Supplementary Information

Design and synthesis of fluorescent 7-deazaadenosine nucleosides containing π-extended diarylacetylene motifs

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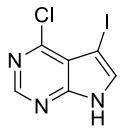
1 Experimental Details

General details

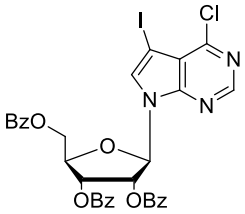
Dry, N_2-saturated solvents were collected from a Grubbs-type solvent system in flame and vacuum-dried glassware. $Pd(OAc)_2$ was purchased from Precious Metals Online (Australia), having a purity >99%. 6-Chloro-7-deazapurine was purchased from Chemos GmbH. All other chemicals were purchased from Sigma-Aldrich or Alfa Aesar. Proton (^{1}H), carbon (^{13}C), boron (^{11}B) and fluorine (^{19}F) NMR were recorded using a Jeol ECX400, ECS400 or Bruker AMX500 spectrometer. ^{13}C and ^{11}B and NMR were proton decoupled. In all cases, the *ipso* carbon of boron-containing compounds was not observed due to quadrupolar coupling. All NMR spectra were processed in MNova software and images generated directly from the program as .jpeg, .bmp, .png or .tif files. Mass spectrometry was recorded using ESI on a Bruker Daltronics micrOTOF machine, or EI on a Waters GCT Premier. Melting points (Mp) were recorded using a Stuart digital SMP3 machine. UV/Vis spectra were recorded using a Jasco V-550 or a Jasco V-560 spectrophotometer. Fluorescence spectra were recorded using a Horiba FluoroMax-3 fluorimeter. Quantum yields were measured using an integrating sphere.[1]

4-Chloro-5-iodo-7H-pyrrolo[2,3-d]pyrimidine 8



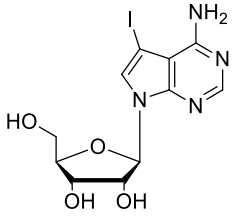
Based on the procedure reported by Wilulski *et al.*[2,3] 4-Chloro-7H-pyrrolo[2,3-d]pyrimidine (2.61 g, 17.1 mmol, 1.0 eq) and KOH (2.39 g, 42.7 mmol, 2.5 eq) were dissolved in DMF (30 ml). Iodine (4.39 g, 17.3 mmol, 1.01 eq) in DMF (30 ml) was added slowly, and the reaction was stirred at room temperature for 30 min. The reaction mixture was then poured onto water and ice (*ca.* 800 ml) containing 0.5% ammonia and 0.1% sodium metabisulfite. A white precipitate formed slowly, and this was filtered off. The precipitate was dissolved in EtOAc, dried over sodium sulfate and filtered. The volatiles were removed *in vacuo* to yield the product as a white solid (3.53 g, 12.7 mmol, 74%). Spectroscopic characterisation was consistent with that previously reported.[3] ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.95 (br s, 1H, NH), 8.60 (s, 1H, C2-H), 7.93 (d, J = 2.5, 1H, C6-H); ^{13}C NMR (101 MHz, DMSO-d_6) δ 151.5, 150.8, 150.5, 133.9, 115.8, 51.8; ESI HRMS $[MH]^+$ 279.9134 (Calcd. for $C_6H_4ClIN_3$ 279.9133).

4-Chloro-5-iodo-7-[(2,3,5-tri-*O*-benzoyl)-β-D-ribofuranosyl]-7H-pyrrolo[2,3-d]pyrimidine 10



Based on the procedure reported by Seela and Ming.[4] 4-Chloro-5-iodo-7H-pyrrolo[2,3-d]pyrimidine (729 mg, 2.61 mmol, 1.0 eq) was stirred with *N*,*O*-bis(trimethylsilyl)acetamide (BSA) (0.77 ml, 3.1 mmol, 0.5 eq) in dry acetonitrile (20 ml) at room temperature for 15 min. 1-*O*-Acetyl-2,3,5-*O*-benzoyl-β- D-ribofuranose (1.45 g, 2.87 mmol, 1.1 eq) and TMSOTf (0.20 ml, 3.1 mmol, 0.5 eq) were added and the reaction mixture was stirred for a further 10 min at rt, followed by 1.5 h at 80 °C. The reaction mixture was allowed to cool to rt, then diluted with EtOAc (40 ml). The reaction mixture was then washed with sat. aq. $NaHCO_3$ (2 x 30 ml) and brine (2 x 30 ml), dried over Na_2SO_4 and filtered. The volatiles were removed *in vacuo* to yield the crude product as a yellow gum. This was redissolved in cyclohexane/EtOAc (20 ml 1:1 v/v) and absorbed on to silica. It was purified by column chromatography on silica gel, eluting with cyclohexane/EtOAc (10:1 v/v) to yield the title compound as a white solid (1.20 g, 1.66 mmol, 71%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.60 (s, 1H, C2-H), 8.30 (s, 1H, C6-H), 7.99 (dd, *J* = 8.4, 1.3 Hz, 2H, ArH), 7.94 (dd, *J* = 8.4, 1.3 Hz, 2H, Ar-H), 7.85 (dd, *J* = 8.4, 1.3 Hz, 2H, Ar-H), 7.71 – 7.61 (m, 3H, Ar-H), 7.57 – 7.39 (m, 6H, Ar-H), 6.71 (d, *J* = 5.1 Hz, 1H, C1′-H), 6.29 (dd, *J* = 6.1, 5.1 Hz, 1H, C2′-H), 6.13 (app t, *J* = 5.8 Hz, 1H, C3′-H), 4.86 (ddd, *J* = 5.8, 5.0, 3.9 Hz, 1H, C4′-H), 4.80 (dd, *J* = 12.1, 3.9 Hz, 1H, C5′-Ha), 4.68 (dd, *J* = 12.1, 5.0 Hz, 1H, C5′-Hb); ^{13}C NMR (101 MHz, DMSO-d_6) δ 166.0, 165.2, 165.0, 152.2, 151.5, 151.2, 134.8, 134.5, 134.5, 134.1, 130.0, 129.9, 129.9, 129.9, 129.8, 129.7, 129.7, 129.4, 129.3, 129.2, 129.2, 129.1, 128.8, 87.0, 79.8, 74.0, 71.2, 63.9, 55.1 (29 of 32 resonances observed); ESI HRMS $[M+H]^+$ 724.0336 (Calcd. for $C_{32}H_{24}ClIN_3O_7$ 724.0342).

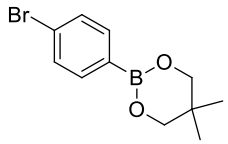
4-Amino-5-iodo-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine 11



Based on the procedure reported by Seela and Ming.[4] **Error! Bookmark not defined.**4-Chloro-5-iodo-7-[(2′,3′,5′-tri-*O*-enzoyl)-β-D-ribofuranosyl]-7H-pyrrolo[2,3-d]pyrimidine (362 mg, 0.500 mmol) was added to a sealed tube and dissolved in aq. NH_3 (5 ml, 25%) and dioxane (5 ml). The reaction was stirred at 60 °C for 3 days. The volatiles were removed *in vacuo* and the crude product was redissolved in methanol and adsorbed on to silica. The product was then purified by column chromatography on silica gel eluting with CH_2Cl_2/MeOH/Et_3N (95:4:1). The product was dried *in vacuo* to yield 4-amino-5-iodo-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine as

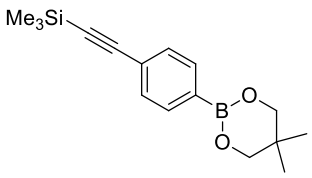
a white solid (171 mg, 0.436 mmol, 87%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.10 (s, 1H, C2-H), 7.67 (s, 1H, C6-H), 6.67 (br s, 2H, NH_2), 6.02 (d, J = 6.4 Hz, 1H, C1′-H), 5.31 (d, J = 6.4 Hz, 1H, C2′-OH), 5.16 (app t, J = 6.0 Hz, 1H, C5′-OH), 5.12 (d, J = 5.0 Hz, 1H, C3′-OH), 4.35 (app dt, J = 6.4, 5.0 Hz, 1H, C2′-H), 4.06 (app dt, J = 5.0, 3.1 Hz, 1H, C3′-H), 3.88 (app q, J = 3.8 Hz, 1H, C4′-H), 3.61 (ddd, J = 12.0, 5.0, 4.0 Hz, 1H, C5′-Ha), 3.52 (ddd, J = 12.0, 6.0, 3.9 Hz, 1H, C5′-Hb); ^{13}C NMR (101 MHz, DMSO-d_6) δ 157.2, 151.9, 150.2, 127.2, 103.3, 86.8, 85.2, 73.9, 70.5, 61.6, 51.9; ESI HRMS $[MH]^+$ 393.0058 (Calcd. for $C_{11}H_{14}IN_4O_4$ 393.0054).

4-Bromophenylboronic acid neopentyl glycol ester {IUPAC name: 2-(4-Bromophenyl)-5,5-dimethyl-1,3,2-dioxaborinane} **13**



Prepared according to Zheng *et al.*[5] 4-Bromophenylboronic acid (1.00 g, 5.00 mmol, 1.0 eq) and 2,2,-dimethylpropanediol (573 mg, 5.50 mmol, 1.1 eq) were dissolved in toluene (50 ml) and heated to reflux in a Dean-Stark apparatus for 16 h (or until production of water ceased). The toluene was removed *in vacuo*. The product was purified by column chromatography on silica gel, eluting with EtOAc/Pet Ether 40-60 (1:4 *v*/*v*). The product was isolated as a white solid (1.31 g, 4.87 mmol, 97%). Mp 107-110 °C (lit. 109-111 °C[5]); ^{1}H NMR (400 MHz, acetone-d_6) δ 7.67 (d, J = 8.4 Hz, 2H, Ar-H), 7.53 (d, J = 8.4 Hz, 2H, Ar-H), 3.80 (s, 4H, $(CH_2)_2$), 1.01 (s, 6H, $(CH_3)_2$); ^{13}C NMR (101 MHz, acetone-d_6) δ 136.5, 131.5, 125.8, 72.8, 32.4, 21.8; ^{11}B NMR (128 MHz, acetone-d_6) δ 25.6 (s); EI MS *m/z* (%) 267 (16) $[^{10}B^{79}BrM]^+$; 268 (100) $[^{11}B^{79}BrM]^+$; 269 (33) $[^{10}B^{81}BrM]^+$; 270 (97); 271 (12) $[^{10}B^{81}BrM]^+$; HRMS $[M]^+$ 268.0276 (Calcd. For $C_{11}H_{14}O_2BBr$ 268.0272); Anal. calcd. for $C_{11}H_{14}O_2BBr$: C 49.13, H 5.25; found: C 48.88, H 5.21.

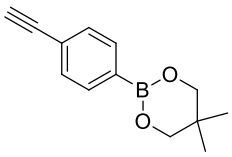
4-(Trimethylsilylethynyl)phenylboronic acid neopentyl glycol ester {IUPAC name: 2-(4-{Trimethylsilylethynyl}phenyl)-5,5-dimethyl-1,3,2-dioxaborinane} **14**



Prepared according to Zheng *et al.*[5] 4-Bromophenylboronic acid neopentyl glycol ester (1.08 g, 4.00 mmol, 1.0 eq), $PdCl_2(PPh_3)_2$ (140 mg, 5 mol%), CuI (38.0 mg, 5 mol%) and PPh_3 (210 mg, 20 mol%) were added to a microwave vial which was sealed with a septum and flushed with argon. DMF (2.2 ml) and Et_2NH (6.5 ml were added and the mixture was sparged with argon and stirred to produce a dark orange solution. Trimethylsilylacetylene (630 μl, 4.4 mmol, 1.1 eq) was added and the reaction mixture formed a pale yellow

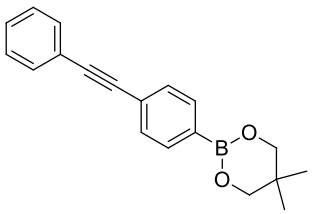
solution. After <2 min, a white precipitate (presumably Et_2NH_2I) was formed. The septum was replaced with a microwave vial cap and the mixture was heated at 120 °C in a microwave for 20 min. The dark orange/brown reaction mixture was then allowed to cool to room temperature and the volatiles removed *in vacuo*. The crude product was then suspended in water (25 ml) and extracted with CH_2Cl_2 (4x25 ml). The combined organic fractions were washed with brine (15 ml) and dried over Na_2SO_4, filtered and the solvent removed *in vacuo*. This crude material was purified by column chromatography on silica gel, eluting with Pet Ether 40-60, followed by Et_2O/Pet Ether 40-60 (1:49 *v*/*v*) to yield the product as a white solid (804 mg, 2.80 mmol, 70%). Mp 94-98 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.1 Hz, 2H, Ar-H), 7.4 (d, *J* = 8.1 Hz, 2H, Ar-H), 3.76 (s, 4H, $(CH_2)_2$), 1.02 (s, 6H, $(CH_3)_2$), 0.25 (s, 9H, $Si(CH_3)_3$); ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.7, 131.2, 125.2, 105.6, 100.1, 95.2, 72.5, 32.0, 22.1, 0.1; ^{11}B NMR (128 MHz, $CDCl_3$) δ 26.4 (br s); EI MS *m/z* (%) 270 (36) [^{10}BM-Me]$^+$; 271 (100) [^{11}BM-Me]$^+$; 285 (7) [^{10}BM]$^+$; 286 (25) [^{11}BM]$^+$; HRMS [M]$^+$ 286.1564 (Calcd. For $C_{16}H_{23}O_2SiB$ 286.1558); Anal. calcd. for $C_{16}H_{23}O_2SiB$: C 66.13, H 8.10; found: C 66.17, H 8.31.

4-Ethynylphenylboronic acid neopentyl glycol ester {IUPAC name: 2-(4-Ethynylphenyl)-5,5-dimethyl-1,3,2-dioxaborinane} **15**



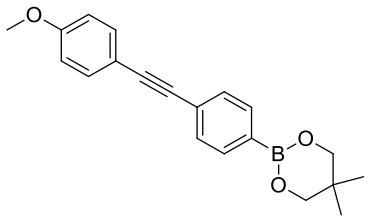
Prepared according to Zheng *et al.*[5] 4-(Trimethylsilylethynyl)phenylboronic acid neopentyl glycol ester (301 mg, 1.05 mmol, 1.0 eq) was dissolved in THF (10.5 ml) and cooled to 0 °C. TBAF (1.05 ml, 1.0 M in THF, 1.0 eq) was added and the reaction mixture stirred at 0 °C for 1 h. The mixture was then allowed to warm to rt and stirred for a further 2 h. Saturated $NaHCO_3$ solution (10 ml) was added and the mixture extracted with Et_2O (3x10 ml). The organic fractions were dried over Na_2SO_4, and the solvent removed *in vacuo*. The crude mixture could be used without further purification, or filtered through a short silica plug (ca. 2 cm) eluting with EtOAc/Pet Ether 40-60 (1:4 *v*/*v*) to give the title compound quantitatively as a white solid. Spectroscopic characterisation was consistent with that previously reported. Mp 75-77 °C (lit. 73-75 °C[6]) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 8.2 Hz, 2H, Ar-H), 7.48 (d, *J* = 8.2 Hz, 2H, Ar-H), 3.77 (s, 4H, $(CH_2)_2$), 3.13 (s, 1H, CCH), 1.02 (s, 6H, $(CH_3)_3$); ^{13}C NMR (101 MHz, $CDCl_3$) 133.8, 131.3, 124.2, 72.5, 32.0, 22.0; ^{11}B NMR (128 MHz, $CDCl_3$) δ 25.8 (br s); EI MS *m/z* (%) 213.1143 (18) [^{10}BM]$^+$; 213.1794 (73) [^{11}BM-H]$^+$; 214 (100) [^{11}BM]$^+$; HRMS [M]$^+$ 214.1163 (Calcd. For $C_{13}H_{15}O_2B$ 214.1168); Anal. calcd. for $C_{13}H_{15}O_2B$: C 72.94, H 7.06; found: C 72.94, H 7.17.

4-(Phenylethynyl)phenylboronic acid neopentyl glycol ester {IUPAC name: 2-(4-{Phenylethynyl}phenyl)-5,5-dimethyl-1,3,2-dioxaborinane} **12a**



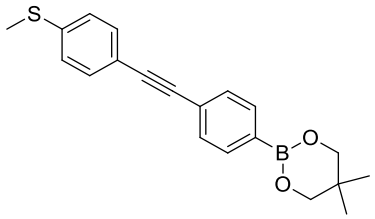
Prepared according to Zheng *et al*.[5] 4-Bromophenyl boronic acid neopentyl glycol ester (538 mg, 2.00 mmol, 1 eq), $PdCl_2(PPh_3)_2$ (70.2 mg, 5 mol%), CuI (19.0 mg, 5 mol%) and PPh_3 (105 mg, 20 mol%) were added to a microwave tube. A septum was used to seal the tube and it was flushed with argon. Diethylamine (3.2 ml) and DMF (1.1 ml) were added, followed by phenylacetylene (264 µl, 2.40 mmol, 1.2 eq). The septum was replaced by a lid and the reaction heated at 120 °C in a microwave (150 W) for 20 min. The solvent was then removed *in vacuo* to give the crude product, which was purified by column chromatography on silica gel eluting with Pet Ether 40-60, followed by EtOAc/Pet Ether 40-60 (1:4 *v*/*v*) to give the product as a pale yellow solid (508 mg, 88%). Mp 125-127 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.8 Hz, 2H, Ar-H), 7.57 – 7.48 (m, 4H, Ar-H), 7.39-7.31 (m, 3H, Ar-H), 3.78 (s, 4H, $(CH_2)_2$), 1.03 (s, 6H, $(CH_3)_2$); ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.8, 131.8, 130.8, 128.5, 128.4, 125.4, 123.4, 90.5, 89.9, 72.5, 32.1, 22.1; ^{11}B NMR (128 MHz, $CDCl_3$) δ 21.5 (br s); EI MS *m/z* (%) 178 (100) $[M\text{-}BO_2C_5H_{16}+H]^+$ 289 (5) $[^{10}BM]^+$; 290 (42) $[^{11}BM]^+$; HRMS $[M]^+$ 290.1443 (Calcd. For $C_{19}H_{19}BO_2$ 290.1482); IR (ATR) $\tilde{\nu}$ (cm^{-1}) = 2901 (br w), 2503 (br), 2159 (br), 2029 (br), 1975, 1603, 1477, 1420, 1305, 1249, 1141, 1124.

4-([4-Methoxyphenyl]ethynyl)phenylboronic acid neopentyl glycol ester {IUPAC name: 2-(4-{[4-Methoxyphenyl]ethynyl}phenyl)-5,5-dimethyl-1,3,2-dioxaborinane} **12b**



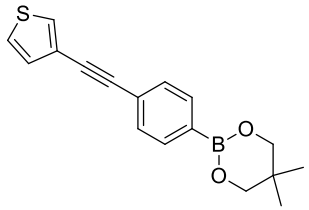
The title compound was prepared as described for **12a** from 4-bromophenyl boronic acid neopentyl glycol ester (40.3 mg, 0.150 mmol) and 4-ethynylanisole (23 µl, 0.18 mmol, 1.2 eq) and isolated as a yellow solid (29.8 mg, 0.0931 mmol, 62%). Mp 116-118 °C (decomp.); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8.3 Hz, 2H, Ar-H), 7.51 – 7.45 (m, 4H, Ar-H), 6.88 (d, *J* = 8.8 Hz, 1H, Ar-H), 3.83 (s, 3H, OCH_3), 3.77 (s, 4H, $(CH_2)_2$), 1.03 (s, 6H, $(CH_3)_2$); ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.8, 133.8, 133.2, 130.7, 125.8, 115.6, 114.1, 90.5, 88.6, 72.5, 55.5, 32.1, 22.1; ^{11}B NMR (128 MHz, $CDCl_3$) δ 26.7 (br s); EI MS *m/z* (%) 319 (24) $[^{10}BM]^+$; 320 (100) $[^{11}BM]^+$; HRMS $[M]^+$ 320.1599 (Calcd. For $C_{20}H_{21}BO_3$ 320.1588); IR (ATR) $\tilde{\nu}$ (cm^{-1}) = 2959, 2918, 2211, 1599, 1476, 1419, 1305, 1245, 1141, 1089.

4-([4-Methylsulfanylphenyl]ethynyl)phenylboronic acid neopentyl glycol ester {IUPAC name: 2-(4-{[4-Methylsulfanylphenyl]ethynyl}phenyl)-5,5-dimethyl-1,3,2-dioxaborinane} **12c**



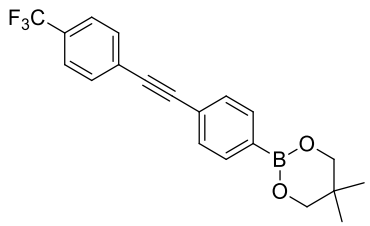
The title compound was prepared as described for **12e** from 4-ethynylphenyl boronic acid neopentyl glycol ester (32.1 mg, 0.150 mmol) and 4-bromothioanisole (45.7 mg, 1.5 eq) and isolated as a pale yellow solid (32.0 mg, 0.0952 mmol, 63%). Mp 148-150 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.1 Hz, 1H, Ar-H), 7.50 (d, *J* = 8.1 Hz, 2H, Ar-H), 7.44 (d, *J* = 8.4 Hz, 2H, Ar-H), 7.21 (d, *J* = 8.4 Hz, 2H, Ar-H), 3.78 (s, 4H, $(CH_2)_2$), 2.50 (s, 3H, SCH_3), 1.03 (s, 6H, $(CH_3)_2$); ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.5, 133.8, 132.1, 130.8, 126.0, 125.5, 119.72, 119.71, 90.3, 90.0, 72.5, 32.1, 22.1, 15.5; ^{11}B NMR (128 MHz, $CDCl_3$) δ 26.7 (br s); EI MS *m/z* (%) 355 (21) [^{10}BM]$^{+}$; 356 (100) [^{11}BM]$^{+}$; HRMS [M]$^{+}$ 336.1359 (Calcd. For $C_{20}H_{21}SO_2B$ 336.1359); IR (ATR) $\tilde{\nu}$ (cm^{-1}) = 2925 (br), 1730, 1603, 1477, 1421, 1342, 1309, 1250, 1128.

4-(3-Thienylethynyl)phenylboronic acid neopentyl glycol ester {IUPAC name: 2-(4-[3-Thienylethynyl]phenyl)-5,5-dimethyl-1,3,2-dioxaborinane} **12d**



The title compound was prepared as described for **12a** from 4-bromophenyl boronic acid neopentyl glycol ester (107 mg, 0.500 mmol) and 3-ethynylthiophene (74 μl, 1.5 eq) and isolated as an off-white solid (101 mg, 0.341 mmol, 68%). Mp 139-142 °C (decomp.); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (d, *J* = 8.3 Hz, 2H, Ar-H), 7.52 (dd, *J* = 3.0, 1.2 Hz, 1H, Ar-H), 7.50 (d, *J* = 8.3 Hz, 2H, Ar-H), 7.30 (dd, *J* = 5.0, 3.0 Hz, 1H, Ar-H), 7.20 (dd, *J* = 5.0, 1.2 Hz, 1H, Ar-H), 3.77 (s, 4H, $(CH_2)_2$), 1.03 (s, 6H, $(CH_3)_2$); ^{13}C NMR (101 MHz, $CDCl_3$) δ 133.8, 130.7, 130.0, 128.8, 125.5, 125.4, 122.5, 89.4, 85.6, 72.5, 32.0, 22.1; ^{11}B NMR (128 MHz, $CDCl_3$) δ 26.4 (br s); EI MS *m/z* (%) 209 (13) [^{10}BM-$CHCHMe_2O$]$^{+}$; 210 (50) [^{11}BM-$CHCHMe_2O$]$^{+}$; 295 (21) [^{10}BM]$^{+}$; 296 (100) [^{11}BM]$^{+}$; HRMS [M]$^{+}$ 296.1050 (Calcd. For $C_{17}H_{17}SO_2B$ 296.1046); IR (ATR) $\tilde{\nu}$ (cm^{-1}) = 3095, 2949, 2897, 2160 (br), 2031 (br), 1976 (br), 1602, 1474, 1418, 1336, 1303, 1246, 1134, 1018.

4-([4-Trifluoromethylphenyl]ethynyl)phenylboronic acid neopentyl glycol ester {IUPAC name: 2-(4-{[4-Trifluoromethylphenyl]ethynyl}phenyl)-5,5-dimethyl-1,3,2-dioxaborinane} **12e**

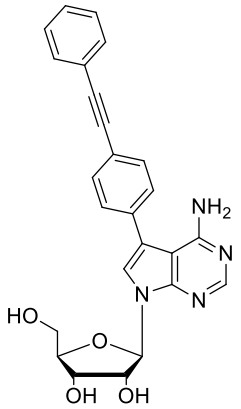


4-Ethynylphenyl boronic acid neopentyl glycol ester (107 mg, 0.500 mmol, 1 eq), $PdCl_2(PPh_3)_2$ (17.5 mg, 5 mol%), CuI (4.8 mg, 5 mol%) and PPh_3 (23.6 mg, 20 mol%) were added to a microwave tube. A septum was used to seal the tube and it was flushed with Ar. Diethylamine (1.5 ml) was added, followed by 4-iodobenzotrifluoride (110 µl, 0.750 mmol, 1.5 eq). The septum was replaced by a lid and the reaction heated to 120 °C in a microwave (150 W) for 25 min. The solvent was then removed *in vacuo* to give the crude product. The resulting solid was then purified by column chromatography on silica gel eluting with Et_2O/Pet Ether 40-60 (5:95 *v*/*v*) to give the product as a pale yellow solid (165 mg, 0.460 mmol, 92%). Mp 156-159 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.1 Hz, 2H, Ar-H), 7.63 (d, *J* = 9.0 Hz, 2H, Ar-H), 7.60 (d, *J* = 9.0 Hz, 2H, Ar-H), 7.53 (d, *J* = 8.1 Hz, 2H, Ar-H), 3.78 (s, 4H, $(CH_2)_2$), 1.03 (s, 6H, $(CH_3)_2$); ^{13}C NMR (101 MHz, $CDCl_3$) 133.9, 132.0, 131.0, 129.9 (q, *J* = 33 Hz), 127.3 (central peaks of q observed, *J* = 1.4 Hz), 125.4 (q, *J* = 4 Hz), 124.7 (central peaks of q observed, *J* = 272 Hz), 124.7, 122.7, 92.3, 89.0, 72.5, 32.1, 22.0; ^{11}B NMR (128 MHz, $CDCl_3$) δ 25.9 (br s); ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.66 (s); EI MS *m/z* (%) 271 (21); 272 (88); 357 (21) $[^{10}BM]^+$; 358 (100) $[^{11}BM]^+$; HRMS $[M]^+$ 358.1301 (Calcd. For $C_{20}H_{18}BO_2F_3$ 358.1356); IR (ATR) $\tilde{\nu}$ (cm^{-1}) = 2954, 2916, 2214, 1739, 1608, 1477, 1422, 1316, 1249, 1104, 1064.

General Procedure for Suzuki-Miyaura Cross-Coupling

4-Amino-5-iodo-7-(β-D-ribofuranosyl)-7*H*-pyrrolo[2,3-d]pyrimidine or 4-Amino-5-iodo-7-(2-deoxy-β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine (1.0 eq), $Pd(OAc)_2$ (2 mol%), TPPTS (5 mol%), caesium carbonate (3.0 eq) and the organoboronate ester (1.2 eq) were added to a Schlenk tube under a N_2 atmosphere. Water/acetonitrile (2:1, *v*/*v*, 0.1 mM) was added and the reaction mixture was stirred at 100 °C for 3 h. The crude product was adsorbed on to silica gel and purified by column chromatography, eluting with MeOH/CH_2Cl_2 (0:100 → 1:9 *v*/*v*). Small-scale reactions (0.050 mmol) were isolated by preparative TLC, eluting with 9:1 CH_2Cl_2/MeOH.

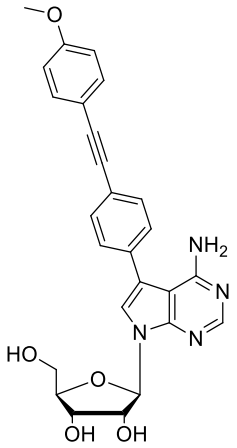
4-Amino-5-(4-[phenylethynyl]phenyl)-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine 4a



The title compound was synthesised from 7-iodo-7-deazaadenosine (196 mg, 0.500 mmol) and **12a** (174 mg, 0.600 mmol, 1.2 eq). The product was isolated as a white solid (164 mg, 0.371 mmol, 74%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.19 (br s, 1H, C2-H), 7.66 (d, J = 9.4 Hz, 3H, Ar-H), 7.61 – 7.50 (m, 4H, Ar-H), 7.46 – 7.42 (m, 3H, Ar-H), 6.28 (br s, 2H, NH_2), 6.13 (d, J = 6.2 Hz, 1H, C1′-H), 5.35 (d, J = 6.2 Hz, 1H, C2′-OH), 5.20 (t, J = 5.6 Hz, 1H, C5′-OH), 5.14 (d, J = 4.8 Hz, 1H, C3′-OH), 4.46 (app q, J = 6.2 Hz, 1H, C2′-H), 4.11 (m, 1H, C3′-H), 3.91 (app q, J = 3.9 Hz, 1H, C4′-H), 3.64 (ddd, J = 11.8, 5.6, 3.9 Hz, 1H, C5′-Ha), 3.53 (ddd, J = 11.8, 5.6, 3.9 Hz, 1H, C5′-Hb); ESI HRMS $[MH]^+$ 443.1706 (Calcd. for $C_{25}H_{23}N_4O_4$ 443.1714).

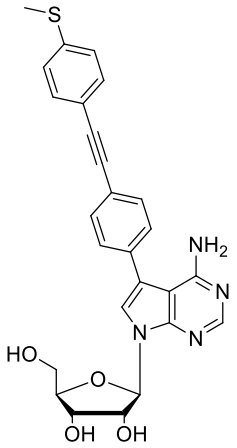
^{1}H NMR (400 MHz, CD_3OD) δ 8.16 (s, 1H, C2-H), 7.63 (d, J = 8.4 Hz, 2H, C), 7.56 – 7.52 (m, 3H), 7.50 (s, 1H), 7.41 – 7.35 (m, 3H), 6.11 (d, J = 6.4 Hz, 1H, C1′-H), 4.67 (dd, J = 6.4, 5.3 Hz, 1H, C2′-H), 4.31 (dd, J = 5.3, 2.8 Hz, 1H, C3′-H), 4.13 (q, J = 2.8 Hz, 1H, C4′-H), 3.87 (dd, J = 12.4, 2.8 Hz, 1H, C5′-Ha), 3.75 (dd, J = 12.4, 2.8 Hz, 1H, C5′-Hb); ^{13}C NMR (101 MHz, CD_3OD) δ 159.0, 152.4, 151.57, 135.8, 133.2, 132.5, 129.9, 129.59, 129.55, 124.5, 123.8, 123.5, 118.04, 102.9, 91.03, 90.99, 89.9, 87.3, 75.6, 72.5, 63.4.

4-Amino-5-(4-[{4-Methoxyphenyl}ethynyl]phenyl)-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine 4b



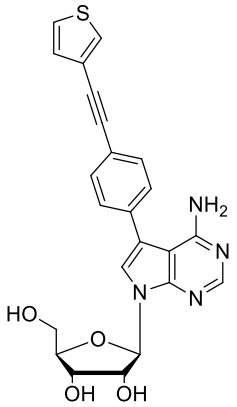
The title compound was synthesised from 7-iodo-7-deazaadenosine (19.6 mg, 0.0500 mmol) and **12b** (19.2 mg, 0.600 mmol, 1.2 eq). The product was obtained as a white solid (23.5 mg, 0.0500 mmol, quant.). ^{1}H NMR (400 MHz, CD_3OD) δ 8.16 (s, 1H, C2-H), 7.60 (d, *J* = 8.5 Hz, 2H, Ar-H), 7.52 (d, *J* = 8.5 Hz, 2H, Ar-H), 7.49 (s, 1H, C6-H), 7.46 (d, *J* = 9.0 Hz, 2H, Ar-H), 6.95 (d, *J* = 9.0 Hz, 2H, Ar-H), 6.11 (d, *J* = 6.3 Hz, 1H, C1′-H), 4.67 (dd, *J* = 6.3, 5.3 Hz, 1H, C2′-H), 4.30 (dd, *J* = 5.3, 2.9 Hz, 1H, C3′-H), 4.13 (app q, *J* = 2.9 Hz, 1H, C4′-H), 3.87 (dd, *J* = 12.3, 2.9 Hz, 1H, C5′-Ha), 3.83 (s, 3H, OCH_3), 3.75 (dd, *J* = 12.3, 2.9 Hz, 1H, C5′-Hb); ESI HRMS $[MH]^+$ 473.1806 (Calcd. for $C_{26}H_{25}N_4O_5$ 473.1819). ^{1}H NMR (500 MHz, DMSO-d_6) δ 8.18 (s, 1H, C2-H), 7.66-7.62 (m, 3H, Ar-H), 7-55-7.47 (m, 4H, Ar-H), 7.02 (d, *J* = 8.9 Hz, 2H, Ar-H), 6.24 (br s, 1H, NH_2), 6.15 (d, *J* = 6.2 Hz, 1H, C1′-H), 5.33 (d, *J* = 6.3 Hz, 1H, C2′-OH), 5.18 (app t, *J* = 5.6 Hz, 1H, C5′-OH), 5.12 (d, *J* = 4.9 Hz, 1H, C3′-OH), 4.48 (app dd, *J* = 11.6, 6.3 Hz, 1H, C2′-H), 4.13 (app dd, *J* = 8.2, 4.9 Hz, 1H, C3′-H), 3.93 (app q, *J* = 3.7 Hz, 1H, C4′-H), 3.66 (app dt, *J* = 12.1, 4.0 Hz, 1H, C5′-Ha), 3.60-3.53 (m, 1H, C5′-Hb); ^{13}C NMR (126 MHz, DMSO-d_6) δ 159.5, 157.3, 151.8, 151.1, 134.4, 132.9, 131.7, 128.5, 121.6, 120.8, 115.8, 114.4, 114.2, 90.0, 88.0, 87.0, 85.1, 73.8, 70.6, 61.6, 55.3.

4-Amino-5-(4-[{4-Methylsulfanylphenyl}ethynyl]phenyl)-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine 4c



The title compound was synthesised from 7-iodo-7-deazaadenosine (19.6 mg, 0.0500 mmol) and **12c** (20.2 mg, 0.600 mmol, 1.2 eq). The product was obtained as a white solid (17.3 mg, 0.0350 mmol, 71%). ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.16 (s, 1H, C2-H), 7.62 (d, J = 8.1 Hz, 2H, Ar-H), 7.53 (d, J = 8.1 Hz, 2H, Ar-H), 7.49 (s, 1H, C6-H), 7.45 (d, J = 8.3 Hz, 2H, Ar-H), 7.27 (d, J = 8.3 Hz, 2H, Ar-H), 6.11 (d, J = 6.3 Hz, 1H, C1′-H), 4.67 (dd, J = 6.2, 5.3 Hz, 1H, C2′-H), 4.31 (dd, J = 5.3, 3.0 Hz, 1H, C3′-H), 4.13 (app q, J = 3.0 Hz, 1H, C4′-H), 3.87 (dd, J = 12.4, 2.6 Hz, 1H, C5′-Ha), 3.75 (dd, J = 12.4, 2.9 Hz, 1H, C5′-Hb); ^{13}C NMR (126 MHz, DMSO-d_6, selected peaks from HSQC) δ 152.2, 132.2, 122.1, 128.9, 132.2, 126.1, 87.5, 73.9, 71.1, 85.7, 62.1, 62.2; ESI HRMS $[MH]^+$ 489.1587 (Calcd. For $C_{26}H_{25}N_4O_4S$ 489.1581).

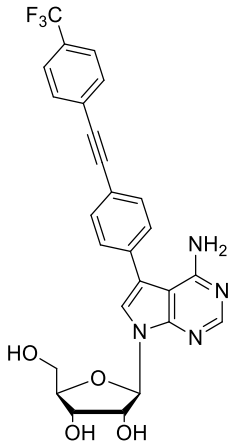
4-Amino-5-(4-[{3-thienyl}ethynyl]phenyl)-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine 4d



The title compound was synthesised from 7-iodo-7-deazaadenosine (19.6 mg, 0.0500 mmol) and **12d** (17.7 mg, 0.600 mmol, 1.2 eq). The product was obtained as a white solid (17.3 mg, 0.0385 mmol, 77%). ^{1}H NMR (400 MHz, CD_3OD) δ 8.15 (s, 1H, C2-H), 7.65 (dd, J = 3.0, 1.2 Hz, 1H, Ar-H), 7.61 (d, J = 8.5 Hz, 2H, Ar-H), 7.53 (d, J = 8.5 Hz, 2H, Ar-H), 7.49 (s, 1H, C6-H), 7.46 (dd, J = 5.0, 3.0 Hz, 1H, Ar-H), 7.21 (dd, J = 5.0, 1.2 Hz, 1H, Ar-H), 6.11 (d, J = 6.3 Hz, 1H, C1′-H), 4.67 (dd, J = 6.3, 5.4 Hz, C2′-H), 4.31 (dd, J = 5.4, 2.9 Hz, 1H, C3′-

H), 4.13 (app dd, *J* = 5.5, 2.9 Hz, 1H, C4′-H), 3.87 (dd, *J* = 12.4 2.7 Hz, 1H, C5′-Ha), 3.75 (dd, *J* = 12.4, 2.9 Hz, 1H, C5′-Hb); ^{13}C NMR (126 MHz, CD_3OD) 159.0, 152.4, 151.6, 135.6, 133.1, 130.7, 129.93, 129.90, 126.9, 123.7, 123.6, 123.5, 118.1, 91.0, 89.2, 87.3, 86.3, 75.6, 72.5, 63.4, 49.4. ESI HRMS $[MH]^+$ 449.1264 (Calcd. for $C_{23}H_{21}N_4O_4S$ 449.1278).

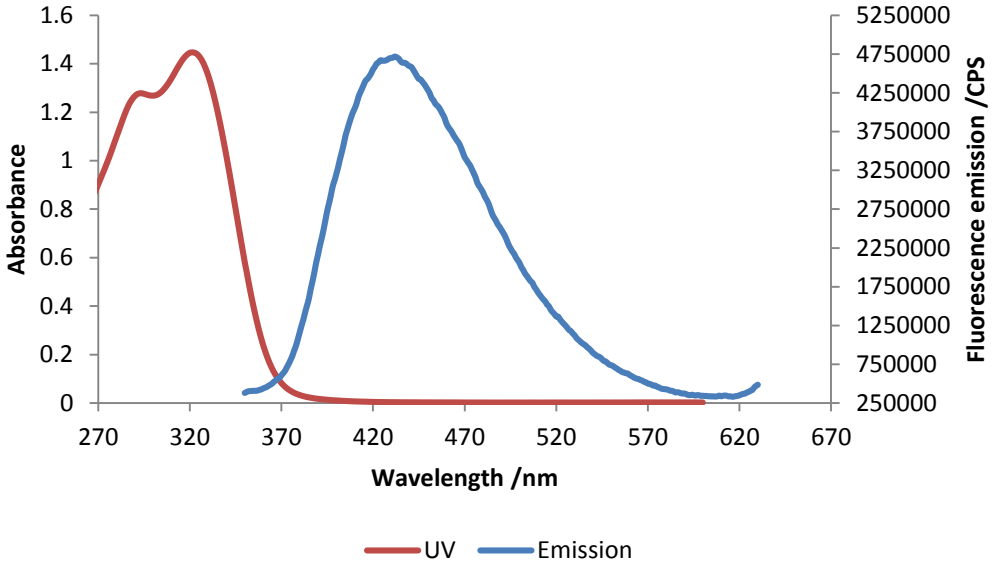
4-Amino-5-(4-[{4-trifluoromethylphenyl}ethynyl]phenyl)-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine 4e

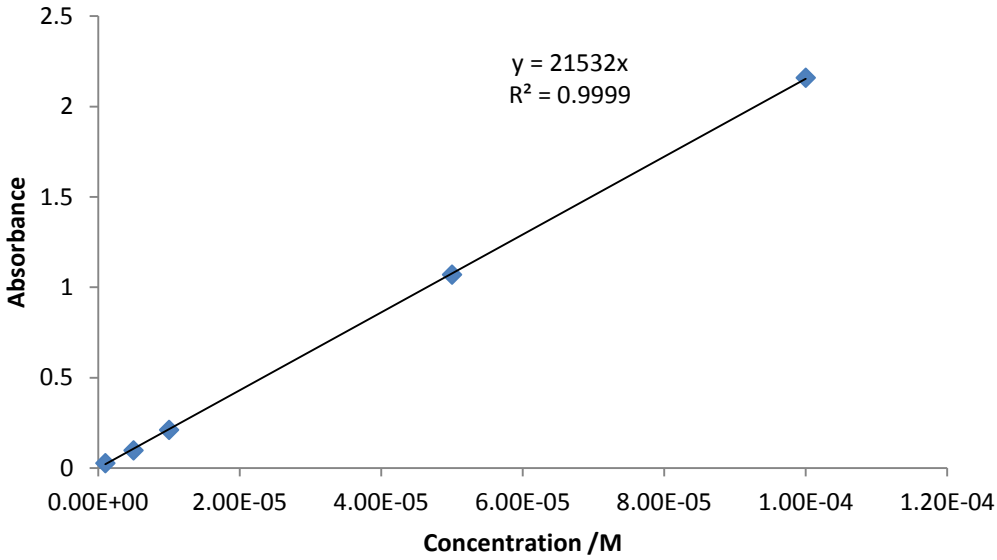


The title compound was synthesised from 7-iodo-7-deazaadenosine (19.6 mg, 0.0500 mmol) and **12e** (21.4 mg, 0.600 mmol, 1.2 eq). The product was obtained as a white solid (17.4 mg, 0.0341 mmol, 68%). ^{1}H NMR (400 MHz, CD_3OD) δ 8.14 (s, 1H, C2-H), 7.70 (d, *J* = 8.8 Hz, 2H, Ar-H), 7.68 (d, *J* = 8.8 Hz, 2H, Ar-H), 7.65 (d, *J* = 8.5 Hz, 2H, Ar-H), 7.55 (d, *J* = 8.5 Hz, 2H, Ar-H), 7.50 (s, 1H, C6-H), 6.09 (d, *J* = 6.3 Hz, 1H, C1′-H), 4.64 (dd, *J* = 6.3, 5.3 Hz, 1H, C2′-H), 4.28 (dd, *J* = 5.3, 2.9 Hz, 1H, C3′-H), 4.10 (app q, *J* = 2.8 Hz, 1H, C4′-H), 3.84 (dd, *J* = 12.4, 2.7 Hz, 1H, C5′-Ha), 3.73 (dd, *J* = 12.4, 2.9 Hz, 1H, C5′-Hb); ^{13}C NMR (101 MHz, CD_3OD) 158.94, 152.37, 151.58, 136.43, 133.43, 133.06, 130.87, 129.9 (q, *J* = 260 Hz, central two peaks of quartet observed), 129.97, 126.83, 126.5 (q, *J* = 3.8 Hz), 123.93, 122.63, 117.92, 92.50, 90.99, 89.41, 87.28, 75.62, 72.50, 69.57, 63.42; ESI HRMS $[MH]^+$ 511.1588 (Calcd. for $C_{26}H_{22}F_3N_4O_4$ 511.1588).

