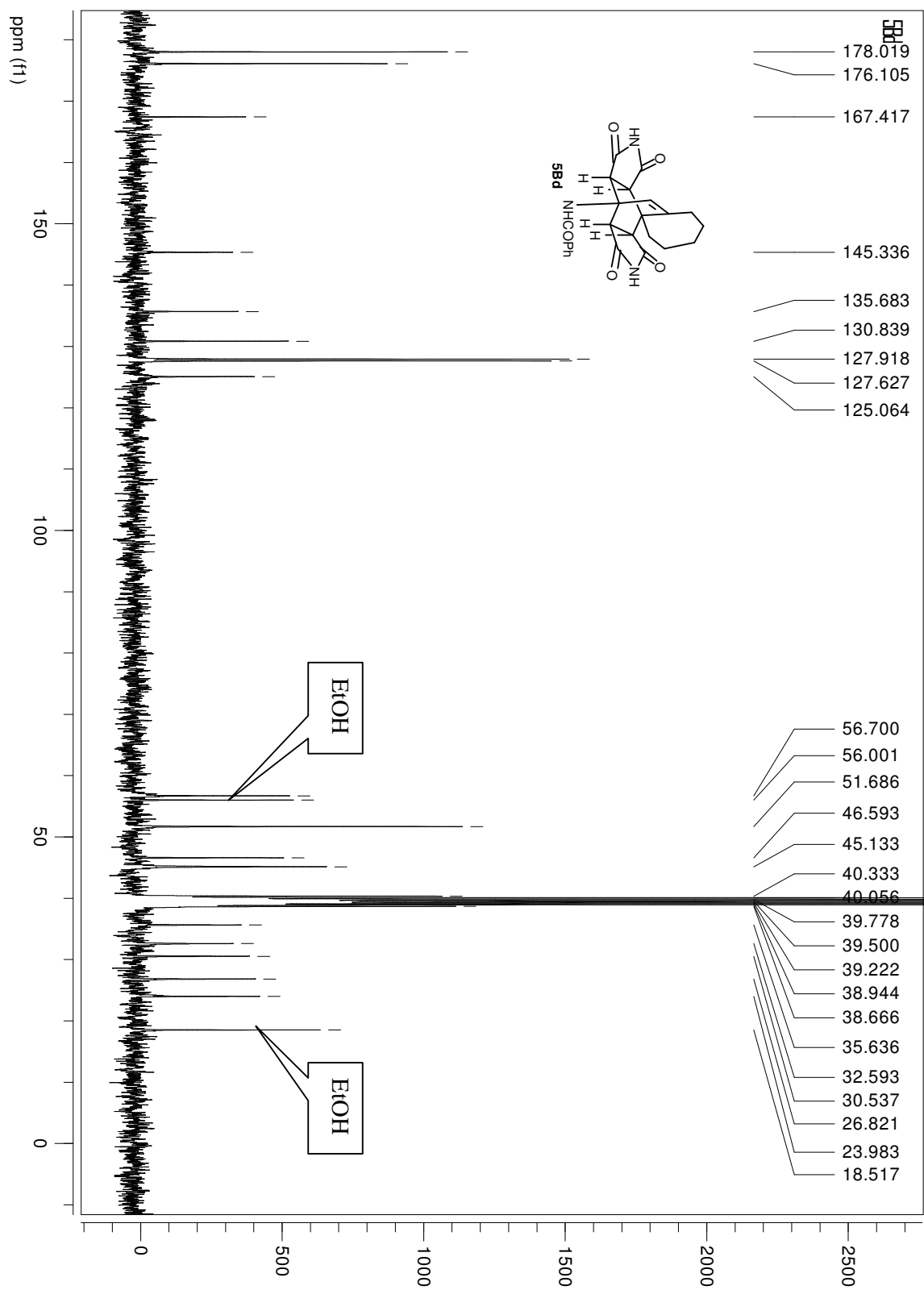


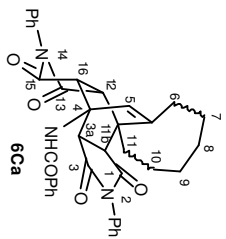


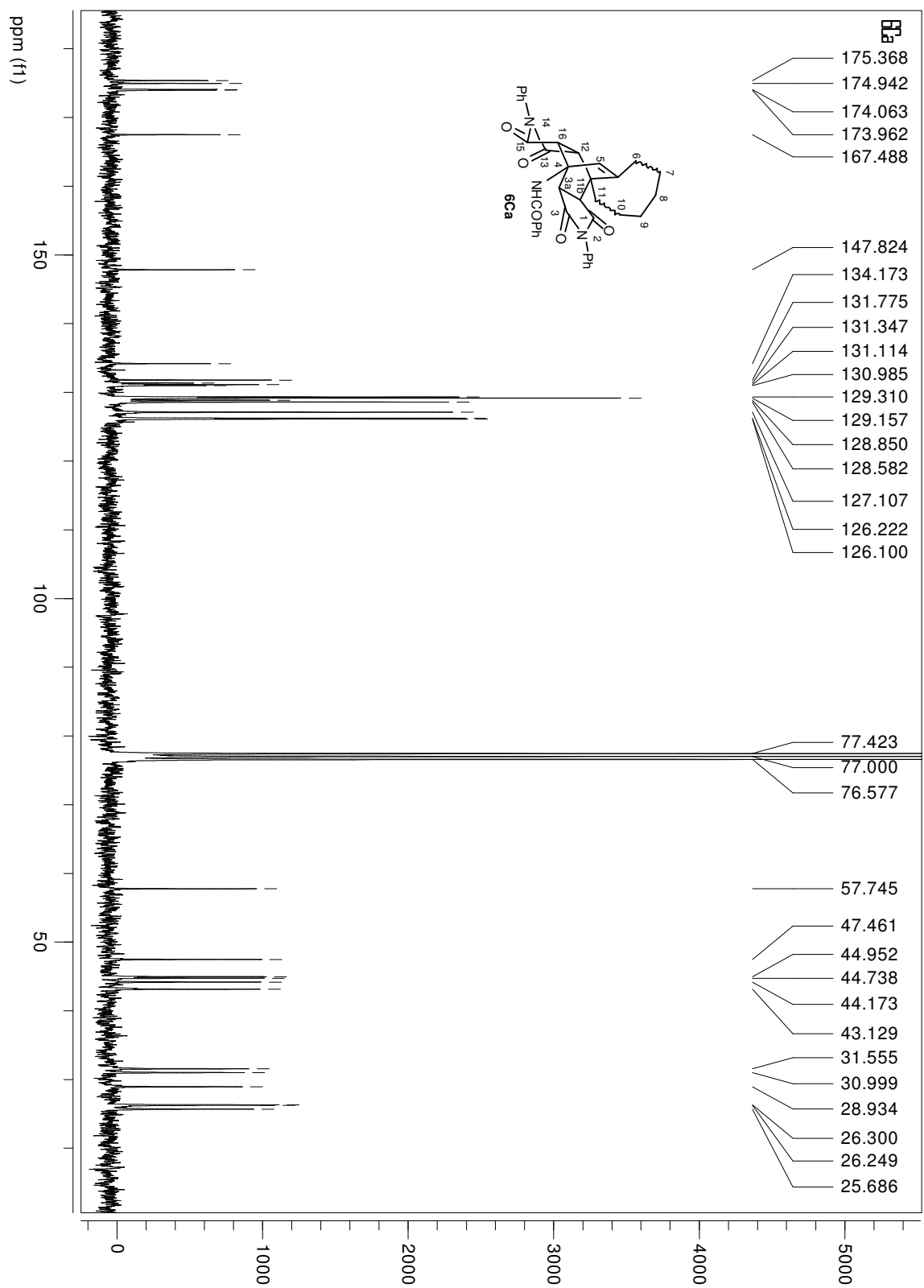


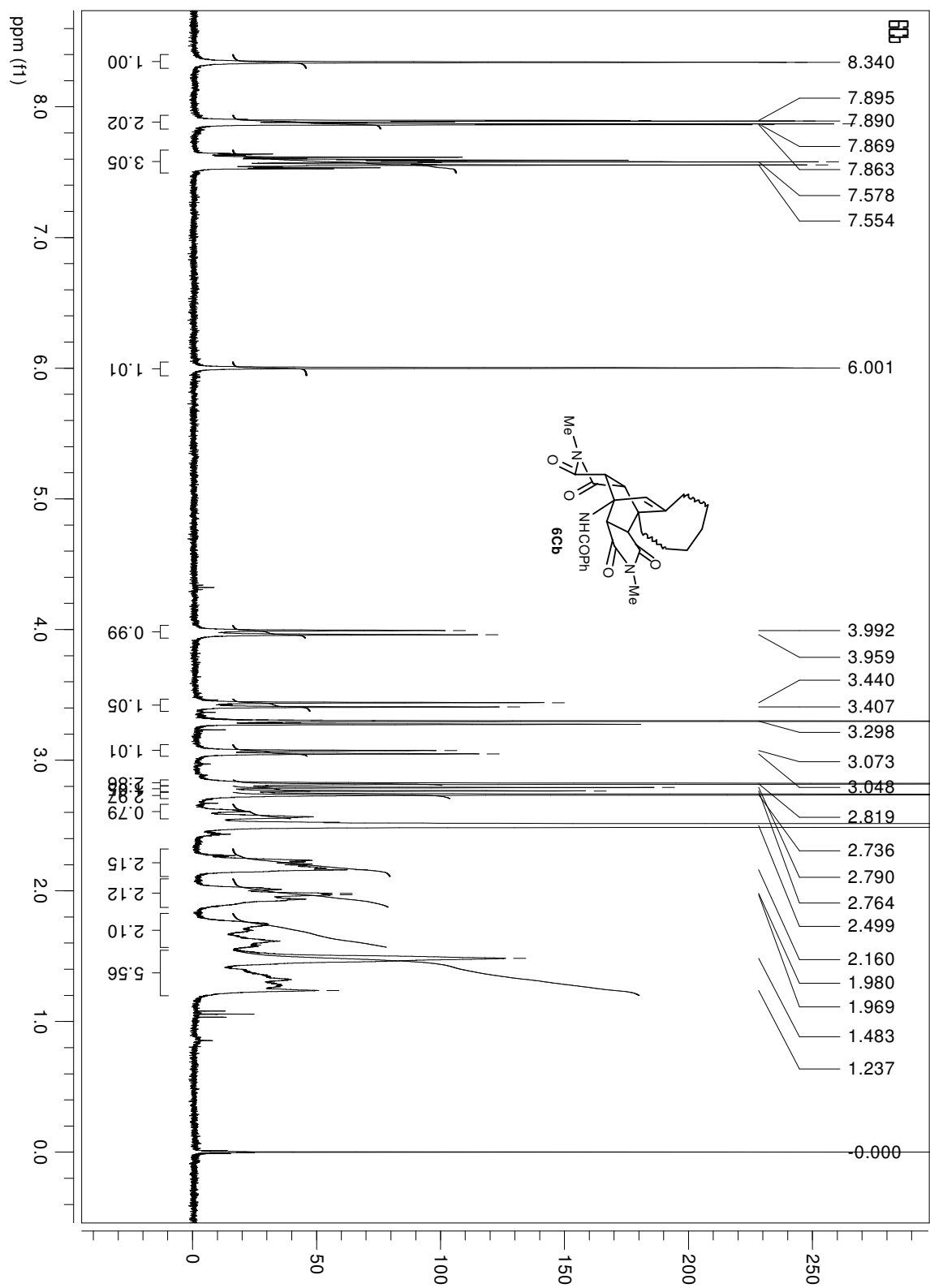


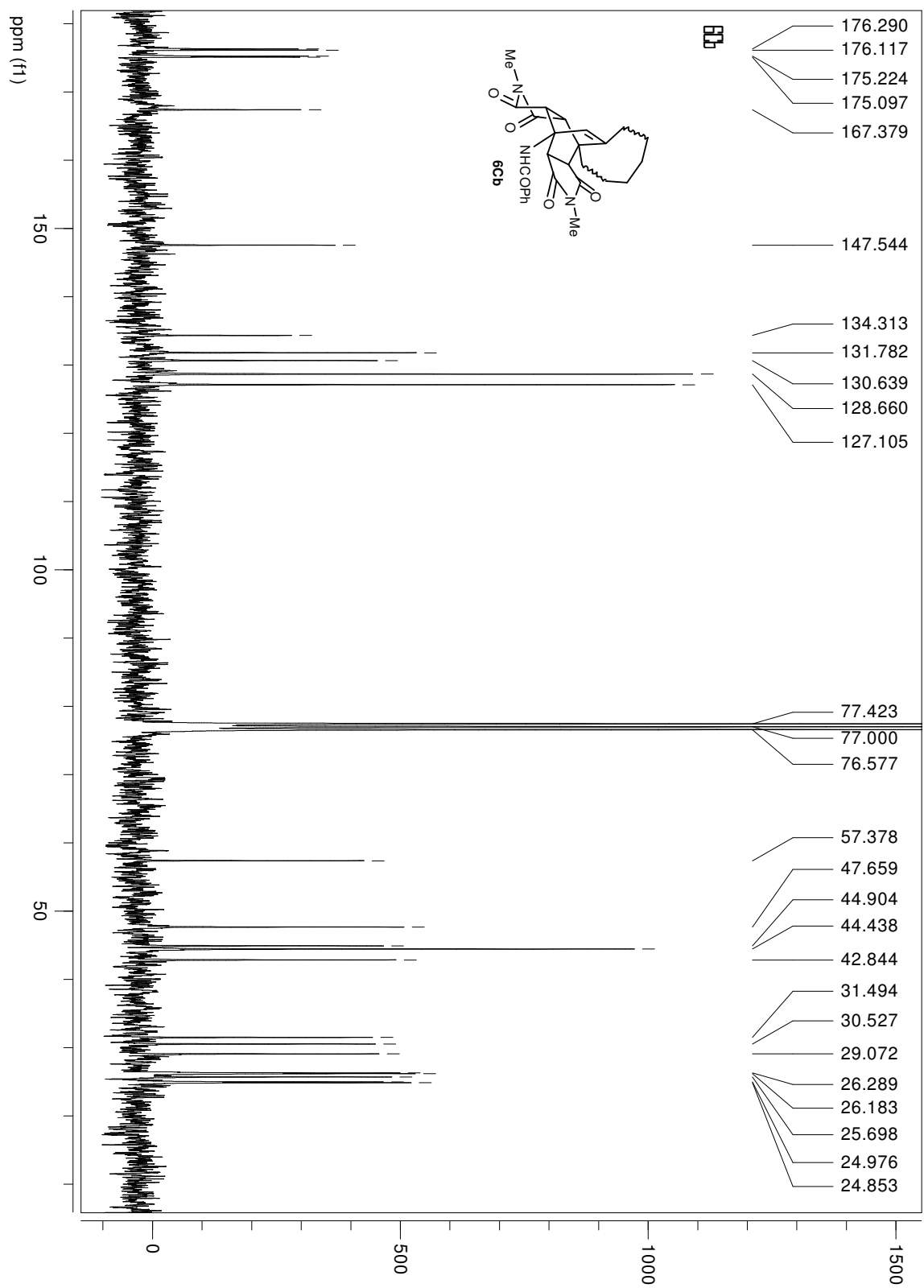


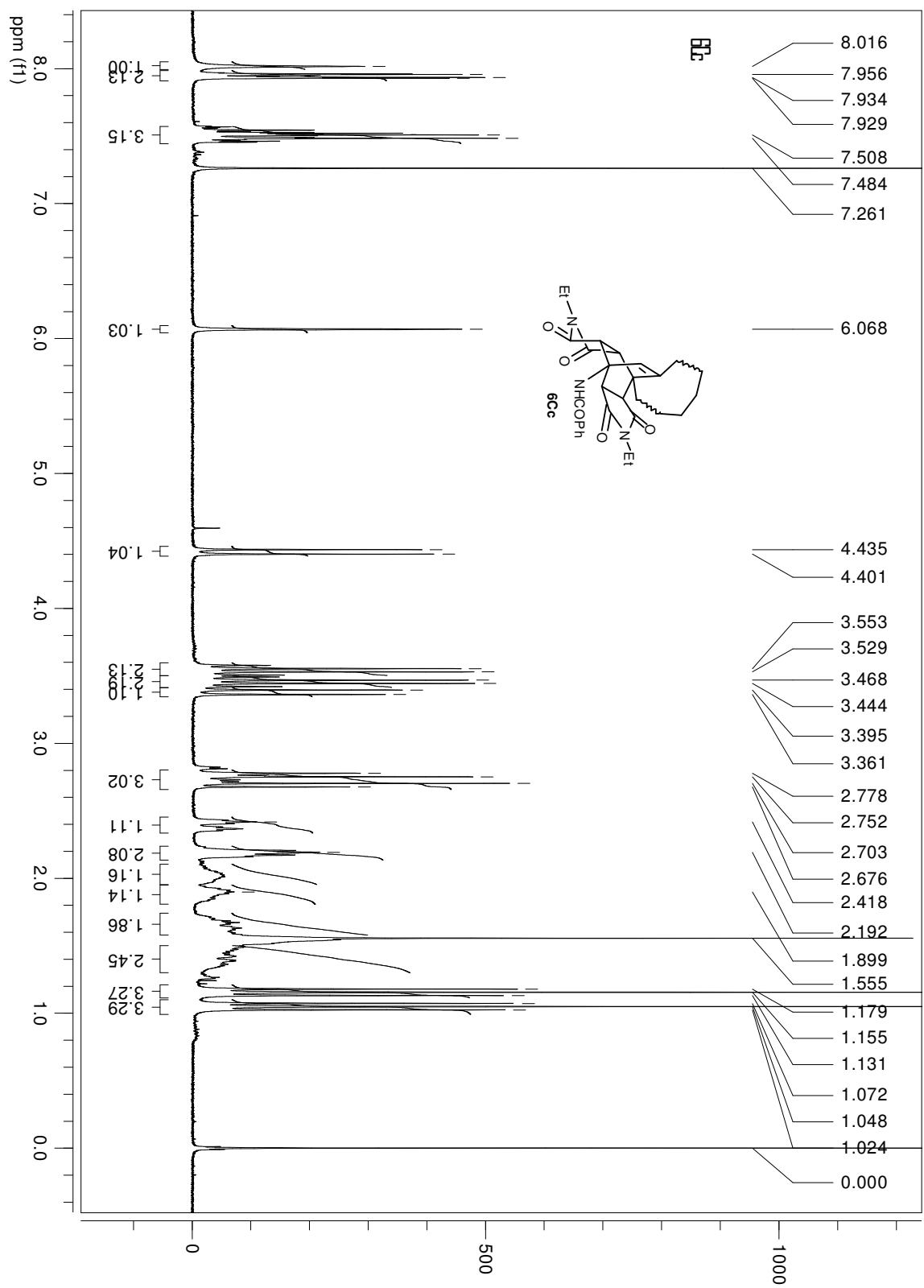


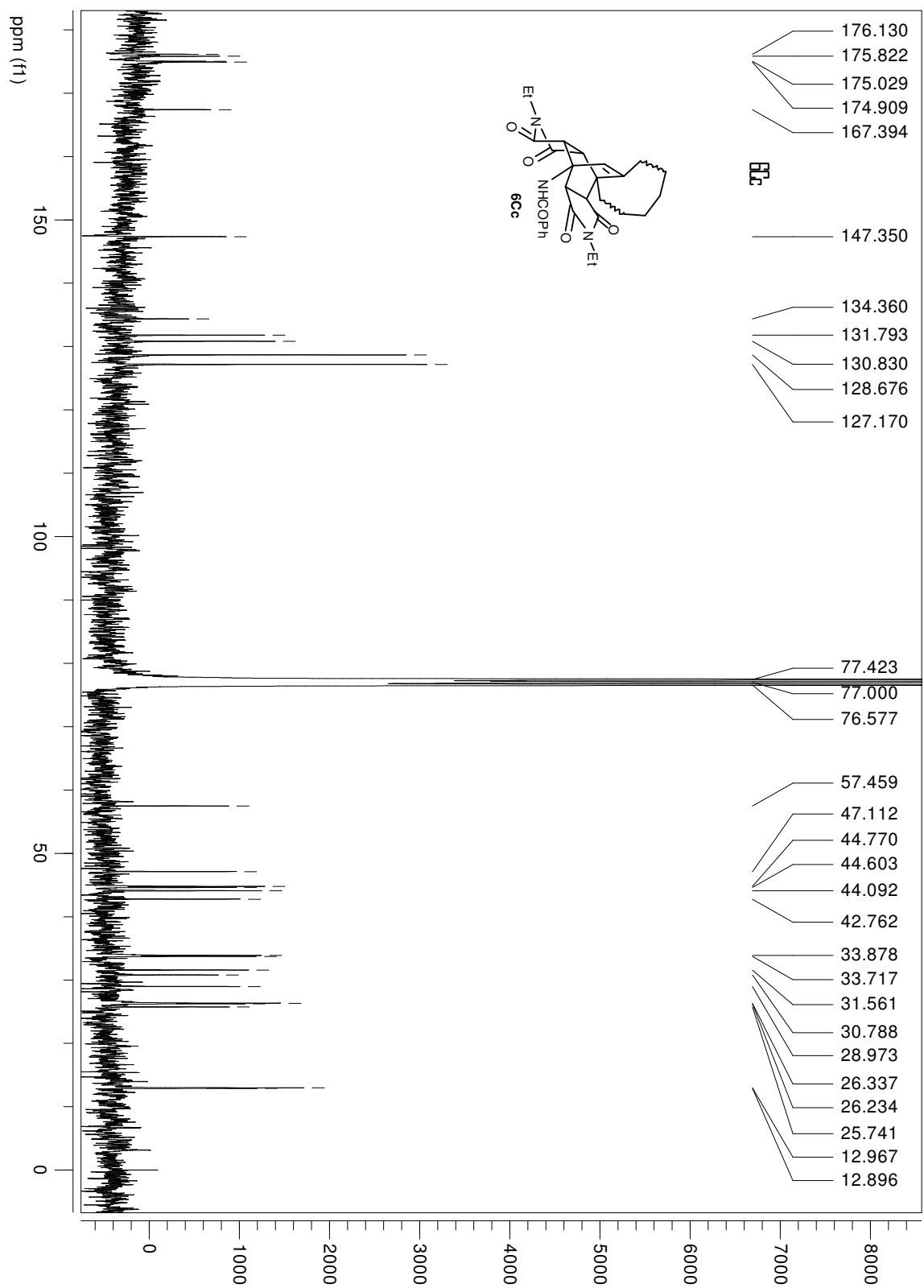


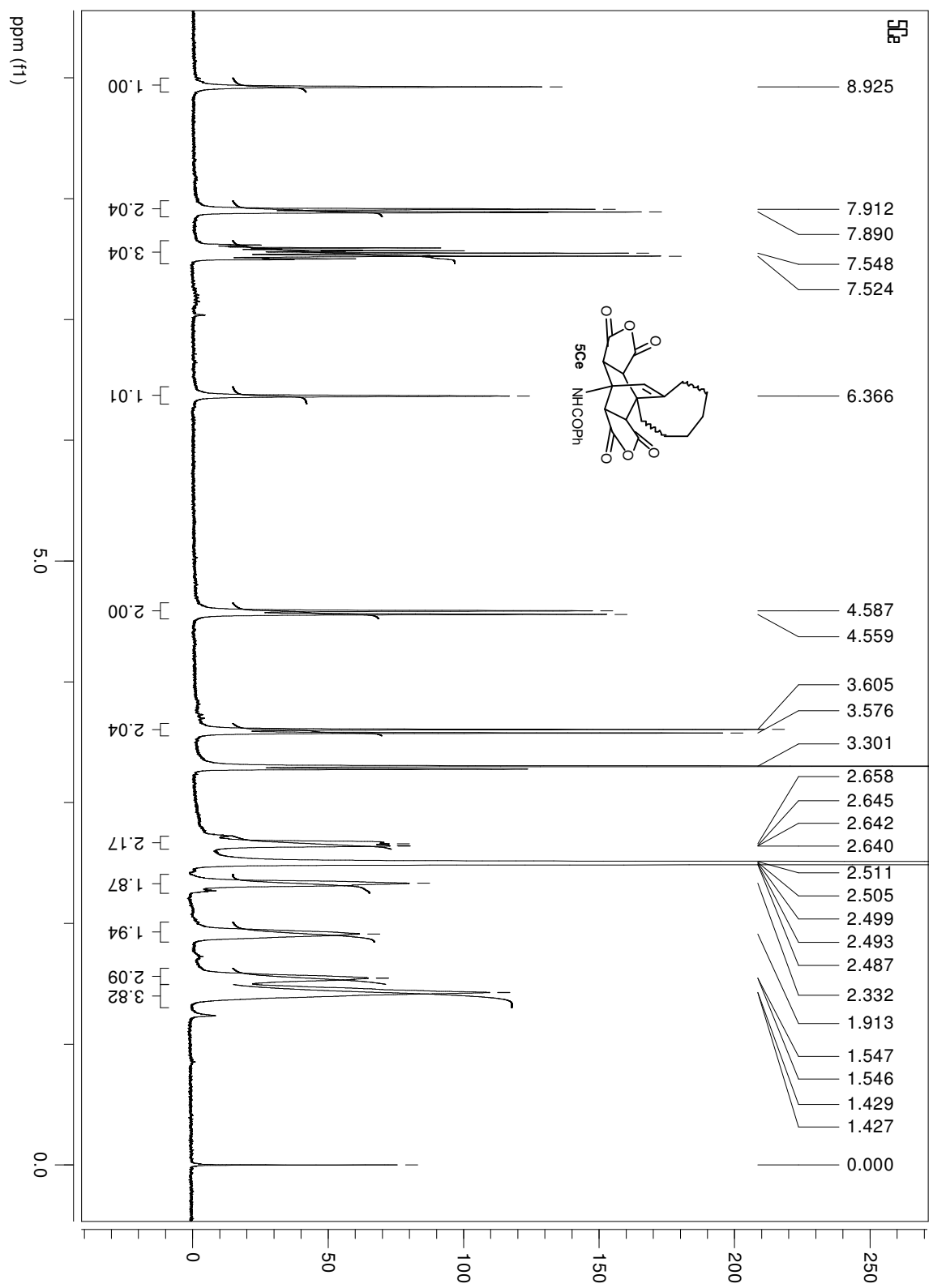


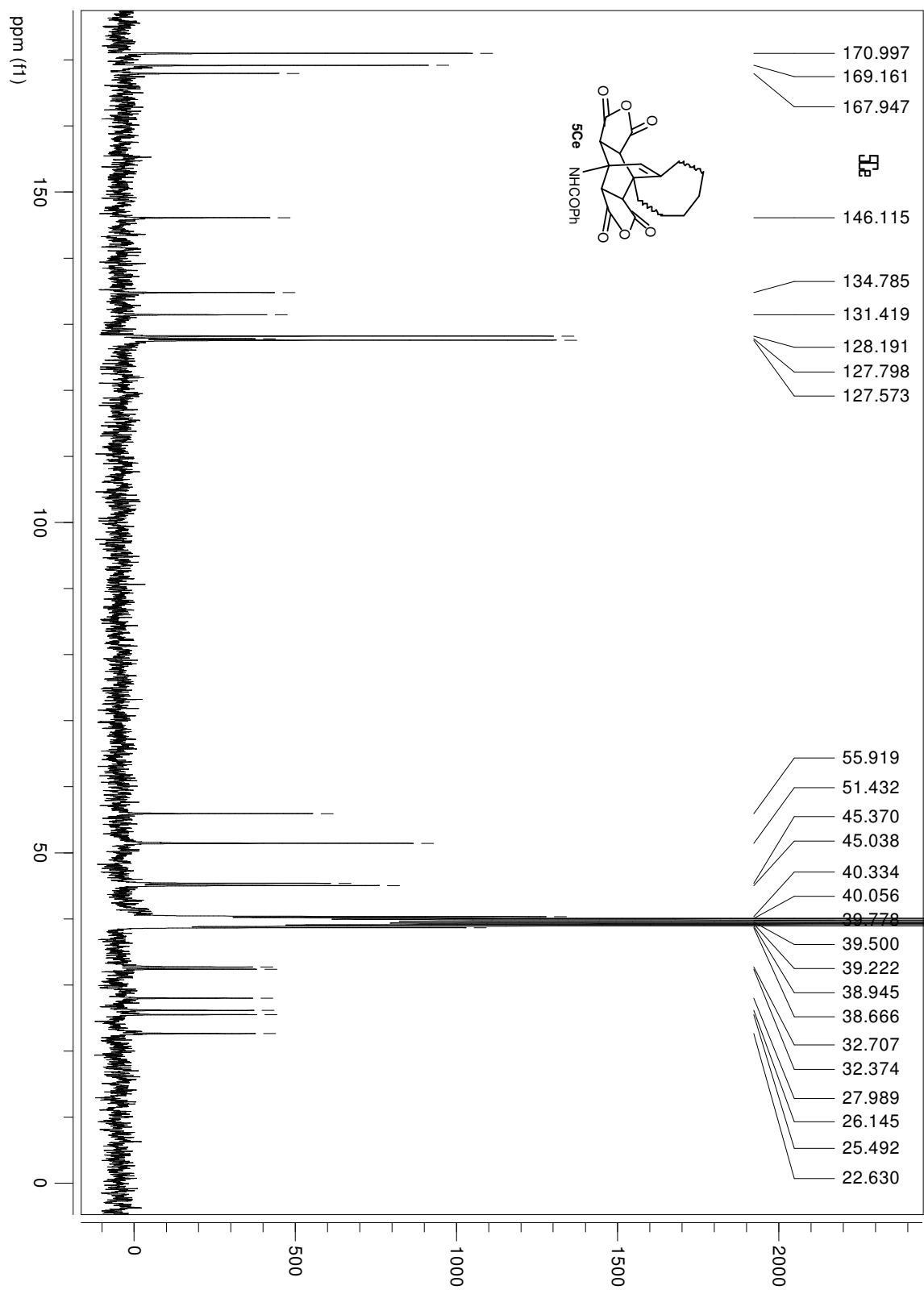


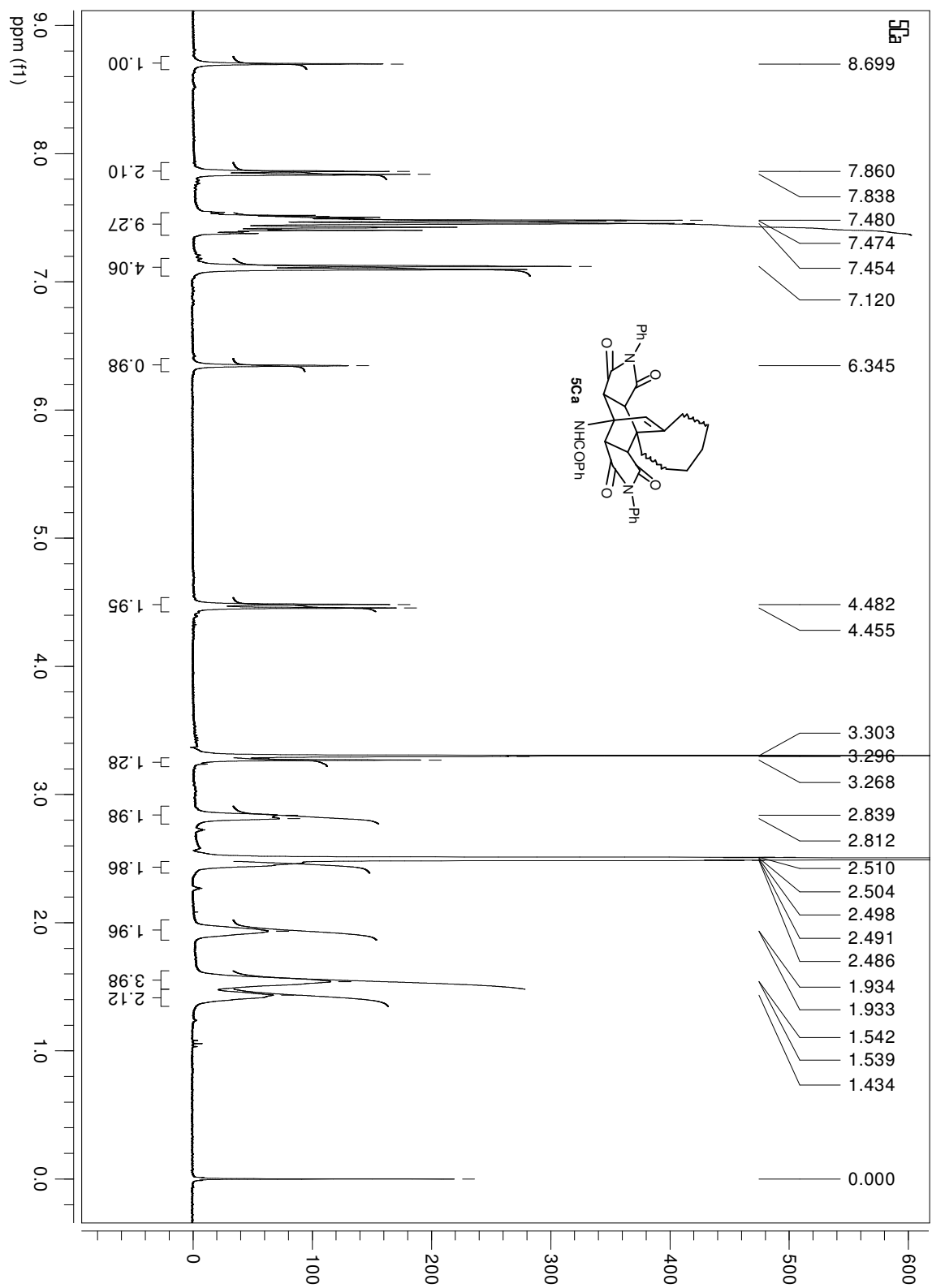


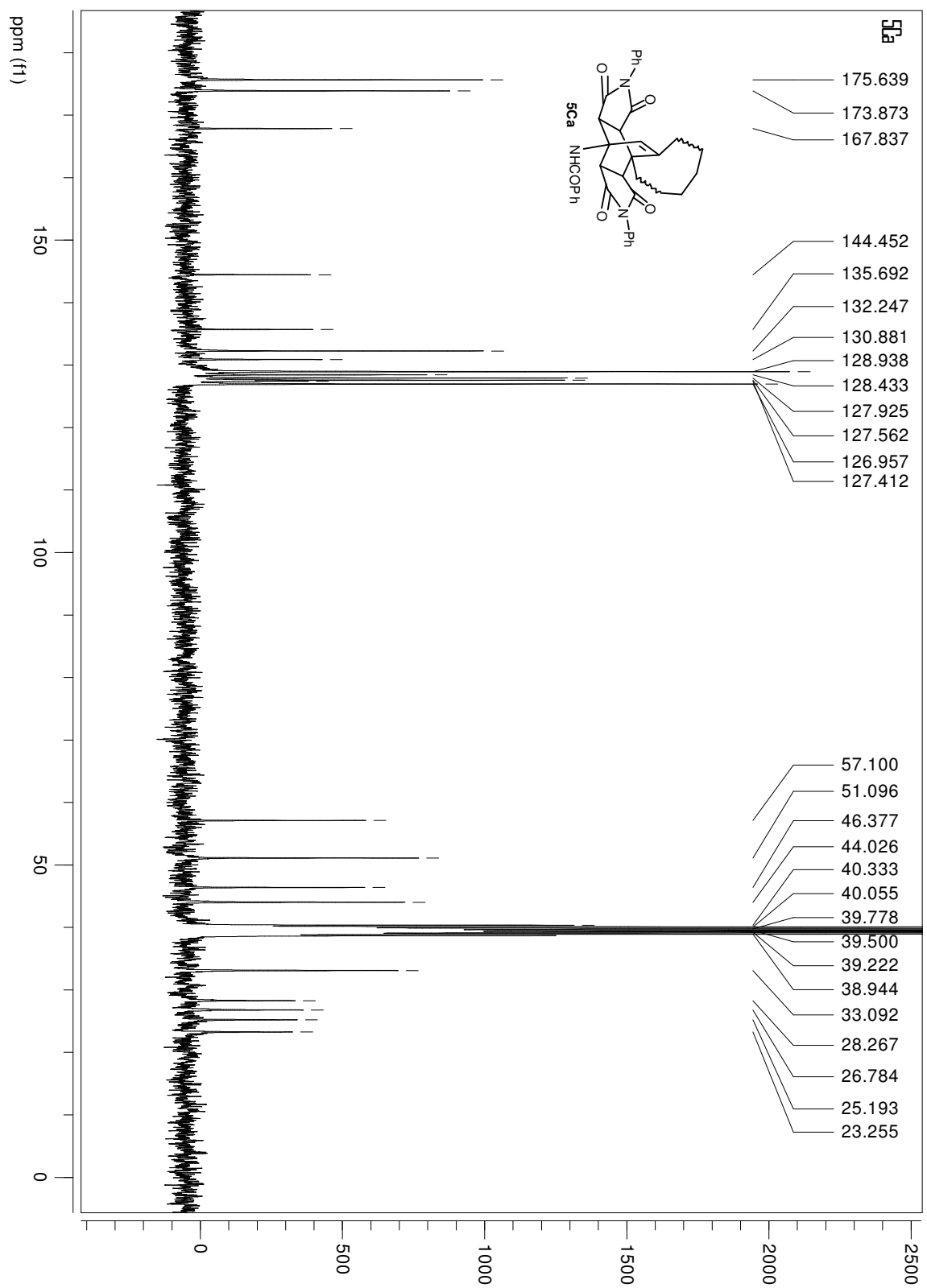


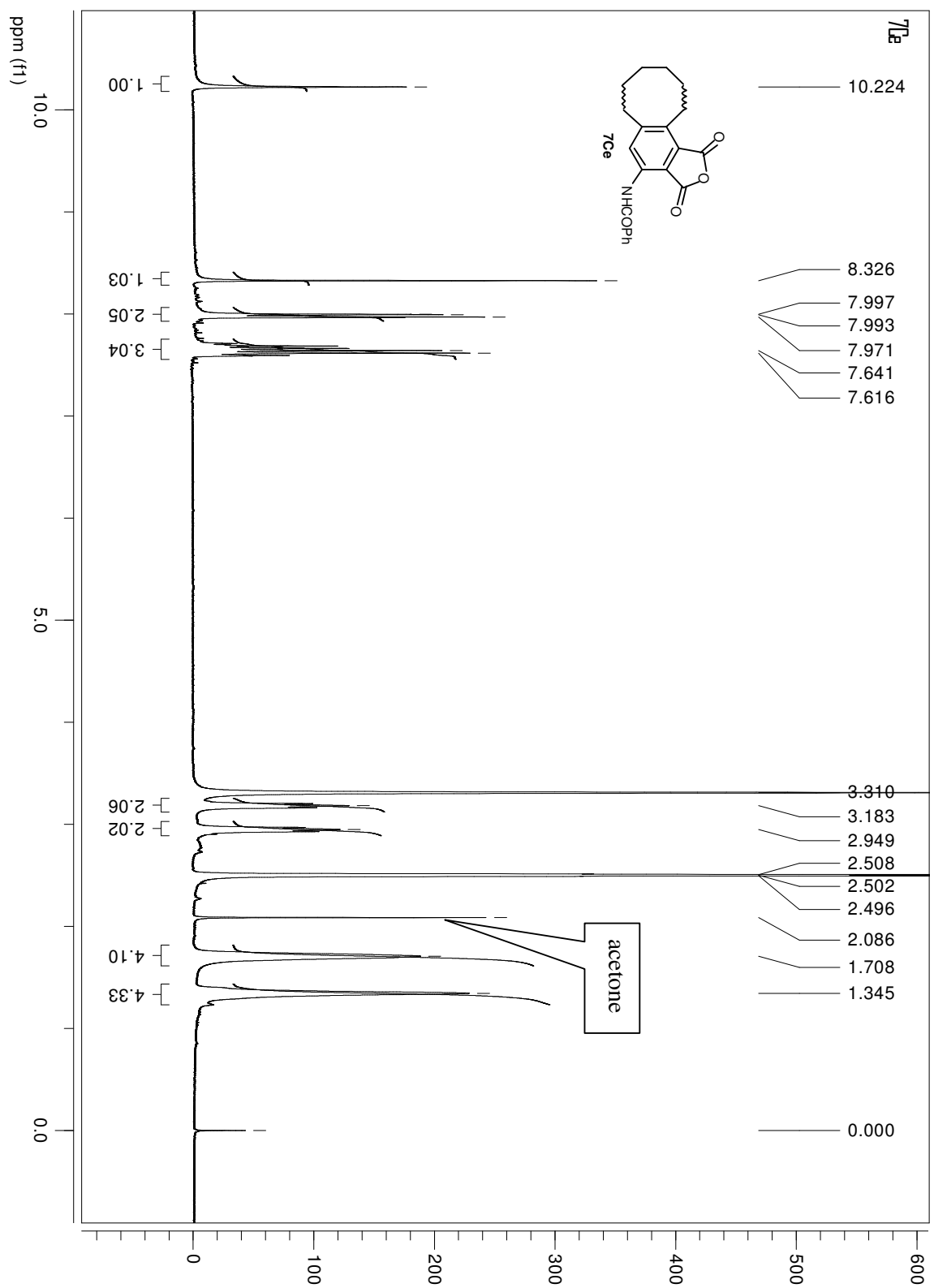


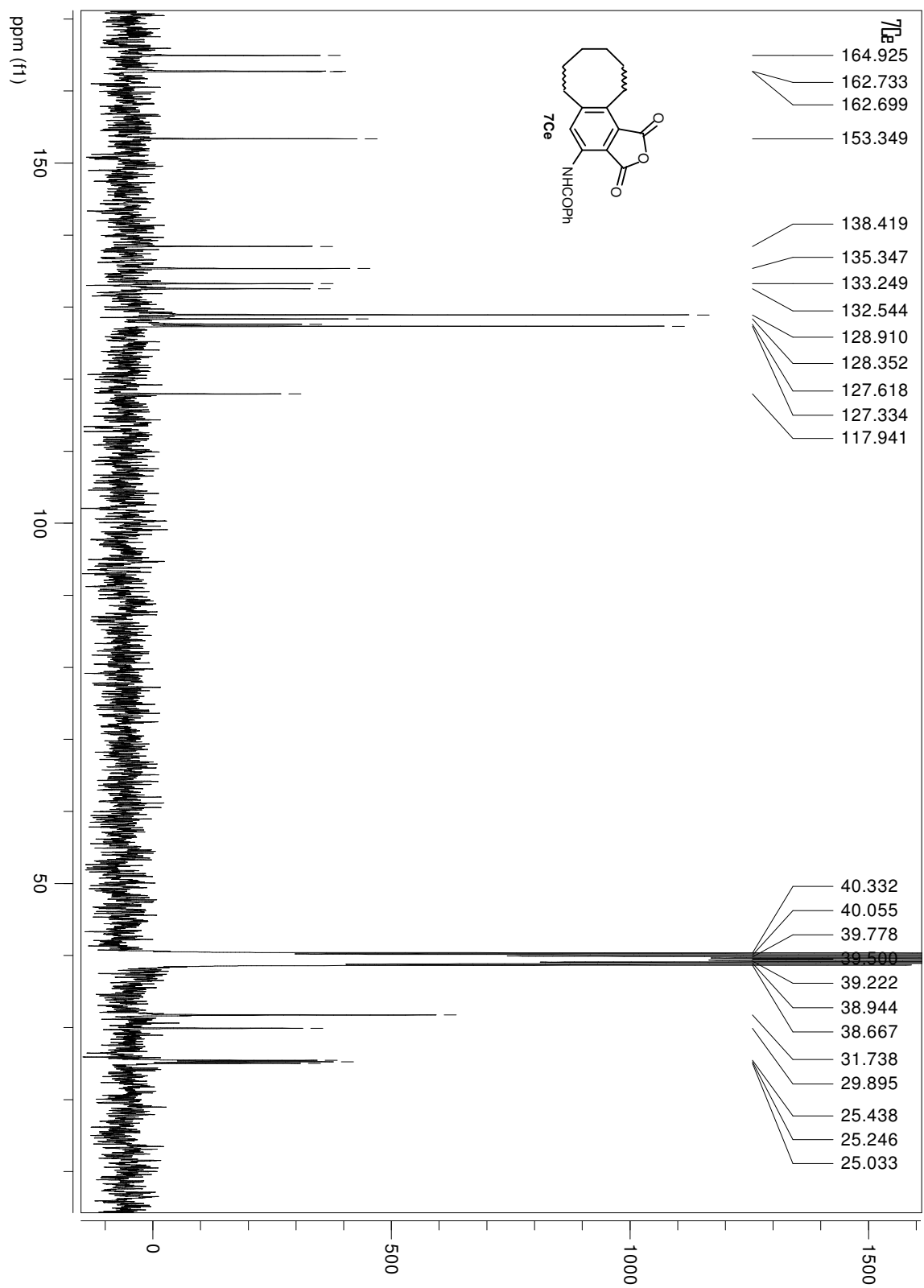












6. Atom coordinates documenting semi-empirical calculations

C-4Cd AM1

C	-0.060959	-0.058343	-0.154534
C	-0.026941	-0.217289	1.234936
C	1.191906	-0.217232	1.919292
C	2.381782	-0.075500	1.206037
C	2.352807	0.075513	-0.180640
C	1.133371	0.089340	-0.858834
C	-1.298945	-0.343875	2.001746
O	-1.572433	0.391425	2.968271
N	-2.151863	-1.361051	1.587420
C	-3.486646	-1.500686	2.016539
C	-6.218302	-1.829494	2.861332
C	-5.772982	-0.437453	2.572067
C	-4.332743	-0.262418	2.043743
C	-3.992258	-2.707037	2.377020
C	-5.368985	-2.881224	2.792803
C	-6.653294	0.228238	1.496445
N	-5.851943	0.599396	0.404590
C	-4.497088	0.315757	0.627421
C	-7.644064	-1.971750	3.275902
C	-8.509075	-2.493197	2.137910
C	-9.129908	-3.847408	2.394827
C	-8.194966	-4.918497	2.917268
C	-6.806126	-4.912988	2.309147
C	-5.756857	-4.264662	3.199084
O	-7.865495	0.453393	1.554017
O	-3.609126	0.528009	-0.205129
H	-6.201106	1.023679	-0.418912
H	-7.708373	-2.658010	4.162661
H	-8.039492	-0.971691	3.603585
H	-3.359611	-3.610831	2.365021
H	-1.870982	-1.932269	0.823189
H	-1.028542	-0.023888	-0.683103
H	1.111201	0.221204	-1.950689
H	3.293312	0.189634	-0.740138
H	3.343160	-0.077512	1.740498
H	1.203338	-0.318117	3.015478
H	-5.893483	0.163573	3.519304
H	-3.805535	0.521190	2.667582
H	-6.824511	-4.412358	1.306886
H	-6.495877	-5.978526	2.131644
H	-8.671650	-5.915954	2.711481
H	-8.121988	-4.832549	4.034697
H	-9.332543	-1.752062	1.947427
H	-7.903931	-2.536137	1.193174
H	-9.970913	-3.730909	3.130654
H	-9.586302	-4.202143	1.430911
H	-4.842652	-4.919789	3.198834
H	-6.118155	-4.231126	4.264126

C-4Cd PM3

C	0.019433	0.137878	-0.282854
C	0.025689	0.093222	1.246592
C	1.524129	0.072332	1.652194
C	2.279633	-0.008795	0.320416
N	1.357796	0.154405	-0.762503
C	-0.776049	1.214810	1.825211
C	-0.238221	2.158857	2.614409
C	1.171892	2.161041	2.969078
C	2.005784	1.200246	2.514546
N	-2.202030	1.282604	1.537608
C	-3.073554	0.249269	2.005110
O	-2.718478	-0.484256	2.914080
C	3.452560	1.154166	2.902535
C	4.267383	2.212837	2.157545
C	4.943206	3.216680	3.075734
C	3.985264	4.012126	3.956354
C	2.604013	4.228810	3.347447
C	1.580781	3.246272	3.917094
O	3.453420	-0.209889	0.089691
O	-0.922315	0.152673	-1.053290
C	-4.426921	0.212062	1.378664
C	-4.561668	-0.002338	0.006171
C	-5.830344	-0.050674	-0.561047
C	-6.959489	0.115941	0.234563
C	-6.822786	0.325185	1.602899
C	-5.557945	0.369426	2.179591
H	1.602045	0.023938	-1.718750
H	3.537219	1.291369	4.001263
H	3.872502	0.147514	2.705414
H	-0.855596	2.962998	3.041300
H	-2.378545	1.572081	0.598548
H	-3.675761	-0.141323	-0.626655
H	-5.938569	-0.221290	-1.637364
H	-7.956612	0.079587	-0.216624
H	-7.711823	0.451590	2.229574
H	-5.448240	0.521177	3.259477
H	1.727691	-0.865760	2.227800
H	-0.448747	-0.867090	1.575562
H	2.653663	4.142206	2.240022
H	2.267683	5.262676	3.552952
H	4.449038	4.989940	4.190712
H	3.865916	3.503744	4.937752
H	5.032422	1.718511	1.528040
H	3.611131	2.772138	1.452870
H	5.684516	2.701916	3.718560
H	5.532640	3.915242	2.448270
H	0.677147	3.804408	4.239324
H	1.983671	2.781569	4.844419

**T-4Cd
AM1**

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.398173
C	1.209195	0.000000	2.102507
C	2.416007	-0.012723	1.404106
C	2.417571	-0.016531	0.009220
C	1.210888	-0.005905	-0.691330
C	-1.271255	0.030400	2.178745
O	-1.436163	0.813886	3.131967
N	-2.251379	-0.869966	1.776425
C	-3.515137	-1.032094	2.370465
C	-3.611509	-0.942532	3.865050
C	-5.032800	-1.071810	4.459882
C	-6.148553	-1.309770	3.503916
C	-5.935380	-1.441232	2.173907
C	-4.611861	-1.291536	1.609701
C	-4.915760	-2.219361	5.483181
N	-3.618595	-2.749574	5.441388
C	-2.801343	-2.074316	4.522324
O	-1.618568	-2.365546	4.325520
O	-5.783302	-2.619778	6.265521
C	-7.515601	-1.314618	4.100769
C	-8.195200	0.034823	3.921479
C	-9.434297	-0.000432	3.054083
C	-9.318235	-0.765396	1.751989
C	-8.008973	-0.580932	1.010535
C	-7.033041	-1.732035	1.204452
H	-3.310396	-3.501627	6.006766
H	-8.129109	-2.127764	3.627798
H	-7.454752	-1.557806	5.196717
H	-4.533947	-1.371290	0.512319
H	-2.068104	-1.429770	0.974134
H	-0.946512	0.023329	-0.560404
H	1.212862	-0.000489	-1.791257