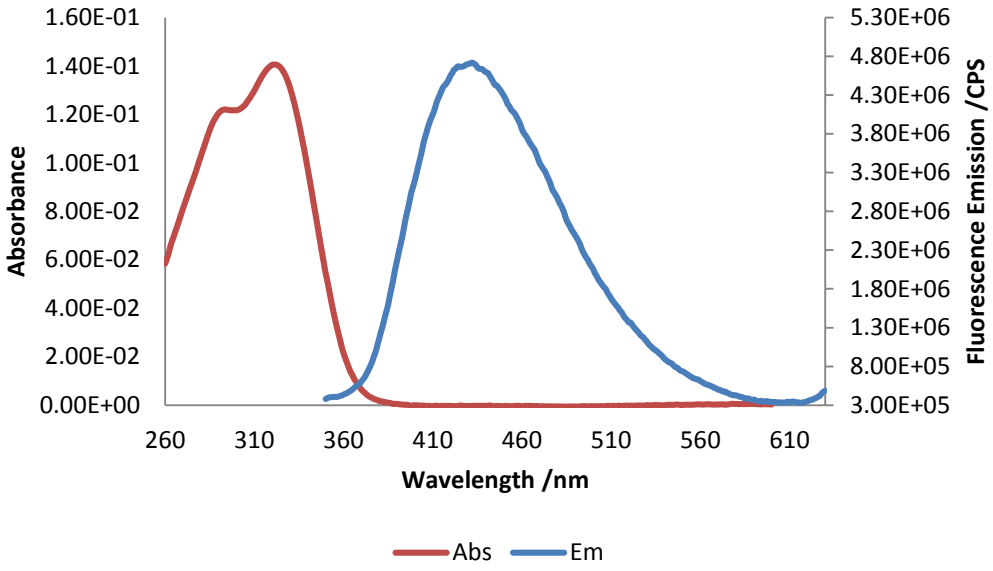
2 UV-Vis and Fluorescence Emission Spectra in DMSO

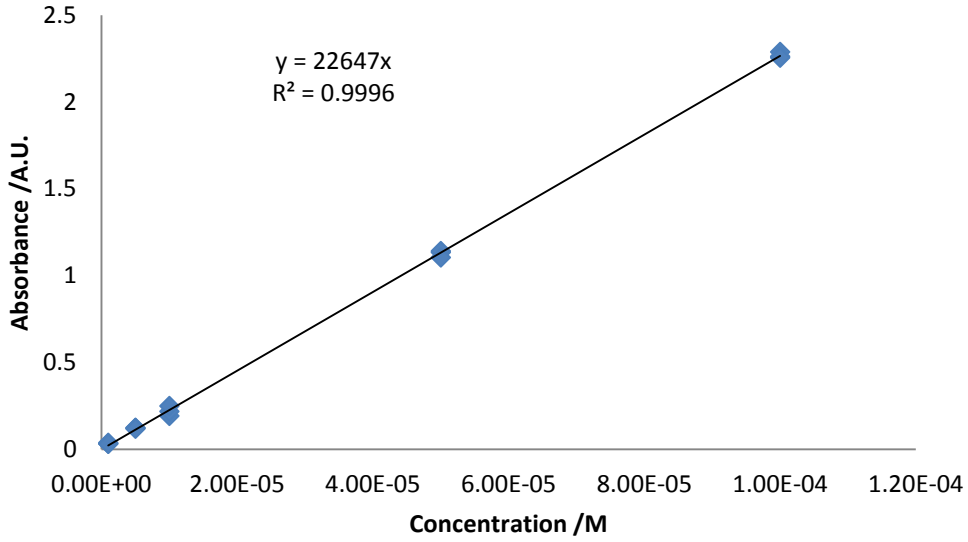
4-Amino-5-(4-[phenylethynyl]phenyl)-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine 4a



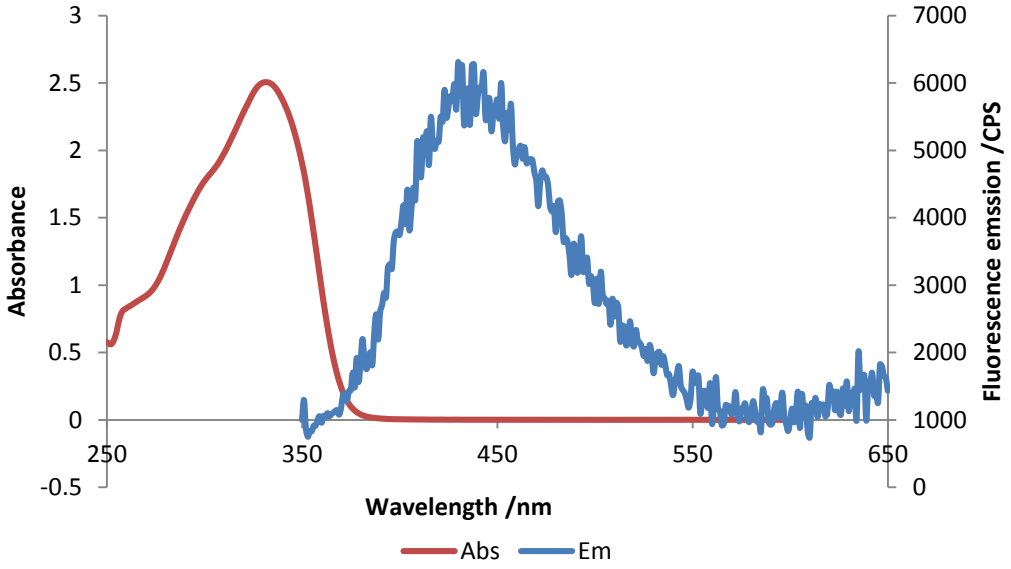


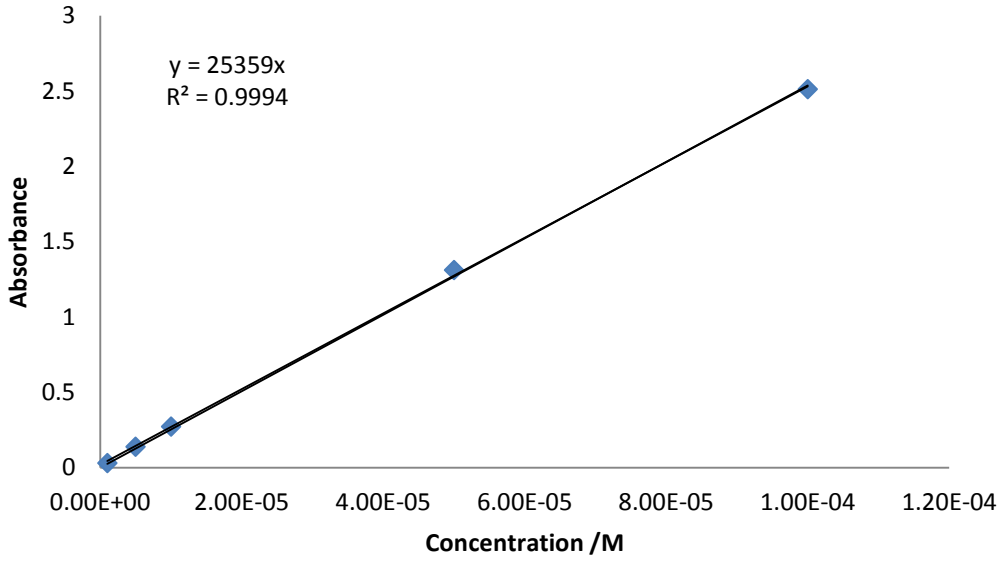
4-Amino-5-(4-[{4-Methoxyphenyl}ethynyl]phenyl)-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine 4b



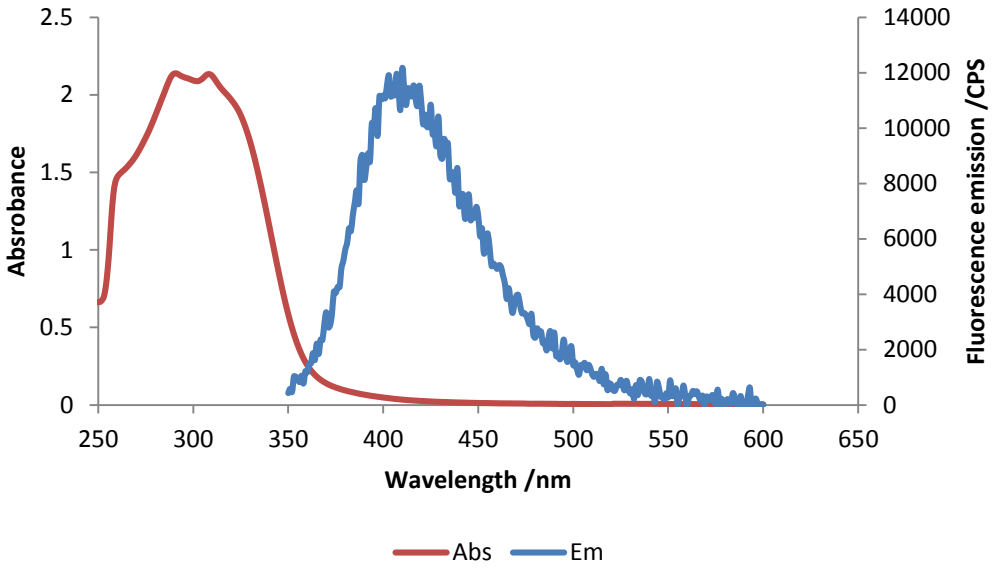


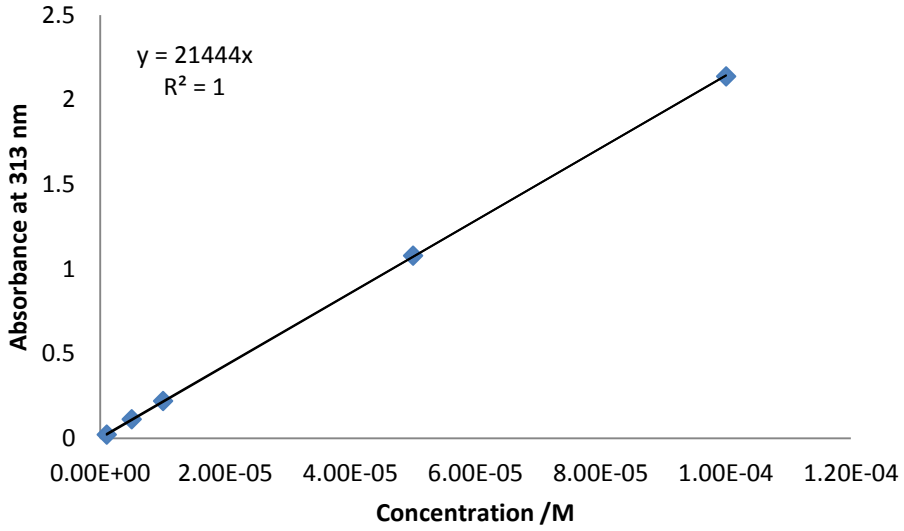
4-Amino-5-(4-[{4-Methylsulfanylphenyl}ethynyl]phenyl)-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine 4c



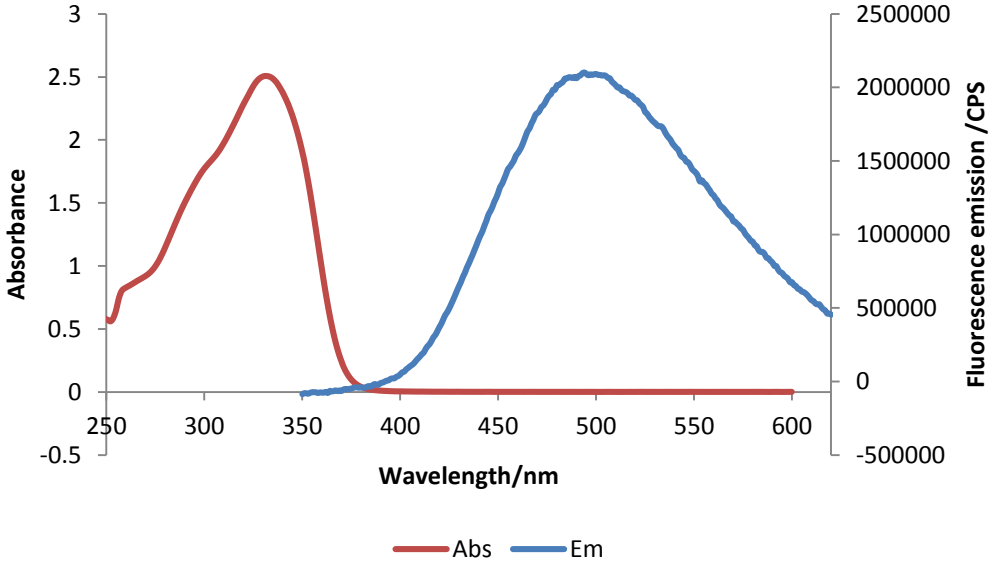


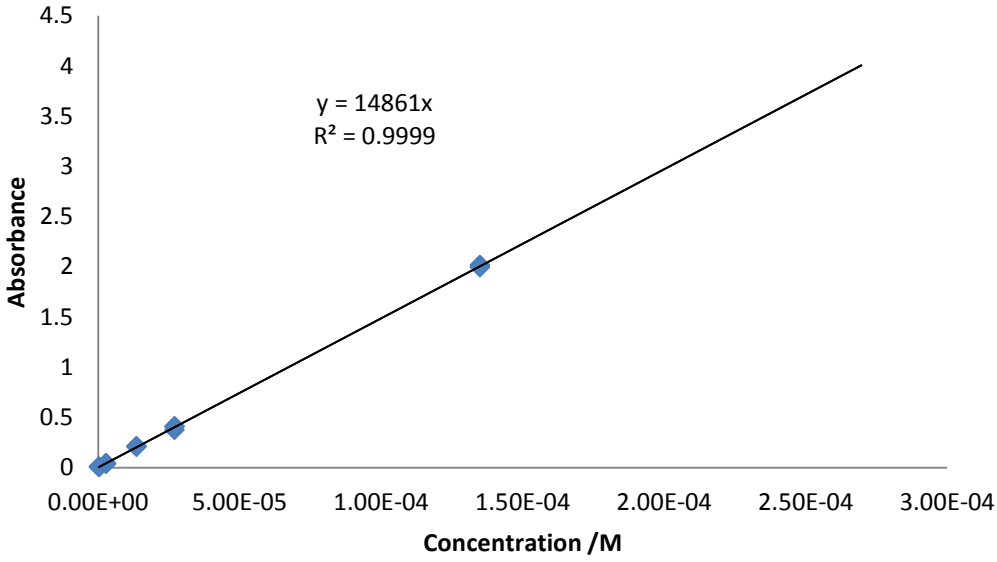
4-Amino-5-(4-[{3-thienyl}ethynyl]phenyl)-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine 4d





4-Amino-5-(4-[{4-trifluoromethylphenyl}ethynyl]phenyl)-7-(β-D-ribofuranosyl)-7H-pyrrolo[2,3-d]pyrimidine 4e





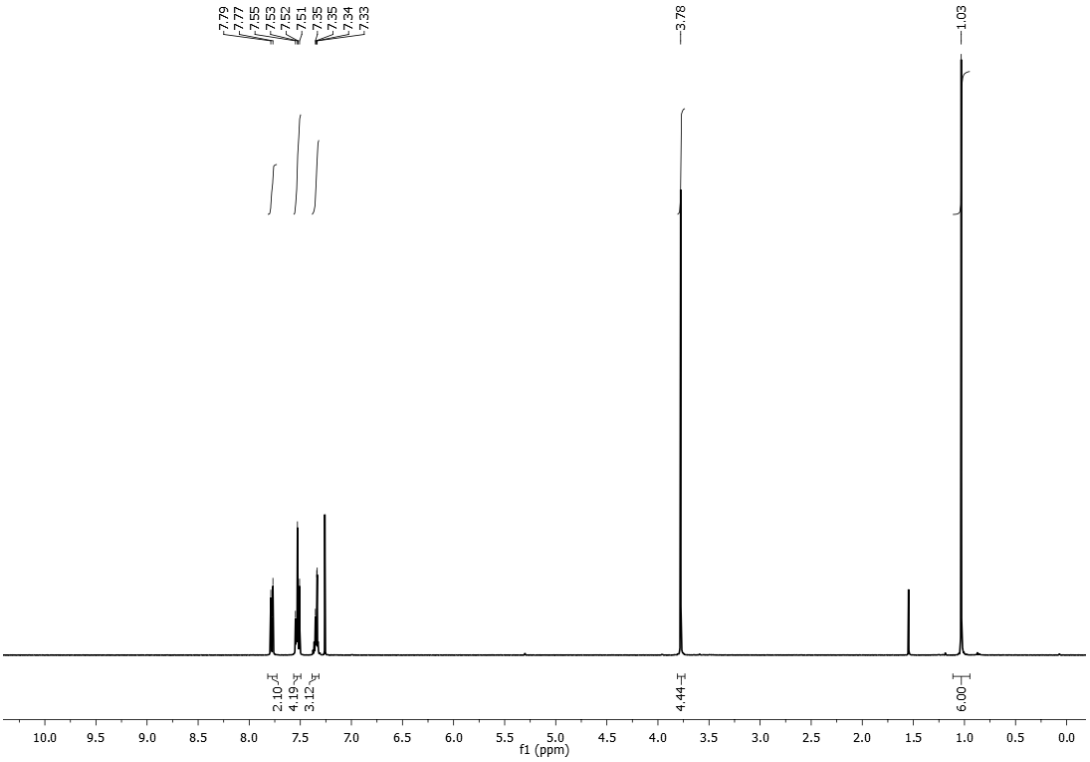
3 Fluorescence Lifetime Measurements

Samples for fluorescence lifetime measurement were prepared so as to have an absorbance of *ca.* 0.1 at their respective absorption maxima. The fluorescence lifetimes were measured by time-correlated single photon counting (TCSPC). The excitation source used was the 3rd harmonic (300 nm) of a mode-locked (900 nm), cavity dumped (APE Pulse switch) Ti:sapphire laser (Coherent MIRA 900), pumped by the 2nd harmonic (532 nm) of a CW Nd:YAG laser (Coherent Verdi V6). The pulse characteristics were as follows: a temporal full width at half maximum (FWHM) of ~150 fs, average power 0.3 mW at a repetition rate of 4 MHz. The fluorescence emission was collected at right angles to the excitation source, with the emission wavelength selected by a monochromator (Jobin Yvon TRIAX 190) and detected by a cooled photomultiplier tube module (IBH TBX-04). The detector was linked to a time-to-amplitude converter (Ortec 567) and a pulse height analyser, PHA, (E.G. & G. Trump Card) controlled by the software Maestro (ver 5.10). Fluorescence decays were recorded to a minimum of 10,000 counts in the peak channel of the PHA with a record length of 1000 channels. The band pass of the monochromator was adjusted to give a signal count rate of 5-20 KHz. The instrument response function (IRF) was measured using a dilute LUDOX® colloidal silica suspension as the scattering sample, giving an IRF of ~200 ps FWHM. Iterative reconvolution of the IRF with one or two decay functions and non-linear least-squares analysis were used to analyse the data in Microsoft Excel using the solver function. The quality of the fit was judged by the calculated value of the reduced χ^2 and Durbin-Watson parameters and visual inspection of both the residuals and the autocorrelated residuals.

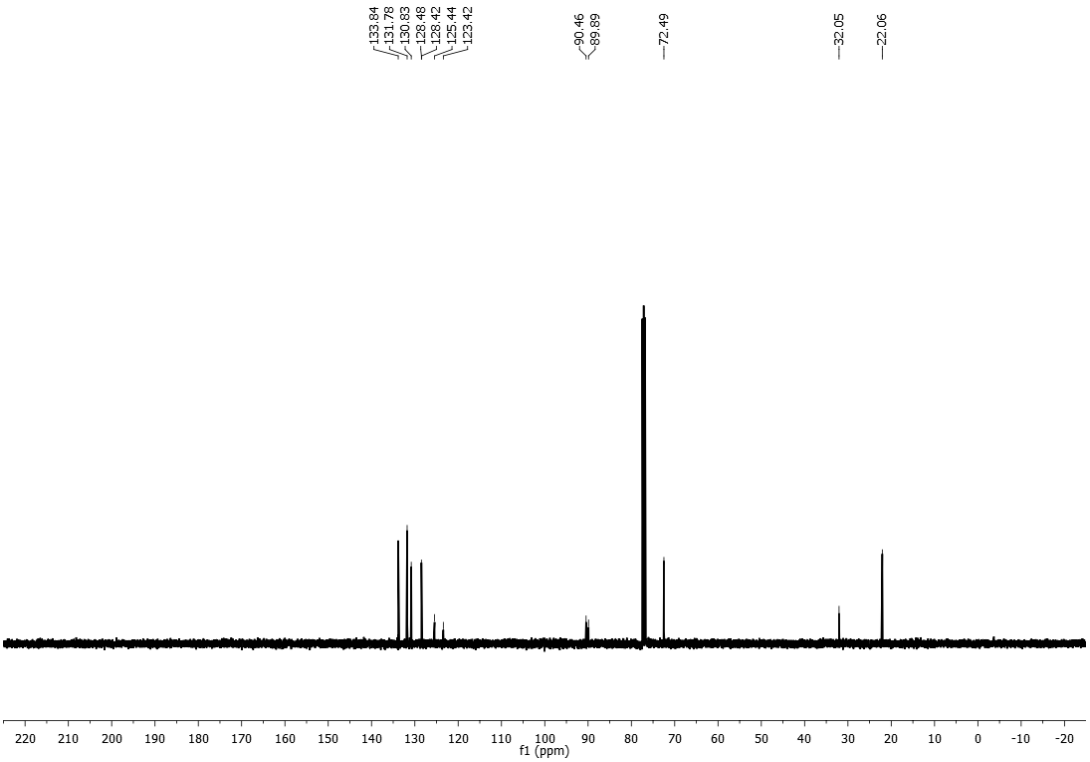
Compound	Emission Wavelength /nm	Fluorescence lifetime /ns	Durbin-Watson parameter
4a	430	2.2 (92%), 0.5 (8%)	1.83
4b	405	1.6 (90%), 0.5 (10%)	1.92
4c	430	2.0 (92%), 0.5 (8%)	1.86
4d	405	1.5 (88%), 0.5 (12%)	1.82
4e	490	2.1 (87%), 0.8 (12%)	1.82

4 NMR Spectra

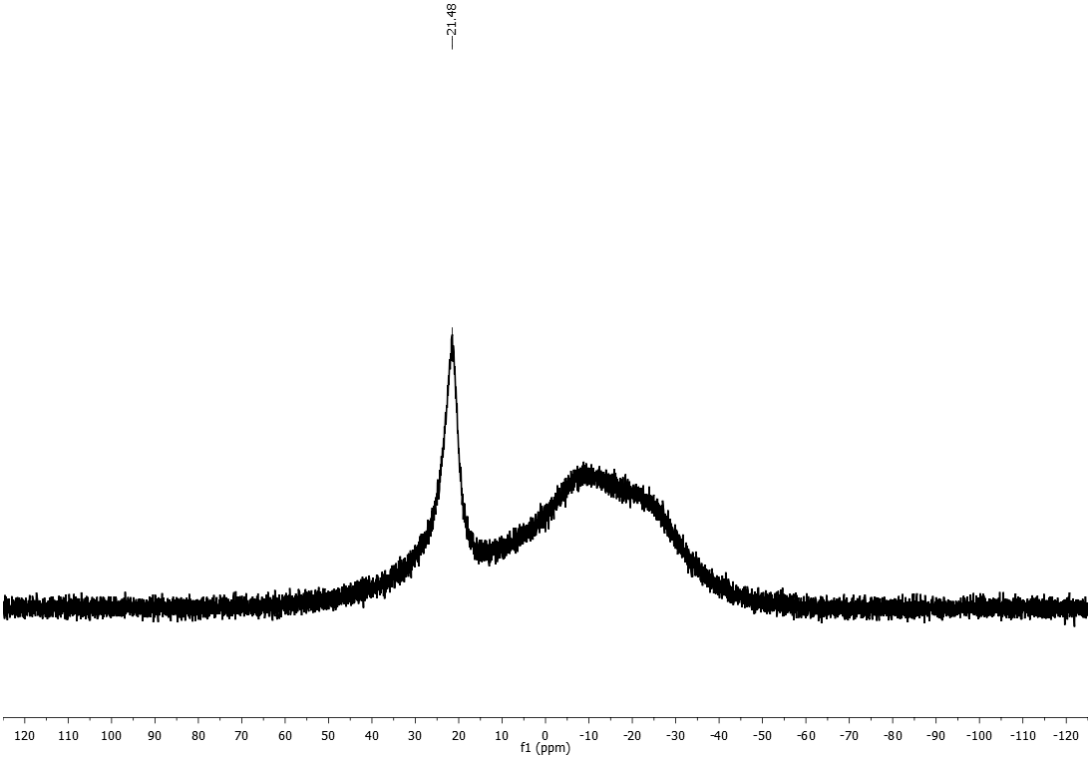
12a – ^{1}H NMR $CDCl_3$ 400 MHz



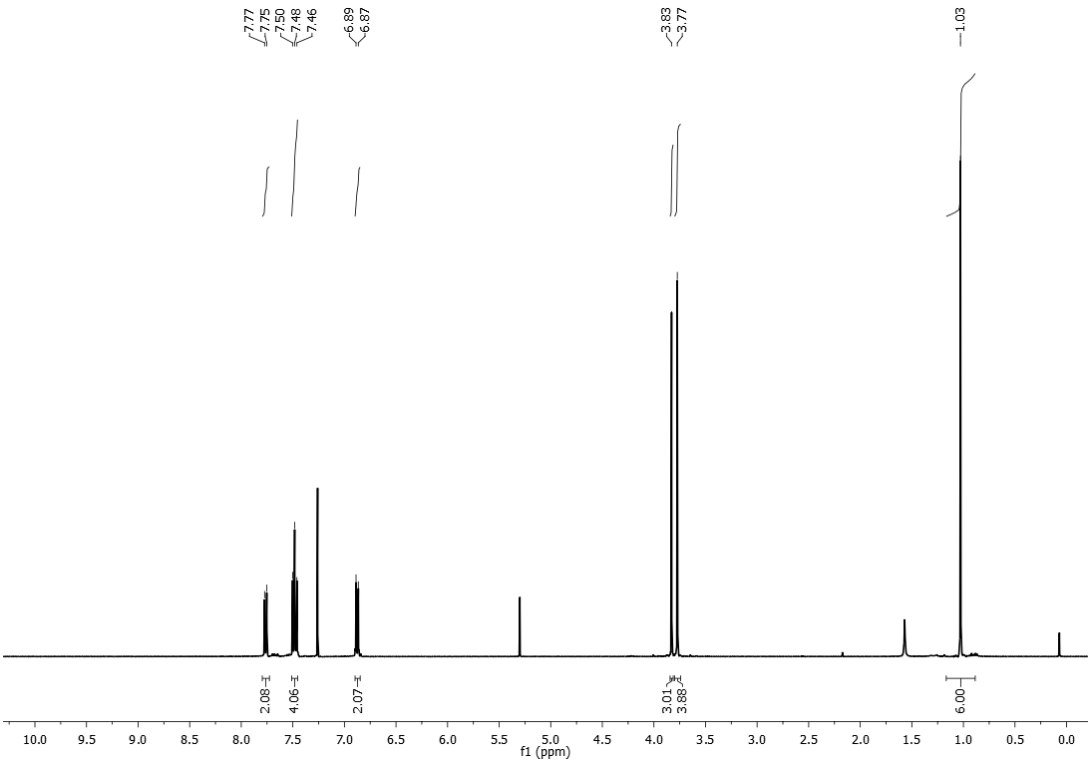
12a – ^{13}C NMR $CDCl_3$ 400 MHz



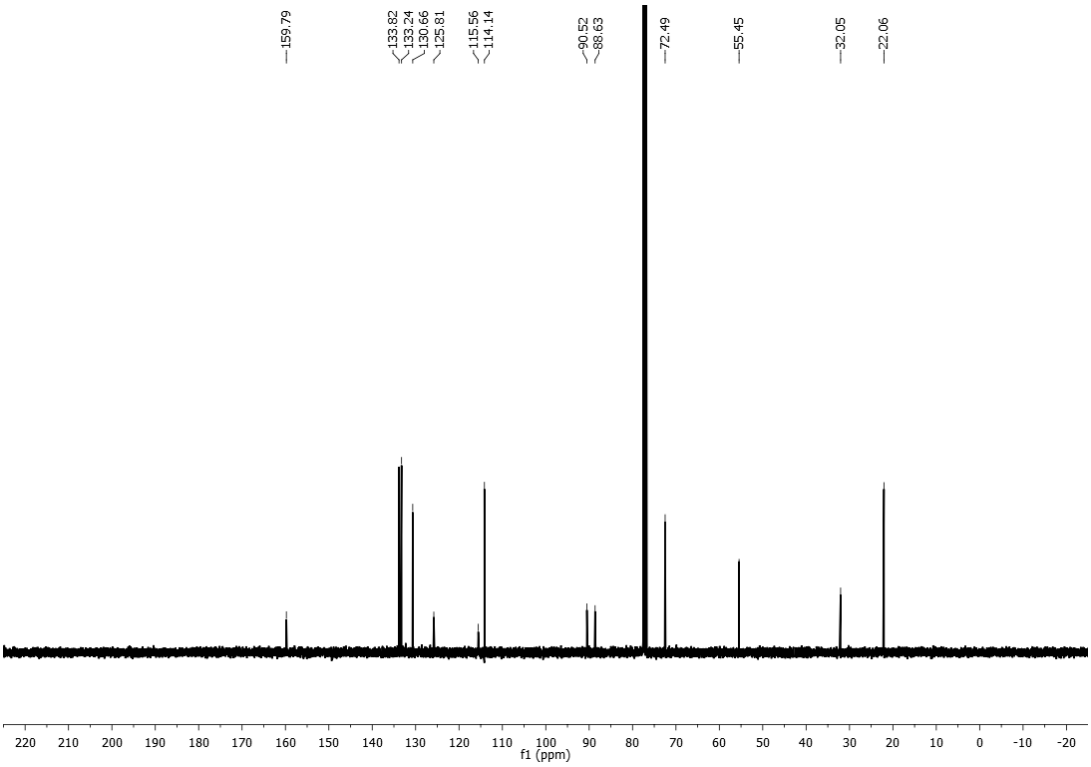
12a – ^{11}B NMR $CDCl_3$ 400 MHz



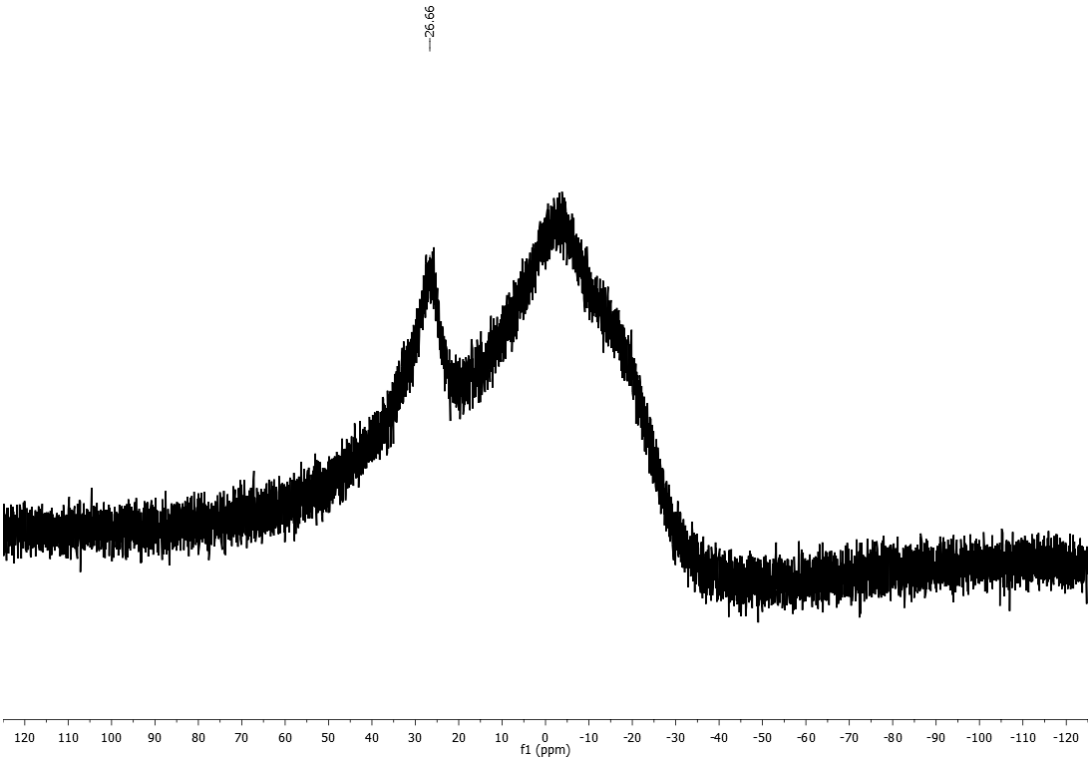
12b – ^{1}H NMR $CDCl_3$ 400 MHz



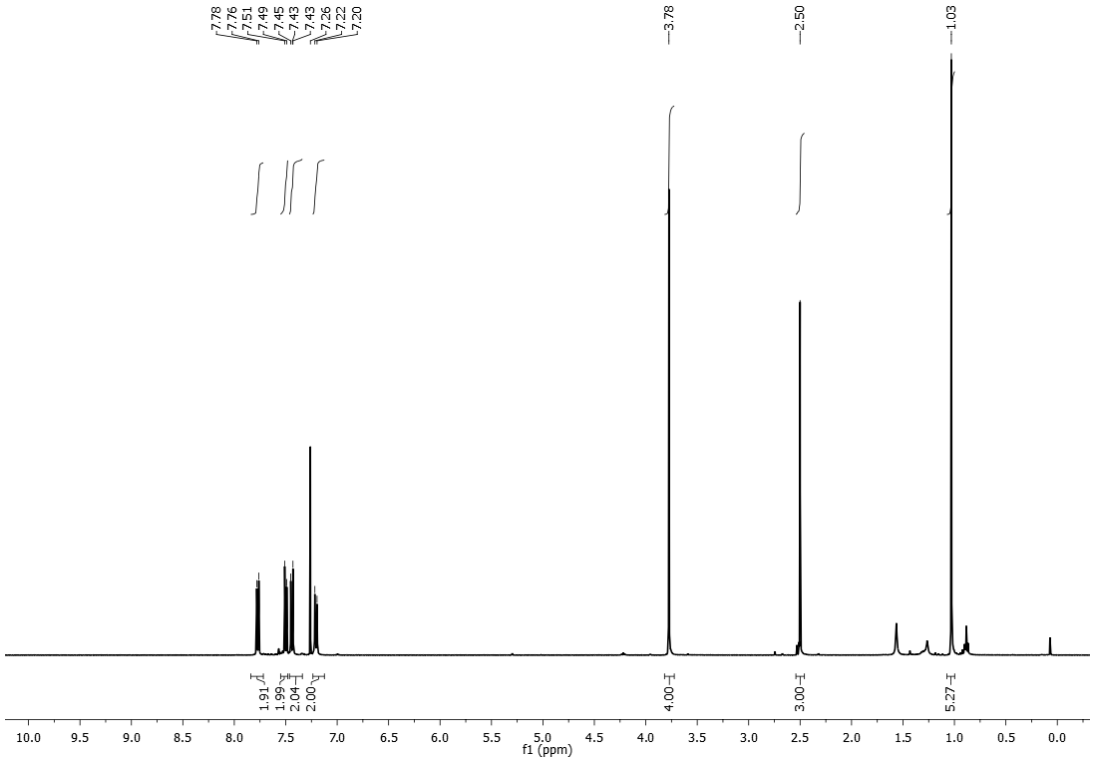
12b – ^{13}C NMR $CDCl_3$ 400 MHz



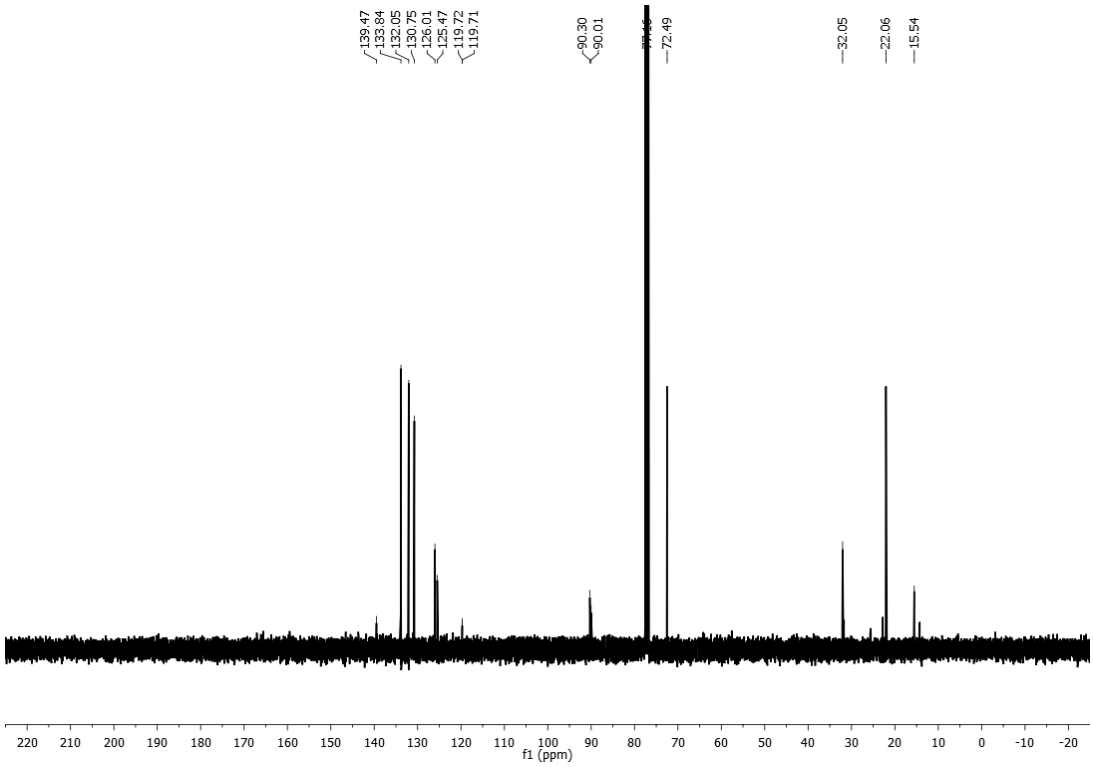
12b – ^{11}B NMR $CDCl_3$ 400 MHz



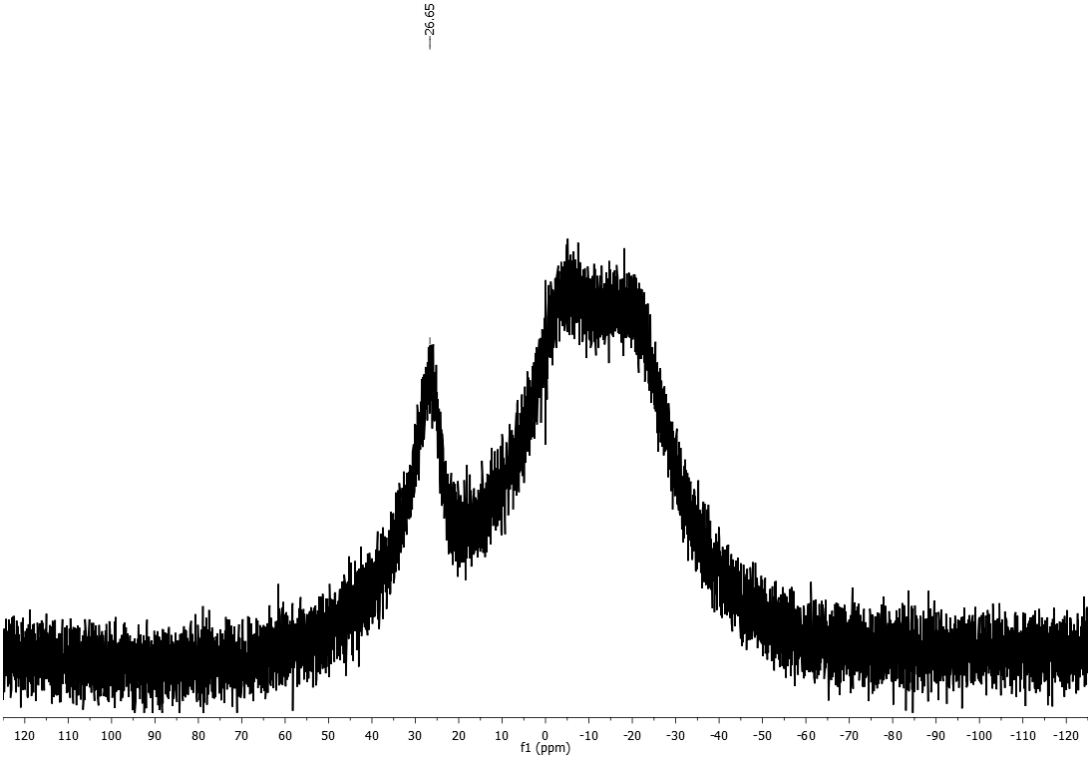
12c – ^{1}H NMR $CDCl_3$ 400 MHz



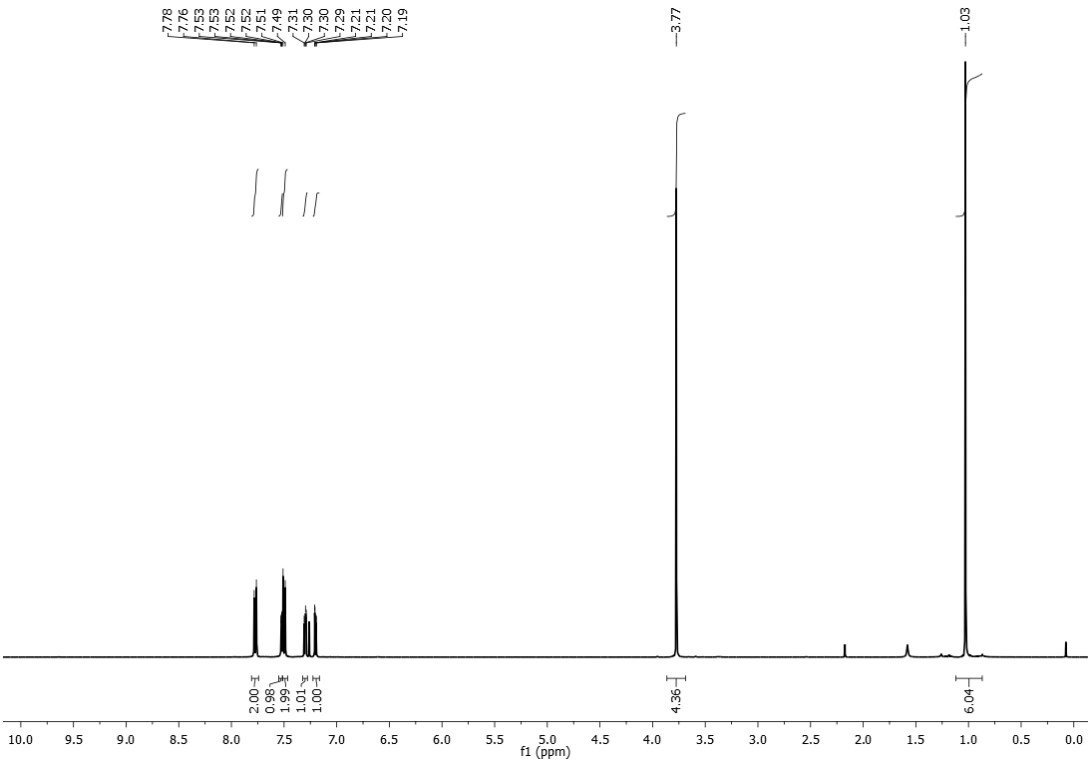
12c – ^{13}C NMR $CDCl_3$ 400 MHz



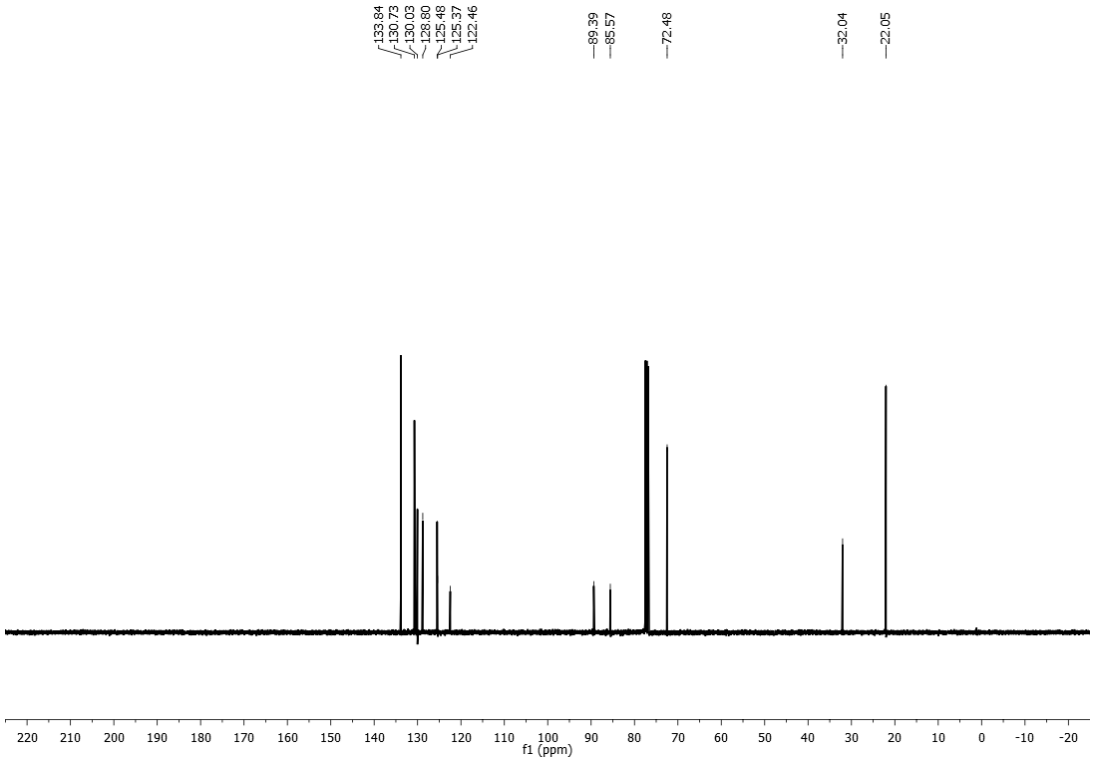
12c – ^{11}B NMR $CDCl_3$ 400 MHz



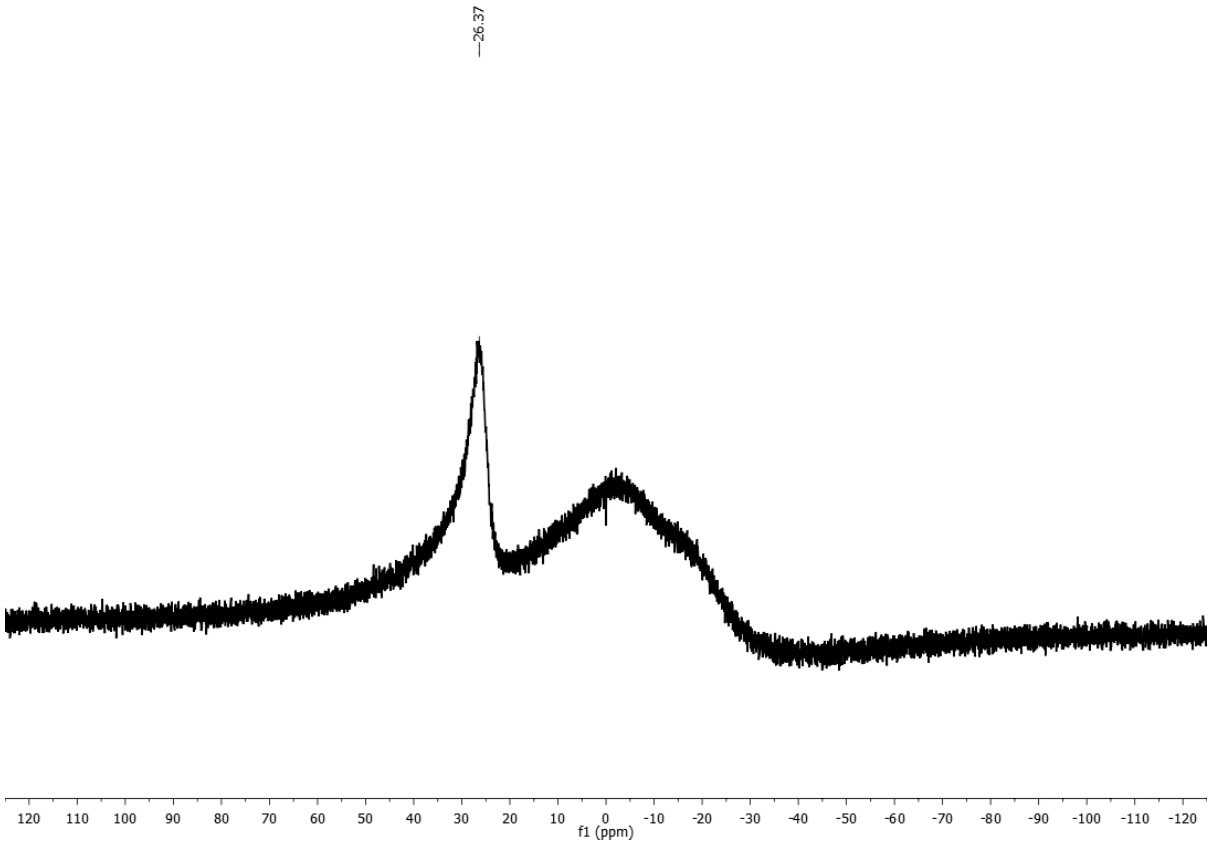
12d – ^{1}H NMR $CDCl_3$ 400 MHz



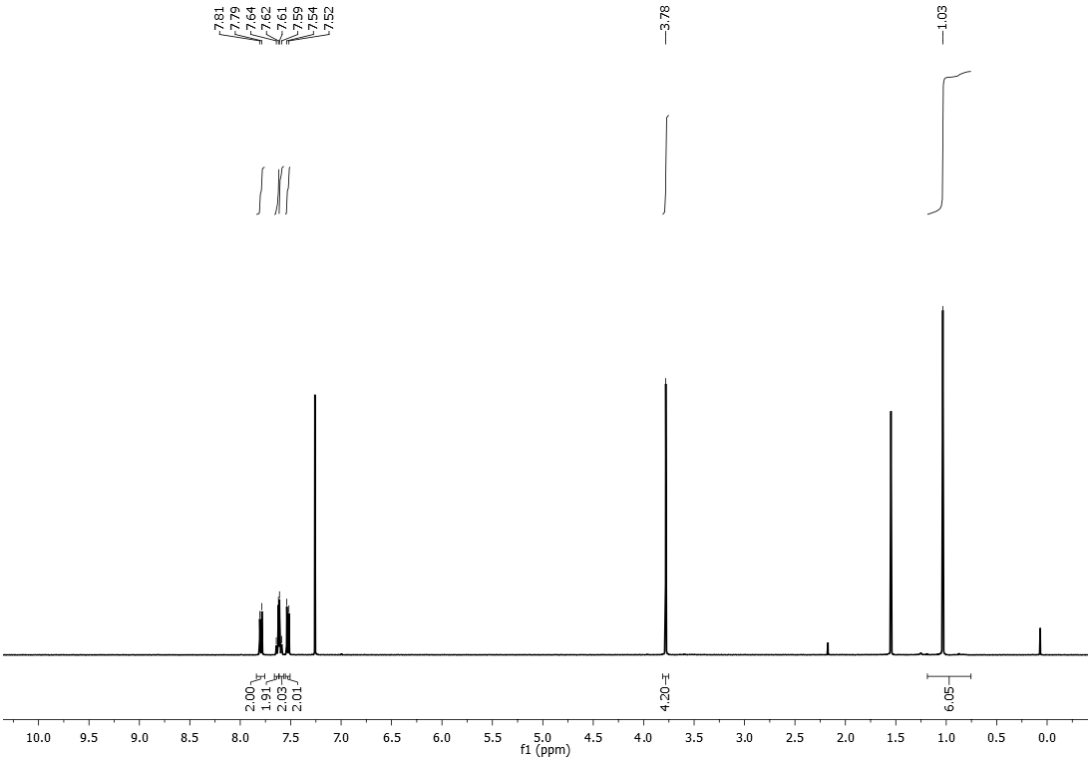
12d – ^{13}C NMR $CDCl_3$ 400 MHz



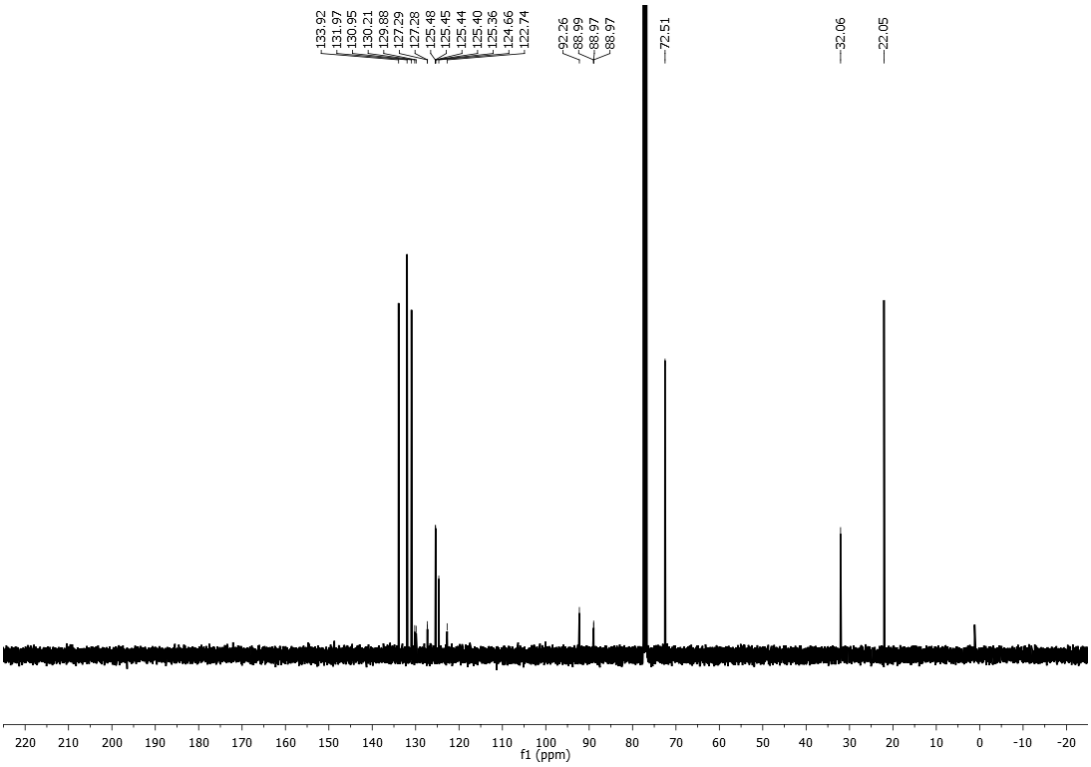
12d – ^{11}B NMR $CDCl_3$ 400 MHz



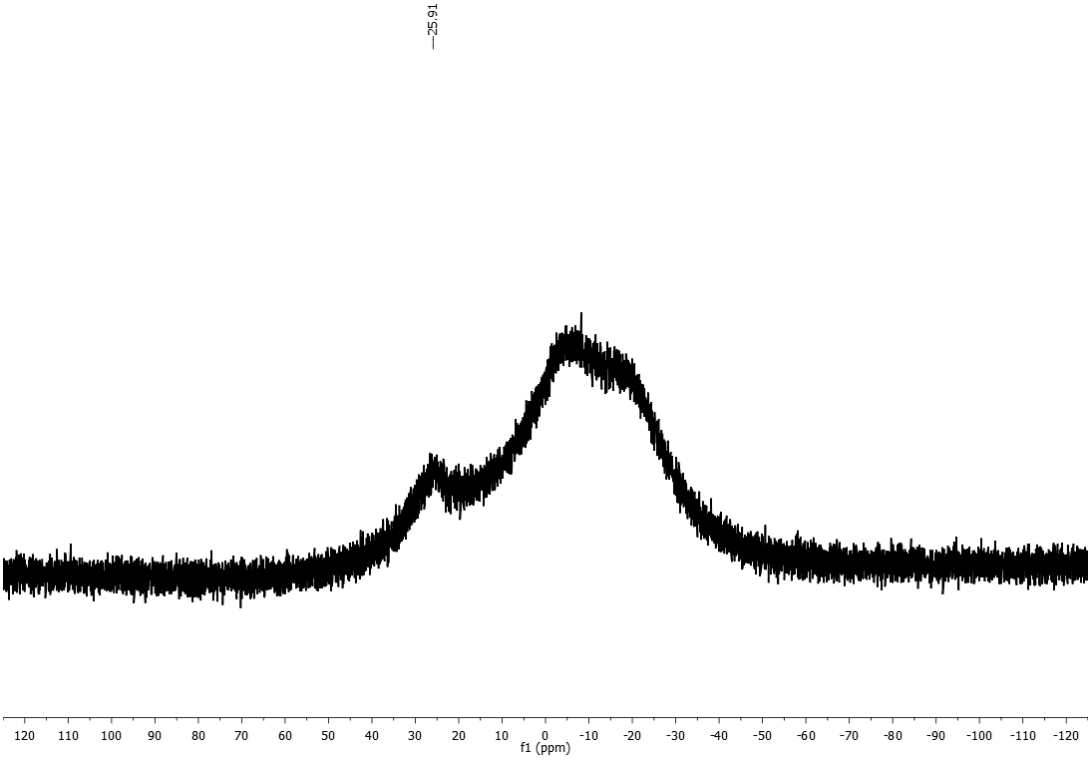
12e – ^{1}H NMR $CDCl_3$ 400 MHz



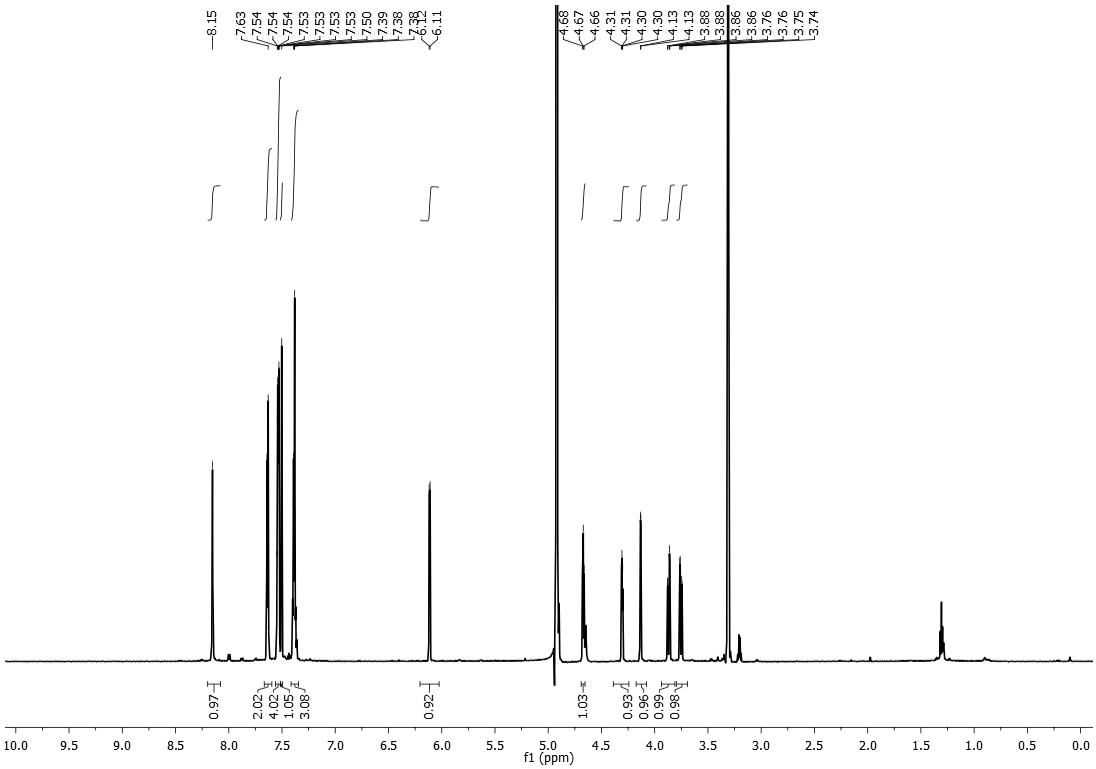
12e – ^{13}C NMR $CDCl_3$ 400 MHz



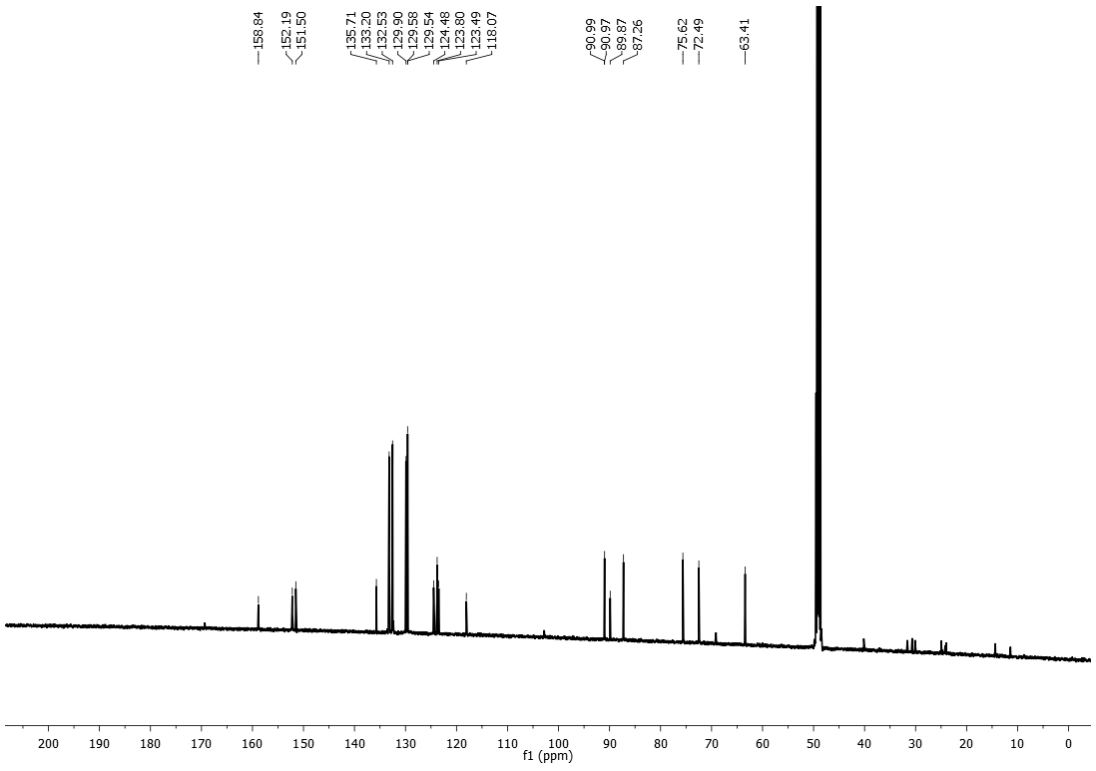
12e – ^{11}B NMR $CDCl_3$ 400 MHz



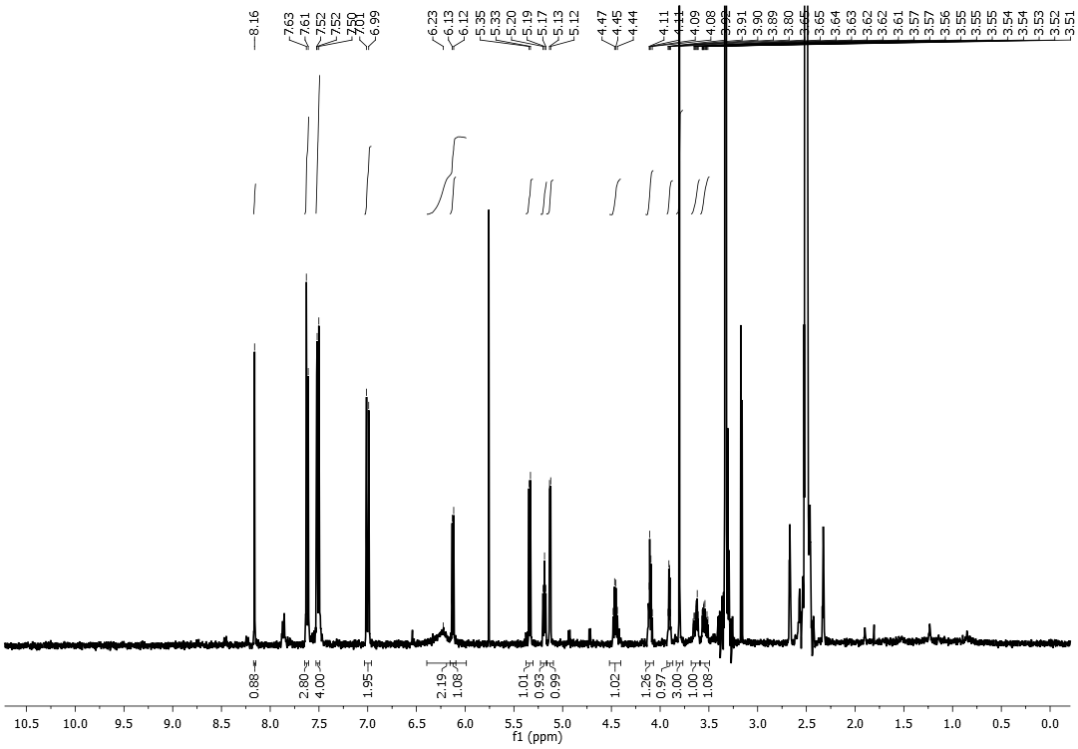
4a – ^{1}H NMR CD_3OD 500 MHz



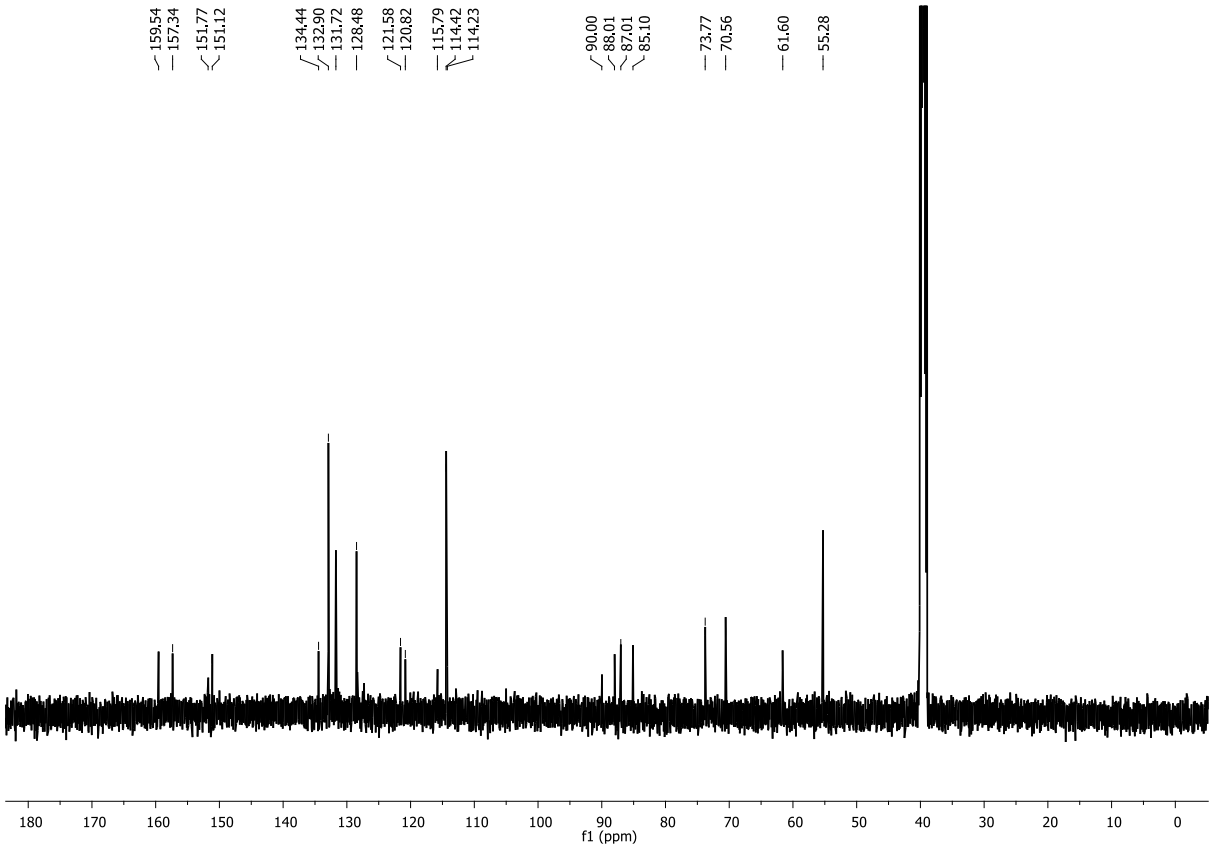
4a – ^{13}C NMR CD_3OD 500 MHz



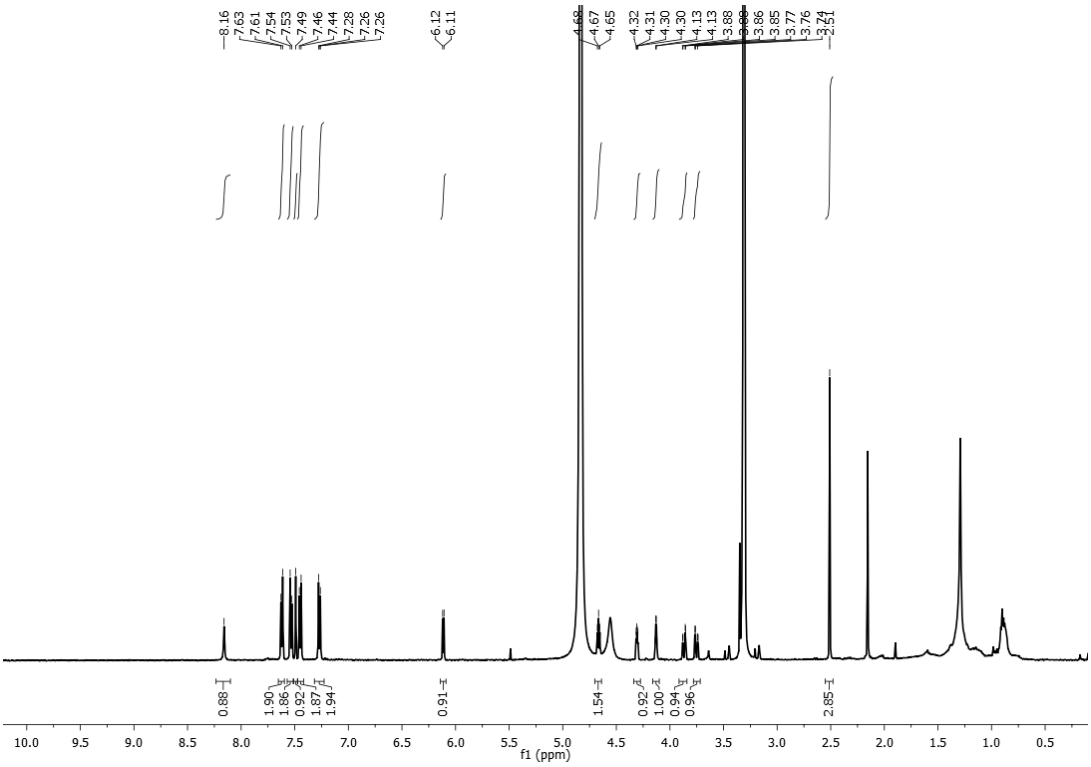
4b – ^{1}H NMR DMSO-d_6 400 MHz



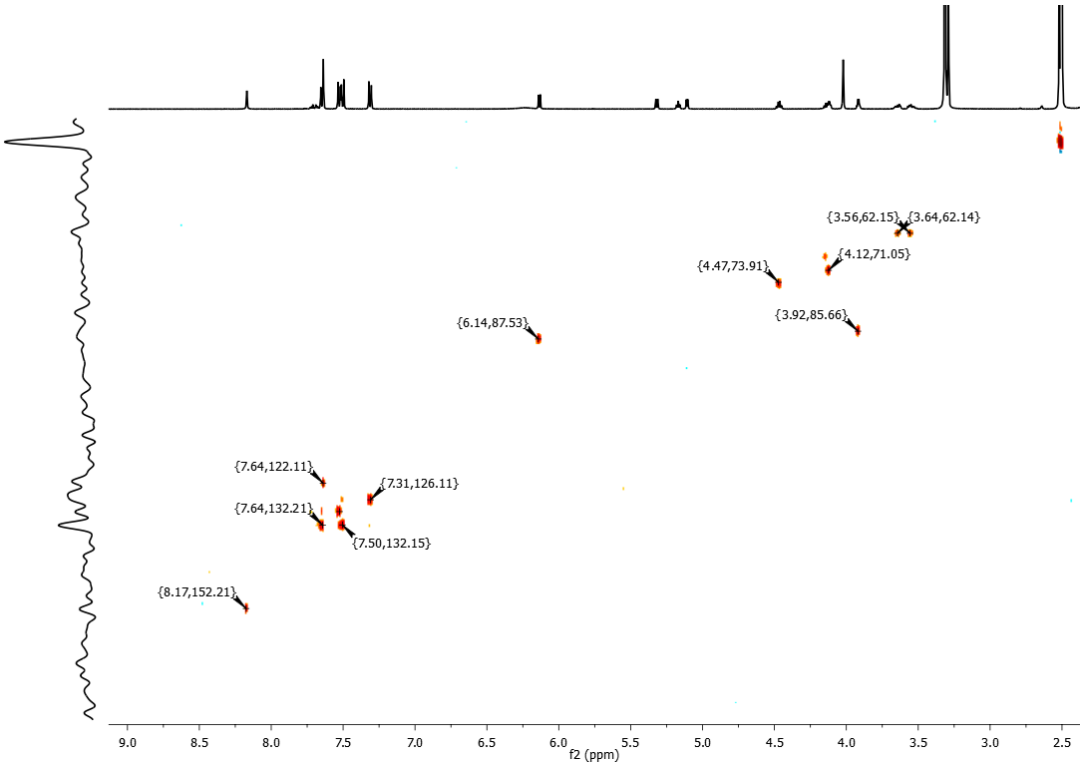
4b – ^{13}C NMR DMSO-d_6 500 MHz



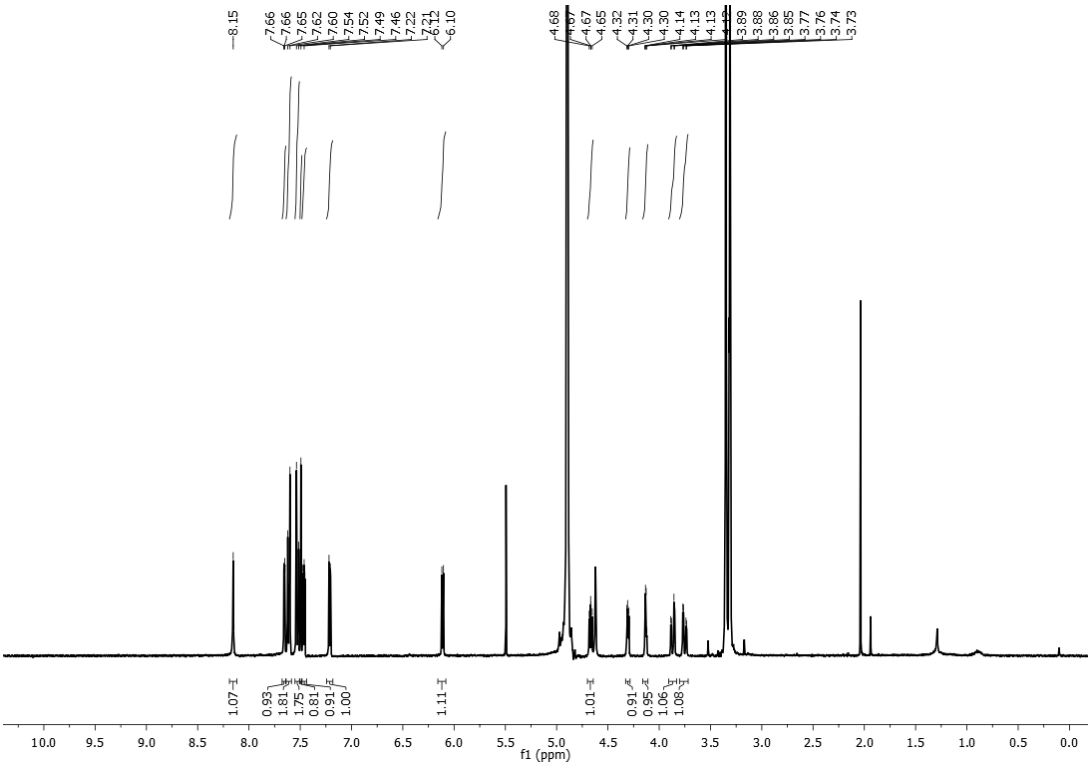
4c – ^{1}H NMR CD_3OD 400 MHz



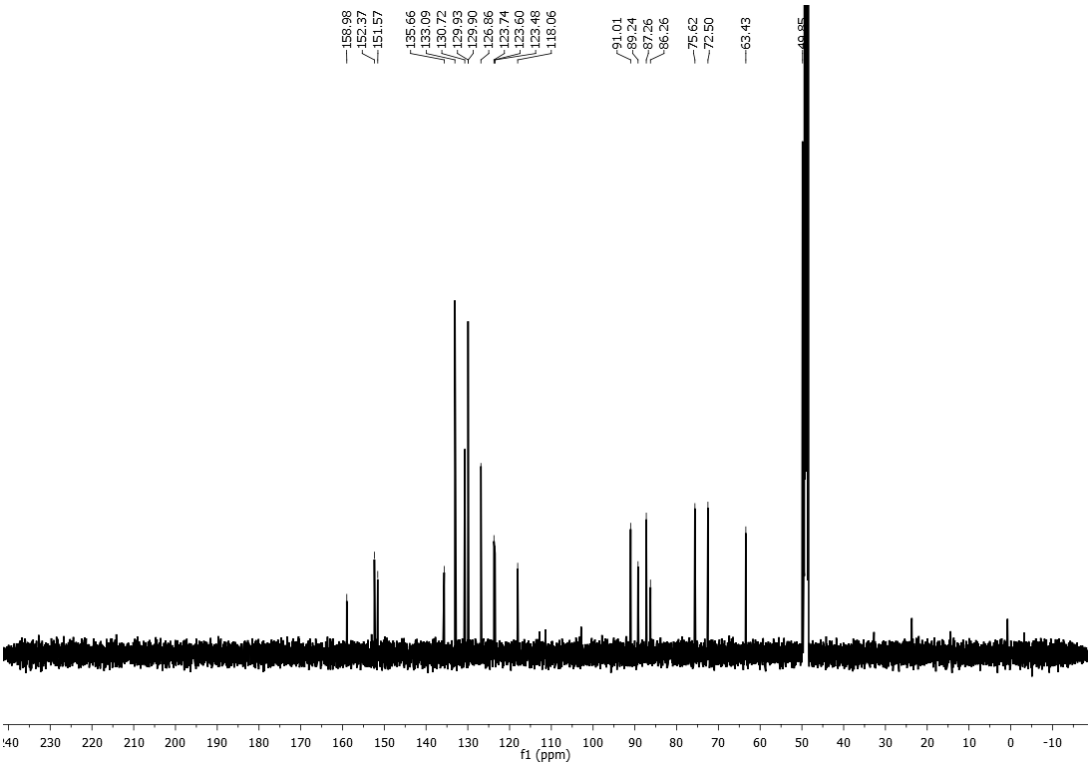
4c – HSQC NMR DMSO-d_6 400 MHz



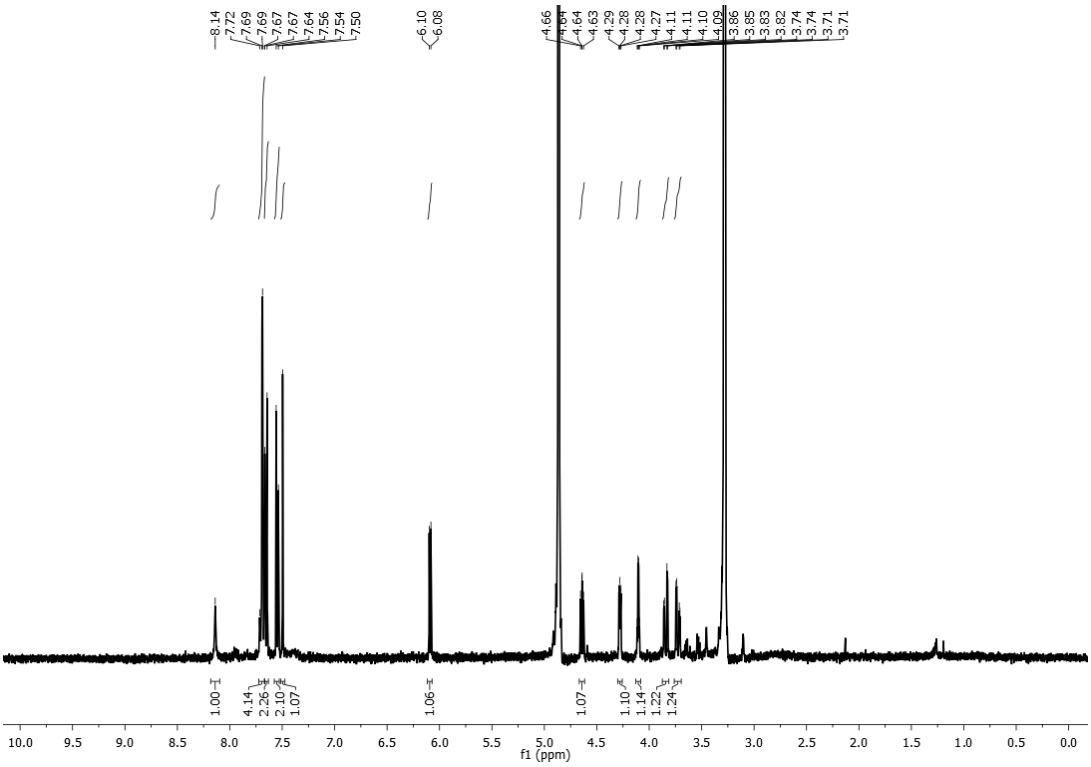
4d – ^{1}H NMR CD_3OD 400 MHz



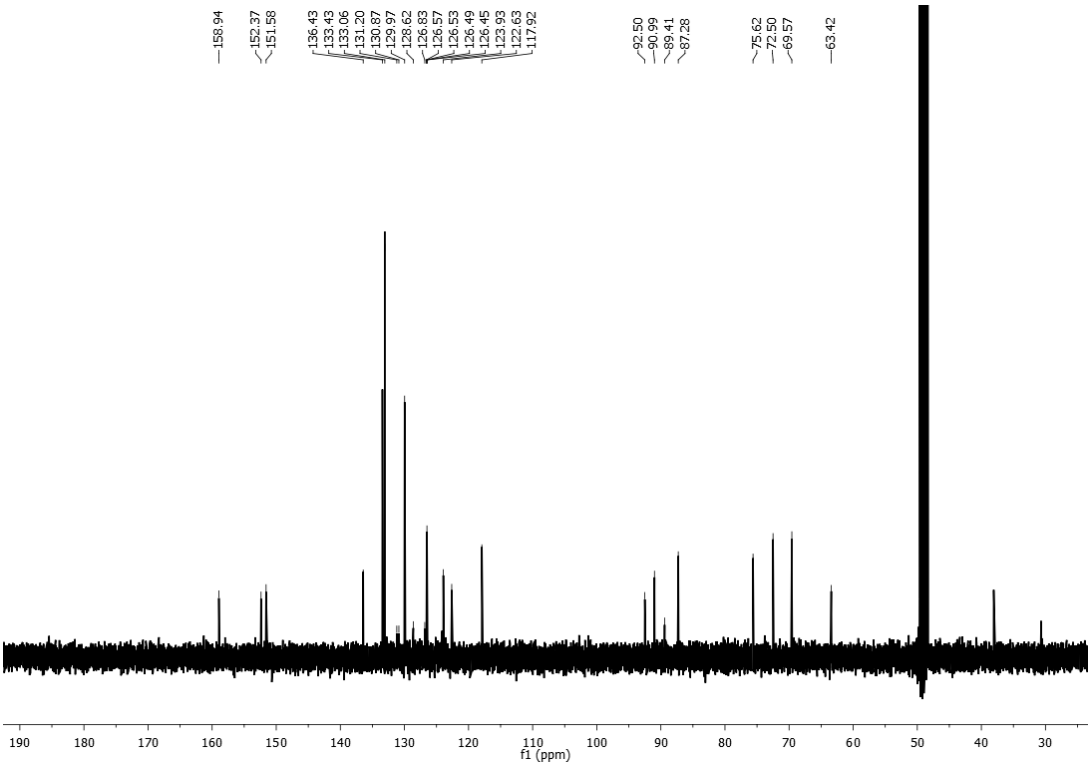
4d – ^{13}C NMR CD_3OD 400 MHz



4e – ^{1}H NMR CD_3OD 400 MHz



4e – ^{13}C NMR CD_3OD 400 MHz



5 Computational Details

Geometry optimisations were performed at the (RI-)BP86/SV(P) and (RI-)BP86/def2-TZVPP levels followed by frequency calculations at the same level. All minima were confirmed as such by the absence of imaginary frequencies. Additional optimisations were also performed at the (RI-)PBE0/def2-TZVPP level using previously optimised structures as the starting points. Vibrational frequency calculations were not performed at this level due to computational expense. However, the absence of negative vibrational modes in the BP86-level optimisations give some confidence that these states are likely to be minima. All calculations were performed using the TURBOMOLE V6.40 package using the resolution of identity (RI) approximation.[6]

Vertical excitation energies were calculated using the ESCF module of TURBOMOLE (full TDDFT) on the (RI-)PBE0/def2-TZVPP optimised structures at the same level of theory. Tight SCF convergence criteria were used in these calculations. 50 singlet excitations were calculated for each state.