H	3.371048	-0.024779	-0.539818
H	3.367089	-0.016933	1.957072
H	1.195869	0.014640	3.204067
H	-5.271316	-0.135769	5.043031
H	-3.158400	0.036092	4.206602
H	-7.528328	0.385522	1.312123
H	-8.234453	-0.501452	-0.087494
H	-10.157621	-0.426340	1.084679
H	-9.496284	-1.857096	1.946368
H	-8.489236	0.429448	4.931400
H	-7.465804	0.772190	3.491164
H	-10.279295	-0.448528	3.643856
H	-9.722020	1.061887	2.826079
H	-6.585231	-1.988448	0.205364
H	-7.580119	-2.652259	1.549099

**T-4Cd
PM3**

C	-0.008010	0.820623	0.072414
C	-0.140558	0.094509	1.255501
C	0.927206	-0.656810	1.746269
C	2.125822	-0.687149	1.041092
C	2.258066	0.027619	-0.145004
C	1.192754	0.781166	-0.627774
C	-1.421570	0.152359	2.019584
O	-1.828940	1.143002	2.601337
N	-2.143212	-1.083486	2.071508
C	-3.485663	-1.165606	2.601904
C	-3.655386	-0.898892	4.065763
C	-5.094314	-1.130506	4.601914
C	-6.166146	-1.370465	3.585382
C	-5.879847	-1.596780	2.285451
C	-4.512464	-1.517031	1.804114
C	-4.968626	-2.305278	5.579574
N	-3.604541	-2.721757	5.648161
C	-2.772133	-1.840722	4.891486
O	-1.564069	-1.912821	4.975738
O	-5.808788	-2.860368	6.257941
C	-7.568400	-1.266895	4.101019
C	-8.124113	0.134086	3.835155
C	-9.266799	0.170285	2.828094
C	-9.152463	-0.839150	1.697720
C	-7.846394	-0.758117	0.914997
C	-6.905886	-1.916849	1.242412
H	-3.255992	-3.337777	6.348336
H	-8.210369	-2.042001	3.622858
H	-7.603732	-1.490537	5.185358
H	-4.362419	-1.728201	0.734906
H	-2.001485	-1.664737	1.273876
H	-0.841576	1.427612	-0.297807
H	1.300162	1.349154	-1.557776
H	3.203244	0.000695	-0.697410
H	2.967452	-1.273781	1.424321
H	0.824820	-1.213976	2.685466
H	-5.402559	-0.228156	5.188645
H	-3.352733	0.160059	4.266554
H	-7.341515	0.212011	1.089889
H	-8.071466	-0.781224	-0.169099
H	-10.011032	-0.704875	1.012174
H	-9.260599	-1.863638	2.125129
H	-8.475089	0.579304	4.786843
H	-7.307964	0.802303	3.490726
H	-10.227243	-0.006265	3.353172
H	-9.342667	1.194219	2.410791
H	-6.388034	-2.237278	0.314384
H	-7.492081	-2.802099	1.570549

**C-4Ca
AM1**

C	0.318508	1.018863	0.353289
C	0.221952	-0.368027	1.012065
C	-1.254972	-0.519415	1.416592
C	-1.864927	0.872068	1.159875
N	-0.914852	1.694860	0.505238
C	0.767433	-1.427098	0.099561
C	-0.030877	-2.404708	-0.398664
C	-1.444820	-2.485050	-0.094365
C	-2.033812	-1.592521	0.735471
N	2.135034	-1.357556	-0.231511
C	3.151170	-1.098298	0.681562
O	2.957585	-1.136928	1.910808
C	-3.485629	-1.645857	1.073152
C	-4.341365	-1.048757	-0.034192
C	-5.275641	-2.032249	-0.701548
C	-4.661741	-3.351586	-1.121962
C	-3.258464	-3.257205	-1.688178
C	-2.175292	-3.641948	-0.692143
O	-2.992312	1.236849	1.502265
O	1.316123	1.483999	-0.206216
C	4.489421	-0.808577	0.092324
C	4.631782	0.206223	-0.860010
C	5.893909	0.487181	-1.381899
C	7.005483	-0.242010	-0.957810
C	6.860508	-1.247969	-0.002021
C	5.603097	-1.531262	0.530166
C	-1.164908	3.019773	0.073081
H	-3.784543	-2.711056	1.267031
H	-3.669874	-1.074314	2.023598
H	0.379008	-3.185350	-1.061871
H	2.352990	-1.329090	-1.201722
H	3.754635	0.796122	-1.174807
H	6.011431	1.288311	-2.126502
H	7.999359	-0.019334	-1.374053
H	7.738783	-1.816258	0.337994
H	5.481192	-2.310363	1.298411
H	-1.318132	-0.706770	2.527949
H	0.858234	-0.335877	1.948372
H	-3.069476	-2.226283	-2.084448
H	-3.184946	-3.957661	-2.564010
H	-5.332521	-3.805432	-1.902080
H	-4.674191	-4.059567	-0.250198
H	-4.953771	-0.212278	0.400476
H	-3.679913	-0.580312	-0.811192
H	-6.131550	-2.252462	-0.007826
H	-5.710789	-1.529006	-1.607458
H	-1.439731	-4.313106	-1.215079
H	-2.615801	-4.251516	0.144727
C	-0.126376	3.975787	0.048428
C	-0.384622	5.273665	-0.383066
C	-1.664500	5.648124	-0.787475
C	-2.695363	4.710727	-0.761499
C	-2.458700	3.405516	-0.340310
H	0.895732	3.699201	0.353372
H	0.435164	6.007625	-0.400595
H	-1.859980	6.676398	-1.123730
H	-3.709758	4.998961	-1.076039
H	-3.291530	2.684583	-0.313816

**C-4Ca
PM3**

C	0.223951	1.172218	0.270791
C	0.259497	-0.222189	0.902970
C	-1.190243	-0.510641	1.358054
C	-1.924798	0.822693	1.158867
N	-1.079003	1.744990	0.439762
C	0.847794	-1.229437	-0.032805
C	0.138193	-2.255015	-0.530851
C	-1.258240	-2.467718	-0.186948
C	-1.891472	-1.655141	0.687339
N	2.246246	-1.105361	-0.418334
C	3.273892	-1.186638	0.572166
O	3.039981	-1.700414	1.654821
C	-3.309551	-1.897832	1.106459
C	-4.295937	-1.472035	0.017588
C	-5.163433	-2.609262	-0.494017
C	-4.386891	-3.772415	-1.102483
C	-3.057179	-3.378535	-1.736718
C	-1.881439	-3.680336	-0.807351
O	-3.027737	1.137738	1.558964
O	1.139885	1.755210	-0.282686
C	4.619561	-0.700412	0.149820
C	4.798499	0.628171	-0.238390
C	6.061984	1.071094	-0.613732
C	7.142110	0.194153	-0.604748
C	6.962333	-1.128389	-0.213198
C	5.703114	-1.578481	0.169159