Energies, geometries and vibrational frequencies (where available) for each state are presented below.

			BP86/SV(P)					BP86/def2-TZVPP					PBE0/def2-TZVPP				
Compound	**Isomer**	**Expt. lamda max. (nm)**	**SCF E (a.u.)**	**ZPE (a.u.)**	**HOMO (eV)**	**LUMO (eV)**	**Gap (eV)**	**SCF E (a.u.)**	**ZPE (a.u.)**	**HOMO (eV)**	**LUMO (eV)**	**Gap (eV)**	**SCF E (a.u.)**	**HOMO (eV)**	**LUMO (eV)**	**Gap (eV)**	**Calc. lamda max. (nm)**
3	iso1	302	-1253.836735	0.343421	-5.101	-2.319	2.782	-1255.286482	0.342595	-5.192	-2.379	2.812	-1253.785395	-5.996	-1.402	4.594	311
3	iso2	302	-1253.836750	0.343561	-5.102	-2.322	2.780	-1255.286467	0.342681	-5.193	-2.387	2.806	-1253.785344	-6.010	-1.393	4.617	310
3	iso3 (C3'-endo)	302	-1253.839332	0.343202	-5.015	-2.246	2.769	-1255.289013	0.342425	-5.110	-2.324	2.786	-1253.788035	-5.877	-1.375	4.502	312
4a Ar = Ph	iso1	321	-1484.728205	0.422124	-5.128	-2.580	2.548	-1486.429872	0.420925	-5.217	-2.628	2.588	-1484.645117	-5.986	-1.727	4.259	336
4a Ar = Ph	iso2	321	-1484.728199	0.422184	-5.128	-2.580	2.549	-1486.429914	0.421168	-5.219	-2.627	2.592	-1484.645127	-5.986	-1.726	4.261	336
4a Ar = Ph	iso3 (C3'-endo)	321	-1484.730871	0.422106	-5.052	-2.524	2.528	-1486.432493	0.420819	-5.145	-2.578	2.568	-1484.647837	-5.912	-1.674	4.238	338
5	Iso 1	302	-797.257052	0.235411	-4.857	-2.157	2.700	-798.148654	0.234754	-4.980	-2.251	2.729	-797.166859	-5.745	-1.321	4.424	318
5	Iso 2	302	-797.257063	0.235399	-4.855	-2.160	2.696	-798.148652	0.234789	-4.981	-2.249	2.731	-797.166864	-5.747	-1.320	4.427	318
6a Ar = Ph	Iso 1	321	-1028.148538	0.314329	-4.902	-2.461	2.441	-1029.291970	0.313386	-5.016	-2.525	2.491	-1028.026485	-5.782	-1.636	4.147	345
6a Ar = Ph	Iso 2	321	-1028.148546	0.314322	-4.902	-2.463	2.438	-1029.291969	0.313355	-5.019	-2.528	2.491	-1028.026503	-5.786	-1.637	4.149	345
6b Ar = p-OMeC$_6$H$_4$	Iso1	321	-1142.592405	0.345846	-4.758	-2.262	2.496	-1143.871650	0.344659	-4.868	-2.327	2.541	-1142.472483	-5.636	-1.443	4.193	341
6b Ar = p-OMeC$_6$H$_4$	Iso2	321	-1142.592417	0.345844	-4.759	-2.262	2.497	-1143.871659	0.344673	-4.866	-2.327	2.539	-1142.472494	-5.637	-1.443	4.194	341
6b Ar = p-OMeC$_6$H$_4$	Iso3	321	-1142.592406	0.345839	-4.759	-2.263	2.496	-1143.871376	0.344278	-4.867	-2.342	2.526	-1142.472488	-5.639	-1.443	4.195	341
6b Ar = p-OMeC$_6$H$_4$	Iso4	321	-1142.592414	0.345863	-4.760	-2.262	2.498	-1143.871662	0.344717	-4.870	-2.327	2.542	-1142.472501	-5.638	-1.443	4.195	341
6c Ar = p-SMeC$_6$H$_4$	Iso2	331	-1465.545065	0.341951	-4.770	-2.376	2.394	-1466.876693	0.340931	-4.869	-2.445	2.424	-1465.374544	-5.631	-1.586	4.045	353
6c Ar = p-SMeC$_6$H$_4$	Iso3	331	-1465.545070	0.341950	-4.772	-2.376	2.395	-1466.876698	0.340947	-4.871	-2.446	2.425	-1465.374555	-5.634	-1.588	4.046	353
6c Ar = p-SMeC$_6$H$_4$	Iso4	331	-1465.545070	0.341984	-4.773	-2.376	2.397	-1466.876694	0.340952	-4.874	-2.445	2.429	-1465.374555	-5.637	-1.587	4.049	353
6c Ar = p-SMeC$_6$H$_4$	Iso5	331	-1465.545074	0.341960	-4.771	-2.378	2.393	-1466.876708	0.340930	-4.870	-2.446	2.424	-1465.374561	-5.633	-1.589	4.045	353
6d Ar = 3-thienyl	Iso1	313	-1348.891698	0.281356	-4.870	-2.354	2.516	-1350.091199	0.280512	-4.982	-2.426	2.556	-1348.734944	-5.761	-1.534	4.226	338
6d Ar = 3-thienyl	Iso2	313	-1348.891701	0.281354	-4.869	-2.353	2.516	-1350.091193	0.280542	-4.983	-2.427	2.556	-1348.734939	-5.761	-1.534	4.227	338
6d Ar = 3-thienyl	Iso3	313	-1348.891701	0.281312	-4.870	-2.355	2.516	-1350.091199	0.280495	-4.985	-2.426	2.558	-1348.734949	-5.761	-1.535	4.227	338
6d Ar = 3-thienyl	Iso4	313	-1348.891698	0.281329	-4.870	-2.353	2.517	-1350.091196	0.280560	-4.984	-2.426	2.558	-1348.734949	-5.761	-1.533	4.228	338
6e Ar = p-CF$_3$C$_6$H$_4$	Iso 1	328	-1364.961265	0.318862	-5.050	-2.808	2.243	-1366.505073	0.317498	-5.179	-2.894	2.284	-1364.905197	-5.938	-2.007	3.932	363
6e Ar = p-CF$_3$C$_6$H$_4$	Iso 2	328	-1364.961368	0.318893	-5.050	-2.804	2.245	-1366.505146	0.317408	-5.179	-2.894	2.285	-1364.905272	-5.939	-2.005	3.934	363

Calculated λ_{max} values are taken to be the most intense excitations > 250 nm, as experimental UV/Vis spectra were only measured from ~ 250 nm.

5.1 (RI-)BP86/SV(P) Level Calculations

6d/iso1

bp86 energy (au): -1348.8916980350

Zero point energy (au): 0.2813557
Entropy (kJ mol-1 K-1): 0.64997
Chemical potential (kJ mol-1): 601.76

XYZ coordinates:

38

C	-5.78670	1.33760	0.96596
C	-5.57400	0.12568	0.23783
C	-6.77206	-0.58917	-0.05164
N	-8.02873	-0.20096	0.21819
C	-8.07571	0.98454	0.83918
N	-7.04337	1.75312	1.23260
N	-4.76959	2.13608	1.41623
C	-4.46606	-0.68688	-0.23037
N	-6.42789	-1.78472	-0.65830
H	-9.08331	1.37714	1.07349
C	-3.02056	-0.40363	-0.22124
C	-5.05023	-1.84140	-0.75787
C	-7.38280	-2.77582	-1.12195
H	-4.56563	-2.69477	-1.24982
H	-3.81552	1.77491	1.46617
H	-5.04233	2.89923	2.04119
H	-7.29821	-2.92832	-2.22060
H	-8.39489	-2.39196	-0.88161
H	-7.22773	-3.74937	-0.60700
C	-0.19839	0.11736	-0.24938
C	-0.70326	-1.18131	0.03533
C	-2.07826	-1.42861	0.05250
C	-2.51240	0.88782	-0.52210
C	-1.13764	1.14651	-0.53016
C	1.20185	0.37838	-0.25157
H	0.00625	-1.99355	0.25942
H	-2.44260	-2.43738	0.30774
H	-3.21371	1.69702	-0.78298
H	-0.76903	2.15570	-0.77344
C	2.41486	0.60264	-0.24844
C	3.80945	0.87642	-0.24676
C	4.38565	2.18655	-0.46395
C	4.80084	-0.08695	-0.03391
H	3.78019	3.08529	-0.65064
C	5.76150	2.18156	-0.41096
S	6.38788	0.59047	-0.09740
H	6.45166	3.02653	-0.53872
H	4.65749	-1.15876	0.15499

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	19.62	0.01475	YES	YES
8	a	24.20	0.19231	YES	YES
9	a	26.30	0.10761	YES	YES
10	a	55.70	3.11067	YES	YES
11	a	63.63	0.53823	YES	YES
12	a	71.36	1.20262	YES	YES
13	a	99.66	0.92368	YES	YES
14	a	119.00	0.68537	YES	YES
15	a	131.54	1.79602	YES	YES
16	a	145.27	0.94448	YES	YES
17	a	160.06	0.04008	YES	YES
18	a	189.59	1.68508	YES	YES
19	a	225.93	0.95948	YES	YES
20	a	231.74	5.02325	YES	YES
21	a	253.30	2.92202	YES	YES
22	a	279.42	0.57886	YES	YES
23	a	319.67	2.43955	YES	YES
24	a	346.52	13.03372	YES	YES
25	a	354.41	176.81983	YES	YES
26	a	385.04	16.92917	YES	YES
27	a	395.31	1.01910	YES	YES
28	a	412.38	11.46188	YES	YES
29	a	444.09	2.99011	YES	YES
30	a	456.74	3.31051	YES	YES
31	a	473.68	2.42067	YES	YES
32	a	521.94	4.99870	YES	YES
33	a	525.25	26.11813	YES	YES
34	a	539.39	0.69934	YES	YES
35	a	544.44	6.50369	YES	YES
36	a	551.70	5.61897	YES	YES
37	a	553.88	3.98046	YES	YES
38	a	580.36	3.60543	YES	YES
39	a	610.69	7.96712	YES	YES
40	a	626.58	7.47973	YES	YES
41	a	631.40	16.70527	YES	YES
42	a	639.76	1.61433	YES	YES
43	a	647.73	11.44518	YES	YES
44	a	648.88	3.25827	YES	YES
45	a	678.25	1.24992	YES	YES
46	a	703.69	10.36660	YES	YES
47	a	738.45	4.11728	YES	YES
48	a	756.50	3.29752	YES	YES
49	a	756.84	59.39956	YES	YES
50	a	768.40	9.78218	YES	YES

6d/iso2

bp86 energy (au): -1348.8917007490

Zero point energy (au): 0.2813543
Entropy (kJ mol-1 K-1): 0.65204
Chemical potential (kJ mol-1): 601.16

XYZ coordinates:

38

C	-5.80282	1.33036	0.98087
C	-5.57883	0.12425	0.24659
C	-6.77165	-0.59315	-0.05815
N	-8.03228	-0.21119	0.20228
C	-8.08923	0.97049	0.82996
N	-7.06334	1.73980	1.23807
N	-4.79292	2.12906	1.44665
C	-4.46378	-0.68083	-0.21750
N	-6.41764	-1.78335	-0.66982
H	-9.10042	1.35826	1.05671
C	-3.01956	-0.39207	-0.19977
C	-5.03894	-1.83392	-0.75789
C	-7.36467	-2.77443	-1.14954
H	-4.54695	-2.68152	-1.25251
H	-3.83824	1.77076	1.50404
H	-5.07452	2.88708	2.07393
H	-7.26909	-2.91862	-2.24843
H	-8.38033	-2.39573	-0.91604
H	-7.21097	-3.75110	-0.64008
C	-0.19834	0.13503	-0.23014
C	-0.70013	-1.16646	0.04767
C	-2.07454	-1.41668	0.06588
C	-2.51485	0.90327	-0.48909
C	-1.14060	1.16480	-0.49861
C	1.20189	0.39668	-0.24261
H	0.01159	-1.97920	0.26303
H	-2.43602	-2.42830	0.31365
H	-3.21814	1.71335	-0.74162
H	-0.77458	2.17659	-0.73511
C	2.41396	0.62581	-0.25658
C	3.81276	0.87644	-0.26963
C	4.82522	-0.12223	0.00127
C	4.38701	2.12136	-0.54632
H	4.58708	-1.16861	0.24155
C	6.10544	0.37906	-0.07483
S	6.11149	2.07044	-0.47679
H	7.05530	-0.14964	0.08318
H	3.86465	3.05619	-0.78725

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	18.13	0.03445	YES	YES
8	a	20.34	0.00152	YES	YES
9	a	25.84	0.03582	YES	YES
10	a	56.72	3.19712	YES	YES
11	a	63.92	0.44597	YES	YES
12	a	71.21	1.47011	YES	YES
13	a	100.30	1.16338	YES	YES
14	a	119.15	0.82222	YES	YES
15	a	131.53	1.70011	YES	YES
16	a	142.12	0.49938	YES	YES
17	a	163.11	0.28984	YES	YES
18	a	189.80	1.28454	YES	YES
19	a	226.00	1.12780	YES	YES
20	a	231.12	4.62978	YES	YES
21	a	253.63	2.91674	YES	YES
22	a	279.62	0.30715	YES	YES
23	a	319.96	2.21873	YES	YES
24	a	345.34	10.69601	YES	YES
25	a	354.40	180.02369	YES	YES
26	a	384.48	17.55577	YES	YES
27	a	397.28	0.93720	YES	YES
28	a	412.72	12.52122	YES	YES
29	a	443.82	3.35084	YES	YES
30	a	455.53	1.80464	YES	YES
31	a	473.59	2.14743	YES	YES
32	a	522.19	4.56554	YES	YES
33	a	525.20	25.49697	YES	YES
34	a	541.24	2.18082	YES	YES
35	a	544.01	5.73489	YES	YES
36	a	551.38	5.17082	YES	YES
37	a	553.59	4.33962	YES	YES
38	a	580.38	3.96001	YES	YES
39	a	610.86	8.14971	YES	YES
40	a	626.55	7.10084	YES	YES
41	a	630.91	15.98515	YES	YES
42	a	639.84	1.58749	YES	YES
43	a	647.67	11.87353	YES	YES
44	a	649.39	3.51442	YES	YES
45	a	678.23	1.20628	YES	YES
46	a	703.65	10.32736	YES	YES
47	a	738.67	4.35940	YES	YES
48	a	756.38	3.20004	YES	YES
49	a	757.08	59.63253	YES	YES
50	a	768.49	9.60001	YES	YES

6d/iso3

bp86 energy (au): -1348.8917014890

Zero point energy (au): 0.2813118
Entropy (kJ mol-1 K-1): 0.65240
Chemical potential (kJ mol-1): 600.94

XYZ coordinates:

38

C	-5.80161	1.30881	1.03788
C	-5.57359	0.08272	0.33892
C	-6.76357	-0.64836	0.05690
N	-8.01167	-0.33887	0.44358
C	-8.06115	0.79794	1.14971
N	-7.04663	1.62965	1.44963
N	-4.80845	2.20268	1.33633
C	-4.47435	-0.62885	-0.28702
N	-6.42442	-1.74935	-0.71027
H	-9.05797	1.10294	1.52079
C	-3.03075	-0.33586	-0.26744
C	-5.05764	-1.73083	-0.91782
C	-7.36971	-2.74810	-1.17712
H	-4.57081	-2.54404	-1.47164
H	-3.90636	2.14908	0.86022
H	-5.11383	3.10184	1.71782
H	-7.37134	-2.80576	-2.28775
H	-8.37408	-2.43732	-0.82450
H	-7.12827	-3.75164	-0.76199
C	-0.20701	0.17892	-0.23169
C	-0.85404	-0.28995	-1.40827
C	-2.22964	-0.53515	-1.42172
C	-2.37888	0.11713	0.90994
C	-1.00388	0.37457	0.92911
C	1.19246	0.44464	-0.21812
H	-0.25716	-0.44505	-2.32107
H	-2.70975	-0.86849	-2.35658
H	-2.96242	0.24197	1.83659
H	-0.52163	0.71866	1.85793
C	2.40391	0.67735	-0.21284
C	3.79852	0.95078	-0.19366
C	4.53032	1.38866	0.97629
C	4.63953	0.83272	-1.30509
H	4.05726	1.54433	1.95674
C	5.87008	1.58589	0.72700
S	6.27358	1.24528	-0.92952
H	6.65236	1.91394	1.42498
H	4.36061	0.52211	-2.32026

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.33	0.15428	YES	YES
8	a	20.97	0.02863	YES	YES
9	a	26.39	0.09854	YES	YES
10	a	53.20	3.48039	YES	YES
11	a	63.93	0.51485	YES	YES
12	a	71.02	1.21742	YES	YES
13	a	104.50	1.52084	YES	YES
14	a	123.86	0.06165	YES	YES
15	a	133.00	1.56829	YES	YES
16	a	145.72	1.03476	YES	YES
17	a	160.30	0.03917	YES	YES
18	a	190.34	1.92264	YES	YES
19	a	226.41	0.84292	YES	YES
20	a	230.44	4.96213	YES	YES
21	a	253.56	3.12770	YES	YES
22	a	279.05	0.57436	YES	YES
23	a	318.92	4.27866	YES	YES
24	a	346.35	41.65872	YES	YES
25	a	348.65	148.74153	YES	YES
26	a	384.54	16.32372	YES	YES
27	a	394.77	0.63459	YES	YES
28	a	411.38	9.20370	YES	YES
29	a	444.08	3.22864	YES	YES
30	a	457.04	3.49616	YES	YES
31	a	473.57	2.06669	YES	YES
32	a	521.92	5.04386	YES	YES
33	a	523.77	25.83666	YES	YES
34	a	539.44	0.24955	YES	YES
35	a	544.19	7.41483	YES	YES
36	a	550.80	4.95956	YES	YES
37	a	553.85	3.80489	YES	YES
38	a	580.26	3.70935	YES	YES
39	a	610.52	7.99196	YES	YES
40	a	626.72	7.76832	YES	YES
41	a	631.04	15.88056	YES	YES
42	a	639.57	1.55017	YES	YES
43	a	648.18	11.78123	YES	YES
44	a	648.77	3.53687	YES	YES
45	a	678.47	1.21788	YES	YES
46	a	703.88	10.32024	YES	YES
47	a	738.35	3.92306	YES	YES
48	a	756.31	3.14319	YES	YES
49	a	756.75	59.63739	YES	YES
50	a	768.14	9.94804	YES	YES

6d/iso4

bp86 energy (au): -1348.8916982150

Zero point energy (au): 0.2813286
Entropy (kJ mol-1 K-1): 0.65017
Chemical potential (kJ mol-1): 601.63

XYZ coordinates:

38

C	-5.81711	1.30905	1.03396
C	-5.57892	0.08398	0.33665
C	-6.76256	-0.65795	0.05635
N	-8.01310	-0.35874	0.44327
C	-8.07210	0.77889	1.14740
N	-7.06475	1.61991	1.44552
N	-4.83149	2.21177	1.33063
C	-4.47373	-0.61926	-0.28799
N	-6.41402	-1.75738	-0.70884
H	-9.07142	1.07575	1.51835
C	-3.03230	-0.31595	-0.26746
C	-5.04751	-1.72740	-0.91668
C	-7.35057	-2.76511	-1.17392
H	-4.55353	-2.53750	-1.46871
H	-3.92808	2.16395	0.85647
H	-5.14404	3.10825	1.71259
H	-7.35590	-2.82107	-2.28465
H	-8.35685	-2.46537	-0.81719
H	-7.09685	-3.76665	-0.76136
C	-0.21075	0.20881	-0.22692
C	-0.85442	-0.26000	-1.40532
C	-2.22903	-0.51031	-1.42105
C	-2.38429	0.14004	0.91087
C	-1.01021	0.40214	0.93243
C	1.18876	0.47356	-0.20961
H	-0.25546	-0.41228	-2.31722
H	-2.70663	-0.84505	-2.35666
H	-2.96977	0.26234	1.83668
H	-0.53049	0.74708	1.86225
C	2.40086	0.70218	-0.19362
C	3.79803	0.96260	-0.19088
C	4.65220	0.85417	-1.35474
C	4.52351	1.35744	0.93770
H	4.28095	0.55710	-2.34625
C	5.96671	1.16197	-1.08442
S	6.19767	1.58892	0.58477
H	6.82217	1.16376	-1.77350
H	4.13903	1.51837	1.95310

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	20.35	0.00060	YES	YES
8	a	22.21	0.03517	YES	YES
9	a	26.23	0.03094	YES	YES
10	a	53.51	3.59163	YES	YES
11	a	64.16	0.49166	YES	YES
12	a	70.76	1.33962	YES	YES
13	a	104.80	1.84994	YES	YES
14	a	124.51	0.10976	YES	YES
15	a	133.12	1.35273	YES	YES
16	a	142.89	0.72517	YES	YES
17	a	163.02	0.29758	YES	YES
18	a	190.36	1.53066	YES	YES
19	a	226.34	1.13541	YES	YES
20	a	229.80	4.58619	YES	YES
21	a	253.61	3.07872	YES	YES
22	a	279.13	0.30952	YES	YES
23	a	319.08	4.32086	YES	YES
24	a	344.64	127.50592	YES	YES
25	a	345.51	66.43348	YES	YES
26	a	383.97	13.82791	YES	YES
27	a	396.89	0.78598	YES	YES
28	a	411.32	9.07850	YES	YES
29	a	444.13	3.41274	YES	YES
30	a	455.79	1.76679	YES	YES
31	a	473.38	2.25690	YES	YES
32	a	522.15	4.74351	YES	YES
33	a	523.84	24.67311	YES	YES
34	a	541.03	1.86708	YES	YES
35	a	543.76	6.51978	YES	YES
36	a	550.66	4.66603	YES	YES
37	a	553.03	3.72327	YES	YES
38	a	580.28	4.09597	YES	YES
39	a	610.54	8.21913	YES	YES
40	a	626.59	7.18435	YES	YES
41	a	630.77	15.59032	YES	YES
42	a	639.90	1.54910	YES	YES
43	a	648.17	12.18722	YES	YES
44	a	649.55	3.66426	YES	YES
45	a	678.47	1.22002	YES	YES
46	a	703.84	10.25979	YES	YES
47	a	738.30	3.99548	YES	YES
48	a	756.39	3.37086	YES	YES
49	a	757.18	59.30356	YES	YES
50	a	768.14	9.92186	YES	YES

6e/iso1

bp86 energy (au): -1364.9612650860

Zero point energy (au): 0.3188616
Entropy (kJ mol-1 K-1): 0.74414
Chemical potential (kJ mol-1): 682.79

XYZ coordinates:

44

C	-5.50843	1.81319	0.33154
C	-5.48132	0.41056	0.05428
C	-6.77335	-0.18449	-0.02584
N	-7.95738	0.44358	0.04845
C	-7.82549	1.76353	0.23394
N	-6.68863	2.46580	0.39185
N	-4.38294	2.56511	0.53788
C	-4.50876	-0.65983	-0.07143
N	-6.61287	-1.55106	-0.18237
H	-8.76273	2.34966	0.28019
C	-3.03888	-0.59347	-0.10381
C	-5.26024	-1.83107	-0.20308
C	-7.70791	-2.49610	-0.31756
H	-4.91049	-2.85922	-0.36271
H	-3.49283	2.11188	0.75105
H	-4.53842	3.52281	0.86402
H	-7.65588	-3.02995	-1.29186
H	-8.64997	-1.91342	-0.26737
H	-7.69346	-3.24215	0.50737
C	-0.17423	-0.48584	-0.17240
C	-0.85265	-1.54252	0.49508
C	-2.24833	-1.58801	0.52924
C	-2.35715	0.44526	-0.79218
C	-0.96045	0.50378	-0.82253
C	1.24742	-0.40962	-0.17543
H	-0.26234	-2.31951	1.00614
H	-2.74896	-2.39832	1.08447
H	-2.93972	1.20755	-1.33427
H	-0.45478	1.31831	-1.36515
C	2.47805	-0.32523	-0.15991
C	3.89656	-0.20422	-0.11547
C	6.71317	0.07962	0.03067
C	5.94359	1.01687	-0.68629
C	4.55423	0.87839	-0.76128
C	4.68761	-1.14784	0.59529
C	6.07675	-1.00433	0.66710
C	8.21744	0.21638	0.08651
H	6.43736	1.86808	-1.18006
H	3.95436	1.61693	-1.31535
H	4.19240	-1.99166	1.10036
H	6.67506	-1.73558	1.23237
F	8.72748	-0.30013	1.23154
F	8.60844	1.51287	0.01420
F	8.82107	-0.43459	-0.94231

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.95	0.17062	YES	YES
8	a	17.84	0.12209	YES	YES
9	a	18.69	0.07707	YES	YES
10	a	23.05	0.02621	YES	YES
11	a	41.75	0.38814	YES	YES
12	a	56.84	0.06640	YES	YES
13	a	62.06	4.58684	YES	YES
14	a	94.01	0.67961	YES	YES
15	a	100.61	1.61499	YES	YES
16	a	114.56	0.27223	YES	YES
17	a	127.46	0.13788	YES	YES
18	a	133.38	1.68493	YES	YES
19	a	152.97	0.83710	YES	YES
20	a	186.92	2.21121	YES	YES
21	a	201.41	0.30283	YES	YES
22	a	223.01	1.53420	YES	YES
23	a	226.24	4.14606	YES	YES
24	a	247.49	1.93378	YES	YES
25	a	278.09	2.35072	YES	YES
26	a	285.71	16.78773	YES	YES
27	a	299.88	2.39041	YES	YES
28	a	341.00	36.98618	YES	YES
29	a	355.98	159.92327	YES	YES
30	a	378.77	2.34339	YES	YES
31	a	387.45	1.21694	YES	YES
32	a	399.38	0.03117	YES	YES
33	a	409.67	3.17638	YES	YES
34	a	414.54	7.78733	YES	YES
35	a	424.11	4.74170	YES	YES
36	a	462.75	2.43595	YES	YES
37	a	468.94	0.80648	YES	YES
38	a	514.44	10.61078	YES	YES
39	a	522.23	9.87622	YES	YES
40	a	526.20	18.14999	YES	YES
41	a	539.39	0.40960	YES	YES
42	a	544.17	7.37736	YES	YES
43	a	552.40	3.35789	YES	YES
44	a	558.16	6.80369	YES	YES
45	a	567.12	0.01064	YES	YES
46	a	588.81	10.86903	YES	YES
47	a	598.73	2.96849	YES	YES
48	a	611.30	6.20017	YES	YES
49	a	625.85	6.16217	YES	YES
50	a	632.48	2.08441	YES	YES

6e/iso2

bp86 energy (au): -1364.9613676280

Zero point energy (au): 0.3188927
Entropy (kJ mol-1 K-1): 0.74376
Chemical potential (kJ mol-1): 683.01

XYZ coordinates:

44

C	-5.50121	1.82534	0.38916
C	-5.47894	0.41553	0.15162
C	-6.77307	-0.17248	0.05540
N	-7.95322	0.43938	0.24221
C	-7.81512	1.74068	0.52827
N	-6.67705	2.45568	0.59576
N	-4.37438	2.60157	0.43294
C	-4.51243	-0.62803	-0.13678
N	-6.61981	-1.50625	-0.28364
H	-8.74842	2.30407	0.71713
C	-3.04135	-0.58129	-0.12274
C	-5.26967	-1.77228	-0.40360
C	-7.71716	-2.44404	-0.44698
H	-4.92342	-2.79009	-0.62518
H	-3.49391	2.25289	0.05067
H	-4.52846	3.61262	0.47317
H	-7.72673	-2.86920	-1.47445
H	-8.65659	-1.88086	-0.27404
H	-7.64507	-3.27460	0.28962
C	-0.17502	-0.55651	-0.07325
C	-0.88506	-1.28554	-1.06674
C	-2.28133	-1.29122	-1.08887
C	-2.32847	0.13560	0.87508
C	-0.93027	0.15355	0.89907
C	1.24839	-0.54073	-0.05706
H	-0.31799	-1.83810	-1.83249
H	-2.80732	-1.83928	-1.88771
H	-2.88739	0.66380	1.66445
H	-0.39962	0.70902	1.68871
C	2.48184	-0.53061	-0.05273
C	3.90580	-0.51710	-0.06305
C	6.73864	-0.47762	-0.10282
C	6.03643	0.18739	0.92116
C	4.63821	0.16974	0.94321
C	4.62921	-1.19128	-1.08476
C	6.02685	-1.17023	-1.10196
C	8.24603	-0.39950	-0.16721
H	6.59138	0.71995	1.70886
H	4.09151	0.68945	1.74528
H	4.07469	-1.73333	-1.86638
H	6.57422	-1.69943	-1.89737
F	8.78726	-1.51407	-0.71785
F	8.79907	-0.24049	1.06006
F	8.65592	0.65290	-0.92417

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.02	0.15767	YES	YES
8	a	17.87	0.07236	YES	YES
9	a	20.31	0.20218	YES	YES
10	a	29.59	0.00857	YES	YES
11	a	41.94	0.35381	YES	YES
12	a	56.42	0.40371	YES	YES
13	a	59.65	4.14687	YES	YES
14	a	92.23	0.66277	YES	YES
15	a	96.74	1.40083	YES	YES
16	a	111.50	0.52698	YES	YES
17	a	126.94	0.60480	YES	YES
18	a	134.44	1.09963	YES	YES
19	a	149.91	0.98536	YES	YES
20	a	186.29	2.10619	YES	YES
21	a	201.45	0.17995	YES	YES
22	a	223.75	1.51128	YES	YES
23	a	225.76	4.95487	YES	YES
24	a	245.51	1.52494	YES	YES
25	a	277.48	3.47917	YES	YES
26	a	289.61	17.01048	YES	YES
27	a	296.41	1.15182	YES	YES
28	a	342.41	46.74859	YES	YES
29	a	355.74	145.78930	YES	YES
30	a	378.45	2.01333	YES	YES
31	a	386.67	0.97326	YES	YES
32	a	399.69	0.08915	YES	YES
33	a	408.91	3.38715	YES	YES
34	a	414.37	16.80177	YES	YES
35	a	425.50	1.95519	YES	YES
36	a	463.15	0.60735	YES	YES
37	a	468.67	0.79382	YES	YES
38	a	514.82	11.48887	YES	YES
39	a	522.63	7.45311	YES	YES
40	a	528.29	18.79599	YES	YES
41	a	539.61	0.25755	YES	YES
42	a	544.22	7.58898	YES	YES
43	a	552.97	3.93312	YES	YES
44	a	557.86	6.38884	YES	YES
45	a	567.38	0.03399	YES	YES
46	a	589.19	10.23611	YES	YES
47	a	598.87	2.76783	YES	YES
48	a	611.07	6.87314	YES	YES
49	a	625.73	6.26330	YES	YES
50	a	632.52	2.11907	YES	YES

6b/iso1

bp86 energy (au): -1142.5924050310

Zero point energy (au): 0.3458462
Entropy (kJ mol-1 K-1): 0.70932
Chemical potential (kJ mol-1): 761.15

XYZ coordinates:

45

C	-4.71905	1.77629	0.15718
C	-4.59983	0.36194	-0.01537
C	-5.85116	-0.31381	-0.10719
N	-7.07147	0.24634	-0.12524
C	-7.02273	1.58093	-0.02638
N	-5.93597	2.35992	0.12523
N	-3.64711	2.60556	0.34917
C	-3.56198	-0.65284	-0.02686
N	-5.60558	-1.67480	-0.16248
H	-7.99323	2.11166	-0.05793
C	-2.09673	-0.50167	-0.00222
C	-4.23791	-1.87285	-0.10945
C	-6.63613	-2.69134	-0.27747
H	-3.82211	-2.88615	-0.18353
H	-2.73840	2.22140	0.61369
H	-3.86648	3.57455	0.59444
H	-6.51242	-3.28146	-1.21218
H	-7.61223	-2.16574	-0.30119
H	-6.61244	-3.38249	0.59381
C	0.76445	-0.25962	0.00971
C	0.10968	-1.28751	0.74335
C	-1.28313	-1.39814	0.73798
C	-1.43974	0.51464	-0.74507
C	-0.04640	0.63909	-0.73607
C	2.18313	-0.13651	0.01918
H	0.71674	-1.99309	1.33243
H	-1.76506	-2.18603	1.34028
H	-2.03690	1.20203	-1.36625
H	0.43910	1.43190	-1.32728
C	3.41271	-0.03068	0.02609
C	4.83167	0.09340	0.03063
C	7.66849	0.34008	0.03821
C	6.86965	1.25693	-0.68656
C	5.48134	1.13645	-0.69064
C	5.64617	-0.81667	0.75205
C	7.04316	-0.70121	0.76023
O	9.01316	0.54313	-0.02216
H	7.37418	2.06254	-1.24283
H	4.87038	1.85561	-1.25863
H	5.16680	-1.63188	1.31686
H	7.63554	-1.42956	1.33334
C	9.87049	-0.33769	0.68458
H	9.67375	-0.31323	1.78262
H	10.90262	0.01883	0.49345
H	9.77496	-1.38824	0.32046

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	14.93	0.20968	YES YES
8	a	18.21	0.01460	YES YES
9	a	22.08	0.09643	YES YES
10	a	45.36	1.90556	YES YES
11	a	59.31	0.42329	YES YES
12	a	61.78	2.96367	YES YES
13	a	91.61	0.70412	YES YES
14	a	101.30	1.62337	YES YES
15	a	116.88	0.60230	YES YES
16	a	126.41	1.27369	YES YES
17	a	135.28	1.58125	YES YES
18	a	146.37	0.27846	YES YES
19	a	181.42	3.44631	YES YES
20	a	200.28	0.69374	YES YES
21	a	226.87	3.40684	YES YES
22	a	235.44	2.76687	YES YES
23	a	245.65	2.03897	YES YES
24	a	254.33	2.29616	YES YES
25	a	276.69	1.07697	YES YES
26	a	283.82	0.29535	YES YES
27	a	320.73	18.96035	YES YES
28	a	337.44	14.96663	YES YES
29	a	349.88	179.92470	YES YES
30	a	392.69	0.87866	YES YES
31	a	405.39	2.21203	YES YES
32	a	411.44	0.27323	YES YES
33	a	412.83	13.71740	YES YES
34	a	441.87	4.74665	YES YES
35	a	469.13	2.76235	YES YES
36	a	480.25	1.26390	YES YES
37	a	519.43	17.98751	YES YES
38	a	523.98	19.59533	YES YES
39	a	533.67	6.26401	YES YES
40	a	537.00	18.84531	YES YES
41	a	544.77	2.17251	YES YES
42	a	549.67	4.16622	YES YES
43	a	557.32	5.05490	YES YES
44	a	561.24	9.70808	YES YES
45	a	610.92	8.22358	YES YES
46	a	625.98	7.98618	YES YES
47	a	634.65	0.18904	YES YES
48	a	648.00	12.14324	YES YES
49	a	669.14	7.56702	YES YES
50	a	678.15	1.13936	YES YES

6b/iso2

bp86 energy (au): -1142.5924171550

Zero point energy (au): 0.3458444
Entropy (kJ mol-1 K-1): 0.70924
Chemical potential (kJ mol-1): 761.17

XYZ coordinates:

45

C	-4.75584	1.76252	0.16764
C	-4.62542	0.34925	-0.00510
C	-5.87131	-0.33755	-0.08795
N	-7.09654	0.21182	-0.09826
C	-7.05897	1.54678	-0.00012
N	-5.97806	2.33549	0.14398
N	-3.68981	2.60131	0.35151
C	-3.57877	-0.65622	-0.02282
N	-5.61411	-1.69635	-0.14358
H	-8.03433	2.06896	-0.02501
C	-2.11482	-0.49226	-0.00876
C	-4.24438	-1.88224	-0.09959
C	-6.63637	-2.72220	-0.25001
H	-3.82009	-2.89192	-0.17537
H	-2.77666	2.22491	0.61181
H	-3.91643	3.56797	0.59945
H	-6.51453	-3.31194	-1.18520
H	-7.61731	-2.20541	-0.26665
H	-6.59962	-3.41237	0.62155
C	0.74417	-0.22624	-0.01806
C	0.10350	-1.25854	0.72182
C	-1.28835	-1.38090	0.72661
C	-1.47189	0.52862	-0.75747
C	-0.07965	0.66460	-0.75892
C	2.16175	-0.09122	-0.01868
H	0.72067	-1.95789	1.30786
H	-1.75914	-2.17223	1.33328
H	-2.07929	1.21036	-1.37482
H	0.39477	1.46072	-1.35458
C	3.39030	0.02596	-0.02076
C	4.80856	0.15825	-0.02303
C	7.64389	0.42226	-0.03013
C	6.84268	1.33502	-0.75233
C	5.44752	1.19902	-0.74454
C	5.63395	-0.75153	0.69898
C	7.02145	-0.62208	0.69524
O	9.00345	0.46219	0.02944
H	7.29581	2.15719	-1.32565
H	4.83035	1.91443	-1.31075
H	5.16147	-1.56868	1.26658
H	7.66103	-1.32440	1.25262
C	9.68903	1.48546	-0.67286
H	9.50128	1.42994	-1.77140
H	10.76836	1.31996	-0.48103
H	9.40469	2.50015	-0.30595

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.38	0.69833	YES	YES
8	a	16.92	0.15375	YES	YES
9	a	21.99	0.29864	YES	YES
10	a	46.26	1.70763	YES	YES
11	a	59.68	0.45942	YES	YES
12	a	61.19	2.75512	YES	YES
13	a	92.11	0.72482	YES	YES
14	a	101.01	1.34339	YES	YES
15	a	116.55	0.57192	YES	YES
16	a	125.14	1.49258	YES	YES
17	a	132.68	1.53180	YES	YES
18	a	149.64	0.70620	YES	YES
19	a	181.39	3.28062	YES	YES
20	a	199.25	0.77695	YES	YES
21	a	225.38	3.40402	YES	YES
22	a	234.43	1.81538	YES	YES
23	a	247.65	2.13634	YES	YES
24	a	253.82	2.65543	YES	YES
25	a	276.50	0.67583	YES	YES
26	a	282.91	0.29601	YES	YES
27	a	321.50	19.52536	YES	YES
28	a	338.77	12.30205	YES	YES
29	a	351.34	182.36350	YES	YES
30	a	389.81	1.69476	YES	YES
31	a	405.84	3.92036	YES	YES
32	a	410.43	2.35558	YES	YES
33	a	413.53	13.30003	YES	YES
34	a	446.72	2.56289	YES	YES
35	a	467.88	2.11561	YES	YES
36	a	477.34	1.43742	YES	YES
37	a	520.29	21.31192	YES	YES
38	a	523.68	16.92792	YES	YES
39	a	535.01	15.28320	YES	YES
40	a	539.02	9.10368	YES	YES
41	a	543.92	0.72135	YES	YES
42	a	546.97	4.86364	YES	YES
43	a	557.55	4.14599	YES	YES
44	a	561.64	10.33120	YES	YES
45	a	610.98	7.98220	YES	YES
46	a	625.87	7.83150	YES	YES
47	a	634.83	1.52813	YES	YES
48	a	647.96	11.99715	YES	YES
49	a	669.06	9.47441	YES	YES
50	a	678.04	1.05012	YES	YES