C	-1.463160	3.077075	0.023679
H	-3.434558	-2.973551	1.352918
H	-3.530912	-1.361191	2.050624
H	0.596912	-2.989548	-1.209138
H	2.383304	-0.382726	-1.093475
H	3.952666	1.327289	-0.241461
H	6.205181	2.113800	-0.916254
H	8.135048	0.546489	-0.903252
H	7.813556	-1.817164	-0.201685
H	5.561682	-2.616716	0.490639
H	-1.188395	-0.751349	2.451272
H	0.915462	-0.175458	1.810960
H	-3.067938	-2.302246	-2.015725
H	-2.921608	-3.932924	-2.684624
H	-5.028020	-4.270227	-1.855687
H	-4.196423	-4.544937	-0.326163
H	-4.944053	-0.659481	0.399131
H	-3.744476	-1.038864	-0.847455
H	-5.807150	-2.990740	0.323203
H	-5.861411	-2.196876	-1.250256
H	-1.104121	-4.238592	-1.369607
H	-2.209857	-4.370777	0.001130
C	-0.552704	3.879881	-0.674216
C	-0.934622	5.151514	-1.081247
C	-2.210491	5.628450	-0.799306
C	-3.111141	4.829757	-0.102156
C	-2.746744	3.555856	0.313346
H	0.460996	3.487460	-0.884214
H	-0.222435	5.778783	-1.627346
H	-2.504825	6.631587	-1.123957
H	-4.115227	5.203350	0.124144
H	-3.448431	2.908612	0.875078

**T-4Ca
AM1**

C	-0.349944	1.300975	0.308790
C	0.015581	-0.121803	0.768327
C	1.545301	-0.106492	0.951000
C	1.956143	1.350292	0.657979
N	0.819027	2.098287	0.271480
C	2.337376	-1.065760	0.132513
C	1.752941	-1.885590	-0.771985
C	0.315527	-1.921118	-0.929435
C	-0.521039	-1.133770	-0.202126
N	-1.914530	-1.229302	-0.361515
C	-2.859368	-1.124932	0.652873
O	-2.542219	-0.943720	1.843095
C	3.797268	-1.118789	0.434068
C	4.122100	-2.283677	1.357674
C	5.019614	-3.335487	0.743675
C	4.653692	-3.794895	-0.652424
C	3.169711	-3.976082	-0.903140
C	2.532142	-2.811557	-1.646325
O	3.091949	1.817283	0.778610
O	-1.483965	1.702223	0.037458
C	-4.285400	-1.241671	0.229749
C	-4.713427	-2.257988	-0.629788
C	-6.059734	-2.344023	-0.982419
C	-6.975426	-1.417085	-0.483227
C	-6.547756	-0.406146	0.377509
C	-5.204264	-0.317664	0.739983
C	0.847338	3.466459	-0.092588
H	4.375802	-1.206258	-0.524574
H	4.125461	-0.158849	0.918159
H	-0.081302	-2.650866	-1.655191
H	-2.239387	-1.414105	-1.283987
H	-4.001323	-3.002231	-1.016469
H	-6.398996	-3.146012	-1.654438
H	-8.036340	-1.486030	-0.766674
H	-7.269931	0.322450	0.774924
H	-4.857151	0.469316	1.428403
H	1.787292	-0.298689	2.036778
H	-0.474894	-0.281476	1.775716
H	2.634201	-4.153763	0.065185
H	3.028344	-4.900956	-1.525607
H	5.168857	-4.778598	-0.830642
H	5.082696	-3.077967	-1.402926
H	4.631143	-1.886114	2.276888
H	3.170848	-2.768949	1.704810
H	6.072434	-2.943965	0.713855
H	5.021198	-4.225869	1.429620
H	1.853449	-3.227497	-2.440604
H	3.319355	-2.216425	-2.185765
C	-0.254740	4.305873	0.179209
C	-0.215650	5.647673	-0.188921
C	0.906699	6.180586	-0.819837
C	1.999957	5.358762	-1.087133
C	1.980221	4.012577	-0.734515
H	-1.157463	3.903660	0.666640
H	-1.083608	6.289377	0.025178
H	0.929914	7.242251	-1.104216
H	2.891434	5.772073	-1.582497
H	2.861174	3.384309	-0.942549

**T-4Ca
PM3**

C	-0.189018	1.428312	0.679506
C	0.152093	-0.057192	0.855230
C	1.697513	-0.109736	0.844469
C	2.142873	1.279233	0.367461
N	0.999971	2.153316	0.308772
C	2.329668	-1.202946	0.041133
C	1.626223	-1.917839	-0.862601
C	0.196728	-1.711698	-1.013590
C	-0.500108	-0.883008	-0.212280
N	-1.928336	-0.730246	-0.381323
C	-2.854351	-1.167427	0.621956
O	-2.469824	-1.492246	1.731614
C	3.766445	-1.479649	0.359112
C	3.871913	-2.640830	1.350324
C	4.508674	-3.898057	0.771261
C	4.188551	-4.159401	-0.691285
C	2.697642	-4.215163	-1.006237
C	2.218640	-2.969037	-1.749334
O	3.265540	1.657922	0.095525
O	-1.264038	1.971534	0.836436
C	-4.286957	-1.133599	0.204361
C	-4.989988	-2.327534	0.047238
C	-6.329913	-2.292750	-0.322941
C	-6.966426	-1.072500	-0.527155
C	-6.264692	0.116872	-0.359428
C	-4.923062	0.091818	0.007126
C	1.046619	3.563097	-0.012068
H	4.327993	-1.708019	-0.575813
H	4.253753	-0.576300	0.775917
H	-0.297917	-2.300359	-1.800365
H	-2.232056	-0.914870	-1.312933
H	-4.492753	-3.287455	0.224891
H	-6.885103	-3.228230	-0.448248
H	-8.022439	-1.048493	-0.816136
H	-6.768630	1.076969	-0.513035
H	-4.370963	1.029061	0.147147
H	2.053569	-0.232766	1.899376
H	-0.230592	-0.410409	1.846543
H	2.105133	-4.367389	-0.082965
H	2.493226	-5.102600	-1.636416
H	4.673557	-5.105830	-0.998237
H	4.663755	-3.359663	-1.306545
H	4.457911	-2.320603	2.234153
H	2.865755	-2.886981	1.748120
H	5.610550	-3.836277	0.878004
H	4.201313	-4.768757	1.384245
H	1.465515	-3.266163	-2.508648
H	3.057074	-2.524282	-2.327428
C	-0.123456	4.330599	0.042038
C	-0.071050	5.680831	-0.277774
C	1.132632	6.271483	-0.648185
C	2.293762	5.507129	-0.697599
C	2.260563	4.155358	-0.381645
H	-1.071798	3.844077	0.343224
H	-0.986319	6.280208	-0.235338
H	1.166316	7.336410	-0.899012
H	3.243356	5.969393	-0.986402
H	3.175829	3.531976	-0.409409