6b/iso3

bp86 energy (au): -1142.5924060710

Zero point energy (au): 0.3458390
Entropy (kJ mol-1 K-1): 0.70842
Chemical potential (kJ mol-1): 761.39

XYZ coordinates:

45

C	-4.75718	1.77543	0.23306
C	-4.61564	0.35893	0.10084
C	-5.85511	-0.34180	0.04854
N	-7.08416	0.18186	0.18555
C	-7.05699	1.50811	0.36968
N	-5.98331	2.31940	0.38660
N	-3.69874	2.64285	0.22343
C	-3.56173	-0.61666	-0.10664
N	-5.58717	-1.67893	-0.18734
H	-8.03591	2.00445	0.51072
C	-2.09965	-0.43542	-0.10116
C	-4.21665	-1.83763	-0.28502
C	-6.59980	-2.71553	-0.27956
H	-3.78392	-2.83590	-0.43148
H	-2.78351	2.33670	-0.11070
H	-3.93292	3.63836	0.18975
H	-6.56469	-3.21948	-1.27041
H	-7.58492	-2.22207	-0.15381
H	-6.46531	-3.47738	0.51997
C	0.75566	-0.13835	-0.06434
C	0.11632	-0.98665	-1.01035
C	-1.27412	-1.12458	-1.02672
C	-1.45789	0.40030	0.85062
C	-0.06736	0.55138	0.86749
C	2.17139	0.01376	-0.04827
H	0.73293	-1.52810	-1.74524
H	-1.74506	-1.76554	-1.79044
H	-2.06446	0.91789	1.61173
H	0.40679	1.19897	1.62217
C	3.39830	0.14598	-0.03152
C	4.81412	0.30030	-0.00640
C	7.64467	0.60640	0.04698
C	6.83283	1.26394	1.00231
C	5.44757	1.11479	0.97630
C	5.64148	-0.35145	-0.95655
C	7.03549	-0.20517	-0.93635
O	8.98502	0.81637	0.15781
H	7.32496	1.89214	1.76140
H	4.82653	1.63134	1.72502
H	5.17467	-0.98609	-1.72649
H	7.63804	-0.72954	-1.69258
C	9.85488	0.18979	-0.77001
H	9.78433	-0.92250	-0.71666
H	10.88079	0.50150	-0.48837
H	9.64843	0.51781	-1.81656

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	15.87	0.20860	YES YES
8	a	19.52	0.05602	YES YES
9	a	21.66	0.07263	YES YES
10	a	45.45	1.94606	YES YES
11	a	57.20	0.22475	YES YES
12	a	62.71	3.29047	YES YES
13	a	92.03	0.76785	YES YES
14	a	102.62	1.60505	YES YES
15	a	118.09	0.46801	YES YES
16	a	125.82	1.38191	YES YES
17	a	135.82	1.77921	YES YES
18	a	146.07	0.21540	YES YES
19	a	182.04	3.27212	YES YES
20	a	199.60	0.74937	YES YES
21	a	226.16	3.12472	YES YES
22	a	235.97	3.19734	YES YES
23	a	245.83	1.83141	YES YES
24	a	254.62	2.29437	YES YES
25	a	277.31	1.18301	YES YES
26	a	284.04	0.42775	YES YES
27	a	320.23	23.74964	YES YES
28	a	336.68	38.72416	YES YES
29	a	346.34	151.14338	YES YES
30	a	392.63	0.99370	YES YES
31	a	405.29	2.50257	YES YES
32	a	411.55	0.61907	YES YES
33	a	412.27	10.91175	YES YES
34	a	442.06	4.96689	YES YES
35	a	468.53	2.66767	YES YES
36	a	480.68	1.22367	YES YES
37	a	519.73	19.08057	YES YES
38	a	523.36	19.46381	YES YES
39	a	533.14	6.95593	YES YES
40	a	536.86	16.27108	YES YES
41	a	545.13	2.31269	YES YES
42	a	549.65	4.58830	YES YES
43	a	557.02	4.08404	YES YES
44	a	561.09	10.78525	YES YES
45	a	610.71	8.17031	YES YES
46	a	625.93	7.81249	YES YES
47	a	634.50	0.14956	YES YES
48	a	648.51	12.54742	YES YES
49	a	668.99	7.57548	YES YES
50	a	678.55	1.32268	YES YES

6b/iso4

bp86 energy (au): -1142.5924135180

Zero point energy (au): 0.3458629
Entropy (kJ mol-1 K-1): 0.70716
Chemical potential (kJ mol-1): 761.79

XYZ coordinates:

45

C	-4.78300	1.76768	0.19569
C	-4.63632	0.35036	0.07890
C	-5.87328	-0.35390	0.01565
N	-7.10531	0.16798	0.13081
C	-7.08378	1.49592	0.30299
N	-6.01235	2.31001	0.32715
N	-3.72638	2.63745	0.19238
C	-3.57728	-0.62433	-0.10519
N	-5.59881	-1.69239	-0.20455
H	-8.06576	1.99110	0.42573
C	-2.11598	-0.43833	-0.08131
C	-4.22665	-1.84848	-0.28185
C	-6.60759	-2.73221	-0.30280
H	-3.78949	-2.84687	-0.41375
H	-2.80611	2.33014	-0.12659
H	-3.96215	3.63205	0.14533
H	-6.55819	-3.24303	-1.28953
H	-7.59549	-2.24041	-0.19359
H	-6.48168	-3.48808	0.50374
C	0.73724	-0.12730	-0.01077
C	0.11390	-0.98639	-0.95781
C	-1.27559	-1.13118	-0.99056
C	-1.49021	0.40728	0.87235
C	-0.10071	0.56502	0.90572
C	2.15182	0.03396	0.01945
H	0.74232	-1.53058	-1.68063
H	-1.73371	-1.78034	-1.75517
H	-2.10885	0.92810	1.62147
H	0.36074	1.22094	1.66114
C	3.37736	0.17669	0.04684
C	4.79191	0.34066	0.07614
C	7.61961	0.67052	0.13397
C	6.80958	1.30431	1.10292
C	5.41814	1.13808	1.06810
C	5.62616	-0.29067	-0.89108
C	7.00997	-0.12890	-0.86267
O	8.97621	0.76583	0.07495
H	7.25261	1.93122	1.89073
H	4.79419	1.63618	1.82701
H	5.16318	-0.91477	-1.67168
H	7.65680	-0.61585	-1.60935
C	9.65011	1.54708	1.04748
H	9.33633	2.61708	1.00778
H	10.72936	1.47703	0.80405
H	9.48314	1.15635	2.07939

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.27	0.17799	YES	YES
8	a	19.89	0.49289	YES	YES
9	a	22.21	0.61450	YES	YES
10	a	46.05	1.55390	YES	YES
11	a	57.43	0.70172	YES	YES
12	a	62.19	2.60266	YES	YES
13	a	92.49	0.88906	YES	YES
14	a	102.74	1.16063	YES	YES
15	a	117.85	0.42763	YES	YES
16	a	126.07	1.62077	YES	YES
17	a	133.69	1.74750	YES	YES
18	a	148.91	0.72745	YES	YES
19	a	183.09	3.22789	YES	YES
20	a	199.61	0.91775	YES	YES
21	a	224.79	3.13385	YES	YES
22	a	236.25	2.46293	YES	YES
23	a	248.10	1.55341	YES	YES
24	a	253.93	2.76849	YES	YES
25	a	276.93	0.74667	YES	YES
26	a	283.73	0.50183	YES	YES
27	a	320.71	23.07399	YES	YES
28	a	338.47	33.76019	YES	YES
29	a	347.85	157.10788	YES	YES
30	a	389.69	1.76237	YES	YES
31	a	405.65	4.41179	YES	YES
32	a	410.53	3.29720	YES	YES
33	a	413.27	9.19094	YES	YES
34	a	446.64	2.33353	YES	YES
35	a	468.71	2.35568	YES	YES
36	a	476.47	1.66283	YES	YES
37	a	520.21	23.99918	YES	YES
38	a	523.18	14.29973	YES	YES
39	a	535.56	16.46159	YES	YES
40	a	538.55	6.97264	YES	YES
41	a	543.80	1.06668	YES	YES
42	a	547.16	4.56530	YES	YES
43	a	557.33	3.81149	YES	YES
44	a	561.63	10.92218	YES	YES
45	a	610.79	7.99050	YES	YES
46	a	625.76	7.60635	YES	YES
47	a	634.82	1.31180	YES	YES
48	a	648.42	12.53906	YES	YES
49	a	668.89	9.11109	YES	YES
50	a	678.52	1.26723	YES	YES

6c/iso1

bp86 energy (au): -1465.5450654660

Zero point energy (au): 0.3419511
Entropy (kJ mol-1 K-1): 0.72962
Chemical potential (kJ mol-1): 746.89

XYZ coordinates:

45

C	-5.06954	1.82461	0.26319
C	-5.01388	0.41382	0.03752
C	-6.29433	-0.20492	-0.05261
N	-7.48965	0.40631	-0.02760
C	-7.38248	1.73342	0.11624
N	-6.26078	2.45981	0.27485
N	-3.96004	2.60069	0.46535
C	-4.02074	-0.64281	-0.02959
N	-6.10830	-1.57245	-0.15926
H	-8.32976	2.30527	0.12168
C	-2.55043	-0.55449	-0.03091
C	-4.74986	-1.82978	-0.13995
C	-7.18343	-2.54027	-0.28753
H	-4.37963	-2.85653	-0.25723
H	-3.06587	2.16877	0.70448
H	-4.13471	3.56748	0.75201
H	-7.10087	-3.10455	-1.24256
H	-8.13630	-1.97323	-0.27694
H	-7.17496	-3.25951	0.56112
C	0.31770	-0.43191	-0.07113
C	-0.36491	-1.46162	0.63406
C	-1.76089	-1.51431	0.65421
C	-1.86589	0.46354	-0.74617
C	-0.46881	0.52975	-0.76234
C	1.73990	-0.36761	-0.08614
H	0.22342	-2.21558	1.18074
H	-2.26336	-2.30589	1.23454
H	-2.44575	1.20045	-1.32537
H	0.03777	1.32541	-1.33147
C	2.97289	-0.31201	-0.10001
C	4.39486	-0.24389	-0.11565
C	7.24720	-0.10557	-0.14127
C	6.46784	0.86175	-0.82533
C	5.07457	0.79471	-0.81310
C	5.18491	-1.20763	0.56464
C	6.58361	-1.14207	0.55404
S	9.00709	0.09279	-0.23157
H	6.96920	1.67722	-1.37326
H	4.48546	1.55497	-1.34990
H	4.68316	-2.02209	1.11117
H	7.15312	-1.91115	1.09690
C	9.65445	-1.30523	0.73575
H	9.33227	-1.25609	1.79787
H	10.75900	-1.20548	0.69259
H	9.36578	-2.28210	0.29196

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.32	0.13858	YES	YES
8	a	18.12	0.08932	YES	YES
9	a	19.79	0.03304	YES	YES
10	a	41.93	1.66615	YES	YES
11	a	56.79	0.46327	YES	YES
12	a	57.85	0.83903	YES	YES
13	a	62.50	3.48042	YES	YES
14	a	99.12	1.20099	YES	YES
15	a	102.79	0.91648	YES	YES
16	a	116.77	0.05996	YES	YES
17	a	133.02	1.54371	YES	YES
18	a	137.24	0.13618	YES	YES
19	a	168.62	1.78605	YES	YES
20	a	191.74	0.62746	YES	YES
21	a	202.22	1.15300	YES	YES
22	a	221.60	0.44181	YES	YES
23	a	226.16	3.96857	YES	YES
24	a	241.42	2.80653	YES	YES
25	a	262.16	0.96127	YES	YES
26	a	279.48	0.86277	YES	YES
27	a	298.36	14.75121	YES	YES
28	a	327.39	7.76688	YES	YES
29	a	347.35	22.24173	YES	YES
30	a	347.68	169.65169	YES	YES
31	a	386.03	5.29490	YES	YES
32	a	394.17	8.29843	YES	YES
33	a	400.11	1.15879	YES	YES
34	a	411.57	10.30995	YES	YES
35	a	452.34	8.51239	YES	YES
36	a	458.93	2.42644	YES	YES
37	a	470.10	1.49134	YES	YES
38	a	519.25	24.26153	YES	YES
39	a	522.56	7.22581	YES	YES
40	a	531.25	19.27814	YES	YES
41	a	543.33	0.69118	YES	YES
42	a	544.60	4.62448	YES	YES
43	a	553.84	4.14449	YES	YES
44	a	558.51	1.70771	YES	YES
45	a	609.54	6.91872	YES	YES
46	a	616.99	2.93430	YES	YES
47	a	625.94	6.38189	YES	YES
48	a	631.28	1.02515	YES	YES
49	a	648.06	12.05017	YES	YES
50	a	678.11	1.19326	YES	YES

6c/iso2

bp86 energy (au): -1465.5450697410

Zero point energy (au): 0.3419498
Entropy (kJ mol-1 K-1): 0.72931
Chemical potential (kJ mol-1): 746.93

XYZ coordinates:

45

C	-3.83840	1.69926	0.49281
C	-3.72253	0.34936	0.03622
C	-4.97327	-0.27134	-0.24766
N	-6.18706	0.30109	-0.20136
C	-6.13298	1.58501	0.17555
N	-5.04826	2.29724	0.53201
N	-2.76886	2.45320	0.89524
C	-2.69319	-0.65853	-0.14003
N	-4.73588	-1.59573	-0.57253
H	-7.09716	2.12653	0.21470
C	-1.22966	-0.53932	-0.02184
C	-3.37379	-1.82385	-0.50177
C	-5.76721	-2.54691	-0.94824
H	-2.96295	-2.80717	-0.76494
H	-1.87855	2.00490	1.11878
H	-2.99237	3.35159	1.33150
H	-5.61168	-2.91567	-1.98630
H	-6.73862	-2.01509	-0.89016
H	-5.78016	-3.41476	-0.25286
C	1.62892	-0.34765	0.16391
C	0.93516	-1.49222	0.64604
C	-0.45653	-1.57885	0.55711
C	-0.53327	0.59575	-0.51505
C	0.85892	0.69459	-0.42106
C	3.04599	-0.25049	0.26284
H	1.51026	-2.31041	1.10801
H	-0.96992	-2.46439	0.96708
H	-1.09786	1.40374	-1.00822
H	1.37541	1.58274	-0.81891
C	4.27452	-0.16742	0.34898
C	5.69144	-0.07510	0.45083
C	8.53367	0.11247	0.65808
C	7.78607	1.15168	0.05871
C	6.39261	1.05687	-0.04167
C	6.45519	-1.11561	1.05162
C	7.84341	-1.02335	1.15275
S	10.29671	0.10751	0.84835
H	8.28458	2.04931	-0.33689
H	5.82483	1.87571	-0.51168
H	5.93637	-2.00568	1.44141
H	8.41103	-1.84402	1.62299
C	10.82189	1.68116	0.10164
H	10.56141	1.73224	-0.97727
H	11.92694	1.70003	0.20396
H	10.39782	2.55557	0.64034

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.21	0.06981	YES	YES
8	a	17.15	1.02687	YES	YES
9	a	18.85	0.24787	YES	YES
10	a	43.12	1.08305	YES	YES
11	a	55.40	1.14146	YES	YES
12	a	57.96	0.45956	YES	YES
13	a	65.03	3.17747	YES	YES
14	a	99.92	0.81508	YES	YES
15	a	102.02	1.09336	YES	YES
16	a	117.02	0.45549	YES	YES
17	a	131.44	0.95103	YES	YES
18	a	142.18	0.97824	YES	YES
19	a	169.82	1.41793	YES	YES
20	a	189.65	1.36565	YES	YES
21	a	200.94	0.28601	YES	YES
22	a	224.46	0.47249	YES	YES
23	a	227.31	3.36888	YES	YES
24	a	241.31	2.98892	YES	YES
25	a	262.30	0.91100	YES	YES
26	a	278.24	1.67071	YES	YES
27	a	300.01	14.92705	YES	YES
28	a	329.26	4.56347	YES	YES
29	a	343.10	5.57439	YES	YES
30	a	353.83	185.00562	YES	YES
31	a	387.67	10.77119	YES	YES
32	a	395.19	6.17384	YES	YES
33	a	399.92	0.49319	YES	YES
34	a	412.17	12.92771	YES	YES
35	a	449.70	8.24020	YES	YES
36	a	457.90	0.47073	YES	YES
37	a	472.39	3.66436	YES	YES
38	a	519.44	24.16807	YES	YES
39	a	522.63	7.34656	YES	YES
40	a	531.15	18.42017	YES	YES
41	a	542.39	1.09966	YES	YES
42	a	544.81	4.58198	YES	YES
43	a	554.14	4.17305	YES	YES
44	a	558.52	1.82746	YES	YES
45	a	609.71	7.02691	YES	YES
46	a	616.81	3.01846	YES	YES
47	a	625.73	6.39964	YES	YES
48	a	631.13	0.94757	YES	YES
49	a	648.12	12.30787	YES	YES
50	a	678.28	1.36141	YES	YES

6c/iso3

bp86 energy (au): -1465.5450700890

Zero point energy (au): 0.3419835
Entropy (kJ mol-1 K-1): 0.72991
Chemical potential (kJ mol-1): 746.88

XYZ coordinates:

45

C	-5.09610	1.81993	0.28281
C	-5.02277	0.39870	0.14661
C	-6.29373	-0.24490	0.12914
N	-7.49342	0.33402	0.29935
C	-7.40121	1.65764	0.48134
N	-6.29161	2.41917	0.46879
N	-3.99923	2.63783	0.24602
C	-4.02061	-0.62353	-0.09057
N	-6.09358	-1.59268	-0.11339
H	-8.35235	2.19797	0.64805
C	-2.55214	-0.51048	-0.12912
C	-4.73537	-1.81336	-0.24998
C	-7.15442	-2.58226	-0.17567
H	-4.35277	-2.82998	-0.40832
H	-3.10890	2.29051	-0.11431
H	-4.18816	3.64312	0.21681
H	-7.16780	-3.08972	-1.16518
H	-8.11241	-2.04410	-0.02640
H	-7.03427	-3.34735	0.62309
C	0.31341	-0.34968	-0.18036
C	-0.44615	0.37341	0.77989
C	-1.84225	0.28909	0.80543
C	-1.78968	-1.23309	-1.08310
C	-0.39462	-1.16117	-1.10994
C	1.73461	-0.26619	-0.21045
H	0.08179	0.99364	1.52178
H	-2.40013	0.83118	1.58643
H	-2.31444	-1.84656	-1.83396
H	0.17275	-1.72665	-1.86608
C	2.96659	-0.19513	-0.23829
C	4.38742	-0.11446	-0.27515
C	7.23726	0.04993	-0.35106
C	6.52720	-0.69108	-1.32970
C	5.13511	-0.77205	-1.29280
C	5.10833	0.62418	0.69960
C	6.50573	0.70632	0.66489
S	9.00324	0.07563	-0.50975
H	7.08206	-1.20939	-2.12977
H	4.60008	-1.35163	-2.06162
H	4.55326	1.14132	1.49839
H	7.02057	1.29042	1.44220
C	9.55260	1.09948	0.88981
H	9.15928	2.13625	0.82130
H	10.65936	1.13158	0.81347
H	9.27447	0.64711	1.86578

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.00	0.54060	YES	YES
8	a	16.91	0.33846	YES	YES
9	a	19.60	0.25320	YES	YES
10	a	43.14	1.23577	YES	YES
11	a	54.25	1.45382	YES	YES
12	a	57.53	0.39778	YES	YES
13	a	63.91	2.85892	YES	YES
14	a	99.82	0.98791	YES	YES
15	a	101.56	0.76304	YES	YES
16	a	114.75	0.27125	YES	YES
17	a	129.86	1.28696	YES	YES
18	a	141.85	1.01128	YES	YES
19	a	170.86	1.47047	YES	YES
20	a	189.54	1.48732	YES	YES
21	a	201.62	0.31156	YES	YES
22	a	225.39	0.49485	YES	YES
23	a	227.30	3.36232	YES	YES
24	a	241.52	3.13971	YES	YES
25	a	262.61	1.00787	YES	YES
26	a	278.29	1.60233	YES	YES
27	a	299.86	15.32317	YES	YES
28	a	329.66	8.89793	YES	YES
29	a	343.34	4.87500	YES	YES
30	a	345.74	184.45764	YES	YES
31	a	388.08	7.77339	YES	YES
32	a	395.03	5.50516	YES	YES
33	a	400.05	0.36949	YES	YES
34	a	411.39	8.81394	YES	YES
35	a	450.48	8.67294	YES	YES
36	a	457.21	0.61869	YES	YES
37	a	472.73	3.75298	YES	YES
38	a	520.01	22.85701	YES	YES
39	a	522.84	7.75079	YES	YES
40	a	532.42	17.38643	YES	YES
41	a	542.67	1.29658	YES	YES
42	a	544.91	4.02492	YES	YES
43	a	554.22	4.51468	YES	YES
44	a	558.52	1.96729	YES	YES
45	a	609.65	7.03829	YES	YES
46	a	617.03	3.02483	YES	YES
47	a	625.52	6.68496	YES	YES
48	a	631.15	0.86077	YES	YES
49	a	648.13	12.10296	YES	YES
50	a	678.37	1.44305	YES	YES

6c/iso4

bp86 energy (au): -1465.5450739330

Zero point energy (au): 0.3419597
Entropy (kJ mol-1 K-1): 0.73079
Chemical potential (kJ mol-1): 746.61

XYZ coordinates:

45

C	-3.84513	1.67692	0.56459
C	-3.73117	0.31271	0.15168
C	-4.98090	-0.30894	-0.13400
N	-6.20256	0.22699	0.02021
C	-6.15498	1.48496	0.47758
N	-5.06481	2.22916	0.73973
N	-2.76697	2.48292	0.81098
C	-2.69067	-0.64348	-0.17920
N	-4.73129	-1.57923	-0.62359
H	-7.12848	1.98251	0.64815
C	-1.22905	-0.52897	-0.03512
C	-3.36233	-1.77268	-0.65435
C	-5.76094	-2.52835	-1.00887
H	-2.94667	-2.73707	-0.97418
H	-1.83721	2.21535	0.48381
H	-2.97220	3.47326	0.96670
H	-5.66716	-2.80371	-2.08251
H	-6.73969	-2.03421	-0.84203
H	-5.70434	-3.45136	-0.39074
C	1.62186	-0.35453	0.25314
C	0.74957	0.16502	1.24842
C	-0.63907	0.07307	1.10781
C	-0.35434	-1.05234	-1.02230
C	1.03384	-0.97377	-0.88457
C	3.03561	-0.25736	0.39094
H	1.18208	0.63063	2.14830
H	-1.28795	0.45033	1.91497
H	-0.78265	-1.50968	-1.92954
H	1.69003	-1.38088	-1.67021
C	4.26099	-0.16937	0.51017
C	5.67370	-0.06399	0.65106
C	8.50749	0.15087	0.93207
C	7.94224	-0.46519	-0.20782
C	6.55242	-0.56913	-0.34306
C	6.25469	0.55385	1.79477
C	7.63894	0.65865	1.93154
S	10.24559	0.34640	1.22467
H	8.58308	-0.87191	-1.00431
H	6.12806	-1.05188	-1.23777
H	5.59526	0.95418	2.58103
H	8.06283	1.14253	2.82753
C	11.02227	-0.40243	-0.23987
H	10.78160	-1.48360	-0.32683
H	12.11521	-0.29135	-0.08160
H	10.74014	0.13010	-1.17333

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	14.24	0.11228	YES YES
8	a	16.95	0.09818	YES YES
9	a	20.01	0.03309	YES YES
10	a	41.25	1.56102	YES YES
11	a	56.27	0.26230	YES YES
12	a	57.90	0.72885	YES YES
13	a	63.00	3.73825	YES YES
14	a	98.52	1.33977	YES YES
15	a	101.04	0.68182	YES YES
16	a	114.51	0.19604	YES YES
17	a	131.71	1.71653	YES YES
18	a	137.19	0.08321	YES YES
19	a	168.20	1.73598	YES YES
20	a	191.34	0.65187	YES YES
21	a	202.10	1.13078	YES YES
22	a	222.04	0.49834	YES YES
23	a	225.30	3.89870	YES YES
24	a	241.34	3.03385	YES YES
25	a	262.07	0.98397	YES YES
26	a	279.50	0.97802	YES YES
27	a	298.36	14.79238	YES YES
28	a	327.34	9.52912	YES YES
29	a	344.50	180.18322	YES YES
30	a	347.43	9.82187	YES YES
31	a	386.10	4.57262	YES YES
32	a	394.11	7.64123	YES YES
33	a	400.11	1.32168	YES YES
34	a	411.55	8.46035	YES YES
35	a	452.02	8.41350	YES YES
36	a	459.00	2.63258	YES YES
37	a	470.11	1.57263	YES YES
38	a	519.84	23.12499	YES YES
39	a	522.88	7.33261	YES YES
40	a	531.81	18.65022	YES YES
41	a	543.08	0.64374	YES YES
42	a	544.72	4.59716	YES YES
43	a	553.99	4.63898	YES YES
44	a	558.52	1.90014	YES YES
45	a	609.70	6.81714	YES YES
46	a	617.23	2.98435	YES YES
47	a	625.50	6.77809	YES YES
48	a	631.12	0.92312	YES YES
49	a	647.94	12.12169	YES YES
50	a	678.65	1.38872	YES YES

6a/iso1

bp86 energy (au): -1028.1485376890

Zero point energy (au): 0.3143286

XYZ coordinates:

41

C	-3.81272	1.75183	0.33625
C	-3.70273	0.35699	0.04157
C	-4.95857	-0.30216	-0.09717
N	-6.17556	0.26356	-0.05862
C	-6.11875	1.58486	0.15267
N	-5.02644	2.34211	0.36299
N	-2.73486	2.55641	0.59124
C	-2.67140	-0.65874	-0.06407
N	-4.72123	-1.65503	-0.27000
H	-7.08641	2.12113	0.17311
C	-1.20547	-0.51865	-0.04179
C	-3.35512	-1.86394	-0.24519
C	-5.75868	-2.65262	-0.46529
H	-2.94590	-2.86934	-0.40864
H	-1.82881	2.14591	0.82329
H	-2.94874	3.50093	0.92248
H	-5.64256	-3.16206	-1.44724
H	-6.73160	-2.12126	-0.43962
H	-5.73517	-3.41517	0.34430
C	1.65501	-0.29524	-0.03923
C	1.00220	-1.38009	0.60869
C	-0.39116	-1.48217	0.60824
C	-0.54995	0.55593	-0.69924
C	0.84411	0.67092	-0.69448
C	3.07503	-0.18215	-0.03202
H	1.61094	-2.13781	1.12720
H	-0.87204	-2.31717	1.14414
H	-1.14919	1.29921	-1.24973
H	1.32918	1.50960	-1.21891
C	4.30487	-0.08587	-0.02496
C	5.72669	0.02393	-0.01675
C	8.55281	0.24055	-0.00067
C	7.77521	1.18717	-0.69247
C	6.37802	1.08472	-0.70343
C	6.52432	-0.92573	0.67834
C	7.92077	-0.81398	0.68328
H	9.65208	0.32434	0.00497
H	8.26454	2.01598	-1.23062
H	5.76842	1.82504	-1.24519
H	6.02864	-1.75134	1.21305
H	8.52462	-1.55909	1.22749

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.26	0.08255	YES	YES
8	a	19.92	0.00619	YES	YES
9	a	25.39	0.08362	YES	YES
10	a	55.50	3.39368	YES	YES
11	a	63.10	0.49670	YES	YES
12	a	70.73	1.71595	YES	YES
13	a	102.76	1.28847	YES	YES
14	a	120.10	0.18690	YES	YES
15	a	128.30	1.53400	YES	YES
16	a	142.73	0.90204	YES	YES
17	a	162.37	0.19117	YES	YES
18	a	189.21	1.69593	YES	YES
19	a	223.16	0.85360	YES	YES
20	a	228.84	4.30363	YES	YES
21	a	251.82	3.93555	YES	YES
22	a	278.96	0.51696	YES	YES
23	a	310.09	1.00640	YES	YES
24	a	340.20	33.79906	YES	YES
25	a	348.36	132.20359	YES	YES
26	a	368.77	43.81117	YES	YES
27	a	395.68	0.86931	YES	YES
28	a	399.76	0.02718	YES	YES
29	a	411.81	9.17892	YES	YES
30	a	446.09	3.68575	YES	YES
31	a	464.91	1.24885	YES	YES
32	a	518.39	18.45431	YES	YES
33	a	522.46	12.01999	YES	YES
34	a	533.29	16.27650	YES	YES
35	a	541.63	1.25005	YES	YES
36	a	544.31	2.88934	YES	YES
37	a	550.46	2.83932	YES	YES
38	a	561.55	0.54545	YES	YES
39	a	572.63	7.06998	YES	YES
40	a	611.23	8.14205	YES	YES
41	a	614.54	0.02717	YES	YES
42	a	626.49	7.56708	YES	YES
43	a	647.77	12.03318	YES	YES
44	a	678.03	1.17141	YES	YES
45	a	690.15	30.97673	YES	YES
46	a	698.14	5.45899	YES	YES
47	a	709.65	9.99733	YES	YES
48	a	740.05	5.02378	YES	YES
49	a	758.78	27.34022	YES	YES
50	a	769.55	9.87438	YES	YES

6a/iso2

bp86 energy (au): -1028.1485461850

Zero point energy (au): 0.3143219
Entropy (kJ mol-1 K-1): 0.65519
Chemical potential (kJ mol-1): 687.67

XYZ coordinates:

41

C	-3.84043	1.75337	0.38324
C	-3.71391	0.34947	0.14398
C	-4.96065	-0.33279	0.04453
N	-6.18364	0.19069	0.22731
C	-6.14223	1.49884	0.51254
N	-5.06035	2.29572	0.58486
N	-2.77399	2.60959	0.43237
C	-2.67134	-0.61834	-0.14258
N	-4.70757	-1.65102	-0.29400
H	-7.11537	1.99227	0.69656
C	-1.20774	-0.45514	-0.12868
C	-3.33999	-1.81559	-0.41089
C	-5.73164	-2.66715	-0.46147
H	-2.91861	-2.80430	-0.63455
H	-1.86471	2.32288	0.06646
H	-3.00055	3.60661	0.47503
H	-5.71237	-3.08585	-1.49166
H	-6.71039	-2.17707	-0.28349
H	-5.59589	-3.49463	0.26957
C	1.64917	-0.19222	-0.08150
C	0.99883	-0.96445	-1.08312
C	-0.39287	-1.08613	-1.10415
C	-0.55428	0.30363	0.87827
C	0.83784	0.43795	0.90082
C	3.06681	-0.05546	-0.06233
H	1.60767	-1.45841	-1.85688
H	-0.87293	-1.66576	-1.90988
H	-1.15331	0.77229	1.67609
H	1.32167	1.02491	1.69779
C	4.29452	0.06359	-0.04521
C	5.71388	0.20160	-0.02500
C	8.53488	0.47668	0.01479
C	7.75261	1.06810	1.02358
C	6.35798	0.93535	1.00844
C	6.51624	-0.39139	-1.03787
C	7.91007	-0.25226	-1.01362
H	9.63196	0.58428	0.02990
H	8.23607	1.64030	1.83284
H	5.74486	1.39812	1.79792
H	6.02623	-0.96182	-1.84277
H	8.51742	-0.71847	-1.80722

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	20.50	0.00474	YES	YES
8	a	21.12	0.10854	YES	YES
9	a	26.28	0.07080	YES	YES
10	a	55.08	3.40239	YES	YES
11	a	62.82	0.60893	YES	YES
12	a	70.25	1.57900	YES	YES
13	a	100.42	1.04023	YES	YES
14	a	118.90	0.39162	YES	YES
15	a	127.98	1.53612	YES	YES
16	a	143.12	0.96111	YES	YES
17	a	162.17	0.19905	YES	YES
18	a	189.42	1.98834	YES	YES
19	a	223.18	1.11458	YES	YES
20	a	227.99	3.99516	YES	YES
21	a	251.56	4.18994	YES	YES
22	a	278.79	0.55063	YES	YES
23	a	309.79	1.18579	YES	YES
24	a	337.80	113.63893	YES	YES
25	a	343.13	68.87339	YES	YES
26	a	367.96	27.06626	YES	YES
27	a	395.59	0.94064	YES	YES
28	a	399.99	0.02762	YES	YES
29	a	411.32	6.76536	YES	YES
30	a	445.93	3.54750	YES	YES
31	a	465.05	1.37482	YES	YES
32	a	518.86	17.32671	YES	YES
33	a	522.73	11.91286	YES	YES
34	a	534.04	15.60703	YES	YES
35	a	541.68	1.46524	YES	YES
36	a	544.49	2.78387	YES	YES
37	a	550.52	2.84014	YES	YES
38	a	561.46	0.59547	YES	YES
39	a	572.61	7.32740	YES	YES
40	a	610.83	8.03959	YES	YES
41	a	614.41	0.02873	YES	YES
42	a	626.34	7.81479	YES	YES
43	a	647.95	12.02942	YES	YES
44	a	678.55	1.29883	YES	YES
45	a	690.47	31.24182	YES	YES
46	a	698.21	5.48450	YES	YES
47	a	709.58	9.83891	YES	YES
48	a	739.32	5.03965	YES	YES
49	a	758.89	27.09791	YES	YES
50	a	768.64	9.67670	YES	YES

4a/iso1

bp86 energy (au): -1484.7282046080

Zero point energy (au): 0.4221237
Entropy (kJ mol-1 K-1): 0.80663
Chemical potential (kJ mol-1): 944.96

XYZ coordinates:

55

C	-1.34160	2.58010	0.69302
C	-1.46022	1.23396	0.22629
C	-2.80005	0.78683	0.03437
N	-3.90542	1.54838	0.17177
C	-3.63931	2.81066	0.54748
N	-2.44504	3.34999	0.82474
N	-0.15253	3.15693	1.02635
C	-0.58415	0.10423	-0.01809
N	-2.75941	-0.55726	-0.29822
H	-4.51434	3.47932	0.64820
C	0.88879	0.03898	-0.01281
C	-1.43153	-0.95673	-0.32550
C	-3.88727	-1.46180	-0.53842
H	-1.17601	-1.98419	-0.61466
H	0.70337	2.60447	1.09523
H	-0.18931	4.09560	1.43080
C	3.75115	-0.13188	-0.04785
C	2.96104	-1.16122	0.53379
C	1.56646	-1.07154	0.55206
C	1.67913	1.05796	-0.60654
C	3.07601	0.98042	-0.61987
C	5.17323	-0.21384	-0.06097
H	3.46365	-2.03174	0.98431
H	0.97851	-1.87026	1.03374
H	1.18316	1.91119	-1.09801
H	3.66762	1.77896	-1.09520
C	6.40463	-0.28371	-0.07351
C	7.82846	-0.36562	-0.08899
C	10.65731	-0.52868	-0.11984
C	10.00573	0.56257	-0.72310
C	8.60744	0.64829	-0.71034
C	8.49923	-1.46305	0.51648
C	9.89807	-1.53881	0.49860
H	11.75789	-0.59198	-0.13187
H	10.59546	1.35709	-1.20986
H	8.09637	1.50227	-1.18244
H	7.90356	-2.25345	0.99998
H	10.40283	-2.39694	0.97276
C	-4.68985	-1.88239	0.72785
C	-6.05716	-1.17198	0.53156
C	-6.14899	-0.98614	-0.99239
C	-6.91712	0.26861	-1.42114
O	-4.88506	-3.28035	0.70601
O	-7.13718	-1.99179	0.98771
O	-4.78761	-0.86325	-1.44330

O	-6.57930	1.40943	-0.67281
H	-3.44280	-2.38953	-0.96554
H	-4.16084	-1.56029	1.65830
H	-6.07314	-0.17197	1.01195
H	-6.61776	-1.89684	-1.43998
H	-8.00524	0.07591	-1.27841
H	-6.74571	0.40564	-2.52123
H	-5.84812	-3.39686	0.92578
H	-7.38168	-1.70762	1.89385
H	-5.58333	1.42116	-0.52960

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	14.49	0.35546	YES YES
8	a	16.74	0.02345	YES YES
9	a	20.63	0.09049	YES YES
10	a	28.97	0.17817	YES YES
11	a	42.52	0.75788	YES YES
12	a	50.15	3.67438	YES YES
13	a	59.61	3.63624	YES YES
14	a	65.96	3.23608	YES YES
15	a	72.26	0.40794	YES YES
16	a	107.38	1.53705	YES YES
17	a	115.39	4.21459	YES YES
18	a	123.78	0.07116	YES YES
19	a	133.50	0.98840	YES YES
20	a	147.74	3.54727	YES YES
21	a	155.92	3.91427	YES YES
22	a	174.95	0.62286	YES YES
23	a	204.12	5.93611	YES YES
24	a	223.16	1.47938	YES YES
25	a	230.70	3.50126	YES YES
26	a	252.14	0.63790	YES YES
27	a	253.50	6.34184	YES YES
28	a	271.75	1.59840	YES YES
29	a	290.66	73.38502	YES YES
30	a	293.04	120.71736	YES YES
31	a	303.79	13.94627	YES YES
32	a	310.15	10.83406	YES YES
33	a	322.63	1.78561	YES YES
34	a	331.19	30.21491	YES YES
35	a	341.83	4.72479	YES YES
36	a	379.18	8.24144	YES YES
37	a	399.75	0.00756	YES YES
38	a	407.18	2.45107	YES YES
39	a	410.02	4.62185	YES YES
40	a	451.12	8.14988	YES YES
41	a	452.87	2.37349	YES YES
42	a	469.42	4.41138	YES YES

43	a	521.61	8.93140	YES	YES
44	a	529.85	13.08297	YES	YES
45	a	541.03	1.93167	YES	YES
46	a	544.72	16.91796	YES	YES
47	a	545.66	9.56385	YES	YES
48	a	555.39	3.09266	YES	YES
49	a	560.79	6.39516	YES	YES
50	a	564.26	0.85827	YES	YES

4a/iso2

bp86 energy (au): -1484.7281993560

Zero point energy (au): 0.4221837
Entropy (kJ mol-1 K-1): 0.80487
Chemical potential (kJ mol-1): 945.50

XYZ coordinates:

55

C	-1.38732	2.67321	0.61592
C	-1.48851	1.30076	0.22866
C	-2.82253	0.82887	0.05298
N	-3.94150	1.54304	0.29312
C	-3.69542	2.79114	0.72525
N	-2.50508	3.38338	0.88677
N	-0.20097	3.33439	0.73896
C	-0.59215	0.22738	-0.15598
N	-2.75844	-0.47100	-0.42210
H	-4.58463	3.40708	0.95498
C	0.88109	0.17606	-0.13174
C	-1.42198	-0.81796	-0.55227
C	-3.86404	-1.40472	-0.66050
H	-1.14973	-1.82770	-0.88513
H	0.66747	2.92719	0.38810
H	-0.25216	4.33972	0.92144
C	3.74377	0.01184	-0.07383
C	2.99942	-0.51730	-1.16382
C	1.60496	-0.43063	-1.18986
C	1.62546	0.68923	0.96281
C	3.02250	0.61691	0.99077
C	5.16583	-0.06610	-0.04845
H	3.53826	-0.98798	-2.00133
H	1.05462	-0.82290	-2.06096
H	1.09246	1.12432	1.82431
H	3.57723	1.01411	1.85568
C	6.39714	-0.13596	-0.02802
C	7.82075	-0.22044	-0.00490
C	10.64891	-0.39373	0.04246
C	9.96116	0.22697	1.10120
C	8.56306	0.31541	1.08268
C	8.52800	-0.84415	-1.06870
C	9.92622	-0.92741	-1.04023
H	11.74908	-0.46174	0.06114
H	10.52190	0.64728	1.95260
H	8.02356	0.80060	1.91150
H	7.96125	-1.26206	-1.91576
H	10.45953	-1.41504	-1.87316
C	-4.55215	-1.96747	0.61637
C	-5.94954	-1.29036	0.59068
C	-6.17107	-0.99009	-0.90121
C	-7.01333	0.26182	-1.16896
O	-4.71147	-3.36279	0.47296
O	-6.96429	-2.17994	1.06511
O	-4.85433	-0.77952	-1.44549

O	-6.66586	1.35133	-0.35223
H	-3.41300	-2.26978	-1.19748
H	-3.96078	-1.71653	1.53120
H	-5.95346	-0.33168	1.14906
H	-6.64228	-1.88149	-1.38315
H	-8.08063	0.01235	-0.96870
H	-6.92666	0.49452	-2.26280
H	-5.64494	-3.53418	0.77016
H	-7.14135	-1.97487	2.00758
H	-5.66303	1.39958	-0.28569

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	13.43	0.06830	YES YES
8	a	19.15	0.20006	YES YES
9	a	19.94	0.04404	YES YES
10	a	28.79	0.26337	YES YES
11	a	42.79	1.44611	YES YES
12	a	51.70	2.80097	YES YES
13	a	60.23	0.22464	YES YES
14	a	64.34	4.21339	YES YES
15	a	75.99	3.31071	YES YES
16	a	109.48	1.61183	YES YES
17	a	117.96	2.93931	YES YES
18	a	124.74	0.08603	YES YES
19	a	134.31	0.40041	YES YES
20	a	149.22	6.13326	YES YES
21	a	156.11	1.08730	YES YES
22	a	171.17	3.55784	YES YES
23	a	205.85	1.93729	YES YES
24	a	225.06	3.42995	YES YES
25	a	231.56	2.25761	YES YES
26	a	252.94	4.54804	YES YES
27	a	261.03	3.28722	YES YES
28	a	273.33	0.50088	YES YES
29	a	280.35	2.74996	YES YES
30	a	295.79	23.30964	YES YES
31	a	310.06	5.01533	YES YES
32	a	318.40	110.73532	YES YES
33	a	325.00	34.25966	YES YES
34	a	329.82	86.33423	YES YES
35	a	342.12	5.25408	YES YES
36	a	377.23	4.53553	YES YES
37	a	399.61	0.01245	YES YES
38	a	408.94	4.13236	YES YES
39	a	428.51	1.87559	YES YES
40	a	431.96	1.51453	YES YES
41	a	460.17	11.07999	YES YES
42	a	467.28	0.90776	YES YES