**C-4Ce
AM1**

C	0.213555	-0.653675	0.336095
C	0.155121	-0.000383	1.572604
C	1.202469	0.831962	1.980058
C	2.300988	1.019044	1.141371
C	2.353858	0.380932	-0.098161
C	1.311954	-0.456032	-0.499022
C	-1.024374	-0.247657	2.449017
O	-1.503690	-1.385720	2.607943
N	-1.570527	0.873744	3.068025
C	-2.684095	0.860983	3.925828
C	-2.735120	-0.209257	4.975902
C	-3.987695	-0.213787	5.873709
C	-4.947387	0.913269	5.706091
C	-4.797446	1.837750	4.729034
C	-3.663338	1.798444	3.830657
C	-3.416664	-0.263537	7.284009
O	-2.025764	-0.162384	7.270504
C	-1.576502	-0.083604	5.950854
O	-0.372614	0.048805	5.810602
O	-3.926026	-0.399535	8.384162
C	-5.804136	2.908674	4.466294
C	-5.930472	3.939122	5.577977
C	-7.153085	3.738794	6.451920
C	-6.887645	3.070673	7.785082
C	-5.879516	1.944224	7.774051
C	-6.089382	0.923626	6.665031
H	-7.041677	1.138522	6.109821
H	-6.199840	-0.095914	7.125485
H	-3.624649	2.577985	3.050857
H	-1.236987	1.769347	2.790434
H	1.178435	1.319612	2.967195
H	3.129274	1.667791	1.463017
H	3.221441	0.533042	-0.757745
H	1.357996	-0.966989	-1.472180
H	-0.604218	-1.328997	0.038910
H	-4.556861	-1.174676	5.705275
H	-2.642657	-1.219242	4.469421
H	-5.002624	3.944566	6.206296
H	-6.002130	4.953623	5.099729
H	-7.611638	4.744062	6.661037
H	-7.930287	3.152263	5.892229
H	-5.927052	1.412417	8.763317
H	-4.844350	2.373234	7.701150
H	-7.865444	2.683118	8.180148
H	-6.524956	3.845508	8.514072
H	-5.532499	3.446744	3.516847
H	-6.798891	2.418599	4.275988

**C-4Ce
PM3**

C	0.011866	0.005704	0.001299
C	0.004181	0.002257	1.396083
C	1.205889	0.009295	2.106005
C	2.412538	0.028015	1.415337
C	2.422290	0.041846	0.024057
C	1.223452	0.030071	-0.681238
C	-1.298005	-0.035303	2.121450
O	-2.148505	-0.896855	1.965942
N	-1.560110	1.076276	2.983359
C	-2.625387	0.997419	3.972028
C	-2.524746	-0.018640	5.062959
C	-3.702289	-0.031436	6.068459
C	-4.799170	0.962094	5.842078
C	-4.783954	1.815647	4.794818
C	-3.671975	1.831806	3.857328
C	-3.003811	0.154597	7.420587
O	-1.631175	0.314846	7.281950
C	-1.299726	0.227425	5.945853
O	-0.124337	0.345702	5.707460
O	-3.373001	0.155226	8.564409
C	-5.904995	2.751174	4.461398
C	-6.147533	3.841382	5.505214
C	-7.414536	3.571624	6.309903
C	-7.167668	2.959209	7.684542
C	-5.923881	2.091695	7.772572
C	-5.939502	0.901175	6.812125
H	-6.894326	0.861719	6.246627
H	-5.905424	-0.046037	7.386746
H	-3.732669	2.556137	3.031543
H	-0.742022	1.514611	3.350998
H	1.207063	-0.009493	3.203230
H	3.356735	0.030910	1.970288
H	3.374882	0.058960	-0.515909
H	1.231573	0.036011	-1.776269
H	-0.933652	-0.016860	-0.552526
H	-4.181535	-1.042514	6.060370
H	-2.430837	-1.028158	4.587132
H	-5.272170	3.933250	6.184740
H	-6.235021	4.819033	4.994558
H	-7.983889	4.512569	6.438743
H	-8.079580	2.907989	5.715596
H	-5.801739	1.729886	8.811887
H	-5.036404	2.733192	7.569942
H	-8.059070	2.374605	7.986892
H	-7.077031	3.768138	8.437250
H	-5.702201	3.223822	3.477927
H	-6.835737	2.159069	4.315199

**T-4Ce
AM1**

C	-0.140440	0.017396	0.245330
C	-0.203119	0.023804	1.764071
C	1.266658	0.169205	2.204765
C	2.024152	0.317610	0.891966
O	1.166177	0.217151	-0.202401
C	1.835025	-0.918552	3.047719
C	1.103353	-1.997506	3.411295
C	-0.285658	-2.123669	3.026208
C	-0.924181	-1.191305	2.271408
N	-2.272628	-1.342972	1.903764
C	-3.229353	-0.331671	1.941313
O	-2.953247	0.821084	2.322034
C	3.234421	-0.696782	3.513316
C	3.260116	-0.132672	4.925936
C	3.893537	-1.046982	5.951654
C	3.466284	-2.499477	5.909500
C	1.988430	-2.729900	5.662844
C	1.664161	-3.115177	4.226966
O	3.195241	0.531703	0.624596
O	-0.983245	-0.109164	-0.626618
C	-4.604251	-0.717421	1.515400
C	-5.688383	-0.259331	2.273010
C	-6.987564	-0.589171	1.890584
C	-7.205976	-1.363147	0.750394
C	-6.124793	-1.805627	-0.012244
C	-4.821395	-1.485839	0.367312
H	3.802721	-1.664579	3.467885
H	3.759622	0.013600	2.817598
H	-0.819753	-3.016528	3.393297
H	-2.582925	-2.273376	1.735070
H	-5.505606	0.368908	3.159014
H	-7.840456	-0.231794	2.486470
H	-8.232641	-1.619613	0.448621
H	-6.298139	-2.404088	-0.918984
H	-3.973886	-1.817871	-0.252609
H	1.386031	1.139360	2.770991
H	-0.778543	0.947312	2.079697
H	1.402255	-1.821795	5.959182
H	1.646421	-3.567413	6.329494
H	3.739552	-2.960671	6.898206
H	4.072204	-3.041953	5.134990
H	3.833798	0.833260	4.920156
H	2.215464	0.118717	5.252233
H	5.010141	-1.012057	5.830373
H	3.662076	-0.630196	6.969503
H	0.927929	-3.964879	4.245976
H	2.583770	-3.507090	3.711385

**T-4Ce
PM3**

C	0.058792	-0.008965	0.024833
C	-0.015710	0.017607	1.555229
C	1.471918	0.043658	1.986419
C	2.225988	-0.073265	0.656400
O	1.365727	-0.086777	-0.427806
C	1.916796	-0.989613	2.971146
C	1.109070	-2.000383	3.357794
C	-0.261111	-2.077683	2.883314
C	-0.800978	-1.144246	2.075608
N	-2.167727	-1.265831	1.622668
C	-3.174019	-0.306269	1.968573
O	-2.871534	0.761772	2.472314
C	3.282803	-0.772137	3.544735
C	3.182225	-0.035590	4.882304
C	3.598279	-0.871365	6.086387
C	3.250262	-2.347582	5.989474
C	1.774620	-2.627631	5.726495
C	1.523051	-3.094109	4.293468
O	3.389484	-0.127559	0.354899
O	-0.761217	0.041266	-0.852933
C	-4.567545	-0.705472	1.615560
C	-5.514366	-0.869405	2.626391
C	-6.818317	-1.222448	2.296790
C	-7.177705	-1.401770	0.964686
C	-6.233662	-1.226546	-0.042003
C	-4.925801	-0.878005	0.278416
H	3.804156	-1.748717	3.671966
H	3.913742	-0.196829	2.838837
H	-0.849959	-2.934940	3.242475
H	-2.495231	-2.207694	1.619200
H	-5.234874	-0.710430	3.673839
H	-7.563894	-1.353377	3.088085
H	-8.206232	-1.676929	0.708170
H	-6.519354	-1.360038	-1.090856
H	-4.184322	-0.732054	-0.516441
H	1.706340	1.042738	2.432598
H	-0.517646	0.964014	1.879965
H	1.157021	-1.738076	5.958730
H	1.425987	-3.416833	6.420814
H	3.567879	-2.850137	6.923153
H	3.861025	-2.803387	5.175109
H	3.809156	0.877118	4.849646
H	2.146452	0.334023	5.029980
H	4.693480	-0.783761	6.235443
H	3.140941	-0.436814	6.997624
H	0.738325	-3.879158	4.299643
H	2.431046	-3.591529	3.889524

**5Cd
AM1**

C	5.382400	0.854522	-0.296166
C	4.354590	-0.052083	-0.020367
C	4.608145	-1.207267	0.727125
C	5.896259	-1.448491	1.203084
C	6.922461	-0.540426	0.939038
C	6.666076	0.608248	0.190135
C	2.990809	0.206834	-0.561449
O	2.787622	0.452926	-1.767580
N	1.955444	0.189607	0.365229
C	0.561252	0.179383	-0.016894
C	0.208585	-1.028063	-0.926201
C	-1.290312	-1.018979	-1.308842
C	-2.036036	0.125226	-0.573918
C	-1.366191	1.407758	-1.158478
C	0.154076	1.429166	-0.860338
C	-1.720746	-2.473454	-1.070563
N	-0.710006	-3.151339	-0.362799
C	0.441497	-2.365169	-0.220441
C	-0.375618	0.139629	1.173705
C	-1.698194	0.151675	0.899457
C	-1.893548	2.715324	-0.553415
N	-0.826798	3.425850	0.013510
C	0.398422	2.743664	-0.117747
H	-0.777508	-4.096464	-0.075410
O	1.462942	-2.735769	0.368881
O	-2.718956	-3.048519	-1.513107
C	-3.524012	0.154935	-0.901676
C	-4.318220	-1.049272	-0.441505
C	-5.493832	-0.712788	0.445612
C	-5.129371	-0.110077	1.786797
C	-3.764260	-0.491578	2.327302
C	-2.681097	0.503133	1.958455
O	-3.054610	3.138085	-0.571517
H	-0.922046	4.312022	0.444733
O	1.468070	3.199003	0.291180
H	-3.963802	1.086531	-0.448987
H	-3.625260	0.256010	-2.016307
H	0.038341	0.170243	2.189126
H	2.154941	-0.162487	1.274914
H	3.799952	-1.933167	0.920028
H	6.101744	-2.358335	1.786073
H	7.936720	-0.732803	1.319608
H	7.476501	1.321309	-0.021249
H	5.171478	1.752330	-0.897773
H	-1.412751	-0.840635	-2.413515
H	0.855580	-0.997696	-1.846940
H	-1.555213	1.446747	-2.263577
H	0.758108	1.442775	-1.809257
H	-3.480715	-1.529108	2.020435
H	-3.836161	-0.509006	3.450545
H	-5.906983	-0.430962	2.532617
H	-5.201938	1.009002	1.718427
H	-4.697186	-1.602926	-1.343688
H	-3.657740	-1.766576	0.111622
H	-6.181085	-0.007377	-0.093091
H	-6.070161	-1.662362	0.618451
H	-2.100409	0.731104	2.898013
H	-3.154244	1.476098	1.634521

**5Cd
PM3**

C	0.451228	2.740368	-0.227411
C	0.135282	1.421054	-0.924589
C	-1.404190	1.433906	-1.160262
C	-1.876310	2.764557	-0.576144
N	-0.772775	3.442123	0.020800
C	0.535867	0.161788	-0.099459
C	0.154001	-1.060964	-0.967896
C	-1.358113	-1.011963	-1.325529
C	-2.072995	0.147841	-0.550236
C	-1.671755	0.157864	0.912385
C	-0.342248	0.135263	1.126348
C	-1.808513	-2.457917	-1.118422
N	-0.843297	-3.149216	-0.311138
C	0.368048	-2.396907	-0.263378
N	1.972598	0.193343	0.294035
C	3.048611	0.121195	-0.639666
O	2.857729	0.289267	-1.834914
C	-3.580448	0.196138	-0.836751
C	-4.409878	-0.983289	-0.346142
C	-5.529051	-0.602255	0.606467
C	-5.045286	-0.071668	1.950562
C	-3.670873	-0.582029	2.373278
C	-2.593321	0.446173	2.051155
O	-2.733397	-3.071229	-1.609065
O	1.364596	-2.843654	0.270491
O	-2.973451	3.286977	-0.594987
O	1.511998	3.234013	0.088522
C	4.393923	-0.092700	-0.030673
C	5.336833	0.933743	-0.072509
C	6.596104	0.732038	0.482942
C	6.914032	-0.488619	1.069250
C	5.972608	-1.512610	1.103019
C	4.709279	-1.318935	0.555315
H	-0.871921	-4.133345	-0.161401
H	-0.811669	4.388634	0.327229
H	-3.992847	1.129489	-0.398934
H	-3.714277	0.300231	-1.933164
H	0.104886	0.166628	2.127115
H	2.150446	-0.300571	1.144169
H	3.970374	-2.129801	0.578208
H	6.225269	-2.474783	1.560724
H	7.907174	-0.644803	1.503310
H	7.338266	1.536746	0.455244
H	5.085398	1.892383	-0.540852
H	-1.488931	-0.794342	-2.415401
H	0.765694	-1.060820	-1.905252
H	-1.624436	1.456652	-2.255845
H	0.674003	1.405104	-1.904496
H	-3.442517	-1.561582	1.902921
H	-3.670078	-0.773144	3.463756
H	-5.794532	-0.324655	2.725184
H	-5.010960	1.039784	1.924073
H	-4.844042	-1.515247	-1.215594
H	-3.767348	-1.726006	0.175849
H	-6.198483	0.144080	0.134657
H	-6.159239	-1.499568	0.771195
H	-1.981764	0.613896	2.962189
H	-3.080951	1.425886	1.838960

**6Cd
AM1**

C	0.313852	-1.473218	2.182332
C	-0.062309	-0.117225	1.579722
C	-1.609073	-0.115521	1.526603
C	-2.012863	-1.491603	2.068910
N	-0.854720	-2.198063	2.447157
C	0.540241	0.083881	0.152928
C	0.045245	1.478105	-0.325549
C	-1.501024	1.512813	-0.334008
C	-2.112190	0.158474	0.088512
C	-1.485699	-0.909448	-0.783065
C	-0.137449	-0.921963	-0.762814
C	-1.866341	2.672294	0.601573
N	-0.687669	3.257800	1.092458
C	0.466458	2.618918	0.599896
N	1.979686	-0.025507	0.183607
C	2.773342	0.057357	-0.947423
O	2.289700	0.350490	-2.060311
C	-3.635483	0.199503	0.074913
C	-4.255554	0.732371	-1.202132
C	-5.221093	-0.226907	-1.860240
C	-4.642214	-1.578561	-2.224397
C	-3.170547	-1.579648	-2.591308
C	-2.266638	-1.986089	-1.441241
O	-2.995259	3.079736	0.892109
O	1.610555	2.971899	0.895725
O	-3.152222	-1.944261	2.204036
O	1.456113	-1.876959	2.428917
C	4.232387	-0.188724	-0.766105
C	5.124351	0.564341	-1.539770
C	6.497170	0.359964	-1.412751
C	6.981839	-0.598582	-0.522584
C	6.092661	-1.355980	0.240096
C	4.717649	-1.153652	0.122783
H	-0.670298	4.062422	1.669347
H	-0.865594	-3.110764	2.831695
H	-4.017061	-0.835463	0.290209
H	-3.966188	0.854570	0.928327
H	0.488991	-1.601389	-1.353649
H	2.395508	-0.261732	1.057122
H	4.029139	-1.767634	0.724911
H	6.474356	-2.116169	0.937657
H	8.065782	-0.759103	-0.423429
H	7.196953	0.954989	-2.017935
H	4.728841	1.308895	-2.249132
H	-1.860035	1.781794	-1.362614
H	0.465979	1.671508	-1.351446
H	-2.032043	0.663073	2.216959
H	0.317224	0.688706	2.262914
H	-2.859961	-0.586653	-3.004061
H	-3.021374	-2.325119	-3.420331
H	-5.227054	-1.977859	-3.097681
H	-4.818569	-2.293833	-1.376245
H	-4.806667	1.682256	-0.960129
H	-3.470908	1.007640	-1.953727
H	-6.102628	-0.387398	-1.183413
H	-5.609999	0.266656	-2.792160
H	-1.537581	-2.752415	-1.830305
H	-2.869282	-2.499233	-0.638519

**6Cd
PM3**

C	4.663681	-1.334163	-0.183133
C	4.247224	-0.152696	-0.798142
C	5.187670	0.778588	-1.238582
C	6.543540	0.529654	-1.053181
C	6.960338	-0.646250	-0.438319
C	6.021091	-1.577562	-0.006502
C	2.795196	0.118732	-1.013362
O	2.298780	0.339445	-2.107950
N	2.009891	0.193849	0.171617
C	0.520109	0.161437	0.167533
C	-0.029381	-0.093683	1.604162
C	-1.587752	-0.126968	1.581453
C	-2.118437	0.085732	0.134300
C	-1.593316	1.472544	-0.337694
C	-0.043421	1.519984	-0.333877
C	-1.966546	-1.465503	2.208836
N	-0.775857	-2.176781	2.554824
C	0.385559	-1.437499	2.200413
C	-0.086409	-0.897882	-0.719935
C	-1.429825	-0.952764	-0.738353
C	-2.026151	2.660355	0.518947
N	-0.869325	3.302560	1.062670
C	0.327846	2.725128	0.522252
O	1.494691	-1.890452	2.410612
O	-3.053858	-1.938775	2.464654
C	-3.653324	0.033810	0.100503
C	-4.275755	0.567576	-1.187816
C	-5.181707	-0.427526	-1.890648
C	-4.483192	-1.699150	-2.359944
C	-2.996104	-1.531943	-2.653641
C	-2.147318	-2.025275	-1.483239
O	-3.133908	3.097077	0.756251
O	1.407388	3.218787	0.767059
H	-0.896835	4.207411	1.477733
H	-0.760843	-3.081926	2.968519
H	-3.982744	-1.011178	0.278603
H	-4.047085	0.613591	0.960350
H	0.559428	-1.563775	-1.302009
H	2.427540	-0.240805	0.967882
H	3.930360	-2.073907	0.158710
H	6.349710	-2.504478	0.475205
H	8.028493	-0.840142	-0.294648
H	7.282995	1.261638	-1.394665
H	4.857261	1.700690	-1.730637
H	-1.984717	1.631191	-1.378237
H	0.336700	1.697399	-1.371069
H	-2.002921	0.681901	2.231310
H	0.332201	0.715926	2.284258
H	-2.761196	-0.471134	-2.890682
H	-2.730277	-2.104703	-3.562345
H	-5.002982	-2.077541	-3.261311
H	-4.604314	-2.497115	-1.595169
H	-4.850496	1.487923	-0.964823
H	-3.477782	0.881606	-1.905360
H	-6.028165	-0.699595	-1.229352
H	-5.641034	0.082257	-2.761534
H	-1.404849	-2.761103	-1.854156
H	-2.787832	-2.588251	-0.767540

**5Ca
AM1**

C	5.503751	-1.334299	-0.594578	H	7.540920	-2.038474	-0.592653
C	4.503670	-0.625574	0.105121	H	5.287036	-1.790234	-1.574263
C	4.815599	-0.065069	1.363186	H	-4.342020	-2.694859	0.884711
C	6.092314	-0.215842	1.896039	H	-6.593374	-2.925977	1.880546
C	7.073198	-0.922859	1.202931	H	-8.255053	-1.069128	1.711746
C	6.771876	-1.479178	-0.038525	H	-7.634391	1.042978	0.532050
N	3.204771	-0.475238	-0.439017	H	-5.388746	1.316703	-0.463907
C	2.401037	0.678147	-0.283289	H	0.312613	-5.690591	2.166712
C	1.114524	0.495355	-1.091176	H	-1.075864	-4.965134	1.284026
C	1.107964	-0.982810	-1.527191	H	1.700633	-4.386939	-1.609072
C	2.547549	-1.438483	-1.249153	H	1.786702	-3.379621	-0.124028
C	-0.148409	0.835510	-0.253274	H	0.054172	-5.904915	-0.482502
C	-1.345631	0.452503	-1.182551	H	1.663204	-5.798742	0.328651
C	-1.319963	-1.056609	-1.506770	H	-0.871149	-1.893747	2.560630
C	-0.072075	-1.746286	-0.869625	H	-1.545021	-2.915944	1.233492
C	-0.180988	-1.444396	0.607779				
C	-0.184403	-0.129009	0.914929				
C	-2.658736	-1.590497	-0.982732				
N	-3.409093	-0.526686	-0.430048				
C	-2.700798	0.702054	-0.518940				
N	-0.177379	2.220702	0.158333				
C	-0.129111	3.275900	-0.744664				
O	-0.299638	3.100217	-1.968073				
C	-0.080283	-3.225734	-1.233619				
C	1.100414	-4.028391	-0.728378				
C	0.720974	-5.225143	0.112011				
C	0.036812	-4.894470	1.422380				
C	0.383678	-3.543369	2.018226				
C	-0.591103	-2.452017	1.621529				
O	-3.142308	1.790172	-0.147740				
C	-4.698245	-0.670221	0.138174				
C	-5.645466	0.372201	0.042476				
C	-6.907361	0.220464	0.610057				
C	-7.254709	-0.956909	1.269641				
C	-6.326085	-1.991691	1.364171				
C	-5.055972	-1.858921	0.810871				
O	-3.051329	-2.758459	-1.063579				
O	2.702703	1.674092	0.382378				
O	3.103911	-2.416661	-1.753834				
C	0.103804	4.625909	-0.159118				
C	1.206676	4.853390	0.671209				
C	1.425567	6.129483	1.188528				
C	0.546734	7.169650	0.883396				
C	-0.549677	6.939370	0.052205				
C	-0.772706	5.667982	-0.475785				
H	-1.032503	-3.678711	-0.841403				
H	-0.121573	-3.300664	-2.354102				
H	-0.276591	0.260436	1.936300				
H	0.118169	2.397644	1.092572				
H	1.910705	4.034669	0.897425				
H	2.294861	6.314523	1.836610				
H	0.721084	8.174296	1.296739				
H	-1.239413	7.760849	-0.191431				
H	-1.628378	5.477804	-1.142203				
H	0.975053	-1.065453	-2.642545				
H	1.159917	1.177762	-1.985637				
H	-1.303716	-1.227534	-2.615902				
H	-1.293894	1.076500	-2.117669				
H	1.436180	-3.251047	1.777137				
H	0.338215	-3.643688	3.138471				
H	4.059144	0.510031	1.920550				
H	6.323304	0.230074	2.875230				
H	8.078426	-1.040028	1.632692				

**5Ca
PM3**

C	5.522600	0.608540	-0.029277
C	4.525454	-0.355168	0.144091
C	4.750730	-1.476895	0.949617
C	5.981037	-1.628171	1.577789
C	6.976451	-0.670313	1.411704
C	6.745680	0.443813	0.612053
N	3.242130	-0.205088	-0.511034
C	2.347041	0.898516	-0.346046
C	1.091666	0.635858	-1.179104
C	1.198093	-0.837152	-1.648754
C	2.670580	-1.176812	-1.412286
C	-0.219103	0.844338	-0.382427
C	-1.383878	0.370190	-1.304822
C	-1.229657	-1.142856	-1.625143
C	0.085082	-1.715082	-0.977818
C	-0.051349	-1.408401	0.501845
C	-0.178874	-0.099702	0.792736
C	-2.529877	-1.788478	-1.143830
N	-3.395170	-0.776177	-0.609127
C	-2.762354	0.519423	-0.662332
N	-0.416737	2.245524	0.084378
C	-0.391562	3.376353	-0.783678
O	-0.470972	3.242337	-1.995995
C	0.221809	-3.199465	-1.344013
C	1.452430	-3.925418	-0.814529
C	1.138884	-5.134104	0.049229
C	0.475622	-4.793750	1.377999
C	0.801321	-3.400394	1.906858
C	-0.315799	-2.421703	1.566338
O	-3.327757	1.521793	-0.286724
C	-4.591266	-1.061721	0.161596
C	-5.824169	-0.569347	-0.274907
C	-6.967627	-0.844949	0.467550
C	-6.885920	-1.606547	1.628248
C	-5.656111	-2.096709	2.056118
C	-4.502666	-1.826445	1.329505
O	-2.885591	-2.945499	-1.238904
O	2.609895	1.868550	0.337389
O	3.359250	-2.003381	-1.970481
C	-0.341417	4.698095	-0.092652
C	0.800750	5.076062	0.613975
C	0.841742	6.317874	1.238231
C	-0.250863	7.175908	1.161127
C	-1.387347	6.796017	0.454829
C	-1.435851	5.558062	-0.177694
H	-0.685057	-3.736612	-0.995115
H	0.203865	-3.278281	-2.450460
H	-0.315852	0.279476	1.812559
H	0.003511	2.417950	0.974453
H	1.665743	4.403421	0.672781
H	1.737628	6.619342	1.791023
H	-0.215112	8.152129	1.655898
H	-2.246227	7.472503	0.393370
H	-2.327651	5.258249	-0.740150
H	1.031661	-0.903135	-2.753672
H	1.107996	1.319946	-2.064567
H	-1.171936	-1.298585	-2.730569
H	-1.368888	0.967360	-2.250084
H	1.779815	-3.040915	1.520827
H	0.918780	-3.443183	3.006871
H	3.972343	-2.240866	1.079504
H	6.165642	-2.506071	2.205792
H	7.943100	-0.794622	1.910825

H	7.530441	1.196779	0.483250
H	5.349116	1.493895	-0.651804
H	-3.537626	-2.224052	1.668893
H	-5.594530	-2.698291	2.968974
H	-7.790679	-1.821409	2.206310
H	-7.936664	-0.459407	0.133439
H	-5.897760	0.037376	-1.184777
H	0.763070	-5.556609	2.126941
H	-0.628781	-4.879231	1.277828
H	2.081778	-4.250733	-1.666523
H	2.087949	-3.238774	-0.210944
H	0.501963	-5.849377	-0.508022
H	2.088361	-5.673887	0.240790
H	-0.611565	-1.886543	2.493115
H	-1.222298	-2.994855	1.258683

**6Ca
AM1**

C	2.095666	5.127337	1.834223	H	4.682545	-4.113595	-3.647225
C	1.075785	4.429128	1.175719	H	2.870872	-3.502153	-2.083323
C	0.229856	5.098633	0.285320	H	-4.838027	-1.232574	-0.677810
C	0.412472	6.461405	0.050912	H	-7.082212	-0.667118	-1.546935
C	1.435071	7.154853	0.698440	H	-7.359992	1.075093	-3.314884
C	2.275049	6.487789	1.590427	H	-5.352463	2.262260	-4.208620
C	0.915151	2.978635	1.479881	H	-3.093470	1.734753	-3.354506
O	1.132847	2.518044	2.619602	H	-3.100299	-3.922830	4.464267
N	0.538742	2.157681	0.431112	H	-3.413925	-3.576235	2.728952
C	0.242384	0.753812	0.588979	H	0.366526	-4.722038	2.119801
C	1.473418	-0.081584	1.045668	H	0.164882	-3.179029	3.016842
C	1.078074	-1.562744	1.198868	H	-1.958527	-5.359367	2.569441
C	-0.420360	-1.796139	0.898803	H	-1.077516	-4.946901	4.090019
C	-0.643825	-1.345888	-0.566426	H	-2.907789	-0.273170	2.893907
C	-0.219477	0.123648	-0.764188	H	-3.125137	-1.708514	1.822016
C	2.019542	-2.319509	0.253815				
N	2.890102	-1.399432	-0.382505				
C	2.617789	-0.068772	0.033471				
C	-0.843966	0.463026	1.610808				
C	-1.205840	-0.827591	1.757495				
C	-2.112283	-1.389202	-1.004635				
N	-2.508649	-0.103514	-1.460335				
C	-1.450498	0.824838	-1.343262				
C	3.927473	-1.764647	-1.274977				
C	3.782523	-2.884802	-2.122116				
C	4.807297	-3.234758	-2.996626				
C	5.981120	-2.485970	-3.053415				
C	6.130564	-1.378226	-2.221220				
C	5.121923	-1.014164	-1.333868				
O	3.224662	0.927963	-0.363823				
O	2.042487	-3.541313	0.082254				
C	-0.806607	-3.261733	1.055602				
C	-0.372482	-3.908251	2.356735				
C	-1.510773	-4.508847	3.149986				
C	-2.618427	-3.544473	3.521528				
C	-2.184065	-2.108898	3.747074				
C	-2.406122	-1.217677	2.538225				
O	-2.839015	-2.384956	-1.000370				
C	-3.799595	0.210456	-1.952776				
C	-3.964449	1.190852	-2.954945				
C	-5.237444	1.493088	-3.429919				
C	-6.358508	0.832140	-2.931476				
C	-6.202219	-0.138865	-1.944166				
C	-4.939607	-0.452325	-1.449167				
O	-1.492995	2.012673	-1.681651				
H	-1.920517	-3.347153	0.933320				
H	-0.340547	-3.831118	0.204166				
H	-1.278892	1.300566	2.169987				
H	0.386326	2.552851	-0.470178				
H	-0.589219	4.568395	-0.226236				
H	-0.254206	6.988570	-0.647511				
H	1.577570	8.228915	0.507142				
H	3.078891	7.034363	2.105265				
H	2.743626	4.592430	2.546925				
H	1.307456	-1.903859	2.243601				
H	1.850476	0.347288	2.016317				
H	-0.065794	-2.026049	-1.249060				
H	0.611766	0.205897	-1.515531				
H	-1.116405	-2.061387	4.079916				
H	-2.796011	-1.691465	4.593576				
H	5.258527	-0.127765	-0.693479				
H	7.054178	-0.780955	-2.259787				
H	6.784405	-2.767992	-3.749146				

**6Ca
PM3**

C	0.195486	5.656238	1.406169
C	-0.629524	4.586458	1.058835
C	-1.836822	4.816943	0.397511
C	-2.212137	6.118015	0.082272
C	-1.386970	7.185655	0.421716
C	-0.185394	6.954366	1.082869
C	-0.217184	3.198451	1.422536
O	0.056426	2.846477	2.560810
N	-0.073830	2.299654	0.329749
C	0.025294	0.821816	0.493085
C	1.437995	0.435604	1.011874
C	1.523898	-1.097092	1.203903
C	0.186047	-1.791118	0.812358
C	-0.077327	-1.441463	-0.682260
C	-0.214110	0.096030	-0.867374
C	2.743614	-1.536096	0.392262
N	3.307115	-0.390940	-0.267633
C	2.583855	0.807000	0.074055
C	-0.964501	0.227853	1.464821
C	-0.906547	-1.106409	1.619677
C	-1.367568	-2.033858	-1.246537
N	-2.225968	-0.965183	-1.694120
C	-1.620156	0.308879	-1.433536
C	4.484080	-0.430667	-1.114789
C	4.434610	-1.132379	-2.323458
C	5.561332	-1.169365	-3.136809
C	6.724987	-0.510100	-2.754216
C	6.768110	0.187339	-1.551629
C	5.651717	0.230649	-0.723612
O	2.912494	1.896435	-0.341636
O	3.242875	-2.638092	0.301136
C	0.268790	-3.310468	1.020563
C	0.852076	-3.729104	2.368386
C	-0.056335	-4.642916	3.171387
C	-1.395502	-4.023751	3.556704
C	-1.371476	-2.505150	3.690740
C	-1.922290	-1.828268	2.437508
O	-1.666815	-3.198348	-1.397487
C	-3.641928	-1.138541	-1.968354
C	-4.131511	-0.845882	-3.243696
C	-5.487078	-1.015689	-3.505945
C	-6.343380	-1.474830	-2.511076
C	-5.848758	-1.767037	-1.243720
C	-4.498031	-1.599403	-0.962794
O	-2.178170	1.356598	-1.691525
H	-0.742922	-3.748608	0.891997
H	0.880398	-3.749328	0.205907
H	-1.678841	0.873089	1.987241
H	-0.531442	2.591628	-0.508375
H	-2.494247	3.981830	0.127940
H	-3.159478	6.300655	-0.435768
H	-1.684905	8.208703	0.169269
H	0.463090	7.794822	1.351628
H	1.137749	5.472288	1.935139
H	1.714450	-1.347038	2.282093
H	1.607371	0.953887	1.988930
H	0.774386	-1.833427	-1.290804
H	0.526828	0.465296	-1.617850
H	-0.339931	-2.149487	3.905949
H	-1.979208	-2.200466	4.563885
H	5.694248	0.790027	0.217960

H	7.684725	0.707090	-1.253367
H	7.608662	-0.541901	-3.399998
H	5.530108	-1.720533	-4.082541
H	3.524891	-1.661884	-2.629379
H	-4.114075	-1.839119	0.037254
H	-6.524882	-2.131087	-0.463007
H	-7.408830	-1.608722	-2.725538
H	-5.879242	-0.786168	-4.502400
H	-3.464963	-0.478898	-4.032514
H	-1.735468	-4.477790	4.507691
H	-2.167790	-4.303381	2.807730
H	1.825732	-4.232585	2.208384
H	1.081533	-2.827679	2.989224
H	-0.236542	-5.582406	2.612258
H	0.486214	-4.946315	4.089419
H	-2.718520	-1.112782	2.729327
H	-2.428953	-2.579248	1.789400

**5Ce
AM1**

C	5.380085	0.855604	-0.325177
C	4.356429	-0.045649	-0.017501
C	4.615934	-1.175272	0.766515
C	5.905704	-1.395546	1.247777
C	6.927574	-0.491939	0.952724
C	6.665408	0.630543	0.166951
C	2.992382	0.189699	-0.564049
O	2.778485	0.404289	-1.774258
N	1.954135	0.178083	0.359359
C	0.562096	0.169588	-0.019373
C	0.208723	-1.033462	-0.938280
C	-1.293248	-1.039718	-1.294586
C	-2.034559	0.117931	-0.577917
C	-1.357675	1.393690	-1.170821
C	0.155043	1.421567	-0.863264
C	-1.697535	-2.474358	-1.011546
O	-0.676060	-3.172428	-0.356413
C	0.451095	-2.359797	-0.257455
C	-0.376845	0.130405	1.169679
C	-1.699968	0.149449	0.896318
C	-1.872160	2.688981	-0.574658
O	-0.836789	3.428172	-0.007031
C	0.367816	2.721691	-0.124110
O	1.413062	-2.835698	0.323629
O	-2.655270	-3.157343	-1.333586
C	-3.519573	0.160007	-0.916925
C	-4.324679	-1.040436	-0.466624
C	-5.503556	-0.694324	0.412503
C	-5.137834	-0.067196	1.742075
C	-3.788101	-0.470664	2.305304
C	-2.680810	0.504296	1.956023
O	-2.978763	3.201656	-0.524824
O	1.344630	3.271994	0.351374
H	-3.952355	1.094356	-0.462025
H	-3.613579	0.266913	-2.031751
H	0.035931	0.156624	2.186214
H	2.159173	-0.071098	1.300275
H	3.812877	-1.899549	0.983264
H	6.116036	-2.285634	1.859216
H	7.943386	-0.667724	1.337711
H	7.472623	1.339735	-0.069135
H	5.165846	1.731924	-0.956538
H	-1.434066	-0.889356	-2.402572
H	0.843060	-0.984639	-1.868604
H	-1.541029	1.423622	-2.278100
H	0.768768	1.439917	-1.807750
H	-3.516663	-1.513838	2.006096
H	-3.878789	-0.484152	3.427383
H	-5.930868	-0.351298	2.486615
H	-5.182894	1.051298	1.646388
H	-4.698534	-1.592378	-1.371414
H	-3.675139	-1.761140	0.095032
H	-6.193404	-0.000463	-0.137557
H	-6.075453	-1.643413	0.601468
H	-2.099164	0.704403	2.901516
H	-3.129539	1.493632	1.646128

**5Ce
PM3**

C	0.367618	2.750616	-0.203255
C	0.127053	1.429815	-0.926145
C	-1.405312	1.418178	-1.177968
C	-1.864318	2.746035	-0.576059
O	-0.813013	3.463904	-0.036382
C	0.538764	0.172434	-0.106754
C	0.170600	-1.041637	-0.992433
C	-1.346606	-1.030049	-1.322804
C	-2.070344	0.133072	-0.565732
C	-1.675002	0.147201	0.898814
C	-0.345368	0.130915	1.115252
C	-1.736557	-2.484036	-1.050011
O	-0.734637	-3.181576	-0.385086
C	0.389601	-2.384550	-0.306183
N	1.972510	0.218163	0.291425
C	3.053769	0.152369	-0.638575
O	2.858779	0.333321	-1.830995
C	-3.574737	0.181205	-0.867653
C	-4.408713	-0.997019	-0.383578
C	-5.534416	-0.611573	0.559311
C	-5.056336	-0.072542	1.902180
C	-3.690198	-0.591759	2.341575
C	-2.601459	0.429289	2.034986
O	-2.651175	-3.187534	-1.388103
O	1.329893	-2.882785	0.257774
O	-2.925348	3.311137	-0.512465
O	1.341156	3.313660	0.218039
C	4.395749	-0.070668	-0.029275
C	5.355251	0.939200	-0.094955
C	6.612467	0.728703	0.461859
C	6.912150	-0.484607	1.072562
C	5.954611	-1.492729	1.129178
C	4.693166	-1.290038	0.580728
H	-3.988759	1.116420	-0.434700
H	-3.698400	0.284428	-1.965496
H	0.097989	0.161361	2.118266
H	2.151781	-0.258525	1.151208
H	3.943482	-2.090256	0.620906
H	6.193182	-2.449671	1.605407
H	7.903782	-0.647789	1.507824
H	7.367409	1.520752	0.415870
H	5.119258	1.891770	-0.583224
H	-1.510692	-0.859945	-2.415768
H	0.774602	-1.023287	-1.934126
H	-1.625346	1.448850	-2.272544
H	0.687509	1.449013	-1.893358
H	-3.461647	-1.573679	1.876048
H	-3.704383	-0.781811	3.432225
H	-5.814247	-0.312207	2.672631
H	-5.012382	1.038432	1.866998
H	-4.833176	-1.532569	-1.255350
H	-3.772625	-1.737342	0.149013
H	-6.202378	0.131150	0.079822
H	-6.164022	-1.508935	0.725903
H	-1.993386	0.583081	2.950847
H	-3.078942	1.415655	1.828971

**6Ce
AM1**

C	0.286090	-1.429072	2.181771
C	-0.068013	-0.090313	1.574390
C	-1.610170	-0.092521	1.518489
C	-1.992285	-1.451453	2.066630
O	-0.857156	-2.167037	2.472211
C	0.541286	0.093589	0.145861
C	0.043968	1.481747	-0.351877
C	-1.498709	1.514462	-0.359512
C	-2.111018	0.163432	0.074599
C	-1.481805	-0.915727	-0.780925
C	-0.133227	-0.924681	-0.758159
C	-1.843559	2.661509	0.568718
O	-0.689789	3.278331	1.054311
C	0.442657	2.621504	0.553913
N	1.980331	-0.009111	0.190222
C	2.781779	0.088781	-0.938671
O	2.304338	0.432508	-2.038659
C	-3.633922	0.208933	0.064558
C	-4.254962	0.713064	-1.223655
C	-5.219727	-0.261357	-1.860410
C	-4.640585	-1.621099	-2.191330
C	-3.171940	-1.627520	-2.569702
C	-2.258547	-2.007684	-1.418500
O	-2.898555	3.142083	0.949466
O	1.512314	3.075240	0.920512
O	-3.057221	-2.017893	2.238427
O	1.358386	-1.943611	2.457106
C	4.233658	-0.189266	-0.759176
C	5.143942	0.588679	-1.485586
C	6.512184	0.356111	-1.357386
C	6.973570	-0.654932	-0.514145
C	6.065803	-1.437189	0.200340
C	4.695413	-1.207008	0.082198
H	-4.016187	-0.820438	0.305186
H	-3.960194	0.886078	0.902648
H	0.495052	-1.613828	-1.336029
H	2.383190	-0.324534	1.044765
H	3.992601	-1.842116	0.643965
H	6.429251	-2.238871	0.860465
H	8.054105	-0.837592	-0.414068
H	7.226731	0.970569	-1.925016
H	4.767366	1.375434	-2.158782
H	-1.862248	1.776393	-1.389586
H	0.466010	1.661156	-1.381685
H	-2.036827	0.693958	2.200429
H	0.308315	0.726602	2.249141
H	-2.866380	-0.643675	-3.007345
H	-3.027700	-2.391329	-3.382873
H	-5.231197	-2.045183	-3.048962
H	-4.808849	-2.313924	-1.323107
H	-4.809218	1.666419	-1.003584
H	-3.469516	0.972448	-1.980315
H	-6.102654	-0.405299	-1.181598
H	-5.606477	0.210720	-2.804338
H	-1.525458	-2.774782	-1.798773
H	-2.851856	-2.513320	-0.603684

**6Ce
PM3**

C	4.642552	-1.354856	-0.188854
C	4.247548	-0.161265	-0.794972
C	5.204030	0.759862	-1.222212
C	6.554921	0.488975	-1.031040
C	6.950478	-0.698468	-0.424294
C	5.995046	-1.620049	-0.006803
C	2.802110	0.133171	-1.014903
O	2.307527	0.364156	-2.106747
N	2.011892	0.220826	0.172171
C	0.522748	0.182463	0.155904
C	-0.030722	-0.022561	1.598367
C	-1.583644	-0.073577	1.573153
C	-2.116651	0.089465	0.121726
C	-1.596905	1.459912	-0.395993
C	-0.049921	1.518550	-0.390355
C	-1.905415	-1.416713	2.221727
O	-0.754884	-2.102194	2.588927
C	0.353412	-1.357842	2.232720
C	-0.077598	-0.907625	-0.698698
C	-1.421061	-0.972273	-0.717591
C	-1.997291	2.668857	0.445880
O	-0.893593	3.372455	0.899147
C	0.265560	2.748765	0.451624
O	1.408535	-1.875145	2.495497
O	-2.925035	-1.986630	2.504176
C	-3.651158	0.034239	0.101952
C	-4.283353	0.520561	-1.200124
C	-5.184467	-0.504428	-1.865186
C	-4.478995	-1.788427	-2.287099
C	-2.996705	-1.619736	-2.603540
C	-2.131174	-2.071810	-1.428875
O	-3.051838	3.146849	0.773582
O	1.277032	3.301966	0.789444
H	-3.976334	-1.003935	0.323026
H	-4.039046	0.646272	0.942228
H	0.573587	-1.588245	-1.257729
H	2.415680	-0.244489	0.958566
H	3.896991	-2.088299	0.139663
H	6.307100	-2.556357	0.468034
H	8.014885	-0.909571	-0.276160
H	7.307223	1.212976	-1.361687
H	4.890922	1.691252	-1.708073
H	-2.000597	1.597394	-1.434305
H	0.341846	1.684329	-1.424579
H	-2.018856	0.733717	2.211404
H	0.330974	0.802756	2.259023
H	-2.771886	-0.565394	-2.876454
H	-2.737177	-2.218703	-3.497077
H	-5.004645	-2.209309	-3.165962
H	-4.584418	-2.554840	-1.488243
H	-4.864985	1.442880	-1.005121
H	-3.490760	0.816811	-1.931267
H	-6.029299	-0.756358	-1.193841
H	-5.646650	-0.029150	-2.753927
H	-1.382211	-2.807465	-1.787069
H	-2.757620	-2.624871	-0.692931