43	a	522.78	9.02681	YES	YES
44	a	527.49	17.89759	YES	YES
45	a	541.90	4.88178	YES	YES
46	a	543.63	19.01376	YES	YES
47	a	549.38	14.58354	YES	YES
48	a	553.93	4.17231	YES	YES
49	a	559.22	0.62675	YES	YES
50	a	565.41	1.51160	YES	YES

4a/iso3

bp86 energy (au): -1484.7308708780

Zero point energy (au): 0.4221057
Entropy (kJ mol-1 K-1): 0.80422
Chemical potential (kJ mol-1): 945.67

XYZ coordinates:

55

C	-1.32251	2.63791	0.54354
C	-1.45647	1.26084	0.18395
C	-2.80094	0.80671	0.06150
N	-3.89968	1.58069	0.18087
C	-3.62334	2.86670	0.45169
N	-2.42012	3.42124	0.64441
N	-0.12332	3.23457	0.79866
C	-0.59070	0.11166	-0.00246
N	-2.77393	-0.55663	-0.18255
H	-4.49540	3.54082	0.53815
C	0.88138	0.03629	-0.01326
C	-1.44929	-0.96274	-0.21687
C	-3.91238	-1.44582	-0.38589
H	-1.20566	-2.00960	-0.43663
H	0.72723	2.68022	0.90925
H	-0.15179	4.19573	1.14750
C	3.74266	-0.15117	-0.06071
C	2.95283	-1.13544	0.59471
C	1.55900	-1.03747	0.61897
C	1.67108	1.00729	-0.68350
C	3.06743	0.92209	-0.70300
C	5.16462	-0.23720	-0.07371
H	3.45549	-1.97506	1.10038
H	0.97165	-1.79710	1.16059
H	1.17454	1.82785	-1.22718
H	3.65859	1.68361	-1.23620
C	6.39603	-0.30832	-0.08130
C	7.81990	-0.38929	-0.08906
C	10.64937	-0.54790	-0.10175
C	9.99809	0.51326	-0.75672
C	8.59962	0.59650	-0.75333
C	8.49047	-1.45658	0.56830
C	9.88949	-1.53034	0.55903
H	11.75010	-0.60921	-0.10623
H	10.58820	1.28609	-1.27676
H	8.08873	1.42709	-1.26563
H	7.89443	-2.22515	1.08529
H	10.39403	-2.36488	1.07372
C	-4.83938	-1.62266	0.85446
C	-6.17891	-1.97408	0.17232
C	-6.12672	-1.17884	-1.14814
C	-6.85167	0.17353	-1.08240
O	-4.40370	-2.59691	1.76353
O	-6.12948	-3.39729	-0.02768
O	-4.72029	-0.95815	-1.43160

O	-6.56843	0.90081	0.08510
H	-3.47043	-2.44122	-0.63531
H	-4.93950	-0.65128	1.37887
H	-7.04660	-1.68434	0.80340
H	-6.54440	-1.79496	-1.97938
H	-7.95095	-0.01711	-1.10345
H	-6.59802	0.73476	-2.01935
H	-4.79144	-3.44023	1.41542
H	-7.04307	-3.74301	-0.09322
H	-5.58845	1.15871	0.07365

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	14.85	0.01229	YES YES
8	a	18.65	0.05908	YES YES
9	a	19.25	0.08303	YES YES
10	a	33.03	0.24970	YES YES
11	a	41.93	1.73985	YES YES
12	a	51.84	0.51186	YES YES
13	a	65.03	3.38482	YES YES
14	a	70.37	0.59644	YES YES
15	a	76.59	5.46464	YES YES
16	a	111.57	5.80039	YES YES
17	a	111.86	1.74179	YES YES
18	a	125.39	0.82450	YES YES
19	a	133.70	0.84471	YES YES
20	a	143.82	1.05649	YES YES
21	a	162.79	1.91084	YES YES
22	a	176.71	2.95685	YES YES
23	a	202.73	6.97583	YES YES
24	a	212.67	4.86240	YES YES
25	a	223.15	4.21998	YES YES
26	a	230.45	68.16749	YES YES
27	a	248.84	3.34648	YES YES
28	a	274.30	2.87827	YES YES
29	a	277.70	0.11332	YES YES
30	a	303.23	0.78883	YES YES
31	a	313.93	5.95602	YES YES
32	a	316.82	169.08395	YES YES
33	a	329.27	29.00945	YES YES
34	a	341.61	10.34615	YES YES
35	a	344.27	6.14063	YES YES
36	a	371.19	6.66908	YES YES
37	a	399.83	0.01043	YES YES
38	a	408.79	2.69820	YES YES
39	a	411.53	0.62201	YES YES
40	a	441.80	3.80475	YES YES
41	a	452.49	2.84498	YES YES
42	a	468.43	1.82260	YES YES

43	a	523.36	13.48590	YES	YES
44	a	523.59	16.23855	YES	YES
45	a	533.76	6.43453	YES	YES
46	a	542.01	3.39503	YES	YES
47	a	543.51	13.21162	YES	YES
48	a	551.43	98.08145	YES	YES
49	a	553.02	5.17141	YES	YES
50	a	556.89	2.49660	YES	YES

5/iso1

bp86 energy (au): -797.2570517510

Zero point energy (au): 0.2354112

XYZ coordinates:

31

C	-1.93367	1.69737	-0.06459
C	-1.86694	0.27506	-0.00546
C	-3.12230	-0.38094	0.01468
N	-4.33028	0.20528	-0.00875
C	-4.24555	1.54293	-0.05886
N	-3.13826	2.30859	-0.08960
N	-0.81954	2.47935	-0.09101
C	-0.83920	-0.74929	0.02877
N	-2.89332	-1.74997	0.06028
H	-5.20620	2.09168	-0.07969
C	0.56347	-0.56532	0.02550
C	-1.53110	-1.97014	0.06767
C	-3.94362	-2.75348	0.09095
H	-1.12552	-2.98868	0.10369
H	0.11021	2.05962	-0.13812
H	-0.94299	3.48892	-0.18516
H	-3.87996	-3.42254	-0.79504
H	-4.91152	-2.21270	0.07385
H	-3.88047	-3.36693	1.01626
C	1.78495	-0.37742	0.02306
C	3.19984	-0.19820	0.01581
C	6.01670	0.14673	-0.00778
C	5.45637	-1.12220	-0.24304
C	4.06669	-1.29805	-0.23366
C	3.78033	1.07754	0.25554
C	5.17143	1.24322	0.24138
H	7.11089	0.28091	-0.01784
H	6.11204	-1.98712	-0.43809
H	3.62911	-2.29134	-0.42068
H	3.12234	1.93799	0.45763
H	5.60216	2.24071	0.42973

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.57	0.02630	YES	YES
8	a	33.96	0.15515	YES	YES

9	a	39.60	0.01573	YES	YES
10	a	88.66	3.03374	YES	YES
11	a	108.91	0.14719	YES	YES
12	a	112.41	1.51910	YES	YES
13	a	130.10	3.77602	YES	YES
14	a	186.19	35.55388	YES	YES
15	a	212.69	16.39416	YES	YES
16	a	215.99	79.32457	YES	YES
17	a	235.83	42.00945	YES	YES
18	a	256.09	9.19623	YES	YES
19	a	270.60	0.23682	YES	YES
20	a	314.02	2.96812	YES	YES
21	a	337.12	4.23207	YES	YES
22	a	399.73	0.01630	YES	YES
23	a	410.70	0.19542	YES	YES
24	a	457.64	0.14422	YES	YES
25	a	514.49	2.00042	YES	YES
26	a	522.99	0.31727	YES	YES
27	a	533.04	4.11787	YES	YES
28	a	540.24	12.86911	YES	YES
29	a	541.07	7.72593	YES	YES
30	a	547.83	3.08264	YES	YES
31	a	577.96	6.66900	YES	YES
32	a	613.45	0.60597	YES	YES
33	a	627.10	3.84146	YES	YES
34	a	632.47	17.65415	YES	YES
35	a	677.64	0.17591	YES	YES
36	a	689.97	31.68906	YES	YES
37	a	700.42	15.00694	YES	YES
38	a	753.20	4.19578	YES	YES
39	a	756.30	28.50607	YES	YES
40	a	761.40	7.22860	YES	YES
41	a	796.87	8.97680	YES	YES
42	a	825.11	0.05589	YES	YES
43	a	831.88	24.22641	YES	YES
44	a	899.27	2.62925	YES	YES
45	a	929.11	2.00991	YES	YES
46	a	952.85	0.00719	YES	YES
47	a	969.19	4.35340	YES	YES
48	a	978.04	0.04556	YES	YES
49	a	981.00	0.24350	YES	YES
50	a	989.88	9.86155	YES	YES

5/iso2

bp86 energy (au): -797.2570628628

Zero point energy (au): 0.2353989
Entropy (kJ mol-1 K-1): 0.55903
Chemical potential (kJ mol-1): 496.96

XYZ coordinates:

31

C	-1.93550	1.68176	-0.22108
C	-1.86717	0.26715	-0.06141
C	-3.12168	-0.38847	-0.00594
N	-4.33007	0.19038	-0.09703
C	-4.24668	1.52032	-0.25037
N	-3.14050	2.28548	-0.31421
N	-0.82250	2.46260	-0.28863
C	-0.83864	-0.74709	0.08007
N	-2.89146	-1.74756	0.16308
H	-5.20767	2.06246	-0.33337
C	0.56376	-0.56110	0.07563
C	-1.52934	-1.96187	0.21539
C	-3.94048	-2.74828	0.25847
H	-1.12288	-2.97252	0.34389
H	0.10735	2.05622	-0.17482
H	-0.94721	3.47335	-0.36587
H	-3.86402	-3.48498	-0.57127
H	-4.90892	-2.21306	0.18569
H	-3.88886	-3.28700	1.22985
C	1.78510	-0.37253	0.06204
C	3.19984	-0.19370	0.05050
C	6.01705	0.14910	0.03054
C	5.17200	1.21457	-0.32924
C	3.78072	1.04976	-0.32172
C	4.06652	-1.26228	0.41143
C	5.45631	-1.08757	0.39910
H	7.11137	0.28215	0.02318
H	5.60277	2.18666	-0.62158
H	3.12282	1.88542	-0.60987
H	3.62897	-2.23042	0.70178
H	6.11200	-1.92795	0.68177

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -

7	a	14.43	0.04913	YES	YES
8	a	34.31	0.10023	YES	YES
9	a	39.42	0.00416	YES	YES
10	a	90.01	2.68849	YES	YES
11	a	110.97	0.34587	YES	YES
12	a	112.15	1.44816	YES	YES
13	a	130.19	4.74849	YES	YES
14	a	181.61	65.45271	YES	YES
15	a	208.99	82.54483	YES	YES
16	a	213.35	4.14655	YES	YES
17	a	234.25	19.48794	YES	YES
18	a	256.32	8.87459	YES	YES
19	a	270.43	0.14199	YES	YES
20	a	314.48	3.19411	YES	YES
21	a	337.14	4.02856	YES	YES
22	a	399.70	0.01932	YES	YES
23	a	410.74	0.18875	YES	YES
24	a	457.98	0.16610	YES	YES
25	a	514.66	1.88079	YES	YES
26	a	523.19	0.38950	YES	YES
27	a	533.97	3.51748	YES	YES
28	a	539.74	13.82211	YES	YES
29	a	541.29	7.57776	YES	YES
30	a	548.62	2.43215	YES	YES
31	a	577.92	6.82970	YES	YES
32	a	613.37	0.60662	YES	YES
33	a	627.29	3.51713	YES	YES
34	a	632.89	18.09543	YES	YES
35	a	677.73	0.17497	YES	YES
36	a	689.91	31.79081	YES	YES
37	a	700.44	15.00537	YES	YES
38	a	753.17	4.26321	YES	YES
39	a	756.12	28.67681	YES	YES
40	a	761.51	7.19266	YES	YES
41	a	797.56	8.86961	YES	YES
42	a	824.98	0.02753	YES	YES
43	a	831.85	24.38669	YES	YES
44	a	898.91	2.67644	YES	YES
45	a	929.47	2.00736	YES	YES
46	a	952.76	0.00518	YES	YES
47	a	969.28	4.36762	YES	YES
48	a	977.95	0.04312	YES	YES
49	a	980.98	0.28905	YES	YES
50	a	989.62	9.70933	YES	YES

3/iso1

bp86 energy (au): -1253.8367346740

Zero point energy (au): 0.3434205
Entropy (kJ mol-1 K-1): 0.70557
Chemical potential (kJ mol-1): 755.82

XYZ coordinates:

45

C	-1.27960	2.57393	0.37539
C	-1.46107	1.19366	0.07228
C	-2.80439	0.76668	-0.08242
N	-3.88468	1.56822	0.02882
C	-3.57341	2.84489	0.31609
N	-2.35801	3.38098	0.49523
N	-0.05051	3.12338	0.55393
C	-0.60347	0.04048	-0.12229
N	-2.78882	-0.59523	-0.36006
H	-4.43047	3.53691	0.41289
C	-1.47285	-1.02320	-0.38560
C	-3.93250	-1.50065	-0.52943
H	-1.23439	-2.07246	-0.59681
H	0.79268	2.54970	0.49188
H	0.00561	4.11763	0.78233
C	0.81029	-0.00444	-0.07143
C	2.04461	-0.02555	-0.02473
C	3.46870	-0.09442	0.02315
C	6.29930	-0.24889	0.11662
C	5.66054	1.00359	0.07625
C	4.26267	1.08482	0.02901
C	4.12763	-1.35397	0.06441
C	5.52587	-1.42410	0.10962
H	7.39937	-0.30948	0.15261
H	6.25944	1.92935	0.07920
H	3.76647	2.06803	-0.00927
H	3.52312	-2.27468	0.06091
H	6.01968	-2.40964	0.14086
C	-4.67199	-1.89187	0.78273
C	-6.03405	-1.15803	0.64937
C	-6.21022	-1.00946	-0.87091
C	-6.98778	0.24323	-1.29005
O	-4.89494	-3.28547	0.78326
O	-7.09955	-1.94408	1.18970
O	-4.87290	-0.91586	-1.39920
O	-6.61204	1.39515	-0.57852
H	-3.51125	-2.43720	-0.96057
H	-4.08757	-1.57164	1.68036
H	-6.00394	-0.14495	1.10187
H	-6.71100	-1.92564	-1.26940
H	-8.06944	0.06084	-1.09552
H	-6.86440	0.35747	-2.39902
H	-5.84158	-3.38183	1.07269
H	-7.28478	-1.63272	2.10104
H	-5.60739	1.42152	-0.51224

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.81	0.11964	YES	YES
8	a	18.52	0.27247	YES	YES
9	a	27.53	0.17676	YES	YES
10	a	40.40	0.43760	YES	YES
11	a	50.33	2.38040	YES	YES
12	a	64.58	3.91462	YES	YES
13	a	95.04	1.23974	YES	YES
14	a	105.31	1.52451	YES	YES
15	a	117.06	3.90321	YES	YES
16	a	143.35	2.47980	YES	YES
17	a	151.84	3.38660	YES	YES
18	a	159.66	3.90226	YES	YES
19	a	191.60	5.71610	YES	YES
20	a	202.98	15.25895	YES	YES
21	a	234.73	3.13139	YES	YES
22	a	249.43	113.79125	YES	YES
23	a	254.89	32.42134	YES	YES
24	a	266.79	4.93267	YES	YES
25	a	274.10	1.31562	YES	YES
26	a	281.47	9.11887	YES	YES
27	a	300.42	21.61079	YES	YES
28	a	306.34	10.46725	YES	YES
29	a	324.44	13.66613	YES	YES
30	a	340.93	14.16392	YES	YES
31	a	357.01	3.26061	YES	YES
32	a	398.90	0.03339	YES	YES
33	a	419.17	3.18762	YES	YES
34	a	444.82	2.91371	YES	YES
35	a	465.47	0.68455	YES	YES
36	a	517.22	1.28443	YES	YES
37	a	523.18	5.84875	YES	YES
38	a	537.77	4.51756	YES	YES
39	a	543.25	6.84855	YES	YES
40	a	548.38	24.38210	YES	YES
41	a	552.75	10.91527	YES	YES
42	a	562.18	2.96108	YES	YES
43	a	596.43	51.31867	YES	YES
44	a	612.19	32.29868	YES	YES
45	a	617.87	14.17229	YES	YES
46	a	629.67	0.33743	YES	YES
47	a	638.93	29.26818	YES	YES
48	a	648.13	10.96126	YES	YES
49	a	678.38	1.62486	YES	YES
50	a	689.48	31.51704	YES	YES

3/iso2

bp86 energy (au): -1253.8367501900

Zero point energy (au): 0.3435610
Entropy (kJ mol-1 K-1): 0.70427
Chemical potential (kJ mol-1): 756.49

XYZ coordinates:

45

C	-1.30826	2.50254	0.80023
C	-1.47333	1.18977	0.27166
C	-2.81250	0.76569	0.07977
N	-3.90396	1.50749	0.36209
C	-3.60791	2.71989	0.86427
N	-2.39753	3.24738	1.09550
N	-0.08469	3.04604	1.02850
C	-0.60128	0.11215	-0.15470
N	-2.78115	-0.52270	-0.44056
H	-4.47437	3.36148	1.11021
C	-1.45892	-0.90662	-0.58335
C	-3.91589	-1.40653	-0.73565
H	-1.20835	-1.89527	-0.98603
H	0.76642	2.53726	0.78205
H	-0.04061	4.00447	1.37971
C	0.81393	0.09421	-0.14638
C	2.04918	0.10002	-0.12594
C	3.47538	0.06995	-0.12052
C	6.31098	-0.00177	-0.11925
C	5.62961	1.03869	0.53773
C	4.22915	1.07787	0.54046
C	4.17708	-0.97636	-0.78024
C	5.57761	-1.00696	-0.77580
H	7.41297	-0.02946	-0.11924
H	6.19686	1.82937	1.05630
H	3.69981	1.89213	1.06107
H	3.60384	-1.76268	-1.29617
H	6.10456	-1.82602	-1.29294
C	-4.62588	-2.01672	0.50698
C	-6.00032	-1.29304	0.51673
C	-6.20593	-0.90034	-0.95554
C	-7.00555	0.39241	-1.15228
O	-4.82992	-3.39574	0.28545
O	-7.04529	-2.17411	0.93733
O	-4.87983	-0.70259	-1.48348
O	-6.63431	1.41763	-0.26601
H	-3.49065	-2.25384	-1.32015
H	-4.02971	-1.83662	1.43517
H	-5.97571	-0.36744	1.12813
H	-6.70309	-1.74643	-1.48998
H	-8.08205	0.16478	-0.97751
H	-6.90004	0.68913	-2.22882
H	-5.76978	-3.55303	0.57030
H	-7.22040	-2.01698	1.88935
H	-5.63017	1.44190	-0.20045

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.27	0.09778	YES	YES
8	a	19.41	0.32774	YES	YES
9	a	27.60	0.09019	YES	YES
10	a	40.76	0.32789	YES	YES
11	a	50.55	2.34339	YES	YES
12	a	64.82	4.14418	YES	YES
13	a	95.13	1.52809	YES	YES
14	a	105.07	1.01378	YES	YES
15	a	116.99	3.87836	YES	YES
16	a	144.16	2.51625	YES	YES
17	a	150.88	3.86349	YES	YES
18	a	159.60	3.11341	YES	YES
19	a	190.71	4.79996	YES	YES
20	a	205.14	8.57518	YES	YES
21	a	234.91	4.38166	YES	YES
22	a	252.99	20.72707	YES	YES
23	a	259.26	101.98783	YES	YES
24	a	269.16	27.74273	YES	YES
25	a	271.27	6.98742	YES	YES
26	a	288.08	15.05690	YES	YES
27	a	301.25	13.69548	YES	YES
28	a	304.33	12.54794	YES	YES
29	a	325.55	16.85790	YES	YES
30	a	337.75	11.19617	YES	YES
31	a	357.38	7.01557	YES	YES
32	a	399.09	0.03814	YES	YES
33	a	424.16	2.25651	YES	YES
34	a	440.73	1.14723	YES	YES
35	a	466.17	2.39306	YES	YES
36	a	516.98	1.81806	YES	YES
37	a	524.18	5.41153	YES	YES
38	a	537.15	6.41653	YES	YES
39	a	543.72	6.18533	YES	YES
40	a	548.95	31.33521	YES	YES
41	a	554.45	4.83423	YES	YES
42	a	562.55	2.45352	YES	YES
43	a	598.87	30.52609	YES	YES
44	a	614.55	17.67183	YES	YES
45	a	620.42	40.71039	YES	YES
46	a	629.64	0.97238	YES	YES
47	a	640.14	35.97517	YES	YES
48	a	648.34	10.59345	YES	YES
49	a	678.24	2.00171	YES	YES
50	a	689.87	31.19319	YES	YES

3/iso3

bp86 energy (au): -1253.8393319810

Zero point energy (au): 0.3432021
Entropy (kJ mol-1 K-1): 0.70860
Chemical potential (kJ mol-1): 754.60

XYZ coordinates:

45

C	-1.30229	2.58482	0.66145
C	-1.47561	1.23300	0.24640
C	-2.81675	0.79470	0.12225
N	-3.90251	1.55432	0.37804
C	-3.60044	2.80470	0.76970
N	-2.38646	3.35176	0.91833
N	-0.07527	3.14626	0.81413
C	-0.61286	0.12381	-0.11455
N	-2.79759	-0.52852	-0.30216
H	-4.46302	3.45911	0.99361
C	-1.47961	-0.92316	-0.44612
C	-3.94498	-1.39588	-0.55324
H	-1.23877	-1.94120	-0.77373
H	0.77199	2.61272	0.61069
H	-0.02413	4.12613	1.09867
C	0.80204	0.09954	-0.12611
C	2.03753	0.09575	-0.12171
C	3.46295	0.04719	-0.12627
C	6.29777	-0.06835	-0.13683
C	5.63697	1.04244	0.41813
C	4.23729	1.10377	0.42605
C	4.14412	-1.06965	-0.68427
C	5.54399	-1.12161	-0.68613
H	7.39914	-0.11348	-0.14043
H	6.21995	1.87148	0.85266
H	3.72463	1.97380	0.86708
H	3.55507	-1.89449	-1.11534
H	6.05418	-1.99635	-1.12273
C	-4.80002	-1.73264	0.70564
C	-6.17280	-2.01019	0.05841
C	-6.19847	-1.04949	-1.14764
C	-6.91748	0.27741	-0.86562
O	-4.30997	-2.80410	1.46430
O	-6.12230	-3.39407	-0.32577
O	-4.80969	-0.78624	-1.48188
O	-6.56625	0.85167	0.36614
H	-3.51625	-2.34763	-0.95022
H	-4.87615	-0.83298	1.34848
H	-7.00640	-1.81654	0.76757
H	-6.66416	-1.55349	-2.02733
H	-8.01619	0.08220	-0.84667
H	-6.72011	0.95537	-1.73626
H	-4.70820	-3.60593	1.03965
H	-7.03518	-3.72553	-0.45091
H	-5.59270	1.12958	0.32656

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.76	0.03977	YES	YES
8	a	20.01	0.16206	YES	YES
9	a	28.05	0.05735	YES	YES
10	a	44.67	2.05769	YES	YES
11	a	52.39	0.95305	YES	YES
12	a	71.74	4.10318	YES	YES
13	a	95.20	0.63636	YES	YES
14	a	108.83	2.04093	YES	YES
15	a	116.41	4.86150	YES	YES
16	a	126.33	2.18634	YES	YES
17	a	158.70	0.87777	YES	YES
18	a	167.13	3.89138	YES	YES
19	a	185.67	3.40620	YES	YES
20	a	205.89	14.49918	YES	YES
21	a	213.79	2.92031	YES	YES
22	a	232.00	75.00820	YES	YES
23	a	252.77	132.39019	YES	YES
24	a	263.61	18.38380	YES	YES
25	a	273.37	12.30000	YES	YES
26	a	279.73	1.37369	YES	YES
27	a	285.24	10.37929	YES	YES
28	a	305.28	1.12679	YES	YES
29	a	340.00	3.92894	YES	YES
30	a	347.52	9.58051	YES	YES
31	a	363.52	1.25883	YES	YES
32	a	398.84	0.02760	YES	YES
33	a	408.55	0.59883	YES	YES
34	a	436.39	0.89423	YES	YES
35	a	464.67	0.62533	YES	YES
36	a	517.49	0.29637	YES	YES
37	a	519.84	4.30896	YES	YES
38	a	530.61	20.87851	YES	YES
39	a	536.99	14.01489	YES	YES
40	a	540.40	94.53717	YES	YES
41	a	546.29	10.94140	YES	YES
42	a	550.37	2.92144	YES	YES
43	a	557.93	2.39221	YES	YES
44	a	590.10	1.48315	YES	YES
45	a	614.97	0.26783	YES	YES
46	a	633.03	21.57231	YES	YES
47	a	634.50	11.91031	YES	YES
48	a	650.48	6.27185	YES	YES
49	a	678.26	5.10983	YES	YES
50	a	689.59	31.10166	YES	YES

5.2 (RI-)BP86/def2-TZVPP Level Calculations

6d/iso1

bp86_def2-tzvpp energy (au): -1350.0911988260

Zero point energy (au): 0.2805118
Entropy (kJ mol-1 K-1): 0.66038
Chemical potential (kJ mol-1): 597.06

XYZ coordinates:

38

C	-5.78959	1.32206	0.98275
C	-5.56818	0.12982	0.24456
C	-6.75304	-0.58428	-0.06815
N	-8.01284	-0.21056	0.19885
C	-8.06877	0.95947	0.84238
N	-7.04558	1.72718	1.25397
N	-4.78247	2.12442	1.43967
C	-4.45383	-0.66652	-0.21891
N	-6.39484	-1.76218	-0.68691
H	-9.06732	1.33599	1.07798
C	-3.01455	-0.38145	-0.18978
C	-5.01802	-1.80844	-0.77022
C	-7.32939	-2.75791	-1.18244
H	-4.52671	-2.64009	-1.26473
H	-3.83701	1.76582	1.48764
H	-5.05522	2.84215	2.10163
H	-7.22427	-2.88506	-2.26842
H	-8.34030	-2.40359	-0.95583
H	-7.16545	-3.72497	-0.68835
C	-0.20958	0.13145	-0.20421
C	-0.71450	-1.15494	0.09357
C	-2.08209	-1.39838	0.10454
C	-2.50634	0.89936	-0.49420
C	-1.13916	1.15420	-0.49728
C	1.18506	0.38572	-0.21326
H	-0.01478	-1.95644	0.32892
H	-2.44682	-2.39237	0.36624
H	-3.19755	1.69776	-0.76548
H	-0.77074	2.14904	-0.74593
C	2.38854	0.59998	-0.22737
C	3.77740	0.86289	-0.24831
C	4.35523	2.14638	-0.54696
C	4.75924	-0.08589	0.01568
H	3.76003	3.02553	-0.78175
C	5.72356	2.13695	-0.50345
S	6.33593	0.57552	-0.09884
H	6.40792	2.95881	-0.68609
H	4.61304	-1.13044	0.26848

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	16.54	0.02715	YES YES
8	a	19.21	0.22672	YES YES
9	a	24.60	0.11706	YES YES
10	a	53.76	2.63779	YES YES
11	a	60.86	0.43894	YES YES
12	a	67.27	0.45889	YES YES
13	a	72.57	0.82183	YES YES
14	a	110.37	1.98526	YES YES
15	a	127.19	1.33478	YES YES
16	a	143.13	0.81812	YES YES
17	a	159.52	0.05050	YES YES
18	a	185.65	0.91764	YES YES
19	a	221.21	0.89823	YES YES
20	a	228.11	4.18614	YES YES
21	a	249.09	3.43904	YES YES
22	a	274.54	0.53188	YES YES
23	a	315.94	5.26857	YES YES
24	a	343.75	151.18281	YES YES
25	a	346.34	34.68331	YES YES
26	a	380.50	12.16405	YES YES
27	a	393.90	1.17008	YES YES
28	a	406.06	3.56582	YES YES
29	a	444.88	3.47331	YES YES
30	a	459.59	2.84684	YES YES
31	a	469.84	2.06236	YES YES
32	a	505.09	31.62413	YES YES
33	a	521.66	5.31211	YES YES
34	a	535.32	6.46706	YES YES
35	a	538.35	2.60125	YES YES
36	a	543.63	4.43345	YES YES
37	a	551.24	2.65864	YES YES
38	a	581.03	2.77473	YES YES
39	a	606.11	7.98851	YES YES
40	a	625.09	17.72085	YES YES
41	a	625.50	9.73148	YES YES
42	a	640.99	1.30474	YES YES
43	a	647.40	9.42697	YES YES
44	a	654.29	3.85466	YES YES
45	a	669.49	1.88239	YES YES
46	a	700.07	10.30402	YES YES
47	a	731.35	3.30233	YES YES
48	a	755.71	3.17243	YES YES
49	a	759.98	60.29449	YES YES
50	a	767.23	15.61876	YES YES

6d/iso2

bp86_def2-tzvpp energy (au): -1350.0911930780

Zero point energy (au): 0.2805416
Entropy (kJ mol-1 K-1): 0.66069
Chemical potential (kJ mol-1): 597.02

XYZ coordinates:

38

C	-5.77942	1.32163	0.98240
C	-5.56430	0.12785	0.24475
C	-6.75167	-0.58780	-0.05461
N	-8.00897	-0.21477	0.22459
C	-8.05950	0.95654	0.86606
N	-7.03297	1.72617	1.26534
N	-4.76849	2.12611	1.42737
C	-4.45394	-0.66902	-0.22746
N	-6.39869	-1.76725	-0.67353
H	-9.05589	1.33266	1.11106
C	-3.01470	-0.38278	-0.21186
C	-5.02264	-1.81299	-0.76983
C	-7.33744	-2.76502	-1.15695
H	-4.53555	-2.64625	-1.26589
H	-3.82242	1.76795	1.46761
H	-5.03554	2.84480	2.09070
H	-7.24246	-2.89573	-2.24345
H	-8.34633	-2.41034	-0.92193
H	-7.16848	-3.73039	-0.66116
C	-0.21087	0.13592	-0.24101
C	-0.71161	-1.15152	0.05912
C	-2.07852	-1.39785	0.07700
C	-2.51060	0.89819	-0.52244
C	-1.14390	1.15583	-0.53287
C	1.18288	0.39463	-0.25119
H	-0.00913	-1.95125	0.29197
H	-2.43981	-2.39217	0.34213
H	-3.20491	1.69514	-0.79022
H	-0.77873	2.15089	-0.78562
C	2.38429	0.62039	-0.26167
C	3.77582	0.86965	-0.26773
C	4.77908	-0.12180	0.01689
C	4.34949	2.10505	-0.54814
H	4.54122	-1.15422	0.26179
C	6.05304	0.37471	-0.05425
S	6.06028	2.05003	-0.46641
H	6.98887	-0.14845	0.11229
H	3.83552	3.02745	-0.79584

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.63	0.04350	YES	YES
8	a	17.98	0.00225	YES	YES
9	a	24.26	0.03705	YES	YES
10	a	53.90	2.75797	YES	YES
11	a	61.21	0.39951	YES	YES
12	a	67.50	0.54464	YES	YES
13	a	72.97	0.89542	YES	YES
14	a	110.65	2.17193	YES	YES
15	a	128.37	1.22077	YES	YES
16	a	140.76	0.52191	YES	YES
17	a	162.07	0.29137	YES	YES
18	a	185.77	0.64110	YES	YES
19	a	221.26	1.11272	YES	YES
20	a	228.32	3.76087	YES	YES
21	a	249.21	3.31646	YES	YES
22	a	274.77	0.35877	YES	YES
23	a	316.30	4.74688	YES	YES
24	a	344.05	46.47124	YES	YES
25	a	347.32	138.91082	YES	YES
26	a	380.46	13.63557	YES	YES
27	a	396.02	1.25264	YES	YES
28	a	406.55	4.47616	YES	YES
29	a	444.99	3.50845	YES	YES
30	a	458.67	1.53484	YES	YES
31	a	470.35	1.89206	YES	YES
32	a	505.38	31.63767	YES	YES
33	a	521.83	5.13553	YES	YES
34	a	536.38	8.63655	YES	YES
35	a	539.88	1.81467	YES	YES
36	a	543.30	3.26248	YES	YES
37	a	550.65	2.64491	YES	YES
38	a	581.00	2.88874	YES	YES
39	a	606.13	8.02354	YES	YES
40	a	625.53	19.51193	YES	YES
41	a	625.64	7.34686	YES	YES
42	a	640.98	2.22615	YES	YES
43	a	647.55	9.22342	YES	YES
44	a	655.18	4.02413	YES	YES
45	a	669.33	1.92863	YES	YES
46	a	699.91	10.16730	YES	YES
47	a	730.04	2.92304	YES	YES
48	a	755.74	3.08335	YES	YES
49	a	760.69	60.11613	YES	YES
50	a	766.94	15.76061	YES	YES

6d/iso3

bp86_def2-tzvpp energy (au): -1350.0911987520

Zero point energy (au): 0.2804953
Entropy (kJ mol-1 K-1): 0.66009
Chemical potential (kJ mol-1): 597.05

XYZ coordinates:

38

C	-5.79641	1.30833	1.02636
C	-5.56434	0.08698	0.34113
C	-6.74221	-0.65262	0.06363
N	-7.99260	-0.34603	0.43859
C	-8.04917	0.79826	1.12661
N	-7.04109	1.63518	1.42494
N	-4.80777	2.19931	1.33585
C	-4.46218	-0.61587	-0.27668
N	-6.39239	-1.75187	-0.68980
H	-9.03727	1.10284	1.48053
C	-3.02631	-0.31166	-0.26329
C	-5.02769	-1.72241	-0.89464
C	-7.31895	-2.77015	-1.15341
H	-4.53724	-2.52563	-1.43483
H	-3.91416	2.14240	0.86323
H	-5.11819	3.10789	1.66114
H	-7.30345	-2.83959	-2.24924
H	-8.32163	-2.47885	-0.82362
H	-7.06735	-3.75054	-0.72637
C	-0.22295	0.20879	-0.23809
C	-0.87222	-0.23418	-1.41313
C	-2.23927	-0.48206	-1.42160
C	-2.37304	0.12175	0.91005
C	-1.00675	0.38106	0.92487
C	1.17077	0.46878	-0.22663
H	-0.28692	-0.36752	-2.32261
H	-2.72112	-0.79405	-2.34901
H	-2.94536	0.22537	1.83235
H	-0.52341	0.70536	1.84607
C	2.37356	0.68744	-0.21969
C	3.76414	0.94163	-0.19783
C	4.49767	1.34242	0.97350
C	4.59771	0.83559	-1.30588
H	4.03274	1.48291	1.94644
C	5.83250	1.52437	0.72897
S	6.22432	1.21430	-0.92250
H	6.60907	1.82304	1.42544
H	4.31696	0.55403	-2.31483

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	15.91	0.08584	YES	YES
8	a	17.81	0.14456	YES	YES
9	a	23.44	0.11258	YES	YES
10	a	51.63	2.99366	YES	YES
11	a	61.42	0.54847	YES	YES
12	a	68.31	0.97739	YES	YES
13	a	90.37	0.48481	YES	YES
14	a	112.46	1.31085	YES	YES
15	a	128.09	1.54155	YES	YES
16	a	142.89	0.81914	YES	YES
17	a	159.69	0.04545	YES	YES
18	a	185.91	1.06544	YES	YES
19	a	221.21	0.91246	YES	YES
20	a	226.90	4.16880	YES	YES
21	a	249.21	3.73796	YES	YES
22	a	274.08	0.77665	YES	YES
23	a	314.22	10.46776	YES	YES
24	a	340.49	162.67673	YES	YES
25	a	346.34	16.27847	YES	YES
26	a	380.17	13.41104	YES	YES
27	a	393.46	1.61883	YES	YES
28	a	405.88	3.24509	YES	YES
29	a	445.30	3.75781	YES	YES
30	a	459.04	2.87941	YES	YES
31	a	469.84	2.18153	YES	YES
32	a	501.61	31.63466	YES	YES
33	a	521.63	5.40099	YES	YES
34	a	534.86	5.03412	YES	YES
35	a	537.41	3.79978	YES	YES
36	a	543.47	4.55978	YES	YES
37	a	550.63	2.53599	YES	YES
38	a	580.84	2.84299	YES	YES
39	a	605.74	8.08042	YES	YES
40	a	624.53	18.03649	YES	YES
41	a	625.75	8.28664	YES	YES
42	a	640.58	1.35694	YES	YES
43	a	647.97	9.81299	YES	YES
44	a	654.73	4.19602	YES	YES
45	a	669.48	1.91022	YES	YES
46	a	700.20	10.17038	YES	YES
47	a	730.84	2.91992	YES	YES
48	a	755.46	3.15249	YES	YES
49	a	760.17	60.78187	YES	YES
50	a	767.60	15.90330	YES	YES

6d/iso4

bp86_def2-tzvpp energy (au): -1350.0911964720

Zero point energy (au): 0.2805601
Entropy (kJ mol-1 K-1): 0.65713
Chemical potential (kJ mol-1): 598.05

XYZ coordinates:

38

C	-5.78464	1.30913	1.01967
C	-5.56020	0.08418	0.33817
C	-6.74342	-0.64431	0.05443
N	-7.99297	-0.32520	0.42155
C	-8.04258	0.82052	1.10765
N	-7.02845	1.64823	1.41066
N	-4.78985	2.19193	1.33172
C	-4.46119	-0.62971	-0.27246
N	-6.39960	-1.74777	-0.69576
H	-9.02978	1.13521	1.45501
C	-3.02322	-0.33628	-0.25220
C	-5.03337	-1.73146	-0.89281
C	-7.33352	-2.75615	-1.16625
H	-4.54747	-2.53977	-1.42963
H	-3.89173	2.12326	0.86938
H	-5.09233	3.10311	1.65704
H	-7.31920	-2.81788	-2.26263
H	-8.33397	-2.46001	-0.83396
H	-7.08842	-3.74122	-0.74632
C	-0.21942	0.18029	-0.21752
C	-0.86489	-0.26370	-1.39416
C	-2.23217	-0.50962	-1.40732
C	-2.37284	0.09330	0.92418
C	-1.00620	0.35068	0.94366
C	1.17220	0.45021	-0.20439
H	-0.27685	-0.39694	-2.30178
H	-2.71143	-0.82021	-2.33650
H	-2.94823	0.19723	1.84464
H	-0.52545	0.67474	1.86633
C	2.37071	0.69057	-0.19185
C	3.75759	0.96471	-0.19215
C	4.60107	0.88052	-1.35467
C	4.48032	1.35094	0.93124
H	4.23224	0.59512	-2.33683
C	5.90622	1.19721	-1.08915
S	6.13688	1.60205	0.57193
H	6.74653	1.21591	-1.77521
H	4.10363	1.49319	1.93829

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.96	0.00699	YES	YES
8	a	20.29	0.03452	YES	YES
9	a	24.51	0.03663	YES	YES
10	a	52.92	3.02645	YES	YES
11	a	61.58	0.53446	YES	YES
12	a	68.87	1.10309	YES	YES
13	a	91.84	0.61419	YES	YES
14	a	113.34	1.47837	YES	YES
15	a	129.15	1.35900	YES	YES
16	a	141.32	0.58133	YES	YES
17	a	161.83	0.31228	YES	YES
18	a	186.06	0.83427	YES	YES
19	a	221.31	1.20226	YES	YES
20	a	227.59	3.91322	YES	YES
21	a	249.08	3.40048	YES	YES
22	a	274.11	0.28679	YES	YES
23	a	315.01	14.73218	YES	YES
24	a	332.85	171.19343	YES	YES
25	a	344.67	8.09607	YES	YES
26	a	380.18	9.44341	YES	YES
27	a	395.49	1.28613	YES	YES
28	a	405.77	2.77409	YES	YES
29	a	445.39	3.61812	YES	YES
30	a	458.82	1.49231	YES	YES
31	a	470.27	2.09905	YES	YES
32	a	502.91	30.59845	YES	YES
33	a	521.71	5.05716	YES	YES
34	a	535.75	8.53681	YES	YES
35	a	539.65	1.59612	YES	YES
36	a	543.40	3.40776	YES	YES
37	a	550.03	2.43334	YES	YES
38	a	580.96	3.05414	YES	YES
39	a	605.82	8.10664	YES	YES
40	a	625.27	19.34957	YES	YES
41	a	625.55	6.56341	YES	YES
42	a	641.20	2.17664	YES	YES
43	a	647.91	9.91715	YES	YES
44	a	655.51	4.24253	YES	YES
45	a	669.56	1.96734	YES	YES
46	a	700.22	10.04933	YES	YES
47	a	731.36	2.41221	YES	YES
48	a	755.81	3.17315	YES	YES
49	a	760.93	60.29944	YES	YES
50	a	767.73	16.11908	YES	YES

6e/iso1

bp86_def2-tzvpp energy (au): -1366.5050732150

Zero point energy (au): 0.3174976
Entropy (kJ mol-1 K-1): 0.75150
Chemical potential (kJ mol-1): 677.63

XYZ coordinates:

44

C	-3.71845	1.74830	0.33016
C	-3.65837	0.35933	0.04104
C	-4.92751	-0.26868	-0.03940
N	-6.12660	0.32313	0.05381
C	-6.02707	1.63999	0.26019
N	-4.91014	2.37045	0.41502
N	-2.61368	2.53018	0.51942
C	-2.65987	-0.67779	-0.09604
N	-4.72828	-1.62205	-0.21060
H	-6.96722	2.19289	0.32757
C	-1.19767	-0.57409	-0.12479
C	-3.37048	-1.86199	-0.23828
C	-5.78853	-2.60529	-0.35440
H	-2.99490	-2.86591	-0.40734
H	-1.72147	2.09707	0.72258
H	-2.78896	3.45490	0.89678
H	-5.72046	-3.11279	-1.32597
H	-6.74305	-2.07275	-0.28980
H	-5.73581	-3.35321	0.44822
C	1.64445	-0.39615	-0.18271
C	0.99517	-1.45465	0.49257
C	-0.39083	-1.53404	0.52240
C	-0.54420	0.46690	-0.81913
C	0.84251	0.55962	-0.84535
C	3.05698	-0.28521	-0.17868
H	1.59727	-2.20047	1.01067
H	-0.86918	-2.33873	1.08185
H	-1.13831	1.19823	-1.36754
H	1.32542	1.37041	-1.39012
C	4.27399	-0.17328	-0.15330
C	5.68225	-0.02418	-0.09453
C	8.47111	0.31060	0.08239
C	7.69727	1.23540	-0.62960
C	6.31960	1.07222	-0.71801
C	6.47884	-0.95668	0.60769
C	7.85598	-0.78942	0.69342
C	9.96657	0.47342	0.15586
H	8.17476	2.09095	-1.10491
H	5.71657	1.79672	-1.26332
H	5.99957	-1.80695	1.09066
H	8.45731	-1.50938	1.24666
F	10.48156	-0.03325	1.30909
F	10.34674	1.77800	0.08524
F	10.59912	-0.17276	-0.86944