**5Bd
AM1**

C	4.505762	-1.065253	0.659528
C	4.172766	0.074307	-0.080670
C	5.141400	1.038642	-0.373678
C	6.446008	0.865565	0.087987
C	6.781702	-0.267416	0.829400
C	5.814273	-1.233005	1.110729
C	2.785969	0.253440	-0.595037
O	2.542907	0.467716	-1.799804
N	1.773833	0.193499	0.354122
C	0.373468	0.118647	0.006133
C	-0.108272	1.337553	-0.834070
C	-1.631196	1.241918	-1.095736
C	-2.235380	-0.057682	-0.490128
C	-1.453574	-1.194158	-1.203503
C	0.055734	-1.120124	-0.884890
C	-2.198841	2.542799	-0.510771
N	-1.155607	3.297554	0.042171
C	0.093693	2.665343	-0.101767
C	-0.534943	0.028622	1.215201
C	-1.860520	-0.068300	0.973169
C	-1.851985	-2.620550	-0.806467
N	-0.756128	-3.254732	-0.193155
C	0.382432	-2.435558	-0.175100
O	1.150169	3.165557	0.288998
O	-3.369724	2.937169	-0.545662
C	-3.714638	-0.130262	-0.865058
C	-4.605529	-0.961520	0.031407
C	-5.166471	-0.172814	1.194535
C	-4.099667	0.617866	1.919740
C	-2.822328	-0.175256	2.100159
O	-2.920371	-3.195449	-1.030916
O	1.459490	-2.767438	0.332226
H	-0.779723	-4.180417	0.157460
H	-1.281673	4.182617	0.467801
H	-4.136874	0.911549	-0.909617
H	-3.776022	-0.550388	-1.907006
H	-0.100645	0.053716	2.222188
H	2.011869	-0.110048	1.271191
H	3.743443	-1.835871	0.865175
H	6.082438	-2.130283	1.687674
H	7.812326	-0.401920	1.190331
H	7.210235	1.624027	-0.136982
H	4.868467	1.923759	-0.969041
H	-1.624810	-1.100196	-2.310250
H	0.667620	-1.060858	-1.826901
H	-1.843655	1.251260	-2.198129
H	0.471512	1.374893	-1.797565
H	-3.068949	-1.261669	2.260535
H	-2.310677	0.178314	3.038929
H	-4.488815	0.916465	2.929086
H	-3.882718	1.564424	1.355002
H	-5.460284	-1.352731	-0.583900
H	-4.049229	-1.857822	0.411581
H	-5.956623	0.534394	0.827720
H	-5.660835	-0.884732	1.907344

**5Bd
PM3**

C	4.629092	-1.146015	0.475213
C	4.212369	0.059492	-0.089712
C	5.073900	1.155019	-0.133523
C	6.354134	1.042743	0.398796
C	6.773292	-0.157097	0.964162
C	5.912612	-1.249731	1.000079
C	2.844528	0.177192	-0.674454
O	2.619179	0.306721	-1.868303
N	1.785901	0.203308	0.281377
C	0.345400	0.087907	-0.079321
C	-0.137457	1.302618	-0.918245
C	-1.677006	1.219257	-1.127694
C	-2.267941	-0.075975	-0.475565
C	-1.514309	-1.242959	-1.196932
C	0.011668	-1.179437	-0.916596
C	-2.212270	2.542705	-0.579996
N	-1.145150	3.284119	0.007718
C	0.112895	2.648075	-0.244075
C	-0.505703	0.026215	1.164886
C	-1.834720	-0.075756	0.976318
C	-1.922323	-2.654636	-0.782492
N	-0.824433	-3.290173	-0.118786
C	0.348517	-2.486269	-0.206638
O	1.148617	3.203933	0.051483
O	-3.328217	3.022027	-0.629712
C	-3.773371	-0.152301	-0.794120
C	-4.658686	-0.858875	0.218289
C	-5.127029	0.062233	1.333031
C	-3.964837	0.699917	2.080993
C	-2.754408	-0.218755	2.140828
O	-2.949661	-3.268176	-0.982318
O	1.408794	-2.878248	0.241151
H	-0.818655	-4.249644	0.146372
H	-1.232279	4.233990	0.293242
H	-4.181024	0.868535	-0.947260
H	-3.889641	-0.653980	-1.777876
H	-0.041389	0.061779	2.157231
H	2.009644	-0.262171	1.136439
H	3.953523	-2.010270	0.499196
H	6.244979	-2.195235	1.441250
H	7.782714	-0.242646	1.379930
H	7.032855	1.901575	0.369476
H	4.742650	2.097424	-0.584832
H	-1.703641	-1.147935	-2.294923
H	0.578779	-1.147151	-1.880426
H	-1.914915	1.190025	-2.219244
H	0.385385	1.303418	-1.906920
H	-3.084263	-1.282085	2.177869
H	-2.192766	-0.038573	3.079469
H	-4.285983	0.960218	3.108231
H	-3.684615	1.661977	1.607667
H	-5.541297	-1.277014	-0.304071
H	-4.130194	-1.729704	0.664435
H	-5.788549	0.853805	0.929037
H	-5.755309	-0.520572	2.035729

**6Bd
AM1**

C	-0.450438	2.583753	-0.123195
C	0.201747	1.488794	0.718306
C	1.717303	1.603921	0.433349
C	1.807309	2.637874	-0.700462
N	0.530610	3.161010	-0.951444
C	-0.298135	0.040677	0.400116
C	0.142061	-0.319886	-1.047692
C	1.681878	-0.254534	-1.194564
C	2.342913	0.224982	0.115836
C	1.880932	-0.711777	1.215066
C	0.539747	-0.822371	1.332117
C	2.091525	-1.667768	-1.627521
N	0.943772	-2.464745	-1.745017
C	-0.227080	-1.762752	-1.408978
N	-1.714891	-0.103627	0.631041
C	-2.725641	0.173151	-0.282291
O	-2.496602	0.637258	-1.413408
C	3.847025	0.370203	-0.089231
C	4.657317	0.481758	1.183422
C	5.158503	-0.867734	1.654487
C	4.082954	-1.930787	1.584462
C	2.767759	-1.446255	2.153642
O	3.227866	-2.080634	-1.882132
O	-1.348962	-2.274952	-1.434229
O	2.819134	3.019508	-1.298354
O	-1.616394	2.976480	-0.064250
C	-4.111061	-0.128194	0.184341
C	-4.592509	0.380268	1.394006
C	-5.901224	0.102040	1.787233
C	-6.723048	-0.684180	0.979077
C	-6.240669	-1.188316	-0.228944
C	-4.935487	-0.909100	-0.632619
H	0.345811	3.876534	-1.610901
H	0.956794	-3.412274	-2.031912
H	4.225111	-0.500900	-0.691882
H	4.026308	1.287173	-0.716082
H	0.043256	-1.477283	2.057641
H	-1.971514	-0.541156	1.485292
H	-3.951857	1.015132	2.024301
H	-6.285613	0.507396	2.734605
H	-7.754417	-0.903104	1.293277
H	-6.890283	-1.803976	-0.868452
H	-4.546400	-1.292545	-1.589336
H	2.253176	2.036496	1.320591
H	-0.017155	1.708500	1.796760
H	1.974210	0.449503	-2.020902
H	-0.363469	0.369121	-1.779514
H	2.968783	-0.774964	3.035828
H	2.202542	-2.336599	2.549218
H	4.421838	-2.827667	2.168535
H	3.939124	-2.264915	0.521683
H	5.539757	1.150363	0.996760
H	4.047500	0.964125	1.991800
H	6.027321	-1.188748	1.021239
H	5.530327	-0.772562	2.708593

**6Bd
PM3**

C	-0.291000	2.670315	-0.078565
C	0.264242	1.481301	0.695211
C	1.797728	1.517832	0.449589
C	1.999779	2.614360	-0.596208
N	0.736048	3.185719	-0.938894
C	-0.288409	0.068536	0.327458
C	0.123824	-0.324756	-1.115451
C	1.672851	-0.297653	-1.265343
C	2.341401	0.107227	0.075826
C	1.816477	-0.825494	1.157444
C	0.473281	-0.855180	1.254546
C	2.044945	-1.681887	-1.791268
N	0.863004	-2.471351	-1.916933
C	-0.284531	-1.750808	-1.478693
N	-1.750925	0.005347	0.619817
C	-2.795125	0.305889	-0.315502
O	-2.571248	0.873161	-1.369612
C	3.866374	0.157320	-0.071947
C	4.581372	0.484086	1.230857
C	5.007283	-0.772378	1.978651
C	4.060299	-1.938486	1.745026
C	2.629777	-1.613105	2.130973
O	3.117630	-2.139155	-2.129930
O	-1.371939	-2.292536	-1.444164
O	3.018873	3.043840	-1.099575
O	-1.365653	3.222858	0.002351
C	-4.160943	-0.069604	0.158712
C	-5.009184	0.914727	0.663872
C	-6.286905	0.565703	1.088912
C	-6.715845	-0.754846	1.003152
C	-5.868785	-1.731944	0.489756
C	-4.588269	-1.393805	0.065511
H	0.649056	4.048670	-1.428373
H	0.850829	-3.421794	-2.212041
H	4.235448	-0.819521	-0.458403
H	4.133066	0.900253	-0.849920
H	-0.062963	-1.477425	1.980261
H	-1.983058	-0.768821	1.207869
H	-4.671920	1.956333	0.718946
H	-6.956916	1.334778	1.487222
H	-7.723319	-1.025184	1.336276
H	-6.210540	-2.769525	0.414948
H	-3.923981	-2.159994	-0.352834
H	2.347116	1.826175	1.380290
H	0.045198	1.653217	1.777710
H	1.975317	0.448197	-2.041296
H	-0.342237	0.379587	-1.848914
H	2.625178	-1.050276	3.088843
H	2.092730	-2.561903	2.339875
H	4.405480	-2.811776	2.332155
H	4.108808	-2.249036	0.677644
H	5.470893	1.109983	1.024789
H	3.920646	1.115944	1.867961
H	6.025251	-1.072535	1.659882
H	5.087912	-0.552783	3.061491

**5Ba
AM1**

C	2.516887	0.316055	-0.361868
C	1.196511	0.224606	-1.130027
C	1.043056	-1.259475	-1.504341
C	2.378614	-1.894161	-1.102255
N	3.164941	-0.941192	-0.402855
C	-0.011922	0.705861	-0.269534
C	-1.260367	0.434172	-1.161933
C	-1.391410	-1.073640	-1.461050
C	-0.216037	-1.883777	-0.840453
C	-0.195857	-1.554053	0.633456
C	-0.100935	-0.235813	0.913513
C	-2.780916	-1.452668	-0.930510
N	-3.399234	-0.316088	-0.361051
C	-2.564427	0.828638	-0.466850
N	0.112000	2.092296	0.117945
C	0.241943	3.123989	-0.803515
O	0.037652	2.944764	-2.021130
C	-0.345478	-3.347362	-1.257756
C	0.319771	-4.370494	-0.363357
C	-0.580769	-4.842856	0.757029
C	-1.234908	-3.692309	1.490047
C	-0.273132	-2.548594	1.734271
O	-3.315089	-2.561660	-1.033821
O	-2.877253	1.957378	-0.086270
O	2.758105	-3.028540	-1.401069
O	2.958574	1.326913	0.194210
C	0.606859	4.455842	-0.244292
C	1.744308	4.595345	0.558259
C	2.086921	5.853565	1.051632
C	1.296637	6.963492	0.750090
C	0.165417	6.820576	-0.053608
C	-0.181311	5.567203	-0.557461
C	4.431028	-1.215957	0.168585
C	-4.686654	-0.313055	0.229360
H	-1.434469	-3.614221	-1.345686
H	0.096944	-3.443037	-2.287958
H	-0.092633	0.170745	1.932277
H	0.430983	2.255776	1.046431
H	2.377865	3.720048	0.780740
H	2.983491	5.969147	1.678277
H	1.568501	7.954015	1.144440
H	-0.454492	7.696732	-0.294474
H	-1.065845	5.445042	-1.201845
H	0.947884	-1.376944	-2.618514
H	1.274031	0.871511	-2.047498
H	-1.401019	-1.258763	-2.568997
H	-1.173506	1.036414	-2.108887
H	0.759413	-2.953655	1.925638
H	-0.585555	-2.013369	2.674580
H	-1.621436	-4.060287	2.477269
H	-2.120461	-3.325797	0.904026
H	0.608481	-5.255538	-0.992241
H	1.271691	-3.956794	0.061841
H	-1.380505	-5.512954	0.344260
H	0.027778	-5.453303	1.475578
C	-4.973281	0.546697	1.312268
C	-6.241364	0.546373	1.885770
C	-7.238474	-0.301727	1.407590
C	-6.962123	-1.154198	0.340569
C	-5.703182	-1.165404	-0.253314
H	-4.204924	1.236747	1.696310
H	-6.452258	1.225692	2.725458
H	-8.236660	-0.297268	1.868347
H	-7.743564	-1.827433	-0.043105

H	-5.505291	-1.855757	-1.089002
C	5.414270	-0.207144	0.257796
C	6.652345	-0.490485	0.827510
C	6.939749	-1.766584	1.307947
C	5.975078	-2.768503	1.218802
C	4.728052	-2.506130	0.659427
H	5.205284	0.811701	-0.106037
H	7.408643	0.306253	0.894101
H	7.921635	-1.982102	1.753267
H	6.195462	-3.779997	1.592256
H	3.985273	-3.316707	0.584746

**5Ba
PM3**

C	-2.541007	0.392573	0.401212
C	-1.227470	0.220707	1.159688
C	-1.131836	-1.287243	1.488097
C	-2.487606	-1.862039	1.080390
N	-3.255662	-0.852940	0.390392
C	0.021523	0.668418	0.346238
C	1.259788	0.331008	1.223502
C	1.333232	-1.197610	1.465974
C	0.119414	-1.936032	0.803954
C	0.107222	-1.538892	-0.658141
C	0.078528	-0.211025	-0.877997
C	2.717226	-1.609707	0.959637
N	3.397081	-0.469465	0.408778
C	2.587253	0.714293	0.573258
N	-0.003610	2.105272	-0.044795
C	-0.163576	3.174555	0.886067
O	-0.046984	2.986616	2.087742
C	0.189781	-3.433733	1.157812
C	-0.393388	-4.410632	0.150929
C	0.599112	-4.803556	-0.931117
C	1.122146	-3.599190	-1.701112
C	0.083204	-2.493536	-1.802965
O	3.250355	-2.700848	1.044921
O	2.980090	1.818971	0.259010
O	-2.939811	-2.961047	1.332915
O	-2.970095	1.407617	-0.117262
C	-0.399849	4.512342	0.268602
C	-1.616261	4.789994	-0.355348
C	-1.831337	6.046614	-0.910541
C	-0.838069	7.018833	-0.846355
C	0.372959	6.738466	-0.222081
C	0.595657	5.486108	0.340907
C	-4.571652	-1.053189	-0.178297
C	4.715830	-0.497030	-0.187062
H	1.242714	-3.730434	1.346492
H	-0.323616	-3.579841	2.131548
H	0.089735	0.232100	-1.880647
H	-0.467679	2.261953	-0.915507
H	-2.402887	4.026612	-0.401705
H	-2.786143	6.269761	-1.398001
H	-1.010957	8.006652	-1.286197
H	1.153343	7.504921	-0.170276
H	1.546548	5.264219	0.838997
H	-1.029487	-1.431394	2.592774
H	-1.288326	0.818525	2.103823
H	1.305354	-1.415469	2.562210
H	1.180618	0.873073	2.199037
H	-0.938996	-2.933893	-1.849731
H	0.220997	-1.936222	-2.751371
H	1.428463	-3.916060	-2.717009
H	2.043702	-3.208283	-1.225440
H	-0.728674	-5.320965	0.685445
H	-1.304097	-3.987979	-0.327593
H	1.449066	-5.362393	-0.492130
H	0.105139	-5.511333	-1.626294
C	5.286743	0.685980	-0.672384
C	6.547259	0.648758	-1.253657
C	7.242179	-0.552040	-1.354408
C	6.674089	-1.724718	-0.867734
C	5.414683	-1.706620	-0.283082
H	4.721314	1.633954	-0.578983
H	6.992777	1.574300	-1.632873
H	8.235414	-0.573719	-1.814026
H	7.219655	-2.671134	-0.942139

H	4.950196	-2.628810	0.118110
C	-5.214630	0.000759	-0.838611
C	-6.472689	-0.204074	-1.389978
C	-7.093017	-1.444963	-1.289205
C	-6.452730	-2.488955	-0.629498
C	-5.195009	-2.302442	-0.071276
H	-4.709983	0.983752	-0.905078
H	-6.975355	0.620598	-1.905972
H	-8.084679	-1.599185	-1.726531
H	-6.939588	-3.466208	-0.545692
H	-4.673864	-3.120717	0.463013

**6Ba
AM1**

C	-2.204016	4.565444	0.078682
C	-2.244468	3.544625	-0.877108
C	-2.750433	3.794690	-2.156023
C	-3.212016	5.070560	-2.478221
C	-3.163772	6.093020	-1.530124
C	-2.661005	5.840182	-0.253639
C	-1.767953	2.185544	-0.487597
O	-2.157472	1.622319	0.552720
N	-0.869612	1.587632	-1.364329
C	-0.216644	0.317603	-1.153125
C	-1.129982	-0.885129	-1.564990
C	-0.419651	-2.217625	-1.257679
C	1.066186	-1.996365	-0.881532
C	1.053444	-1.217683	0.453017
C	0.257311	0.095916	0.314764
C	-1.278146	-2.856276	-0.151503
N	-2.432943	-2.069786	0.060953
C	-2.455051	-0.948590	-0.810664
C	1.007101	0.124933	-2.034887
C	1.641058	-1.063691	-1.930114
C	2.440143	-0.789022	0.946982
N	2.465829	0.615954	1.120539
C	1.222515	1.196920	0.765637
O	-3.419230	-0.204005	-0.985688
O	-1.038681	-3.917008	0.434021
C	1.759380	-3.341146	-0.692261
C	2.159090	-4.038782	-1.973771
C	3.581252	-3.708091	-2.376818
C	3.880434	-2.229534	-2.248725
C	2.778404	-1.374335	-2.834063
O	3.386398	-1.540598	1.199007
O	0.967998	2.401763	0.833379
C	-3.409598	-2.308859	1.058296
C	3.587664	1.344448	1.585569
H	2.671023	-3.202660	-0.048677
H	1.066645	-4.012577	-0.113426
H	1.314346	0.922171	-2.721618
H	-0.508157	2.144551	-2.103842
H	-2.805711	2.986146	-2.900381
H	-3.617525	5.268268	-3.481292
H	-3.526850	7.098909	-1.788573
H	-2.627076	6.645121	0.495310
H	-1.814657	4.351235	1.086568
H	-0.459551	-2.902716	-2.146790
H	-1.359668	-0.794137	-2.659733
H	0.606125	-1.877293	1.247204
H	-0.633768	0.106399	1.002360
H	2.362369	-1.879874	-3.750970
H	3.229718	-0.401897	-3.179753
H	4.838278	-2.005898	-2.790025
H	4.041059	-1.959227	-1.170154
H	2.073549	-5.148622	-1.827169
H	1.455126	-3.763703	-2.802507
H	4.298373	-4.280671	-1.731239
H	3.747817	-4.038596	-3.435831
C	3.413964	2.511438	2.360878
C	4.524263	3.221706	2.808269
C	5.814497	2.790244	2.506301
C	5.993265	1.636860	1.744890
C	4.897561	0.915010	1.280584
H	2.402698	2.877042	2.601849
H	4.374359	4.131712	3.408711

H	6.685654	3.355586	2.867113
H	7.008784	1.287106	1.505404
H	5.061819	-0.002274	0.692541
C	-3.761888	-3.623876	1.425773
C	-4.724223	-3.833558	2.410179
C	-5.349675	-2.756188	3.034111
C	-5.004541	-1.454209	2.673920
C	-4.040569	-1.219051	1.698609
H	-3.267466	-4.487699	0.953676
H	-4.989286	-4.863471	2.692535
H	-6.110970	-2.931699	3.807692
H	-5.494012	-0.598662	3.163411
H	-3.781464	-0.181745	1.418260

**6Ba
PM3**

C	-0.406529	4.983264	0.461174
C	0.800309	4.294938	0.581332
C	1.947559	4.949331	1.027704
C	1.879782	6.296897	1.366089
C	0.676952	6.986524	1.252853
C	-0.463236	6.331199	0.798630
C	0.875341	2.852554	0.200044
O	1.365350	2.445970	-0.838281
N	0.381415	1.958101	1.205212
C	0.137945	0.497806	1.016222
C	1.411566	-0.309107	1.425591
C	1.135116	-1.824460	1.281043
C	-0.364352	-2.093191	0.950032
C	-0.639244	-1.448094	-0.436417
C	-0.356957	0.075256	-0.393287
C	2.151834	-2.315489	0.247962
N	3.028528	-1.236709	-0.120002
C	2.688305	-0.051181	0.633675
C	-0.908322	0.008804	1.995094
C	-1.154031	-1.315583	1.992976
C	-2.072380	-1.577226	-0.950190
N	-2.644983	-0.267152	-1.126368
C	-1.680222	0.739274	-0.775354
O	3.398464	0.931650	0.665490
O	2.285350	-3.439822	-0.198691
C	-0.634038	-3.601628	0.915098
C	-0.432153	-4.275426	2.264484
C	-1.733018	-4.382017	3.049284
C	-2.689381	-3.238560	2.750903
C	-2.075404	-1.878846	3.024468
O	-2.678065	-2.592406	-1.234866
O	-1.939908	1.928093	-0.798094
C	4.151732	-1.348936	-1.026465
C	-3.985342	-0.002786	-1.605856
H	-1.675487	-3.785757	0.566695
H	0.016058	-4.073395	0.151629
H	-1.397699	0.710170	2.680731
H	-0.316342	2.384129	1.780229
H	2.896149	4.405404	1.105234
H	2.777720	6.815412	1.718113
H	0.628231	8.047953	1.517590
H	-1.407542	6.877085	0.702382
H	-1.301002	4.468151	0.090091
H	1.341666	-2.365852	2.244487
H	1.629659	-0.059454	2.493697
H	0.025995	-1.947154	-1.184340
H	0.410604	0.344749	-1.161512
H	-1.509017	-1.916211	3.979548
H	-2.893310	-1.146832	3.190679
H	-3.601490	-3.355737	3.368129
H	-3.026872	-3.301213	1.692566
H	-0.005033	-5.286379	2.119468
H	0.334219	-3.715806	2.848506
H	-2.238506	-5.338850	2.810734
H	-1.511803	-4.425510	4.133919
C	-4.435869	1.317420	-1.727079
C	-5.723544	1.561300	-2.186201
C	-6.563449	0.505139	-2.523748
C	-6.112537	-0.805232	-2.403072
C	-4.827748	-1.068186	-1.946472
H	-3.752407	2.145983	-1.456797
H	-6.074397	2.594051	-2.282392
H	-7.577168	0.704913	-2.885412
H	-6.770222	-1.639005	-2.670042

H	-4.450576	-2.105099	-1.847917
C	4.413053	-2.565605	-1.668250
C	5.481294	-2.657934	-2.550731
C	6.288472	-1.552562	-2.798123
C	6.028561	-0.346408	-2.155698
C	4.965847	-0.235613	-1.268645
H	3.763022	-3.436693	-1.455872
H	5.684352	-3.609610	-3.052638
H	7.127505	-1.631868	-3.496665
H	6.662833	0.525398	-2.347143
H	4.751119	0.715638	-0.744469

**5Be
AM1**

C	0.382410	-2.425317	-0.222585
C	0.052502	-1.117364	-0.902946
C	-1.457573	-1.202694	-1.200763
C	-1.825626	-2.608666	-0.771530
O	-0.729832	-3.266584	-0.202669
C	0.373011	0.113018	0.003060
C	-0.105410	1.337794	-0.833575
C	-1.620565	1.239379	-1.105973
C	-2.234538	-0.055920	-0.499689
C	-1.864589	-0.071034	0.965138
C	-0.538840	0.019317	1.209347
C	-2.173957	2.526139	-0.524297
O	-1.161956	3.306103	0.030528
C	0.066957	2.647454	-0.100292
N	1.770960	0.181647	0.350385
C	2.787431	0.236866	-0.594726
O	2.537058	0.424317	-1.802382
C	-3.712753	-0.105558	-0.881148
C	-4.613696	-0.945984	-0.003842
C	-5.172679	-0.171300	1.169924
C	-4.106918	0.610170	1.906646
C	-2.831788	-0.186585	2.086021
O	-3.293213	3.012517	-0.491345
O	1.028793	3.235915	0.360110
O	-2.834736	-3.284087	-0.880787
O	1.400727	-2.868197	0.283441
C	4.172599	0.076573	-0.074680
C	4.507401	-1.038064	0.702124
C	5.815983	-1.188661	1.158812
C	6.781738	-0.230821	0.846319
C	6.444477	0.876621	0.067879
C	5.139828	1.032289	-0.399706
H	-4.121745	0.943077	-0.899724
H	-3.775932	-0.496159	-1.934105
H	-0.107181	0.035961	2.218115
H	2.007727	-0.023340	1.294048
H	3.748319	-1.804405	0.932131
H	6.085676	-2.066702	1.764319
H	7.812613	-0.351647	1.211935
H	7.207596	1.628614	-0.181991
H	4.866843	1.896527	-1.024964
H	-1.642820	-1.130987	-2.308061
H	0.653110	-1.038122	-1.852341
H	-1.826451	1.246180	-2.210651
H	0.484662	1.382375	-1.792361
H	-3.080257	-1.274778	2.233691
H	-2.323755	0.157417	3.030329
H	-4.500147	0.898431	2.917663
H	-3.885691	1.563960	1.355886
H	-5.469848	-1.318625	-0.628806
H	-4.066407	-1.853018	0.364047
H	-5.963044	0.540746	0.812787
H	-5.667150	-0.892818	1.873088

**5Be
PM3**

C	0.354387	-2.470468	-0.251999
C	0.028508	-1.152926	-0.945655
C	-1.496115	-1.244868	-1.211361
C	-1.839892	-2.660415	-0.753027
O	-0.745451	-3.305355	-0.190872
C	0.347816	0.103481	-0.086632
C	-0.147833	1.319100	-0.914288
C	-1.679345	1.212039	-1.140990
C	-2.263793	-0.086988	-0.495068
C	-1.836452	-0.093062	0.959174
C	-0.508796	0.019020	1.153092
C	-2.203243	2.531690	-0.573161
O	-1.190395	3.309943	-0.043531
C	0.025564	2.659743	-0.208248
N	1.784415	0.233095	0.279073
C	2.848341	0.213338	-0.672280
O	2.618862	0.358632	-1.863358
C	-3.766534	-0.167814	-0.823883
C	-4.655034	-0.885307	0.177763
C	-5.130932	0.025123	1.298053
C	-3.975719	0.654166	2.064308
C	-2.760854	-0.259017	2.116548
O	-3.286233	3.056741	-0.542457
O	0.970329	3.279090	0.199697
O	-2.820687	-3.351195	-0.826775
O	1.360369	-2.924040	0.229963
C	4.212918	0.081567	-0.086903
C	4.603187	-1.116475	0.512722
C	5.884793	-1.234113	1.038869
C	6.770184	-0.162793	0.969975
C	6.377844	1.029092	0.369643
C	5.099710	1.154952	-0.164700
H	-4.174843	0.854088	-0.969753
H	-3.874102	-0.660378	-1.813181
H	-0.049217	0.048840	2.148339
H	2.008320	-0.211522	1.145324
H	3.910276	-1.965797	0.561936
H	6.196429	-2.174017	1.506724
H	7.777996	-0.259106	1.387643
H	7.076084	1.870970	0.314051
H	4.790770	2.090773	-0.644535
H	-1.706658	-1.182777	-2.307126
H	0.595339	-1.105775	-1.908508
H	-1.916283	1.194908	-2.232328
H	0.395091	1.360701	-1.890830
H	-3.084229	-1.325099	2.135436
H	-2.204419	-0.089920	3.060342
H	-4.304644	0.893127	3.094379
H	-3.697029	1.627318	1.613116
H	-5.534163	-1.300255	-0.353059
H	-4.127639	-1.758961	0.619654
H	-5.788820	0.821462	0.897292
H	-5.765781	-0.565185	1.988532

**6Be
AM1**

C	-4.985872	-0.815196	-0.666761
C	-4.124142	-0.129856	0.197211
C	-4.573336	0.293238	1.451760
C	-5.884003	0.022725	1.843181
C	-6.741581	-0.670688	0.988310
C	-6.292951	-1.087815	-0.264932
C	-2.739445	0.160252	-0.273159
O	-2.505705	0.606744	-1.409992
N	-1.722073	-0.110381	0.637704
C	-0.307456	0.038762	0.406030
C	0.193328	1.487780	0.726439
C	1.714486	1.595102	0.488053
C	2.335146	0.223548	0.130947
C	1.669369	-0.222991	-1.190436
C	0.134657	-0.299929	-1.047646
C	1.833657	2.649102	-0.595962
O	0.590037	3.195252	-0.905284
C	-0.402859	2.573755	-0.135767
C	0.530067	-0.836260	1.327521
C	1.871694	-0.733786	1.210739
C	2.066362	-1.613118	-1.644285
O	0.947851	-2.429646	-1.797340
C	-0.204012	-1.724192	-1.430922
O	-1.521845	3.040033	-0.241778
O	2.781663	3.118657	-1.205278
C	3.837587	0.367439	-0.086499
C	4.662305	0.439157	1.179459
C	5.151849	-0.926557	1.614298
C	4.064648	-1.976949	1.535568
C	2.759712	-1.492325	2.128195
O	3.139122	-2.127268	-1.917464
O	-1.244736	-2.354741	-1.492511
H	4.202138	-0.490948	-0.716131
H	4.013675	1.300669	-0.690431
H	0.031282	-1.502657	2.041684
H	-1.974754	-0.543211	1.496256
H	-3.908622	0.857326	2.122820
H	-6.242081	0.361126	2.826606
H	-7.774522	-0.884193	1.301710
H	-6.970584	-1.629145	-0.941875
H	-4.624897	-1.127456	-1.659915
H	2.233095	1.985884	1.405730
H	-0.056349	1.716818	1.797568
H	1.958177	0.502318	-2.001300
H	-0.375207	0.400345	-1.769780
H	2.974878	-0.839167	3.020565
H	2.190193	-2.385293	2.511679
H	4.400924	-2.888165	2.098880
H	3.906232	-2.291584	0.468874
H	5.550909	1.101299	0.998273
H	4.066403	0.910604	2.004552
H	6.009555	-1.243602	0.963904
H	5.537702	-0.857746	2.665516

**6Be
PM3**

C	4.563306	-1.406011	-0.109460
C	4.163964	-0.070915	-0.168994
C	5.037070	0.909850	-0.637506
C	6.311271	0.546524	-1.061159
C	6.712048	-0.784645	-1.009811
C	5.840485	-1.758357	-0.531865
C	2.803307	0.318265	0.304745
O	2.576726	0.881448	1.359451
N	1.754452	0.035093	-0.633040
C	0.293429	0.087828	-0.337585
C	-0.276151	1.485477	-0.732833
C	-1.811706	1.502352	-0.515837
C	-2.338285	0.103836	-0.086383
C	-1.660506	-0.247377	1.263707
C	-0.115215	-0.257591	1.117763
C	-2.009830	2.631677	0.493154
O	-0.823168	3.278901	0.783939
C	0.210839	2.689990	0.063342
C	-0.460443	-0.871125	-1.235340
C	-1.803896	-0.858345	-1.136980
C	-1.973705	-1.640732	1.803632
O	-0.829856	-2.410480	1.944175
C	0.267864	-1.678050	1.526068
O	1.254515	3.277839	0.137472
O	-2.970648	3.096021	1.050601
C	-3.861845	0.143689	0.074562
C	-4.590155	0.409434	-1.234589
C	-5.000802	-0.880808	-1.931434
C	-4.034163	-2.022843	-1.662429
C	-2.611945	-1.692670	-2.074482
O	-2.981194	-2.194390	2.157372
O	1.306277	-2.285455	1.555513
H	-4.213574	-0.821330	0.505081
H	-4.128514	0.916724	0.822971
H	0.083191	-1.511610	-1.939932
H	1.986173	-0.718057	-1.248403
H	4.723277	1.959827	-0.663832
H	7.000886	1.312784	-1.430703
H	7.717107	-1.066235	-1.341296
H	6.160603	-2.804480	-0.482685
H	3.881748	-2.170602	0.282920
H	-2.362308	1.772312	-1.457097
H	-0.027806	1.665665	-1.806722
H	-1.983474	0.500261	2.028947
H	0.351085	0.466558	1.832049
H	-2.622780	-1.166186	-3.052750
H	-2.062508	-2.640939	-2.251336
H	-4.371525	-2.922952	-2.212525
H	-4.068400	-2.294209	-0.583766
H	-5.488069	1.028983	-1.046230
H	-3.942506	1.027169	-1.898724
H	-6.011591	-1.184591	-1.593658
H	-5.093004	-0.702518	-3.020933

5Ad AM1

C	4.344977	-1.076127	0.574827
C	3.993849	0.081486	-0.128004
C	4.953352	1.056832	-0.414330
C	6.267405	0.876298	0.016702
C	6.621308	-0.274796	0.720814
C	5.662704	-1.251073	0.995385
C	2.596389	0.268345	-0.609793
O	2.327603	0.506376	-1.804544
N	1.604593	0.185435	0.358494
C	0.197348	0.118798	0.040496
C	-0.302458	1.358606	-0.760353
C	-1.829393	1.266087	-0.999783
C	-2.413724	-0.043756	-0.413365
C	-1.655911	-1.171596	-1.155206
C	-0.139749	-1.101610	-0.873339
C	-2.396203	2.539441	-0.356690
N	-1.345083	3.287399	0.191609
C	-0.095343	2.667359	0.004685
C	-0.684186	0.000608	1.268811
C	-2.010746	-0.089678	1.041958
C	-2.063471	-2.584468	-0.721150
N	-0.944630	-3.240859	-0.178006
C	0.202562	-2.432582	-0.200284
C	-2.992030	-0.236970	2.143083
C	-4.412893	0.066151	1.720938
C	-4.739670	-0.664431	0.439433
C	-3.909550	-0.132958	-0.708317
O	0.966088	3.162669	0.388734
O	-3.573971	2.912265	-0.339066
O	-3.167441	-3.120520	-0.849629
O	1.297164	-2.783562	0.253607
H	-0.965692	-4.163943	0.179502
H	-1.467880	4.155613	0.651356
H	-4.295305	0.887645	-0.980589
H	-4.068140	-0.797811	-1.600213
H	-0.233608	-0.000941	2.268195
H	1.863053	-0.124668	1.267537
H	3.589130	-1.854637	0.774491
H	5.945093	-2.162405	1.542748
H	7.659317	-0.415067	1.057578
H	7.024671	1.643201	-0.203129
H	4.665998	1.956478	-0.980381
H	-1.859394	-1.081425	-2.255722
H	0.450375	-1.018442	-1.826888
H	-2.061982	1.306360	-2.096831
H	0.261864	1.423273	-1.731309
H	-2.936954	-1.295659	2.522800
H	-2.700853	0.433651	2.996545
H	-5.825328	-0.531270	0.191304
H	-4.555772	-1.764913	0.565117
H	-4.539289	1.171147	1.566483
H	-5.116417	-0.247641	2.534789

5Ad PM3

C	4.454198	-1.178266	0.387883
C	4.033036	0.042175	-0.140486
C	4.901262	1.132529	-0.181042
C	6.192970	0.999832	0.317812
C	6.616659	-0.214980	0.846651
C	5.749076	-1.302239	0.879400
C	2.652499	0.182033	-0.689431
O	2.399514	0.337139	-1.874562
N	1.617468	0.197049	0.292572
C	0.168064	0.100347	-0.034948
C	-0.324982	1.335927	-0.840754
C	-1.871291	1.273039	-1.008619
C	-2.447702	-0.033008	-0.376415
C	-1.730212	-1.193521	-1.133314
C	-0.196822	-1.147035	-0.891527
C	-2.382190	2.574013	-0.387890
N	-1.286702	3.303064	0.160709
C	-0.042942	2.666658	-0.150197
C	-0.652367	0.023038	1.230476
C	-1.984333	-0.058833	1.062732
C	-2.147985	-2.599694	-0.708700
N	-1.028314	-3.268651	-0.121544
C	0.147119	-2.471382	-0.218656
C	-2.916437	-0.185004	2.214762
C	-4.352924	0.146481	1.857004
C	-4.756471	-0.600609	0.601737
C	-3.967750	-0.107152	-0.598014
O	1.006185	3.211678	0.117463
O	-3.503619	3.040002	-0.345020
O	-3.204382	-3.181459	-0.841534
O	1.215029	-2.881518	0.193761
H	-1.035247	-4.220828	0.168098
H	-1.360041	4.239232	0.491387
H	-4.357798	0.890881	-0.885295
H	-4.186671	-0.758285	-1.469380
H	-0.171094	0.039287	2.214232
H	1.857840	-0.289578	1.131194
H	3.773076	-2.038233	0.409045
H	6.084917	-2.259466	1.291711
H	7.635048	-0.316520	1.236114
H	6.877113	1.854427	0.290898
H	4.566251	2.086828	-0.603701
H	-1.951249	-1.086152	-2.223614
H	0.345990	-1.097370	-1.868415
H	-2.143230	1.283921	-2.091976
H	0.170921	1.347790	-1.842959
H	-2.851155	-1.227501	2.590645
H	-2.569542	0.458404	3.047957
H	-5.838104	-0.465258	0.405767
H	-4.613722	-1.690538	0.745706
H	-4.476064	1.238096	1.709536
H	-5.019076	-0.122205	2.699260

6Ad AM1

C	4.029250	0.198344	0.135967
C	2.510107	0.131875	0.239794
C	1.986292	-0.716161	1.380457
C	2.861164	-1.387805	2.372042
C	4.340447	-1.326018	2.061392
C	4.713071	0.015142	1.471809
C	1.921568	1.543699	0.457558
C	0.391369	1.488130	0.676070
C	-0.137908	0.032583	0.445509
C	0.340797	-0.439363	-0.957136
C	1.885389	-0.401303	-1.064060
C	0.642040	-0.785698	1.466399
C	2.285498	-1.838521	-1.419705
N	1.132013	-2.632595	-1.497390
C	-0.036479	-1.900456	-1.223892
C	-0.186356	2.533770	-0.275980
N	0.852696	3.034090	-1.084448
C	2.100679	2.503483	-0.727913
N	-1.564880	-0.057676	0.636995
C	-2.539050	0.167957	-0.328702
O	-2.264071	0.533053	-1.485567
O	3.418935	-2.269897	-1.654019
O	-1.162644	-2.404026	-1.228114
O	3.156459	2.821490	-1.285524
O	-1.344344	2.951750	-0.313147
C	-3.946044	-0.059919	0.114949
C	-4.446575	0.544243	1.271765
C	-5.774017	0.331392	1.642394
C	-6.596003	-0.484711	0.864583
C	-6.094706	-1.084294	-0.290982
C	-4.770477	-0.870981	-0.672187
H	0.721348	3.709385	-1.796965
H	1.139312	-3.594967	-1.729805
H	4.391539	-0.602970	-0.565147
H	4.331271	1.183486	-0.311298
H	0.107243	-1.372342	2.221653
H	-1.860056	-0.425965	1.511360
H	-3.805595	1.202514	1.877203
H	-6.172896	0.811756	2.547788
H	-7.642168	-0.652029	1.161095
H	-6.744232	-1.723498	-0.907061
H	-4.366318	-1.329783	-1.588617
H	2.433239	2.004145	1.344824
H	0.129547	1.796260	1.722874
H	2.212424	0.258250	-1.913677
H	-0.132799	0.199426	-1.753375
H	2.677755	-0.901855	3.371800
H	2.547557	-2.463184	2.471336
H	5.823505	0.072015	1.326443
H	4.421470	0.838528	2.174820
H	4.611968	-2.138968	1.336461
H	4.922069	-1.508240	3.002377

6Ad PM3

C	4.045935	0.080751	0.202300
C	2.512857	0.072515	0.248746
C	1.929338	-0.815665	1.332707
C	2.746445	-1.567168	2.324570
C	4.240847	-1.548392	2.060921
C	4.675629	-0.186541	1.556215
C	1.971690	1.501129	0.547286
C	0.427696	1.485108	0.734419
C	-0.126071	0.065236	0.395780
C	0.342194	-0.380181	-1.015372
C	1.897326	-0.371814	-1.105004
C	0.585666	-0.833381	1.386721
C	2.272621	-1.778220	-1.568044
N	1.091387	-2.571896	-1.673864
C	-0.067686	-1.814019	-1.344442
C	-0.085527	2.650570	-0.101480
N	0.976968	3.121912	-0.943968
C	2.221011	2.550266	-0.537773
N	-1.599892	0.026931	0.628135
C	-2.600966	0.305943	-0.359613
O	-2.327261	0.836564	-1.421012
O	3.347813	-2.253050	-1.872561
O	-1.164823	-2.337025	-1.353741
O	3.260688	2.944322	-1.028277
O	-1.155089	3.218118	-0.078454
C	-3.989175	-0.041695	0.068602
C	-4.845901	0.965445	0.510610
C	-6.143797	0.641946	0.892462
C	-6.583977	-0.676069	0.826551
C	-5.727980	-1.676163	0.376177
C	-4.427462	-1.363540	-0.004672
H	0.916153	3.963351	-1.473226
H	1.074628	-3.514866	-1.991934
H	4.413549	-0.680495	-0.515954
H	4.413547	1.047914	-0.194904
H	0.020794	-1.426308	2.114084
H	-1.865559	-0.723576	1.232325
H	-4.499302	2.004690	0.549899
H	-6.820618	1.428955	1.241131
H	-7.607203	-0.926327	1.125613
H	-6.078230	-2.711907	0.316769
H	-3.755460	-2.148210	-0.373530
H	2.470333	1.856021	1.482335
H	0.169286	1.697016	1.801044
H	2.240812	0.343665	-1.891759
H	-0.086571	0.302790	-1.790497
H	2.539240	-1.125774	3.321984
H	2.383616	-2.613272	2.379369
H	5.778432	-0.143116	1.468104
H	4.398993	0.603664	2.282867
H	4.514182	-2.328651	1.322293
H	4.785216	-1.811991	2.988240