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.60	0.16881	YES	YES
8	a	16.34	0.05606	YES	YES
9	a	17.61	0.16909	YES	YES
10	a	27.89	0.05902	YES	YES
11	a	40.50	0.32511	YES	YES
12	a	55.76	0.06741	YES	YES
13	a	59.87	4.03235	YES	YES
14	a	86.90	0.43344	YES	YES
15	a	92.00	0.75632	YES	YES
16	a	106.39	1.69584	YES	YES
17	a	125.62	0.46986	YES	YES
18	a	131.17	1.27927	YES	YES
19	a	151.64	0.66897	YES	YES
20	a	183.79	1.34988	YES	YES
21	a	200.44	0.28576	YES	YES
22	a	220.83	0.64397	YES	YES
23	a	221.86	3.59724	YES	YES
24	a	244.24	2.40438	YES	YES
25	a	273.74	1.34712	YES	YES
26	a	284.16	21.13246	YES	YES
27	a	297.56	2.05337	YES	YES
28	a	336.01	45.01634	YES	YES
29	a	351.28	142.73039	YES	YES
30	a	373.98	3.19930	YES	YES
31	a	385.13	1.23261	YES	YES
32	a	395.25	0.02218	YES	YES
33	a	404.61	1.60973	YES	YES
34	a	408.88	3.16126	YES	YES
35	a	421.79	4.38177	YES	YES
36	a	456.08	2.46028	YES	YES
37	a	471.24	0.51188	YES	YES
38	a	499.29	34.70290	YES	YES
39	a	509.84	10.10977	YES	YES
40	a	522.39	4.34123	YES	YES
41	a	536.91	0.38502	YES	YES
42	a	541.60	6.91195	YES	YES
43	a	543.93	4.50153	YES	YES
44	a	552.26	4.72667	YES	YES
45	a	558.43	0.25159	YES	YES
46	a	578.60	11.00138	YES	YES
47	a	597.62	3.21127	YES	YES
48	a	606.66	6.30224	YES	YES
49	a	625.38	8.48103	YES	YES
50	a	634.89	1.95473	YES	YES

6e/iso2

bp86_def2-tzvpp energy (au): -1366.5051462130

Zero point energy (au): 0.3174080
Entropy (kJ mol-1 K-1): 0.75832
Chemical potential (kJ mol-1): 675.54

XYZ coordinates:

44

C	-5.45453	1.81579	0.38078
C	-5.45048	0.41396	0.15559
C	-6.74372	-0.15902	0.05489
N	-7.91711	0.46776	0.22040
C	-7.76366	1.76861	0.48702
N	-6.61902	2.46835	0.56153
N	-4.31921	2.57313	0.44550
C	-4.49578	-0.63578	-0.12135
N	-6.60038	-1.49078	-0.27106
H	-8.67975	2.34136	0.65088
C	-3.02963	-0.60044	-0.10865
C	-5.25405	-1.76915	-0.38137
C	-7.69836	-2.42827	-0.43584
H	-4.91848	-2.77916	-0.59301
H	-3.44947	2.20674	0.07934
H	-4.45712	3.57745	0.42898
H	-7.68777	-2.86505	-1.44313
H	-8.63085	-1.87263	-0.29181
H	-7.63796	-3.23450	0.30797
C	-0.18209	-0.58812	-0.06870
C	-0.89269	-1.28108	-1.07503
C	-2.28119	-1.28056	-1.09270
C	-2.31584	0.08010	0.90133
C	-0.92581	0.09132	0.92177
C	1.23471	-0.57193	-0.05784
H	-0.33558	-1.80540	-1.85086
H	-2.80728	-1.79512	-1.89742
H	-2.86557	0.58090	1.69865
H	-0.39551	0.61553	1.71637
C	2.45694	-0.55268	-0.05361
C	3.87395	-0.52548	-0.06540
C	6.68700	-0.45820	-0.10594
C	5.98419	0.19847	0.91175
C	4.59453	0.16497	0.93489
C	4.59822	-1.18682	-1.08303
C	5.98736	-1.15072	-1.10210
C	8.18895	-0.36917	-0.16696
H	6.52816	0.73220	1.68960
H	4.04804	0.67327	1.72794
H	4.05396	-1.72678	-1.85636
H	6.53385	-1.66610	-1.89061
F	8.74924	-1.47557	-0.72728
F	8.74803	-0.21397	1.06339
F	8.59878	0.69758	-0.91848

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.81	0.19778	YES	YES
8	a	15.51	0.05500	YES	YES
9	a	16.76	0.23209	YES	YES
10	a	27.83	0.01845	YES	YES
11	a	40.45	0.31179	YES	YES
12	a	54.53	0.30656	YES	YES
13	a	57.17	3.46839	YES	YES
14	a	76.85	0.39300	YES	YES
15	a	90.36	0.79099	YES	YES
16	a	104.73	2.01276	YES	YES
17	a	124.47	0.84763	YES	YES
18	a	131.91	0.65586	YES	YES
19	a	148.22	0.67085	YES	YES
20	a	182.74	1.37433	YES	YES
21	a	200.42	0.25726	YES	YES
22	a	220.29	2.08133	YES	YES
23	a	222.58	3.17034	YES	YES
24	a	241.06	2.06056	YES	YES
25	a	272.52	2.97203	YES	YES
26	a	288.03	20.00805	YES	YES
27	a	293.89	0.64282	YES	YES
28	a	335.71	89.66999	YES	YES
29	a	348.64	93.75664	YES	YES
30	a	373.78	2.89588	YES	YES
31	a	384.70	0.77825	YES	YES
32	a	395.53	0.07275	YES	YES
33	a	403.84	2.07321	YES	YES
34	a	408.15	11.41686	YES	YES
35	a	422.49	1.90145	YES	YES
36	a	456.34	0.57652	YES	YES
37	a	471.07	0.62411	YES	YES
38	a	501.69	33.10576	YES	YES
39	a	510.43	10.16075	YES	YES
40	a	522.30	3.96263	YES	YES
41	a	536.96	0.31480	YES	YES
42	a	541.63	7.40321	YES	YES
43	a	543.79	3.87826	YES	YES
44	a	551.69	4.67868	YES	YES
45	a	558.28	0.29006	YES	YES
46	a	578.64	10.19142	YES	YES
47	a	597.61	2.85226	YES	YES
48	a	606.24	7.22552	YES	YES
49	a	625.07	8.57140	YES	YES
50	a	634.92	1.96260	YES	YES

6b/iso1

bp86_def2-tzvpp energy (au): -1143.8716496360

Zero point energy (au): 0.3446594
Entropy (kJ mol-1 K-1): 0.71994
Chemical potential (kJ mol-1): 755.61

XYZ coordinates:

45

C	-3.92645	1.70033	0.14536
C	-3.75500	0.30336	-0.04028
C	-4.97101	-0.41888	-0.14834
N	-6.21142	0.09040	-0.16153
C	-6.21391	1.42106	-0.03840
N	-5.16082	2.23961	0.12479
N	-2.88879	2.56866	0.33367
C	-2.68008	-0.66368	-0.05225
N	-4.66907	-1.76134	-0.21747
H	-7.19236	1.90766	-0.05791
C	-1.22753	-0.45671	-0.00872
C	-3.29689	-1.90239	-0.15530
C	-5.64681	-2.82631	-0.35816
H	-2.84283	-2.88475	-0.23597
H	-1.97845	2.21340	0.59861
H	-3.14280	3.50324	0.63313
H	-5.49291	-3.37652	-1.29634
H	-6.63935	-2.36399	-0.36859
H	-5.58192	-3.52692	0.48515
C	1.60370	-0.11202	0.03697
C	0.98131	-1.14269	0.77823
C	-0.39841	-1.30332	0.75655
C	-0.60246	0.56433	-0.75573
C	0.77713	0.73817	-0.73182
C	3.01011	0.06239	0.06283
H	1.59917	-1.80623	1.38265
H	-0.85596	-2.08727	1.36140
H	-1.21009	1.21053	-1.39005
H	1.23729	1.52845	-1.32448
C	4.22361	0.21301	0.08467
C	5.63030	0.38923	0.10560
C	8.43486	0.73952	0.14377
C	7.62398	1.58319	-0.63617
C	6.24923	1.41139	-0.65460
C	6.45830	-0.44652	0.88174
C	7.84222	-0.27939	0.90547
O	9.77647	0.99060	0.09276
H	8.09946	2.36959	-1.22162
H	5.62852	2.06926	-1.26184
H	6.00305	-1.23945	1.47434
H	8.44711	-0.94549	1.51724
C	10.63965	0.16155	0.87082
H	10.41096	0.24020	1.94528
H	11.65317	0.53134	0.68672
H	10.57272	-0.89259	0.55878

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.05	0.13168	YES	YES
8	a	15.10	0.05464	YES	YES
9	a	20.77	0.10519	YES	YES
10	a	44.67	1.74294	YES	YES
11	a	57.41	0.98652	YES	YES
12	a	60.12	1.75639	YES	YES
13	a	80.14	0.33472	YES	YES
14	a	90.36	0.36229	YES	YES
15	a	107.80	2.19212	YES	YES
16	a	122.91	1.43401	YES	YES
17	a	132.29	1.82639	YES	YES
18	a	145.50	0.16475	YES	YES
19	a	176.65	2.03696	YES	YES
20	a	194.06	0.60397	YES	YES
21	a	221.83	1.53789	YES	YES
22	a	224.56	2.09373	YES	YES
23	a	239.27	4.12992	YES	YES
24	a	249.98	2.02500	YES	YES
25	a	269.44	0.75882	YES	YES
26	a	279.39	0.83289	YES	YES
27	a	319.34	25.93745	YES	YES
28	a	333.78	12.67597	YES	YES
29	a	345.54	169.00414	YES	YES
30	a	391.94	1.77979	YES	YES
31	a	400.99	3.97355	YES	YES
32	a	407.32	6.37620	YES	YES
33	a	408.78	0.11839	YES	YES
34	a	441.80	3.52816	YES	YES
35	a	462.53	2.87966	YES	YES
36	a	480.83	1.31888	YES	YES
37	a	505.25	37.27649	YES	YES
38	a	519.48	13.69248	YES	YES
39	a	523.92	19.74970	YES	YES
40	a	531.90	3.38140	YES	YES
41	a	542.62	2.02882	YES	YES
42	a	543.99	3.17655	YES	YES
43	a	548.13	3.10985	YES	YES
44	a	558.39	14.07740	YES	YES
45	a	606.13	8.51850	YES	YES
46	a	625.03	10.21806	YES	YES
47	a	636.31	0.12494	YES	YES
48	a	647.88	9.87922	YES	YES
49	a	667.57	10.10021	YES	YES
50	a	669.46	0.71619	YES	YES

6b/iso2

bp86_def2-tzvpp energy (au): -1143.8716591980

Zero point energy (au): 0.3446727
Entropy (kJ mol-1 K-1): 0.71834
Chemical potential (kJ mol-1): 756.12

XYZ coordinates:

45

C	-4.73268	1.75914	0.15478
C	-4.60278	0.35531	-0.01197
C	-5.84010	-0.33281	-0.09953
N	-7.06534	0.21184	-0.11277
C	-7.02854	1.54383	-0.01194
N	-5.95105	2.33379	0.13232
N	-3.66986	2.59978	0.32746
C	-3.55636	-0.64267	-0.01813
N	-5.57779	-1.68448	-0.14957
H	-7.99248	2.05846	-0.03435
C	-2.09821	-0.47786	0.00429
C	-4.20986	-1.86446	-0.09648
C	-6.58742	-2.72269	-0.26251
H	-3.78535	-2.86078	-0.16627
H	-2.76847	2.22268	0.59240
H	-3.89575	3.54560	0.61381
H	-6.45169	-3.30015	-1.18694
H	-7.56559	-2.23106	-0.28304
H	-6.54233	-3.40386	0.59793
C	0.74274	-0.22009	0.00138
C	0.10156	-1.22775	0.75809
C	-1.28262	-1.34565	0.76052
C	-1.45457	0.52085	-0.75706
C	-0.07025	0.65260	-0.75642
C	2.15415	-0.09122	-0.00107
H	0.70882	-1.90759	1.35506
H	-1.75353	-2.11248	1.37701
H	-2.05226	1.18214	-1.38512
H	0.40390	1.42547	-1.36076
C	3.37205	0.01976	-0.00953
C	4.78401	0.14836	-0.01888
C	7.59885	0.40484	-0.03822
C	6.80309	1.32695	-0.73530
C	5.41534	1.19434	-0.72169
C	5.60604	-0.77041	0.67804
C	6.98596	-0.64528	0.66843
O	8.96322	0.44085	0.01463
H	7.25266	2.14838	-1.28947
H	4.80200	1.91286	-1.26449
H	5.13923	-1.58692	1.22788
H	7.61773	-1.35307	1.20435
C	9.62971	1.49183	-0.68461
H	9.42361	1.44897	-1.76561
H	10.69879	1.33336	-0.51155
H	9.33843	2.48030	-0.29610

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	14.51	0.22328	YES YES
8	a	15.89	0.50887	YES YES
9	a	20.00	0.39231	YES YES
10	a	45.12	1.58909	YES YES
11	a	58.46	0.48897	YES YES
12	a	58.98	2.12535	YES YES
13	a	82.42	0.21505	YES YES
14	a	89.78	0.39623	YES YES
15	a	107.80	2.23382	YES YES
16	a	121.98	1.40412	YES YES
17	a	129.16	1.51223	YES YES
18	a	148.84	0.63327	YES YES
19	a	176.22	2.09030	YES YES
20	a	193.93	0.73507	YES YES
21	a	221.09	1.97379	YES YES
22	a	223.20	1.76119	YES YES
23	a	240.49	3.60737	YES YES
24	a	250.50	2.01711	YES YES
25	a	269.39	0.37504	YES YES
26	a	278.06	0.49902	YES YES
27	a	319.53	29.87175	YES YES
28	a	334.08	30.90275	YES YES
29	a	342.08	148.70785	YES YES
30	a	388.91	1.69904	YES YES
31	a	401.35	5.72234	YES YES
32	a	406.45	1.74001	YES YES
33	a	408.76	4.84202	YES YES
34	a	446.41	2.15371	YES YES
35	a	461.18	2.37892	YES YES
36	a	477.86	1.45397	YES YES
37	a	503.72	36.25434	YES YES
38	a	520.61	13.24695	YES YES
39	a	523.86	19.52946	YES YES
40	a	535.83	4.45342	YES YES
41	a	541.19	1.03357	YES YES
42	a	543.94	2.75986	YES YES
43	a	545.67	3.78887	YES YES
44	a	559.17	13.65738	YES YES
45	a	606.15	8.25939	YES YES
46	a	625.13	9.69716	YES YES
47	a	636.49	1.68435	YES YES
48	a	647.81	9.62895	YES YES
49	a	667.37	12.06672	YES YES
50	a	669.47	0.41919	YES YES

6b/iso3

bp86_def2-tzvpp energy (au): -1143.8713761060

Zero point energy (au): 0.3442783
Entropy (kJ mol-1 K-1): 0.72478
Chemical potential (kJ mol-1): 753.85

XYZ coordinates:

45

C	-4.71639	1.76973	0.16323
C	-4.58814	0.35824	0.07137
C	-5.82372	-0.33557	0.04084
N	-7.04865	0.19616	0.16747
C	-7.00992	1.52365	0.32039
N	-5.93390	2.32824	0.31639
N	-3.66390	2.62656	0.06395
C	-3.54211	-0.62030	-0.11714
N	-5.56018	-1.67255	-0.16543
H	-7.97254	2.02352	0.45477
C	-2.08569	-0.43994	-0.11037
C	-4.19243	-1.83689	-0.26436
C	-6.56846	-2.71578	-0.23392
H	-3.76632	-2.82748	-0.38647
H	-2.71060	2.28814	0.04948
H	-3.84654	3.60971	0.22152
H	-6.53289	-3.22849	-1.20448
H	-7.54631	-2.23767	-0.11378
H	-6.42343	-3.45212	0.56825
C	0.74992	-0.13265	-0.06853
C	0.11663	-0.94519	-1.03701
C	-1.26530	-1.08841	-1.05597
C	-1.44971	0.35996	0.86306
C	-0.06772	0.51641	0.88396
C	2.15881	0.02198	-0.04939
H	0.72842	-1.45112	-1.78344
H	-1.73124	-1.69701	-1.83188
H	-2.05140	0.82938	1.64305
H	0.40101	1.13018	1.65290
C	3.37466	0.15199	-0.02956
C	4.78396	0.30394	-0.00188
C	7.59347	0.60641	0.05624
C	6.78977	1.24849	1.01514
C	5.41255	1.10016	0.98624
C	5.60475	-0.33210	-0.95475
C	6.99113	-0.18724	-0.93208
O	8.93811	0.81576	0.17115
H	7.27274	1.86094	1.77601
H	4.79731	1.60097	1.73288
H	5.14193	-0.94930	-1.72413
H	7.59040	-0.69446	-1.68541
C	9.79459	0.18569	-0.78143
H	9.70901	-0.91126	-0.73475
H	10.81211	0.48313	-0.50940
H	9.57520	0.52617	-1.80569

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	13.39	0.11612	YES YES
8	a	17.78	0.13218	YES YES
9	a	20.41	0.10623	YES YES
10	a	44.36	2.30080	YES YES
11	a	51.11	2.10087	YES YES
12	a	60.75	2.30403	YES YES
13	a	82.66	0.47902	YES YES
14	a	88.51	5.49383	YES YES
15	a	100.26	3.86082	YES YES
16	a	120.97	1.66318	YES YES
17	a	130.16	0.34161	YES YES
18	a	145.66	0.88727	YES YES
19	a	150.70	93.11628	YES YES
20	a	187.93	15.72093	YES YES
21	a	196.54	19.81511	YES YES
22	a	221.63	7.46056	YES YES
23	a	228.35	4.58646	YES YES
24	a	239.18	4.94238	YES YES
25	a	250.11	4.83489	YES YES
26	a	269.67	1.24112	YES YES
27	a	280.45	8.03755	YES YES
28	a	319.63	18.47579	YES YES
29	a	335.55	2.04877	YES YES
30	a	391.43	0.75728	YES YES
31	a	400.64	1.62567	YES YES
32	a	406.82	1.78260	YES YES
33	a	408.36	0.09173	YES YES
34	a	441.95	3.38666	YES YES
35	a	461.67	1.84629	YES YES
36	a	481.43	2.91699	YES YES
37	a	515.89	11.36164	YES YES
38	a	521.76	10.41224	YES YES
39	a	528.11	8.25564	YES YES
40	a	532.06	10.60332	YES YES
41	a	542.59	3.15188	YES YES
42	a	545.11	3.02245	YES YES
43	a	548.36	2.11443	YES YES
44	a	558.49	18.42070	YES YES
45	a	604.66	8.86346	YES YES
46	a	624.96	9.25666	YES YES
47	a	636.43	0.16755	YES YES
48	a	648.57	10.04007	YES YES
49	a	667.82	6.91155	YES YES
50	a	670.33	2.58952	YES YES

6b/iso4

bp86_def2-tzvpp energy (au): -1143.8716616010

Zero point energy (au): 0.3447173
Entropy (kJ mol-1 K-1): 0.71575
Chemical potential (kJ mol-1): 756.95

XYZ coordinates:

45

C	-4.75865	1.76195	0.18676
C	-4.61359	0.35370	0.08194
C	-5.84257	-0.35194	0.02610
N	-7.07448	0.16764	0.13143
C	-7.05288	1.49516	0.28419
N	-5.98396	2.30933	0.30426
N	-3.70370	2.62947	0.19285
C	-3.55519	-0.61460	-0.09661
N	-5.56362	-1.68508	-0.18140
H	-8.02320	1.98631	0.39269
C	-2.09951	-0.42597	-0.08120
C	-4.19311	-1.83592	-0.25904
C	-6.56065	-2.73773	-0.26911
H	-3.75632	-2.82175	-0.38165
H	-2.79393	2.31726	-0.12289
H	-3.93569	3.61093	0.09079
H	-6.49074	-3.25982	-1.23266
H	-7.54576	-2.26724	-0.18321
H	-6.43389	-3.46468	0.54475
C	0.73522	-0.11725	-0.02342
C	0.11103	-0.95362	-0.97718
C	-1.27059	-1.09721	-1.00402
C	-1.47284	0.39975	0.87619
C	-0.09130	0.55588	0.90448
C	2.14336	0.04234	0.00290
H	0.72899	-1.47756	-1.70579
H	-1.72922	-1.72488	-1.76907
H	-2.08173	0.90109	1.62936
H	0.37022	1.19202	1.65943
C	3.35771	0.18513	0.03049
C	4.76613	0.34599	0.06246
C	7.57399	0.66341	0.12810
C	6.77250	1.28371	1.09877
C	5.38814	1.12331	1.06021
C	5.59394	-0.27094	-0.90694
C	6.97036	-0.11529	-0.87530
O	8.93560	0.75405	0.07214
H	7.21492	1.89143	1.88544
H	4.77036	1.60667	1.81649
H	5.13428	-0.87628	-1.68751
H	7.60648	-0.59019	-1.62167
C	9.59358	1.52841	1.07474
H	9.27671	2.58254	1.04047
H	10.66234	1.46241	0.84842
H	9.40726	1.12305	2.08180

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.99	0.11439	YES	YES
8	a	18.67	0.47546	YES	YES
9	a	21.86	0.75306	YES	YES
10	a	44.93	1.31860	YES	YES
11	a	55.60	0.61343	YES	YES
12	a	60.13	2.13864	YES	YES
13	a	85.21	0.25978	YES	YES
14	a	90.54	0.51009	YES	YES
15	a	107.31	1.66729	YES	YES
16	a	122.02	1.63006	YES	YES
17	a	129.66	1.96799	YES	YES
18	a	147.89	0.60348	YES	YES
19	a	178.19	1.75474	YES	YES
20	a	194.84	1.07572	YES	YES
21	a	219.58	2.34302	YES	YES
22	a	228.41	1.61321	YES	YES
23	a	240.62	3.16997	YES	YES
24	a	250.57	2.21504	YES	YES
25	a	269.66	0.46578	YES	YES
26	a	278.62	0.92730	YES	YES
27	a	317.88	40.59904	YES	YES
28	a	333.37	58.87967	YES	YES
29	a	340.62	108.22270	YES	YES
30	a	388.91	2.02130	YES	YES
31	a	400.94	5.90877	YES	YES
32	a	406.55	2.43848	YES	YES
33	a	409.18	2.08219	YES	YES
34	a	446.21	1.64912	YES	YES
35	a	461.81	2.81009	YES	YES
36	a	477.40	1.87866	YES	YES
37	a	503.13	35.53862	YES	YES
38	a	520.57	12.89415	YES	YES
39	a	524.27	18.87792	YES	YES
40	a	535.96	4.90020	YES	YES
41	a	541.55	1.66999	YES	YES
42	a	543.82	1.89555	YES	YES
43	a	545.56	4.40771	YES	YES
44	a	559.24	13.97653	YES	YES
45	a	606.06	8.41714	YES	YES
46	a	625.38	9.49107	YES	YES
47	a	636.63	1.41034	YES	YES
48	a	648.54	10.18671	YES	YES
49	a	667.51	11.94835	YES	YES
50	a	669.83	0.64351	YES	YES

6c/iso1

bp86_def2-tzvpp energy (au): -1466.8766929310

Zero point energy (au): 0.3409313
Entropy (kJ mol-1 K-1): 0.74116
Chemical potential (kJ mol-1): 741.49

XYZ coordinates:

45

C	-5.03057	1.81392	0.27384
C	-4.98623	0.41444	0.03913
C	-6.26290	-0.19840	-0.04111
N	-7.45492	0.41376	0.01042
C	-7.33905	1.73542	0.17181
N	-6.21424	2.45596	0.31746
N	-3.91675	2.58539	0.44921
C	-3.99950	-0.63932	-0.04428
N	-6.08000	-1.55885	-0.16135
H	-8.27215	2.30339	0.20479
C	-2.53430	-0.55647	-0.05140
C	-4.72392	-1.81757	-0.15807
C	-7.15049	-2.53256	-0.28857
H	-4.35962	-2.83180	-0.28505
H	-3.03150	2.14665	0.67010
H	-4.08021	3.52706	0.78728
H	-7.07137	-3.07739	-1.23903
H	-8.09883	-1.98580	-0.26235
H	-7.12378	-3.25079	0.54218
C	0.31534	-0.44262	-0.09543
C	-0.36422	-1.45119	0.62589
C	-1.75226	-1.49907	0.64870
C	-1.85275	0.43997	-0.78228
C	-0.46367	0.50175	-0.80152
C	1.73098	-0.37896	-0.10826
H	0.21711	-2.18667	1.18128
H	-2.25179	-2.26783	1.23955
H	-2.42621	1.15823	-1.36897
H	0.03967	1.27651	-1.37936
C	2.95279	-0.32062	-0.11608
C	4.36780	-0.24914	-0.12461
C	7.20133	-0.10290	-0.13598
C	6.42743	0.85604	-0.82123
C	5.04285	0.78504	-0.81620
C	5.15133	-1.20408	0.55708
C	6.54178	-1.13438	0.55300
S	8.95185	0.09576	-0.21606
H	6.92409	1.66348	-1.36109
H	4.45953	1.53441	-1.35025
H	4.65390	-2.01005	1.09599
H	7.10715	-1.89200	1.09242
C	9.58910	-1.28929	0.76059
H	9.25974	-1.23167	1.80513
H	10.68028	-1.19099	0.72686
H	9.30618	-2.25481	0.32381

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	10.61	0.07537	YES YES
8	a	14.30	0.11030	YES YES
9	a	18.06	0.04346	YES YES
10	a	40.32	1.61719	YES YES
11	a	55.77	0.19732	YES YES
12	a	56.83	1.81647	YES YES
13	a	61.00	2.19630	YES YES
14	a	87.00	0.37892	YES YES
15	a	97.33	0.81575	YES YES
16	a	107.88	1.25234	YES YES
17	a	128.85	1.70946	YES YES
18	a	136.33	0.03183	YES YES
19	a	164.15	1.28925	YES YES
20	a	187.45	0.41720	YES YES
21	a	198.12	1.04492	YES YES
22	a	210.82	0.27811	YES YES
23	a	221.17	2.81659	YES YES
24	a	237.33	3.37022	YES YES
25	a	257.77	0.67147	YES YES
26	a	275.25	1.14161	YES YES
27	a	296.58	18.49378	YES YES
28	a	322.01	22.67341	YES YES
29	a	337.81	161.19595	YES YES
30	a	344.83	6.74750	YES YES
31	a	383.93	9.55797	YES YES
32	a	390.53	3.82590	YES YES
33	a	395.90	1.17407	YES YES
34	a	406.04	3.39238	YES YES
35	a	446.97	6.05192	YES YES
36	a	456.48	5.28455	YES YES
37	a	472.49	0.98156	YES YES
38	a	499.81	35.18955	YES YES
39	a	515.69	19.98548	YES YES
40	a	522.92	4.74340	YES YES
41	a	540.88	1.70428	YES YES
42	a	543.15	0.65927	YES YES
43	a	543.81	4.25400	YES YES
44	a	552.68	3.91648	YES YES
45	a	605.08	7.31617	YES YES
46	a	617.24	2.82620	YES YES
47	a	625.38	8.43785	YES YES
48	a	633.58	0.67596	YES YES
49	a	648.02	9.94129	YES YES
50	a	669.37	1.86007	YES YES

6c/iso2

bp86_def2-tzvpp energy (au): -1466.8766980650

Zero point energy (au): 0.3409465
Entropy (kJ mol-1 K-1): 0.74008
Chemical potential (kJ mol-1): 741.81

XYZ coordinates:

45

C	-3.81896	1.68960	0.49907
C	-3.70207	0.35303	0.03508
C	-4.94410	-0.27178	-0.24538
N	-6.16040	0.28925	-0.18123
C	-6.10970	1.56542	0.21237
N	-5.02783	2.28110	0.56306
N	-2.75109	2.45055	0.88270
C	-2.67034	-0.64297	-0.14976
N	-4.69852	-1.58534	-0.58109
H	-7.06513	2.09267	0.27186
C	-1.21262	-0.52131	-0.02883
C	-3.33671	-1.80326	-0.51768
C	-5.71654	-2.54961	-0.96132
H	-2.92348	-2.77003	-0.78623
H	-1.86608	2.00476	1.09065
H	-2.97468	3.31391	1.36469
H	-5.55768	-2.90020	-1.99023
H	-6.68742	-2.04720	-0.89664
H	-5.70799	-3.41195	-0.28137
C	1.62698	-0.33200	0.16137
C	0.93528	-1.46078	0.65809
C	-0.44821	-1.54609	0.56749
C	-0.51823	0.59874	-0.53369
C	0.86575	0.69667	-0.43813
C	3.03740	-0.23688	0.26143
H	1.50258	-2.26288	1.12951
H	-0.95969	-2.41370	0.98620
H	-1.07500	1.38964	-1.03718
H	1.37981	1.56801	-0.84318
C	4.25491	-0.15692	0.34835
C	5.66520	-0.06902	0.45238
C	8.48939	0.10640	0.66253
C	7.75249	1.13782	0.05701
C	6.36675	1.04944	-0.04503
C	6.41779	-1.10222	1.06023
C	7.79766	-1.01584	1.16262
S	10.24254	0.09862	0.85344
H	8.25302	2.01934	-0.33960
H	5.80879	1.85754	-0.51745
H	5.89874	-1.97676	1.45118
H	8.35520	-1.82585	1.63505
C	10.76806	1.65558	0.09281
H	10.50885	1.69132	-0.97236
H	11.85945	1.67400	0.19332
H	10.34884	2.52317	0.61690

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.26	0.08758	YES	YES
8	a	14.30	1.00877	YES	YES
9	a	16.96	0.25677	YES	YES
10	a	42.01	1.07173	YES	YES
11	a	54.57	1.03024	YES	YES
12	a	56.58	0.80843	YES	YES
13	a	63.57	2.39744	YES	YES
14	a	86.23	0.34049	YES	YES
15	a	97.84	0.75668	YES	YES
16	a	106.42	1.13285	YES	YES
17	a	124.04	1.78820	YES	YES
18	a	140.35	0.69677	YES	YES
19	a	165.89	0.81532	YES	YES
20	a	185.08	1.18284	YES	YES
21	a	197.01	0.38427	YES	YES
22	a	214.07	0.27654	YES	YES
23	a	222.18	2.10727	YES	YES
24	a	236.35	3.77523	YES	YES
25	a	257.98	0.76690	YES	YES
26	a	273.85	2.12397	YES	YES
27	a	297.94	17.64798	YES	YES
28	a	324.27	14.92988	YES	YES
29	a	340.66	20.33881	YES	YES
30	a	343.45	152.07221	YES	YES
31	a	384.93	13.60289	YES	YES
32	a	392.10	2.32253	YES	YES
33	a	395.49	0.71458	YES	YES
34	a	405.84	4.44969	YES	YES
35	a	446.04	7.40844	YES	YES
36	a	455.05	2.56614	YES	YES
37	a	474.10	2.75268	YES	YES
38	a	501.77	35.07415	YES	YES
39	a	516.00	18.97555	YES	YES
40	a	523.12	4.82197	YES	YES
41	a	540.87	2.23873	YES	YES
42	a	543.13	0.41535	YES	YES
43	a	543.97	4.38334	YES	YES
44	a	553.00	3.81691	YES	YES
45	a	605.39	7.59166	YES	YES
46	a	617.13	2.87258	YES	YES
47	a	625.62	8.34836	YES	YES
48	a	633.45	0.61631	YES	YES
49	a	648.16	10.00270	YES	YES
50	a	669.75	1.98868	YES	YES

6c/iso3

bp86_def2-tzvpp energy (au): -1466.8766938540

Zero point energy (au): 0.3409518
Entropy (kJ mol-1 K-1): 0.74005
Chemical potential (kJ mol-1): 741.86

XYZ coordinates:

45

C	-5.06493	1.81266	0.26899
C	-4.99754	0.39990	0.14803
C	-6.26298	-0.24011	0.12836
N	-7.46187	0.34211	0.27771
C	-7.36587	1.66549	0.43844
N	-6.25548	2.42228	0.43000
N	-3.96584	2.62345	0.24910
C	-3.99809	-0.62042	-0.07491
N	-6.06145	-1.58413	-0.09826
H	-8.30510	2.20576	0.58108
C	-2.53488	-0.50902	-0.11479
C	-4.70447	-1.80546	-0.22438
C	-7.11436	-2.58308	-0.15607
H	-4.32442	-2.81140	-0.37018
H	-3.08481	2.26722	-0.09991
H	-4.14898	3.61657	0.16116
H	-7.09099	-3.11576	-1.11594
H	-8.07127	-2.06043	-0.05479
H	-7.01038	-3.30909	0.66203
C	0.31183	-0.35056	-0.17178
C	-0.43846	0.35099	0.79886
C	-1.82643	0.26856	0.82603
C	-1.78147	-1.20943	-1.08005
C	-0.39445	-1.13868	-1.10941
C	1.72601	-0.26631	-0.20592
H	0.08691	0.95058	1.54176
H	-2.37664	0.79073	1.60951
H	-2.30412	-1.80016	-1.83327
H	0.16464	-1.68285	-1.87001
C	2.94652	-0.19235	-0.23914
C	4.36038	-0.10899	-0.27933
C	7.19150	0.05815	-0.35987
C	6.48387	-0.66106	-1.34467
C	5.10049	-0.74353	-1.30560
C	5.07791	0.60832	0.70106
C	6.46715	0.69151	0.66376
S	8.94761	0.08927	-0.51806
H	7.03136	-1.15816	-2.14665
H	4.56865	-1.30300	-2.07451
H	4.52985	1.10424	1.50181
H	6.98051	1.25480	1.44079
C	9.49089	1.08339	0.89416
H	9.09936	2.10656	0.84175
H	10.58407	1.11794	0.82216
H	9.21279	0.61651	1.84692

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.19	0.18209	YES	YES
8	a	15.27	0.63480	YES	YES
9	a	17.48	0.35261	YES	YES
10	a	41.96	1.10501	YES	YES
11	a	52.51	1.13575	YES	YES
12	a	55.69	0.91324	YES	YES
13	a	62.86	2.04992	YES	YES
14	a	84.28	0.27056	YES	YES
15	a	98.38	0.84368	YES	YES
16	a	105.36	1.07711	YES	YES
17	a	124.09	1.80422	YES	YES
18	a	139.88	0.71166	YES	YES
19	a	167.07	0.80535	YES	YES
20	a	184.88	1.24633	YES	YES
21	a	197.61	0.40002	YES	YES
22	a	217.34	0.33211	YES	YES
23	a	221.87	2.08651	YES	YES
24	a	236.68	3.77994	YES	YES
25	a	258.03	0.73298	YES	YES
26	a	273.70	1.96802	YES	YES
27	a	297.65	18.20111	YES	YES
28	a	324.45	23.04799	YES	YES
29	a	338.79	160.64953	YES	YES
30	a	341.20	4.92222	YES	YES
31	a	384.98	10.83974	YES	YES
32	a	392.14	2.11639	YES	YES
33	a	395.67	0.62821	YES	YES
34	a	406.03	3.08171	YES	YES
35	a	446.20	7.35310	YES	YES
36	a	454.48	3.08838	YES	YES
37	a	474.26	2.99347	YES	YES
38	a	503.53	34.63758	YES	YES
39	a	515.75	17.65687	YES	YES
40	a	523.05	4.66154	YES	YES
41	a	540.69	2.62091	YES	YES
42	a	541.93	0.27998	YES	YES
43	a	543.89	4.11802	YES	YES
44	a	553.23	3.89659	YES	YES
45	a	605.06	7.83948	YES	YES
46	a	617.15	2.87124	YES	YES
47	a	625.22	8.39644	YES	YES
48	a	633.42	0.50964	YES	YES
49	a	648.19	10.07760	YES	YES
50	a	669.45	2.24910	YES	YES

6c/iso4

bp86_def2-tzvpp energy (au): -1466.8767080390

Zero point energy (au): 0.3409303
Entropy (kJ mol-1 K-1): 0.74258
Chemical potential (kJ mol-1): 741.16

XYZ coordinates:

45

C	-3.83560	1.66923	0.55726
C	-3.71354	0.31317	0.15493
C	-4.95123	-0.32044	-0.12465
N	-6.17611	0.20599	0.02003
C	-6.13675	1.46704	0.46125
N	-5.05441	2.21961	0.72146
N	-2.76580	2.47858	0.81442
C	-2.66685	-0.62976	-0.17019
N	-4.68833	-1.58584	-0.60223
H	-7.10151	1.95587	0.61814
C	-1.21101	-0.50202	-0.03460
C	-3.31959	-1.76396	-0.63191
C	-5.69973	-2.55895	-0.97758
H	-2.89722	-2.71451	-0.94119
H	-1.84530	2.21409	0.48625
H	-2.97192	3.46608	0.91446
H	-5.57942	-2.85883	-2.02722
H	-6.67841	-2.08518	-0.84686
H	-5.64038	-3.45052	-0.33861
C	1.62187	-0.31641	0.23939
C	0.75789	0.18071	1.24116
C	-0.62278	0.08403	1.10655
C	-0.34443	-0.99870	-1.03084
C	1.03595	-0.91496	-0.89975
C	3.02915	-0.21852	0.37351
H	1.18820	0.62993	2.13581
H	-1.26331	0.44012	1.91399
H	-0.77108	-1.43748	-1.93364
H	1.68395	-1.29982	-1.68678
C	4.24363	-0.13288	0.49145
C	5.65006	-0.04129	0.63647
C	8.46653	0.12848	0.93465
C	7.90317	-0.44936	-0.21536
C	6.52086	-0.53170	-0.35939
C	6.22861	0.54175	1.78930
C	7.60489	0.62413	1.93461
S	10.19659	0.28724	1.23751
H	8.53813	-0.84109	-1.00783
H	6.09864	-0.98416	-1.25630
H	5.57652	0.92826	2.57193
H	8.02618	1.07671	2.83333
C	10.96177	-0.44809	-0.22934
H	10.69730	-1.50741	-0.33402
H	12.04247	-0.36723	-0.06495
H	10.69935	0.10311	-1.14062

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.46	0.11757	YES	YES
8	a	14.31	0.09762	YES	YES
9	a	18.29	0.02864	YES	YES
10	a	40.03	1.46143	YES	YES
11	a	55.14	0.24128	YES	YES
12	a	56.75	1.30961	YES	YES
13	a	60.65	2.11716	YES	YES
14	a	71.34	0.73751	YES	YES
15	a	97.32	0.83872	YES	YES
16	a	105.66	1.65599	YES	YES
17	a	127.31	1.71389	YES	YES
18	a	136.59	0.02442	YES	YES
19	a	163.44	1.16431	YES	YES
20	a	186.29	0.41809	YES	YES
21	a	198.26	1.04937	YES	YES
22	a	208.87	0.32430	YES	YES
23	a	220.20	2.61482	YES	YES
24	a	236.80	3.63594	YES	YES
25	a	257.59	0.68846	YES	YES
26	a	275.09	1.32364	YES	YES
27	a	296.90	18.43221	YES	YES
28	a	322.06	22.99843	YES	YES
29	a	337.58	159.77215	YES	YES
30	a	344.94	7.23213	YES	YES
31	a	384.48	8.82932	YES	YES
32	a	390.61	3.68260	YES	YES
33	a	396.90	1.02487	YES	YES
34	a	406.49	2.71856	YES	YES
35	a	447.04	7.47401	YES	YES
36	a	456.81	4.52443	YES	YES
37	a	472.74	1.09239	YES	YES
38	a	501.93	34.91514	YES	YES
39	a	516.11	19.28145	YES	YES
40	a	523.19	4.61682	YES	YES
41	a	541.40	3.09082	YES	YES
42	a	543.18	0.27723	YES	YES
43	a	543.76	3.62397	YES	YES
44	a	552.96	3.99799	YES	YES
45	a	605.69	7.55806	YES	YES
46	a	617.44	2.90628	YES	YES
47	a	625.58	8.56051	YES	YES
48	a	633.70	0.65309	YES	YES
49	a	648.21	9.93464	YES	YES
50	a	669.92	2.06975	YES	YES

6a/iso1

bp86_def2-tzvpp energy (au): -1029.2919698880

Zero point energy (au): 0.3133864

XYZ coordinates:

41

C	-3.79434	1.74222	0.33192
C	-3.68611	0.35765	0.03721
C	-4.93412	-0.30220	-0.10100
N	-6.15113	0.25869	-0.05596
C	-6.09412	1.57581	0.16364
N	-5.00408	2.33366	0.37055
N	-2.71832	2.54942	0.57169
C	-2.65531	-0.65129	-0.06599
N	-4.69264	-1.64802	-0.27326
H	-7.05033	2.10409	0.19425
C	-1.19509	-0.51126	-0.04059
C	-3.32788	-1.85190	-0.24697
C	-5.71900	-2.65745	-0.46941
H	-2.91913	-2.84401	-0.40908
H	-1.82327	2.13690	0.80325
H	-2.93068	3.46693	0.94710
H	-5.59421	-3.15697	-1.43967
H	-6.68932	-2.15058	-0.44493
H	-5.68273	-3.40938	0.33056
C	1.64746	-0.29295	-0.03524
C	0.99663	-1.35962	0.62574
C	-0.38883	-1.45887	0.62462
C	-0.54120	0.54580	-0.70888
C	0.84482	0.65812	-0.70388
C	3.06090	-0.18195	-0.02798
H	1.59750	-2.10078	1.15207
H	-0.86762	-2.27419	1.16827
H	-1.13265	1.27163	-1.26747
H	1.32743	1.47829	-1.23476
C	4.27964	-0.08673	-0.02172
C	5.69484	0.02287	-0.01528
C	8.50369	0.23899	-0.00377
C	7.72943	1.17731	-0.69393
C	6.34047	1.07524	-0.70269
C	6.48826	-0.91853	0.67838
C	7.87646	-0.80691	0.68094
H	9.59050	0.32220	0.00004
H	8.21209	1.99504	-1.22977
H	5.73597	1.80518	-1.24004
H	5.99817	-1.73294	1.21086
H	8.47421	-1.54169	1.22093