**5Aa
AM1**

C	-0.337177	-3.484391	-1.186235	C	-6.237711	0.364251	1.951714
C	-0.229295	-2.003438	-0.829580	C	-7.225675	-0.507422	1.497640
C	-0.201676	-1.665416	0.642464	C	-6.948107	-1.368233	0.437661
C	-0.259203	-2.696723	1.705526	C	-5.697229	-1.364327	-0.172988
C	-0.739663	-4.041669	1.206369	H	-4.216918	1.088401	1.726763
C	0.005496	-4.424145	-0.051033	H	-6.449536	1.050035	2.785902
C	1.031601	-1.388864	-1.487766	H	-8.217583	-0.514927	1.971701
C	1.171149	0.102433	-1.138957	H	-7.722243	-2.060209	0.072978
C	-0.035334	0.583491	-0.270639	H	-5.497870	-2.062059	-1.002148
C	-1.290001	0.298245	-1.152290				
C	-1.409727	-1.210992	-1.448251				
C	-0.111185	-0.349050	0.922546				
C	-2.783273	-1.609120	-0.890802				
N	-3.411081	-0.475878	-0.323604				
C	-2.592056	0.678614	-0.445189				
C	2.498465	0.219187	-0.386561				
N	3.142707	-1.041551	-0.377374				
C	2.345985	-2.023968	-1.020319				
N	0.083647	1.973189	0.103858				
C	0.198077	2.999339	-0.825293				
O	-0.009149	2.808943	-2.040660				
O	-3.292353	-2.731634	-0.964337				
O	-2.913867	1.805818	-0.067010				
O	2.689446	-3.192535	-1.213044				
O	2.948450	1.250275	0.123543				
C	0.552422	4.338548	-0.276898				
C	1.698107	4.495750	0.510477				
C	2.031129	5.760330	0.994046				
C	1.223286	6.858945	0.697625				
C	0.083918	6.698333	-0.091085				
C	-0.253560	5.438442	-0.584914				
C	4.411443	-1.291877	0.199895				
C	-4.689796	-0.487742	0.285026				
H	-1.384352	-3.709806	-1.527657				
H	0.347685	-3.704750	-2.049639				
H	-0.095650	0.059618	1.939664				
H	0.393017	2.148900	1.033015				
H	2.344987	3.629088	0.728367				
H	2.934112	5.889938	1.608616				
H	1.487730	7.854577	1.084069				
H	-0.549916	7.565598	-0.327842				
H	-1.144487	5.302556	-1.217596				
H	0.964338	-1.534073	-2.599650				
H	1.229818	0.737719	-2.065544				
H	-1.428913	-1.399779	-2.554828				
H	-1.217650	0.900355	-2.100347				
H	0.773077	-2.809876	2.141011				
H	-0.928881	-2.341751	2.535364				
H	-0.267609	-5.469175	-0.353102				
H	1.112420	-4.406690	0.136588				
H	-1.841266	-3.999631	0.992566				
H	-0.575644	-4.812886	2.002654				
C	5.399491	-0.283845	0.225046				
C	6.641547	-0.540495	0.798447				
C	6.928493	-1.789482	1.345849				
C	5.959201	-2.790434	1.320519				
C	4.707983	-2.554060	0.758606				
H	5.190950	0.714474	-0.192083				
H	7.401311	0.255563	0.814580				
H	7.913546	-1.984350	1.793688				
H	6.178888	-3.780709	1.747460				
H	3.962053	-3.364770	0.736050				
C	-4.977549	0.380012	1.361226				

**5Aa
PM3**

C	0.083323	-3.582159	1.040275
C	0.075374	-2.068940	0.766365
C	0.074933	-1.657964	-0.688742
C	0.045620	-2.634374	-1.810107
C	0.445789	-4.035880	-1.389525
C	-0.320965	-4.439177	-0.146079
C	-1.151237	-1.395520	1.459913
C	-1.195832	0.119789	1.154129
C	0.063052	0.534761	0.336192
C	1.292329	0.144490	1.207790
C	1.322706	-1.390756	1.419617
C	0.086274	-0.329891	-0.901457
C	2.674457	-1.839908	0.858332
N	3.395363	-0.703769	0.352095
C	2.630768	0.501823	0.565978
C	-2.507868	0.349306	0.408992
N	-3.260650	-0.873045	0.372289
C	-2.517241	-1.924891	1.023514
N	0.085573	1.975983	-0.036861
C	-0.033452	3.038625	0.908154
O	0.080702	2.831834	2.106816
O	3.151461	-2.959444	0.859078
O	3.062487	1.602787	0.291819
O	-2.989505	-3.026935	1.220464
O	-2.909056	1.389724	-0.080872
C	-0.224547	4.391327	0.307757
C	-1.435594	4.721876	-0.300603
C	-1.608157	5.991953	-0.839800
C	-0.578063	6.925029	-0.775081
C	0.627512	6.591896	-0.166362
C	0.807978	5.325696	0.380570
C	-4.578024	-1.022171	-0.208945
C	4.709497	-0.755819	-0.252505
H	1.091716	-3.902801	1.373661
H	-0.581903	-3.810635	1.898493
H	0.111990	0.118121	-1.900687
H	-0.378815	2.159117	-0.902200
H	-2.251034	3.989370	-0.347080
H	-2.558535	6.256673	-1.314946
H	-0.717560	7.923607	-1.202301
H	1.436898	7.327622	-0.114063
H	1.754599	5.062199	0.866408
H	-1.059278	-1.564709	2.561293
H	-1.227733	0.705812	2.106968
H	1.315414	-1.631948	2.510696
H	1.226964	0.669603	2.193454
H	-0.984329	-2.643122	-2.224356
H	0.698445	-2.278610	-2.632220
H	-0.130740	-5.503618	0.093577
H	-1.411431	-4.365936	-0.332176
H	1.536840	-4.089876	-1.201388
H	0.245690	-4.744987	-2.215648
C	-5.193969	0.070279	-0.831511
C	-6.455435	-0.083877	-1.391498
C	-7.105910	-1.312177	-1.336260
C	-6.492008	-2.394833	-0.714885
C	-5.231225	-2.259255	-0.148798
H	-4.664547	1.042133	-0.862515
H	-6.937079	0.770971	-1.877559
H	-8.099979	-1.426456	-1.780330
H	-7.002440	-3.362446	-0.667322
H	-4.730565	-3.109129	0.354885
C	5.321583	0.424259	-0.692992
C	6.578318	0.364993	-1.280559

C	7.229333	-0.855023	-1.431597
C	6.620424	-2.024951	-0.989760
C	5.363930	-1.984947	-0.399813
H	4.791028	1.387567	-0.559444
H	7.055885	1.288305	-1.624561
H	8.219920	-0.894047	-1.895752
H	7.131171	-2.986699	-1.104053
H	4.866646	-2.905545	-0.036126

**6Aa
AM1**

C	1.374217	4.765963	-0.321902	C	5.082948	-3.312184	-2.345894
C	1.595572	3.818199	0.683219	C	5.505183	-2.196162	-3.065245
C	2.086657	4.214493	1.930639	C	4.975562	-0.941444	-2.766643
C	2.350744	5.562335	2.172090	C	4.028147	-0.791968	-1.758706
C	2.121160	6.510749	1.174888	H	3.809189	-4.082823	-0.779250
C	1.634153	6.112533	-0.070236	H	5.494149	-4.305837	-2.578959
C	1.326979	2.382629	0.378051	H	6.251797	-2.304337	-3.865043
O	1.758066	1.836565	-0.655009	H	5.304399	-0.055729	-3.331048
N	0.574175	1.695354	1.323907	H	3.622766	0.210027	-1.528188
C	0.125107	0.328819	1.202548				
C	1.236512	-0.690731	1.625849				
C	0.734976	-2.135117	1.432750				
C	-0.774138	-2.166792	1.096813				
C	-0.921287	-1.481557	-0.276651				
C	-0.360902	-0.045123	-0.229937				
C	-1.453664	-1.281864	2.121526				
C	-2.488924	-1.766800	3.066432				
C	-2.965232	-3.181019	2.818091				
C	-1.819463	-4.069238	2.389782				
C	-1.278035	-3.604506	1.056888				
C	-1.019010	-0.004925	2.149414				
C	2.518890	-0.596703	0.803282				
N	2.642577	-1.767695	0.007615				
C	1.642229	-2.711206	0.333082				
C	-2.367959	-1.325412	-0.759588				
N	-2.646004	0.045297	-0.983161				
C	-1.518165	0.849944	-0.683746				
O	-3.165034	-2.243468	-0.971082				
O	-1.484241	2.077953	-0.793932				
O	3.355774	0.302640	0.875974				
O	1.549956	-3.838674	-0.162458				
C	3.602680	-1.920029	-1.022193				
C	-3.883703	0.544171	-1.457365				
H	-2.092991	-3.694846	0.287393				
H	-0.445622	-4.284015	0.729522				
H	-1.423521	0.765152	2.815511				
H	0.151003	2.227885	2.048678				
H	2.285564	3.467420	2.713683				
H	2.744307	5.875803	3.150114				
H	2.328431	7.573520	1.369805				
H	1.457708	6.859526	-0.858196				
H	1.000254	4.438362	-1.304822				
H	0.901762	-2.743621	2.361729				
H	1.500457	-0.497010	2.699332				
H	-0.381344	-2.101136	-1.045139				
H	0.487591	0.082086	-0.958850				
H	-2.056945	-1.704573	4.105118				
H	-3.369629	-1.068016	3.038578				
H	-2.174345	-5.128489	2.292495				
H	-1.010222	-4.053645	3.165749				
H	-3.754823	-3.182647	2.020188				
H	-3.434170	-3.581368	3.754431				
C	-3.928302	1.696166	-2.272471				
C	-5.151118	2.180198	-2.728186				
C	-6.340822	1.535297	-2.395584				
C	-6.303915	0.394831	-1.595741				
C	-5.093174	-0.102767	-1.122736				
H	-3.001199	2.228528	-2.539772				
H	-5.171152	3.081434	-3.359441				
H	-7.301831	1.922666	-2.763109				
H	-7.238323	-0.123077	-1.331861				
H	-5.086787	-1.014909	-0.504948				
C	4.141451	-3.186976	-1.327551				

6Aa
PM3

C	-0.707046	4.853888	0.229612
C	0.536823	4.242540	0.383625
C	1.648469	4.987256	0.775189
C	1.507818	6.348473	1.024843
C	0.267920	6.961813	0.877588
C	-0.836663	6.216028	0.478224
C	0.689825	2.784478	0.097255
O	1.195140	2.337600	-0.916910
N	0.253481	1.932410	1.164082
C	0.091217	0.451802	1.074014
C	1.413297	-0.255321	1.513874
C	1.225064	-1.791763	1.464167
C	-0.260768	-2.163376	1.178597
C	-0.590311	-1.628139	-0.241931
C	-0.391952	-0.090750	-0.299168
C	-1.080722	-1.361833	2.173518
C	-1.957523	-1.966097	3.213981
C	-2.130642	-3.469840	3.105933
C	-0.830626	-4.126988	2.686255
C	-0.463101	-3.680005	1.284041
C	-0.915649	-0.029258	2.098752
C	2.665232	0.026466	0.691157
N	3.059748	-1.178421	-0.003573
C	2.246675	-2.280504	0.433049
C	-2.022804	-1.864662	-0.719952
N	-2.667272	-0.600820	-0.971137
C	-1.752730	0.475444	-0.705523
O	-2.579480	-2.925563	-0.927370
O	-2.074643	1.645022	-0.805519
O	3.322603	1.045335	0.661421
O	2.426998	-3.416578	0.034555
C	4.170080	-1.277226	-0.927391
C	-4.026396	-0.439256	-1.443706
H	-1.259575	-4.011837	0.586626
H	0.448109	-4.215312	0.950273
H	-1.439406	0.679618	2.749096
H	-0.463136	2.356394	1.716879
H	2.626209	4.502711	0.879714
H	2.377571	6.937858	1.333432
H	0.161755	8.034111	1.072519
H	-1.810341	6.701534	0.354904
H	-1.573655	4.266812	-0.098218
H	1.496753	-2.247863	2.447986
H	1.626543	0.070715	2.562212
H	0.089159	-2.139897	-0.967495
H	0.352746	0.169472	-1.092571
H	-1.517219	-1.712591	4.201126
H	-2.947427	-1.467401	3.191220
H	-0.931641	-5.229289	2.710177
H	-0.021716	-3.881917	3.403589
H	-2.929671	-3.716832	2.378154
H	-2.476350	-3.874967	4.076556
C	-4.547438	0.844660	-1.645519
C	-5.852636	0.990089	-2.096831
C	-6.640569	-0.128449	-2.347597
C	-6.119671	-1.402585	-2.147099
C	-4.816432	-1.567314	-1.696824
H	-3.904678	1.723815	-1.443809
H	-6.258555	1.994448	-2.256243
H	-7.668525	-0.006237	-2.703551

H	-6.736341	-2.285379	-2.345574
H	-4.383736	-2.574309	-1.535650
C	4.483282	-2.509181	-1.514443
C	5.539273	-2.590197	-2.412656
C	6.283027	-1.458445	-2.729749
C	5.971549	-0.236801	-2.141831
C	4.920230	-0.136868	-1.240014
H	3.883511	-3.400955	-1.247305
H	5.782972	-3.553921	-2.871664
H	7.112753	-1.529126	-3.440238
H	6.555628	0.655954	-2.388499
H	4.665014	0.827186	-0.759314

**5Ae
AM1**

C	-0.005679	-0.033113	0.000807
C	-0.005801	-0.010527	1.527195
C	1.348477	-0.000265	2.197547
C	2.621470	0.032976	1.439264
C	2.463077	-0.329123	-0.021074
C	1.296460	0.420039	-0.621961
C	-0.801152	1.209707	2.051771
C	-0.830865	1.232427	3.591954
C	-0.063035	0.004181	4.180988
C	-0.826885	-1.233539	3.616566
C	-0.774880	-1.240009	2.074198
C	1.313994	0.001121	3.546158
C	-0.125161	-2.568504	1.739037
O	0.173776	-3.288186	2.894120
C	-0.192516	-2.543717	4.022255
C	-0.179054	2.544480	3.962671
O	0.132025	3.285697	2.821253
C	-0.201692	2.550359	1.679791
N	-0.024293	0.030918	5.621757
C	-1.164547	0.074182	6.413481
O	-2.298654	-0.095513	5.922305
O	0.142249	-3.121153	0.684418
O	0.033094	-3.073277	5.095749
O	0.000186	3.109573	0.615478
O	0.107348	3.059980	5.030863
C	-0.943423	0.317637	7.864934
C	-0.207747	1.430436	8.287260
C	-0.032730	1.660533	9.651100
C	-0.584079	0.783244	10.586071
C	-1.320549	-0.322512	10.160561
C	-1.507220	-0.557062	8.798535
H	-0.220592	-1.079285	-0.352651
H	-0.835161	0.623182	-0.376766
H	2.209630	-0.004335	4.179091
H	0.857378	0.213930	6.043063
H	0.210956	2.133846	7.548259
H	0.539222	2.537783	9.988200
H	-0.440392	0.966502	11.661595
H	-1.758909	-1.010776	10.898409
H	-2.097304	-1.420133	8.453167
H	-1.844250	1.169067	1.635118
H	-1.886558	1.223781	3.983319
H	-1.810945	-1.240187	1.640235
H	-1.888070	-1.214166	3.994013
H	3.046970	1.073056	1.518530
H	3.361229	-0.662805	1.921186
H	1.252049	0.233388	-1.727082
H	1.428885	1.524982	-0.472055
H	2.296771	-1.434552	-0.126009
H	3.407075	-0.074210	-0.569038

**5Ae
PM3**

C	-0.014824	0.001424	0.001825
C	-0.010446	-0.000865	1.539337
C	1.349846	-0.000757	2.201313
C	2.624136	0.046209	1.436506
C	2.458889	-0.341654	-0.020843
C	1.300020	0.421499	-0.630418
C	-0.806930	1.218238	2.092631
C	-0.801864	1.226508	3.642653
C	-0.045751	-0.022443	4.181936
C	-0.818189	-1.252770	3.629240
C	-0.773197	-1.249796	2.077275
C	1.324405	-0.022460	3.546100
C	-0.125823	-2.595312	1.747440
O	0.177812	-3.319150	2.886085
C	-0.197562	-2.593182	4.008832
C	-0.132399	2.550393	3.992755
O	0.147908	3.300760	2.865816
C	-0.231182	2.586972	1.736239
N	0.068448	-0.062346	5.664606
C	-1.047467	0.048802	6.547879
O	-2.186822	-0.088244	6.129144
O	0.133866	-3.167582	0.720998
O	0.004963	-3.160444	5.048028
O	-0.080976	3.189123	0.706993
O	0.181749	3.066962	5.034095
C	-0.696029	0.262441	7.980706
C	-0.137319	1.473952	8.389652
C	0.169139	1.669155	9.731727
C	-0.077097	0.661319	10.659107
C	-0.636053	-0.544145	10.247589
C	-0.951516	-0.747155	8.908082
H	-0.276178	-1.009488	-0.373841
H	-0.825361	0.662505	-0.367966
H	2.230175	-0.045780	4.162314
H	0.897761	0.379599	6.003870
H	0.050927	2.273623	7.662347
H	0.604260	2.619928	10.057492
H	0.167739	0.818596	11.714913
H	-0.831456	-1.335901	10.978568
H	-1.398555	-1.693565	8.582612
H	-1.851781	1.168894	1.700899
H	-1.846290	1.236504	4.041940
H	-1.804477	-1.247611	1.649896
H	-1.874080	-1.233386	3.995792
H	3.024452	1.079214	1.510893
H	3.376325	-0.605399	1.924730
H	1.252148	0.238980	-1.721823
H	1.461201	1.512586	-0.517513
H	2.293650	-1.433509	-0.117762
H	3.395087	-0.127865	-0.571550

**6Ae
AM1**

C	0.015522	-0.065402	-0.005335
C	0.009008	0.014290	1.391941
C	1.212732	0.083748	2.099693
C	2.422538	0.081152	1.406435
C	2.431304	0.013806	0.012718
C	1.229400	-0.060453	-0.691410
C	-1.306895	-0.012147	2.092528
O	-2.200723	-0.822645	1.791726
N	-1.475301	0.935182	3.098596
C	-2.664611	1.145941	3.884554
C	-2.699850	0.231395	5.157333
C	-3.967339	0.515582	5.991532
C	-4.785234	1.682548	5.394426
C	-5.217434	1.236566	3.982803
C	-3.990633	0.909085	3.104483
C	-3.806408	2.827163	5.237394
C	-3.959766	4.133139	5.922464
C	-5.276022	4.321904	6.644279
C	-5.720210	3.038700	7.308810
C	-6.001579	1.986045	6.260763
C	-2.741596	2.556261	4.455393
C	-2.758102	-1.251072	4.877988
O	-3.949142	-1.802527	5.371542
C	-4.693266	-0.814638	6.011949
C	-5.961241	2.295147	3.194153
O	-5.302818	2.587803	2.001208
C	-4.128092	1.832644	1.913763
O	-7.007414	2.894078	3.383133
O	-3.448911	2.034537	0.922462
O	-1.976181	-2.042636	4.385351
O	-5.755196	-1.176604	6.492970
H	-6.842537	2.347500	5.606357
H	-6.353924	1.040924	6.755316
H	-1.952844	3.282131	4.225983
H	-0.752107	1.605609	3.225123
H	1.213965	0.117482	3.199336
H	3.371069	0.128224	1.961358
H	3.388008	0.014142	-0.530877
H	1.235885	-0.119914	-1.790004
H	-0.939424	-0.138058	-0.550272
H	-3.698347	0.781815	7.049889
H	-1.775223	0.435667	5.761780
H	-5.891408	0.340222	4.079360
H	-4.028834	-0.157786	2.740416
H	-3.118114	4.228783	6.665294
H	-3.826856	4.960210	5.171749
H	-6.652703	3.221166	7.904519
H	-4.930290	2.679411	8.018855
H	-6.063873	4.657506	5.918265
H	-5.161373	5.131752	7.411219

**6Ae
PM3**

C	-0.010065	0.080937	-0.010706
C	-0.000437	0.006191	1.382066
C	1.204522	-0.063348	2.079883
C	2.404876	-0.043431	1.377162
C	2.400726	0.037410	-0.011617
C	1.195241	0.096318	-0.704070
C	-1.290277	-0.034657	2.131659
O	-1.759271	-1.035652	2.640507
N	-1.924240	1.245109	2.274433
C	-3.318781	1.470587	2.752459
C	-3.314828	1.745629	4.288334
C	-4.755257	2.074941	4.766147
C	-5.742265	2.146291	3.567716
C	-5.760205	0.744210	2.905144
C	-4.337132	0.347232	2.425363
C	-5.101812	3.109729	2.585181
C	-5.720758	4.394593	2.160285
C	-7.157170	4.584186	2.612347
C	-7.346551	4.061580	4.023006
C	-7.140283	2.558882	4.044189
C	-3.878068	2.748606	2.159865
C	-2.888235	0.603255	5.201924
O	-3.935906	0.177029	6.012155
C	-5.037926	0.983585	5.797944
C	-6.601847	0.633715	1.635006
O	-5.838337	0.267769	0.537434
C	-4.518109	0.125308	0.925915
O	-7.772544	0.759794	1.390181
O	-3.764003	-0.137968	0.025680
O	-1.843485	0.057580	5.427603
O	-5.989586	0.704106	6.480556
H	-7.916075	2.083679	3.409143
H	-7.327418	2.169458	5.064976
H	-3.290472	3.340615	1.449362
H	-1.670132	1.879466	1.544691
H	1.204341	-0.140881	3.173313
H	3.354283	-0.097281	1.920312
H	3.347766	0.049618	-0.561424
H	1.193118	0.150069	-1.797860
H	-0.960840	0.110446	-0.556826
H	-4.785305	3.061576	5.288851
H	-2.630237	2.607079	4.479896
H	-6.154496	0.006923	3.646024
H	-4.017630	-0.613688	2.901398
H	-5.090334	5.212968	2.567081
H	-5.654470	4.485246	1.057273
H	-8.363590	4.301529	4.388998
H	-6.647381	4.564496	4.721065
H	-7.852723	4.066344	1.921421
H	-7.425159	5.656947	2.556305