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	15.61	0.07161	YES YES
8	a	17.81	0.01849	YES YES
9	a	23.92	0.08363	YES YES
10	a	52.97	3.25737	YES YES
11	a	61.52	0.51144	YES YES
12	a	67.86	1.23393	YES YES
13	a	88.61	0.40656	YES YES
14	a	112.03	1.26200	YES YES
15	a	125.55	1.37293	YES YES
16	a	141.87	0.84060	YES YES
17	a	161.82	0.18270	YES YES
18	a	185.59	0.85620	YES YES
19	a	219.63	0.82632	YES YES
20	a	225.17	3.40633	YES YES
21	a	248.06	4.46869	YES YES
22	a	274.31	0.59820	YES YES
23	a	306.06	2.65691	YES YES
24	a	336.44	83.80017	YES YES
25	a	344.88	82.19835	YES YES
26	a	363.57	34.55123	YES YES
27	a	394.44	1.83277	YES YES
28	a	394.90	0.02263	YES YES
29	a	405.78	3.53594	YES YES
30	a	440.60	3.70574	YES YES
31	a	468.01	0.70549	YES YES
32	a	499.00	35.09265	YES YES
33	a	518.41	13.94182	YES YES
34	a	523.11	9.00941	YES YES
35	a	540.56	1.30749	YES YES
36	a	543.52	3.05892	YES YES
37	a	545.83	1.21930	YES YES
38	a	550.12	0.98722	YES YES
39	a	573.13	6.46843	YES YES
40	a	606.33	8.31891	YES YES
41	a	616.76	0.11619	YES YES
42	a	626.12	9.44841	YES YES
43	a	647.69	9.64902	YES YES
44	a	669.16	1.67414	YES YES
45	a	683.89	34.34613	YES YES
46	a	696.11	6.37981	YES YES
47	a	707.14	8.79225	YES YES
48	a	730.62	4.06845	YES YES
49	a	750.37	36.63822	YES YES
50	a	768.70	15.27019	YES YES

6a/iso2

bp86_def2-tzvpp energy (au): -1029.2919687440

Zero point energy (au): 0.3133548
Entropy (kJ mol-1 K-1): 0.66320
Chemical potential (kJ mol-1): 683.36

XYZ coordinates:

41

C	-3.80582	1.74771	0.36812
C	-3.69198	0.35024	0.14485
C	-4.93621	-0.32250	0.04254
N	-6.15576	0.21178	0.20217
C	-6.10469	1.52134	0.46473
N	-5.01833	2.30844	0.54224
N	-2.73301	2.59003	0.43686
C	-2.65669	-0.62179	-0.12552
N	-4.68788	-1.63963	-0.27755
H	-7.06331	2.02167	0.62291
C	-1.19756	-0.46515	-0.11280
C	-3.32235	-1.81186	-0.38288
C	-5.70831	-2.66025	-0.44329
H	-2.90807	-2.79280	-0.59212
H	-1.83261	2.28810	0.08648
H	-2.94552	3.58107	0.42061
H	-5.66778	-3.09058	-1.45284
H	-6.68158	-2.18112	-0.29357
H	-5.58112	-3.46269	0.29612
C	1.64096	-0.20922	-0.07417
C	0.98966	-0.95318	-1.08423
C	-0.39441	-1.07164	-1.10113
C	-0.54298	0.26559	0.90160
C	0.84135	0.39598	0.92114
C	3.05209	-0.07135	-0.06051
H	1.58827	-1.42324	-1.86402
H	-0.87526	-1.62471	-1.90882
H	-1.13244	0.71154	1.70334
H	1.32528	0.95831	1.71938
C	4.26820	0.05241	-0.04839
C	5.67992	0.19914	-0.02945
C	8.48133	0.49344	0.00984
C	7.70098	1.05898	1.02346
C	6.31568	0.91657	1.00869
C	6.47933	-0.36794	-1.04724
C	7.86386	-0.21917	-1.02310
H	9.56518	0.60785	0.02470
H	8.17588	1.61559	1.83184
H	5.70632	1.35627	1.79759
H	5.99700	-0.92279	-1.85125
H	8.46640	-0.66243	-1.81636

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.97	0.00265	YES	YES
8	a	20.13	0.12249	YES	YES
9	a	24.89	0.08115	YES	YES
10	a	52.93	2.97161	YES	YES
11	a	60.47	0.61560	YES	YES
12	a	67.53	1.01719	YES	YES
13	a	77.57	0.42495	YES	YES
14	a	110.92	1.65137	YES	YES
15	a	124.86	1.20598	YES	YES
16	a	141.86	0.85836	YES	YES
17	a	161.40	0.18635	YES	YES
18	a	185.28	1.04471	YES	YES
19	a	219.41	0.94844	YES	YES
20	a	223.55	3.22813	YES	YES
21	a	247.16	4.87694	YES	YES
22	a	273.60	0.50944	YES	YES
23	a	305.82	4.13840	YES	YES
24	a	328.97	156.89102	YES	YES
25	a	341.23	21.88927	YES	YES
26	a	363.09	18.23125	YES	YES
27	a	394.24	1.39091	YES	YES
28	a	395.02	0.03093	YES	YES
29	a	405.78	2.14785	YES	YES
30	a	440.46	3.37884	YES	YES
31	a	468.19	0.90516	YES	YES
32	a	501.70	32.87651	YES	YES
33	a	518.61	12.42942	YES	YES
34	a	523.12	9.15400	YES	YES
35	a	540.42	1.64436	YES	YES
36	a	543.50	2.71968	YES	YES
37	a	545.83	1.40855	YES	YES
38	a	550.24	0.96475	YES	YES
39	a	573.14	6.98399	YES	YES
40	a	605.98	8.60067	YES	YES
41	a	616.95	0.14503	YES	YES
42	a	625.87	9.40982	YES	YES
43	a	648.20	9.85219	YES	YES
44	a	669.71	2.08227	YES	YES
45	a	684.21	34.42062	YES	YES
46	a	696.22	6.34874	YES	YES
47	a	707.12	8.64277	YES	YES
48	a	731.56	3.56562	YES	YES
49	a	750.60	36.33560	YES	YES
50	a	768.35	14.89494	YES	YES

4a/iso1

bp86_def2-tzvpp energy (au): -1486.4298716420

Zero point energy (au): 0.4209254
Entropy (kJ mol-1 K-1): 0.82363
Chemical potential (kJ mol-1): 938.10

XYZ coordinates:

55

C	-3.75026	1.81995	0.54525
C	-3.69419	0.46136	0.13593
C	-4.95820	-0.15200	-0.05586
N	-6.15272	0.46124	0.03960
C	-6.05078	1.75437	0.37683
N	-4.93911	2.44970	0.64493
N	-2.64970	2.55835	0.85061
C	-2.68393	-0.55586	-0.04843
N	-4.74507	-1.48703	-0.33736
H	-6.99088	2.30604	0.44904
C	-1.21984	-0.44397	-0.01016
C	-3.37957	-1.71810	-0.32752
C	-5.73945	-2.53784	-0.54596
H	-2.99719	-2.70436	-0.56858
H	-1.74561	2.11799	0.96402
H	-2.80974	3.47050	1.26138
C	1.62405	-0.27563	0.02636
C	0.94957	-1.35426	0.64228
C	-0.43760	-1.42958	0.62622
C	-0.54331	0.62425	-0.63603
C	0.84472	0.71239	-0.61558
C	3.03907	-0.18926	0.05144
H	1.53298	-2.12501	1.14500
H	-0.93577	-2.25640	1.13380
H	-1.11741	1.37754	-1.17661
H	1.34625	1.54168	-1.11363
C	4.25900	-0.11657	0.07480
C	5.67596	-0.03429	0.10216
C	8.48709	0.12766	0.15672
C	7.73819	1.12466	-0.47665
C	6.34780	1.04943	-0.50655
C	6.44368	-1.03519	0.73879
C	7.83356	-0.95009	0.76290
H	9.57508	0.19010	0.17762
H	8.24173	1.96731	-0.95108
H	5.76266	1.82505	-0.99948
H	5.93290	-1.87443	1.20968
H	8.41188	-1.73077	1.25768
C	-6.55054	-2.95214	0.70978
C	-7.98602	-2.46589	0.39202
C	-8.01986	-2.39608	-1.14103
C	-8.91300	-1.29717	-1.70775
O	-6.51797	-4.36860	0.82225
O	-8.97519	-3.39554	0.86208
O	-6.65846	-2.12444	-1.54441

O	-8.76579	-0.04867	-1.05511
H	-5.17084	-3.42169	-0.87893
H	-6.13606	-2.48228	1.61716
H	-8.15956	-1.46417	0.80624
H	-8.33841	-3.37669	-1.53981
H	-9.96329	-1.60841	-1.59228
H	-8.70746	-1.21910	-2.79207
H	-7.43845	-4.62791	1.03679
H	-9.35776	-3.04549	1.68111
H	-7.80961	0.08819	-0.83388

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	10.27	0.35005	YES	YES
8	a	14.59	0.02590	YES	YES
9	a	16.26	0.10032	YES	YES
10	a	27.65	0.15051	YES	YES
11	a	40.05	0.98693	YES	YES
12	a	46.37	4.24701	YES	YES
13	a	56.06	2.84119	YES	YES
14	a	63.31	1.14979	YES	YES
15	a	68.77	0.54337	YES	YES
16	a	99.62	3.00331	YES	YES
17	a	111.62	1.81996	YES	YES
18	a	122.22	0.84380	YES	YES
19	a	131.47	0.36889	YES	YES
20	a	136.62	6.34756	YES	YES
21	a	152.65	2.35137	YES	YES
22	a	172.85	0.30873	YES	YES
23	a	201.54	6.08800	YES	YES
24	a	219.48	4.32131	YES	YES
25	a	226.10	8.17430	YES	YES
26	a	227.35	7.81137	YES	YES
27	a	250.88	6.44644	YES	YES
28	a	260.49	48.69963	YES	YES
29	a	268.30	17.81490	YES	YES
30	a	276.36	123.33621	YES	YES
31	a	294.77	0.93024	YES	YES
32	a	302.40	6.97644	YES	YES
33	a	314.24	16.58015	YES	YES
34	a	317.55	4.54064	YES	YES
35	a	340.64	9.88850	YES	YES
36	a	373.99	4.96788	YES	YES
37	a	394.20	0.00246	YES	YES
38	a	403.14	1.48927	YES	YES
39	a	405.19	3.64608	YES	YES
40	a	447.03	1.39755	YES	YES
41	a	449.24	8.49302	YES	YES
42	a	470.93	2.96080	YES	YES

43	a	515.00	16.25388	YES	YES
44	a	518.87	24.23466	YES	YES
45	a	528.48	35.87887	YES	YES
46	a	535.86	28.22450	YES	YES
47	a	542.83	2.38615	YES	YES
48	a	545.55	18.14779	YES	YES
49	a	548.75	10.38167	YES	YES
50	a	555.22	6.36498	YES	YES

4a/iso2

bp86_def2-tzvpp energy (au): -1486.4299144010

Zero point energy (au): 0.4211681
Entropy (kJ mol-1 K-1): 0.81948
Chemical potential (kJ mol-1): 939.80

XYZ coordinates:

55

C	-1.36403	2.64228	0.67013
C	-1.46690	1.27915	0.28661
C	-2.79434	0.80801	0.12374
N	-3.91459	1.51586	0.35845
C	-3.66576	2.76438	0.77750
N	-2.47650	3.35740	0.93505
N	-0.17917	3.29777	0.80480
C	-0.57518	0.20962	-0.10096
N	-2.73190	-0.49018	-0.34321
H	-4.54145	3.37913	0.99842
C	0.89309	0.16111	-0.09366
C	-1.39763	-0.83506	-0.48123
C	-3.83454	-1.42303	-0.56569
H	-1.12872	-1.83493	-0.80554
H	0.67670	2.89173	0.44811
H	-0.22761	4.30123	0.93697
C	3.73744	0.00138	-0.06838
C	2.98908	-0.49499	-1.15975
C	1.60225	-0.41088	-1.16970
C	1.64206	0.64543	0.99941
C	3.03099	0.57329	1.01306
C	5.15327	-0.07288	-0.05823
H	3.51588	-0.93553	-2.00566
H	1.04878	-0.77429	-2.03632
H	1.12077	1.05403	1.86592
H	3.58844	0.94483	1.87241
C	6.37394	-0.13605	-0.04817
C	7.79150	-0.21268	-0.03704
C	10.60364	-0.36735	-0.01445
C	9.92103	0.17497	1.07919
C	8.53055	0.25400	1.07317
C	8.49262	-0.75826	-1.13582
C	9.88328	-0.83213	-1.11953
H	11.69188	-0.42764	-0.00555
H	10.47684	0.53873	1.94377
H	7.99708	0.67575	1.92442
H	7.92977	-1.11987	-1.99576
H	10.40958	-1.25567	-1.97532
C	-4.59023	-1.88571	0.70745
C	-5.99272	-1.24759	0.55175
C	-6.12796	-1.01640	-0.96008
C	-6.94493	0.21339	-1.34406
O	-4.68265	-3.30371	0.68859
O	-7.03008	-2.13289	1.00463
O	-4.77898	-0.83297	-1.44602

O	-6.63042	1.36743	-0.58522
H	-3.37936	-2.31598	-1.02366
H	-4.06970	-1.54431	1.61784
H	-6.04212	-0.28440	1.07485
H	-6.57172	-1.91652	-1.42386
H	-8.01045	-0.01088	-1.17769
H	-6.80740	0.38653	-2.42819
H	-5.60776	-3.50169	0.94491
H	-7.32113	-1.83873	1.88132
H	-5.65355	1.38880	-0.42171

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	11.78	0.04854	YES YES
8	a	16.09	0.15428	YES YES
9	a	18.12	0.05800	YES YES
10	a	28.61	0.20476	YES YES
11	a	39.66	3.42871	YES YES
12	a	49.31	2.26496	YES YES
13	a	52.20	0.73057	YES YES
14	a	61.22	2.67768	YES YES
15	a	71.41	1.77667	YES YES
16	a	100.61	2.64827	YES YES
17	a	113.60	1.08681	YES YES
18	a	120.39	0.60475	YES YES
19	a	132.27	0.70326	YES YES
20	a	138.89	6.94263	YES YES
21	a	153.36	1.23262	YES YES
22	a	165.94	2.32463	YES YES
23	a	204.00	2.31942	YES YES
24	a	220.87	2.97156	YES YES
25	a	227.34	2.60751	YES YES
26	a	231.94	10.89997	YES YES
27	a	258.09	8.51982	YES YES
28	a	266.72	5.44035	YES YES
29	a	273.62	10.04957	YES YES
30	a	281.49	1.33635	YES YES
31	a	293.07	177.47098	YES YES
32	a	302.96	10.03822	YES YES
33	a	314.02	9.28628	YES YES
34	a	320.42	19.98292	YES YES
35	a	340.42	7.15517	YES YES
36	a	372.59	1.39587	YES YES
37	a	394.88	0.00628	YES YES
38	a	404.25	1.20151	YES YES
39	a	422.02	1.67521	YES YES
40	a	428.73	1.84580	YES YES
41	a	455.44	10.79680	YES YES
42	a	469.73	0.49792	YES YES

43	a	514.62	17.89721	YES	YES
44	a	517.66	44.05265	YES	YES
45	a	524.87	9.56678	YES	YES
46	a	537.51	27.33256	YES	YES
47	a	542.90	6.15660	YES	YES
48	a	544.51	16.39943	YES	YES
49	a	548.94	9.53035	YES	YES
50	a	558.14	3.65380	YES	YES

4a/iso3

bp86_def2-tzvpp energy (au): -1486.4324934270

Zero point energy (au): 0.4208187
Entropy (kJ mol-1 K-1): 0.82194
Chemical potential (kJ mol-1): 938.48

XYZ coordinates:

55

C	-1.31016	2.63397	0.58826
C	-1.44423	1.27005	0.21739
C	-2.78162	0.81709	0.09648
N	-3.88232	1.58013	0.23114
C	-3.60540	2.85789	0.52291
N	-2.40408	3.41341	0.71557
N	-0.11278	3.23313	0.82718
C	-0.57878	0.12959	0.01591
N	-2.75079	-0.53956	-0.16397
H	-4.46581	3.52268	0.62732
C	0.88781	0.05317	0.00150
C	-1.42626	-0.93948	-0.20734
C	-3.87754	-1.43704	-0.36776
H	-1.18182	-1.97086	-0.43748
H	0.73242	2.68402	0.91752
H	-0.13825	4.16944	1.21305
C	3.72979	-0.14174	-0.05673
C	2.94582	-1.11328	0.60594
C	1.56052	-1.01146	0.63599
C	1.67226	1.01319	-0.67211
C	3.06003	0.92392	-0.69824
C	5.14460	-0.23250	-0.07582
H	3.44390	-1.94106	1.10979
H	0.97917	-1.75617	1.18073
H	1.17986	1.82245	-1.21260
H	3.64521	1.67240	-1.23175
C	6.36456	-0.30753	-0.08869
C	7.78142	-0.39442	-0.10253
C	10.59275	-0.56478	-0.12695
C	9.94726	0.49300	-0.77545
C	8.55744	0.58207	-0.76650
C	8.44524	-1.45850	0.54833
C	9.83562	-1.53795	0.53322
H	11.68073	-0.63035	-0.13593
H	10.53184	1.25476	-1.29192
H	8.05295	1.40556	-1.27084
H	7.85373	-2.21568	1.06192
H	10.33273	-2.36535	1.04020
C	-4.82475	-1.59565	0.85077
C	-6.15225	-1.96401	0.16346
C	-6.08603	-1.20989	-1.17559
C	-6.84002	0.12063	-1.18188
O	-4.37899	-2.54272	1.79714
O	-6.12489	-3.39767	-0.00911
O	-4.67366	-0.96509	-1.44146

O	-6.59123	0.91495	-0.03870
H	-3.43109	-2.42126	-0.60047
H	-4.93578	-0.62654	1.35289
H	-7.01806	-1.65770	0.76594
H	-6.46775	-1.85450	-1.98591
H	-7.92190	-0.09088	-1.20345
H	-6.58857	0.64962	-2.12061
H	-4.73748	-3.39945	1.49194
H	-7.03572	-3.72219	-0.06075
H	-5.62167	1.15314	-0.01796

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -
7	a	12.57	0.00853	YES YES
8	a	14.24	0.09462	YES YES
9	a	15.45	0.06588	YES YES
10	a	30.32	0.22766	YES YES
11	a	39.88	1.48145	YES YES
12	a	49.88	0.55524	YES YES
13	a	61.97	4.01160	YES YES
14	a	66.74	0.84801	YES YES
15	a	71.31	5.32095	YES YES
16	a	104.88	7.31218	YES YES
17	a	108.50	1.15891	YES YES
18	a	123.74	0.85914	YES YES
19	a	131.87	0.63725	YES YES
20	a	139.28	3.95895	YES YES
21	a	156.86	6.91204	YES YES
22	a	167.45	3.57867	YES YES
23	a	181.70	49.29169	YES YES
24	a	201.82	4.79964	YES YES
25	a	210.72	11.14877	YES YES
26	a	219.36	1.78436	YES YES
27	a	244.38	4.75202	YES YES
28	a	256.35	129.92218	YES YES
29	a	267.23	4.61281	YES YES
30	a	273.27	40.79855	YES YES
31	a	293.08	3.13941	YES YES
32	a	307.79	5.49349	YES YES
33	a	321.82	3.93108	YES YES
34	a	337.50	5.28173	YES YES
35	a	339.94	9.13033	YES YES
36	a	366.00	2.59317	YES YES
37	a	394.56	0.00133	YES YES
38	a	403.38	0.59549	YES YES
39	a	406.48	0.12941	YES YES
40	a	437.39	3.81241	YES YES
41	a	448.09	1.80719	YES YES
42	a	470.43	2.24790	YES YES

43	a	473.73	78.40501	YES	YES
44	a	514.74	22.84825	YES	YES
45	a	521.06	17.71797	YES	YES
46	a	525.15	13.02989	YES	YES
47	a	530.59	12.46912	YES	YES
48	a	541.33	0.77610	YES	YES
49	a	545.58	0.49666	YES	YES
50	a	552.45	1.66012	YES	YES

5/iso1

bp86_def2-tzvpp energy (au): -798.1486536287

Zero point energy (au): 0.2347541

XYZ coordinates:

31

C	-1.92487	1.68800	-0.06030
C	-1.86015	0.27613	-0.00284
C	-3.10708	-0.38119	0.01558
N	-4.31479	0.20169	-0.00822
C	-4.22916	1.53647	-0.05891
N	-3.12397	2.30237	-0.08934
N	-0.81135	2.46858	-0.06631
C	-0.83252	-0.73950	0.02817
N	-2.87275	-1.74330	0.05708
H	-5.17764	2.07876	-0.08181
C	0.56232	-0.55261	0.02486
C	-1.51175	-1.95702	0.06360
C	-3.91100	-2.76015	0.08261
H	-1.10622	-2.96232	0.09624
H	0.09837	2.04436	-0.20075
H	-0.93234	3.45712	-0.24817
H	-3.83453	-3.41461	-0.79587
H	-4.87686	-2.24451	0.06709
H	-3.83782	-3.36756	0.99442
C	1.77272	-0.36674	0.02417
C	3.18125	-0.19227	0.01624
C	5.98205	0.14033	-0.01127
C	5.42054	-1.12202	-0.22903
C	4.03851	-1.29195	-0.21758
C	3.76182	1.07663	0.23959
C	5.14534	1.23603	0.22329
H	7.06427	0.26905	-0.02289
H	6.06553	-1.98210	-0.41103
H	3.60180	-2.27494	-0.39007
H	3.11437	1.93155	0.43249
H	5.57437	2.22312	0.39771

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	13.00	0.00860	YES	YES
8	a	32.55	0.15166	YES	YES

9	a	37.68	0.03276	YES	YES
10	a	78.36	1.03265	YES	YES
11	a	95.63	2.02062	YES	YES
12	a	110.94	1.62306	YES	YES
13	a	121.63	2.63383	YES	YES
14	a	187.93	5.72405	YES	YES
15	a	210.60	3.57844	YES	YES
16	a	221.35	9.73557	YES	YES
17	a	250.85	54.42929	YES	YES
18	a	260.65	71.76825	YES	YES
19	a	266.58	31.35220	YES	YES
20	a	310.65	2.28345	YES	YES
21	a	330.17	5.59116	YES	YES
22	a	395.13	0.01225	YES	YES
23	a	410.64	0.06578	YES	YES
24	a	446.70	0.24778	YES	YES
25	a	513.86	4.86516	YES	YES
26	a	517.69	1.13839	YES	YES
27	a	521.87	1.96660	YES	YES
28	a	527.70	8.29626	YES	YES
29	a	540.10	6.98425	YES	YES
30	a	543.45	12.45085	YES	YES
31	a	577.57	7.23737	YES	YES
32	a	615.11	1.26569	YES	YES
33	a	622.59	13.87522	YES	YES
34	a	625.97	8.15202	YES	YES
35	a	667.13	0.20071	YES	YES
36	a	683.37	34.11455	YES	YES
37	a	696.50	13.96867	YES	YES
38	a	747.63	36.55254	YES	YES
39	a	750.31	3.69039	YES	YES
40	a	758.60	14.47249	YES	YES
41	a	788.99	7.61355	YES	YES
42	a	821.58	0.06807	YES	YES
43	a	829.45	21.78183	YES	YES
44	a	893.99	3.09926	YES	YES
45	a	932.18	4.07494	YES	YES
46	a	946.98	0.01144	YES	YES
47	a	960.44	3.78216	YES	YES
48	a	965.24	0.03366	YES	YES
49	a	987.05	2.54269	YES	YES
50	a	989.30	12.30597	YES	YES

5/iso2

bp86_def2-tzvpp energy (au): -798.1486521452

Zero point energy (au): 0.2347886
Entropy (kJ mol-1 K-1): 0.56369
Chemical potential (kJ mol-1): 494.25

XYZ coordinates:

31

C	-1.92642	1.67775	-0.21273
C	-1.86040	0.27203	-0.06932
C	-3.10684	-0.38421	-0.01267
N	-4.31491	0.19327	-0.09000
C	-4.23043	1.52210	-0.22705
N	-3.12596	2.28726	-0.28805
N	-0.81334	2.45436	-0.30020
C	-0.83230	-0.73525	0.05934
N	-2.87148	-1.73775	0.14345
H	-5.17942	2.05971	-0.29528
C	0.56236	-0.54702	0.05537
C	-1.51060	-1.94683	0.18781
C	-3.90861	-2.75151	0.23854
H	-1.10427	-2.94526	0.30541
H	0.09399	2.05622	-0.09041
H	-0.93829	3.45832	-0.26081
H	-3.83131	-3.46618	-0.59182
H	-4.87514	-2.23950	0.18619
H	-3.83524	-3.29360	1.19053
C	1.77306	-0.36357	0.04378
C	3.18183	-0.19040	0.03812
C	5.98293	0.13906	0.03441
C	5.15112	1.18272	-0.38315
C	3.76730	1.02447	-0.38470
C	4.03426	-1.23790	0.45646
C	5.41659	-1.06986	0.45165
H	7.06535	0.26647	0.03363
H	5.58418	2.12734	-0.71326
H	3.12323	1.83679	-0.72054
H	3.59365	-2.17893	0.78382
H	6.05807	-1.88913	0.77745

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number	IR intensity	selection rules
#		cm**(-1)	km/mol	IR RAMAN
1		0.00	0.00000	- -
2		0.00	0.00000	- -
3		0.00	0.00000	- -
4		0.00	0.00000	- -
5		0.00	0.00000	- -
6		0.00	0.00000	- -

7	a	12.46	0.01264	YES	YES
8	a	31.44	0.13746	YES	YES
9	a	37.46	0.01616	YES	YES
10	a	81.82	1.08327	YES	YES
11	a	95.89	1.99167	YES	YES
12	a	110.70	1.58648	YES	YES
13	a	124.04	2.92491	YES	YES
14	a	188.08	5.55507	YES	YES
15	a	210.60	3.42496	YES	YES
16	a	222.43	8.70143	YES	YES
17	a	251.61	43.89579	YES	YES
18	a	261.25	68.93696	YES	YES
19	a	267.24	46.16806	YES	YES
20	a	309.96	2.11610	YES	YES
21	a	330.83	5.64774	YES	YES
22	a	395.57	0.00876	YES	YES
23	a	410.67	0.06230	YES	YES
24	a	446.70	0.37446	YES	YES
25	a	513.90	4.70741	YES	YES
26	a	517.76	1.18034	YES	YES
27	a	522.00	2.25913	YES	YES
28	a	527.86	8.31657	YES	YES
29	a	540.24	8.10373	YES	YES
30	a	543.85	11.30441	YES	YES
31	a	577.53	7.26756	YES	YES
32	a	614.99	1.23165	YES	YES
33	a	622.72	13.47037	YES	YES
34	a	625.61	8.75143	YES	YES
35	a	667.17	0.20644	YES	YES
36	a	683.87	34.20113	YES	YES
37	a	696.46	13.93690	YES	YES
38	a	747.87	36.27688	YES	YES
39	a	750.15	3.77768	YES	YES
40	a	758.57	14.53409	YES	YES
41	a	789.77	7.55776	YES	YES
42	a	822.37	0.04555	YES	YES
43	a	829.28	21.94431	YES	YES
44	a	894.57	3.12794	YES	YES
45	a	932.50	4.08991	YES	YES
46	a	947.81	0.01114	YES	YES
47	a	960.40	3.79611	YES	YES
48	a	965.59	0.03851	YES	YES
49	a	987.07	2.61551	YES	YES
50	a	989.38	12.21548	YES	YES

3/iso1

bp86_def2-tzvpp energy (au): -1255.2864818270

Zero point energy (au): 0.3425949
Entropy (kJ mol-1 K-1): 0.71956
Chemical potential (kJ mol-1): 750.76

XYZ coordinates:

45

C	-1.26587	2.54923	0.48241
C	-1.44852	1.18672	0.14874
C	-2.78526	0.76270	0.00406
N	-3.86812	1.55086	0.14445
C	-3.55426	2.81660	0.46041
N	-2.33900	3.35121	0.64016
N	-0.03663	3.09799	0.64272
C	-0.59418	0.04478	-0.08073
N	-2.76979	-0.58856	-0.30243
H	-4.39855	3.49880	0.58384
C	-1.45511	-1.01161	-0.35234
C	-3.90955	-1.49059	-0.47131
H	-1.21955	-2.04421	-0.58382
H	0.78812	2.50990	0.64157
H	0.02037	4.05193	0.97643
C	0.81308	0.00258	-0.05116
C	2.03680	-0.01836	-0.02765
C	3.45513	-0.08648	-0.00847
C	6.26920	-0.24086	0.02673
C	5.63464	0.99905	-0.09622
C	4.24429	1.08058	-0.11588
C	4.10871	-1.33360	0.11535
C	5.49938	-1.40397	0.13056
H	7.35735	-0.30065	0.03960
H	6.22783	1.90980	-0.18154
H	3.75332	2.04746	-0.22397
H	3.50878	-2.23907	0.19971
H	5.98699	-2.37453	0.22610
C	-4.69905	-1.82143	0.82287
C	-6.07549	-1.14907	0.59172
C	-6.17691	-1.02498	-0.93498
C	-6.93855	0.20442	-1.42178
O	-4.84090	-3.23175	0.91844
O	-7.15067	-1.96282	1.08734
O	-4.81353	-0.92823	-1.40673
O	-6.59407	1.39588	-0.73827
H	-3.48641	-2.43463	-0.85167
H	-4.17962	-1.42452	1.71107
H	-6.10102	-0.14779	1.04067
H	-6.64677	-1.93936	-1.34147
H	-8.01460	0.03225	-1.26190
H	-6.77503	0.29454	-2.51232
H	-5.77839	-3.37743	1.16511
H	-7.44714	-1.59584	1.93434
H	-5.61449	1.40804	-0.58475

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.82	0.01247	YES	YES
8	a	17.00	0.29379	YES	YES
9	a	25.55	0.26243	YES	YES
10	a	39.72	0.75937	YES	YES
11	a	45.22	4.14634	YES	YES
12	a	53.71	1.01672	YES	YES
13	a	93.39	0.67216	YES	YES
14	a	98.17	2.66838	YES	YES
15	a	112.36	2.48030	YES	YES
16	a	135.24	1.95537	YES	YES
17	a	141.55	5.23861	YES	YES
18	a	158.62	2.31234	YES	YES
19	a	186.78	15.99831	YES	YES
20	a	198.50	23.47979	YES	YES
21	a	222.47	22.03853	YES	YES
22	a	230.23	0.83279	YES	YES
23	a	233.73	114.69728	YES	YES
24	a	261.33	2.50982	YES	YES
25	a	267.34	1.25967	YES	YES
26	a	274.13	18.38742	YES	YES
27	a	279.82	2.39989	YES	YES
28	a	298.90	2.47016	YES	YES
29	a	314.37	21.73641	YES	YES
30	a	335.01	5.56588	YES	YES
31	a	351.68	0.95756	YES	YES
32	a	394.84	0.00369	YES	YES
33	a	413.81	4.16686	YES	YES
34	a	443.31	3.79460	YES	YES
35	a	455.11	0.91541	YES	YES
36	a	512.90	28.45230	YES	YES
37	a	516.01	3.41036	YES	YES
38	a	526.08	2.70456	YES	YES
39	a	533.30	29.69912	YES	YES
40	a	539.46	6.05092	YES	YES
41	a	544.80	10.38581	YES	YES
42	a	550.65	55.12686	YES	YES
43	a	557.69	8.79970	YES	YES
44	a	601.53	0.42978	YES	YES
45	a	617.76	0.40454	YES	YES
46	a	620.21	4.74467	YES	YES
47	a	628.62	15.76664	YES	YES
48	a	643.00	9.85617	YES	YES
49	a	670.51	2.66456	YES	YES
50	a	684.10	28.71628	YES	YES

3/iso2

bp86_def2-tzvpp energy (au): -1255.2864674680

Zero point energy (au): 0.3426813
Entropy (kJ mol-1 K-1): 0.71757
Chemical potential (kJ mol-1): 751.42

XYZ coordinates:

45

C	-1.29498	2.48759	0.84355
C	-1.46169	1.18347	0.32158
C	-2.79394	0.75807	0.14323
N	-3.88677	1.49019	0.43098
C	-3.58777	2.70082	0.92667
N	-2.37783	3.23307	1.14544
N	-0.07171	3.02574	1.07505
C	-0.59327	0.11509	-0.11585
N	-2.76239	-0.52405	-0.38175
H	-4.44072	3.33654	1.17497
C	-1.44202	-0.90123	-0.53767
C	-3.89021	-1.41279	-0.66456
H	-1.19435	-1.87724	-0.93915
H	0.76040	2.55269	0.74301
H	-0.02549	4.00189	1.33971
C	0.81465	0.10193	-0.12483
C	2.03885	0.10716	-0.11929
C	3.45836	0.07539	-0.13218
C	6.27603	-0.00105	-0.16834
C	5.60877	0.99033	0.55779
C	4.21673	1.03140	0.58020
C	4.14489	-0.92203	-0.86154
C	5.53699	-0.95541	-0.87485
H	7.36540	-0.03049	-0.18253
H	6.17745	1.73619	1.11364
H	3.70076	1.79953	1.15577
H	3.56925	-1.66380	-1.41404
H	6.04989	-1.73210	-1.44264
C	-4.63982	-1.95895	0.57872
C	-6.02806	-1.27686	0.49431
C	-6.17656	-0.92459	-0.99228
C	-6.97183	0.34792	-1.26731
O	-4.76762	-3.36767	0.44639
O	-7.08001	-2.17012	0.89239
O	-4.82865	-0.73050	-1.47902
O	-6.62812	1.43020	-0.42111
H	-3.46031	-2.27571	-1.19879
H	-4.09943	-1.70478	1.50588
H	-6.04780	-0.35546	1.09054
H	-6.64315	-1.77631	-1.52049
H	-8.03983	0.13113	-1.10790
H	-6.84113	0.60479	-2.33552
H	-5.69331	-3.56443	0.70137
H	-7.35344	-1.93863	1.79330
H	-5.64618	1.43408	-0.28486

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.32	0.05134	YES	YES
8	a	17.25	0.28878	YES	YES
9	a	25.88	0.08549	YES	YES
10	a	39.50	1.07634	YES	YES
11	a	44.70	3.92088	YES	YES
12	a	55.27	1.32379	YES	YES
13	a	94.13	0.99416	YES	YES
14	a	98.95	1.92890	YES	YES
15	a	112.41	2.27527	YES	YES
16	a	136.68	3.71962	YES	YES
17	a	139.70	5.21826	YES	YES
18	a	158.23	1.67471	YES	YES
19	a	188.36	5.29673	YES	YES
20	a	202.98	8.81590	YES	YES
21	a	227.18	14.78551	YES	YES
22	a	230.49	4.42415	YES	YES
23	a	254.96	108.64032	YES	YES
24	a	262.95	0.68584	YES	YES
25	a	265.93	28.99132	YES	YES
26	a	276.67	30.85723	YES	YES
27	a	290.06	6.51067	YES	YES
28	a	295.18	1.96090	YES	YES
29	a	312.98	18.15469	YES	YES
30	a	330.88	3.32518	YES	YES
31	a	352.14	3.41365	YES	YES
32	a	394.80	0.00933	YES	YES
33	a	419.96	2.35598	YES	YES
34	a	436.76	0.77395	YES	YES
35	a	457.32	4.33900	YES	YES
36	a	514.26	27.20923	YES	YES
37	a	515.78	1.57126	YES	YES
38	a	525.08	17.62754	YES	YES
39	a	532.45	5.85323	YES	YES
40	a	540.75	11.47373	YES	YES
41	a	541.77	20.14277	YES	YES
42	a	552.24	60.58571	YES	YES
43	a	557.83	6.27646	YES	YES
44	a	601.89	0.34416	YES	YES
45	a	617.90	0.09718	YES	YES
46	a	619.04	2.36517	YES	YES
47	a	628.59	18.76796	YES	YES
48	a	643.03	10.45841	YES	YES
49	a	670.12	3.19757	YES	YES
50	a	684.63	32.81392	YES	YES

3/iso3

bp86_def2-tzvpp energy (au): -1255.2890127420

Zero point energy (au): 0.3424254
Entropy (kJ mol-1 K-1): 0.72326
Chemical potential (kJ mol-1): 749.53

XYZ coordinates:

45

C	-1.29252	2.55317	0.76015
C	-1.46624	1.21755	0.32813
C	-2.79959	0.78040	0.20351
N	-3.88706	1.52989	0.46606
C	-3.58328	2.77144	0.87287
N	-2.37090	3.31788	1.02981
N	-0.06714	3.10670	0.92852
C	-0.60405	0.12383	-0.05711
N	-2.77632	-0.53289	-0.24017
H	-4.43327	3.41864	1.10058
C	-1.45895	-0.91675	-0.39967
C	-3.91388	-1.40025	-0.51225
H	-1.21776	-1.91609	-0.74273
H	0.76484	2.59975	0.65193
H	-0.01281	4.09077	1.15860
C	0.80329	0.10689	-0.08558
C	2.02758	0.10610	-0.10178
C	3.44594	0.05789	-0.13638
C	6.26246	-0.05756	-0.21442
C	5.61870	1.06403	0.31743
C	4.22786	1.12540	0.35926
C	4.10920	-1.07049	-0.67084
C	5.50030	-1.12229	-0.70597
H	7.35095	-0.10205	-0.24445
H	6.20512	1.89765	0.70464
H	3.73178	1.99923	0.78096
H	3.51590	-1.89955	-1.05493
H	5.99424	-2.00122	-1.12108
C	-4.81758	-1.70558	0.71138
C	-6.17274	-1.98003	0.03260
C	-6.14820	-1.06751	-1.20512
C	-6.89259	0.25520	-1.02081
O	-4.34736	-2.76464	1.51562
O	-6.16710	-3.38141	-0.31777
O	-4.74343	-0.79468	-1.48817
O	-6.60999	0.89470	0.20880
H	-3.48069	-2.34745	-0.88154
H	-4.90279	-0.80577	1.33295
H	-7.01231	-1.74491	0.69948
H	-6.56071	-1.60701	-2.07459
H	-7.97609	0.05178	-1.04065
H	-6.66183	0.89943	-1.88970
H	-4.72334	-3.57539	1.11901
H	-7.08078	-3.70134	-0.33435
H	-5.64186	1.13649	0.22976

Vibrational Spectrum (first 50 lines):

# mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	6.82	0.17829	YES	YES
8	a	20.23	0.13270	YES	YES
9	a	25.76	0.06700	YES	YES
10	a	43.83	2.55864	YES	YES
11	a	52.23	0.36551	YES	YES
12	a	62.25	5.49099	YES	YES
13	a	92.82	0.12844	YES	YES
14	a	102.74	3.89250	YES	YES
15	a	112.92	4.34213	YES	YES
16	a	124.53	4.17691	YES	YES
17	a	150.35	4.53971	YES	YES
18	a	158.73	0.22440	YES	YES
19	a	167.63	106.15538	YES	YES
20	a	182.35	46.48490	YES	YES
21	a	189.35	23.96105	YES	YES
22	a	211.67	3.33731	YES	YES
23	a	214.11	34.84253	YES	YES
24	a	257.18	1.14261	YES	YES
25	a	268.46	7.30371	YES	YES
26	a	274.47	0.52230	YES	YES
27	a	280.56	9.72553	YES	YES
28	a	296.83	1.69723	YES	YES
29	a	333.53	2.18474	YES	YES
30	a	343.25	3.35091	YES	YES
31	a	359.95	1.09614	YES	YES
32	a	393.82	0.02942	YES	YES
33	a	404.82	0.44730	YES	YES
34	a	435.17	0.93589	YES	YES
35	a	454.37	0.33947	YES	YES
36	a	480.74	73.16338	YES	YES
37	a	517.26	2.03236	YES	YES
38	a	518.20	4.25844	YES	YES
39	a	525.66	9.66355	YES	YES
40	a	529.63	19.66487	YES	YES
41	a	537.66	5.46983	YES	YES
42	a	543.46	14.74020	YES	YES
43	a	553.28	7.16241	YES	YES
44	a	587.82	1.71894	YES	YES
45	a	617.04	0.84877	YES	YES
46	a	623.95	14.62491	YES	YES
47	a	629.05	17.66201	YES	YES
48	a	645.74	8.91730	YES	YES
49	a	669.79	3.61721	YES	YES
50	a	683.01	33.37372	YES	YES

5.3 (RI-)PBE0/def2-TZVPP Level Calculations

6d/iso1

pbe0_def2-tzvpp energy (au): -1348.7349442970

XYZ coordinates:

38

C	-5.75692	1.31025	0.97657
C	-5.54588	0.12428	0.24535
C	-6.72137	-0.58029	-0.06124
N	-7.96833	-0.20191	0.21118
C	-8.01648	0.95350	0.84859
N	-6.99793	1.71205	1.25020
N	-4.75086	2.10043	1.42188
C	-4.44296	-0.66885	-0.22368
N	-6.37401	-1.74438	-0.67856
H	-9.00580	1.33074	1.08991
C	-3.00828	-0.38560	-0.20086
C	-5.00861	-1.79395	-0.76935
C	-7.30345	-2.72971	-1.16671
H	-4.52354	-2.62233	-1.26166
H	-3.81391	1.74358	1.45756
H	-5.01077	2.82042	2.07247
H	-7.20670	-2.85352	-2.24682
H	-8.30769	-2.38106	-0.93582
H	-7.13859	-3.69262	-0.68025
C	-0.23159	0.12458	-0.21963
C	-0.72726	-1.14528	0.09911
C	-2.08611	-1.38883	0.11310
C	-2.50796	0.87921	-0.52796
C	-1.14965	1.13312	-0.53349
C	1.16231	0.38148	-0.22543
H	-0.03084	-1.93526	0.35035
H	-2.44977	-2.37088	0.39130
H	-3.19701	1.66707	-0.80823
H	-0.78300	2.11741	-0.79629
C	2.35204	0.59666	-0.23190
C	3.74008	0.86189	-0.24415
C	4.31021	2.14141	-0.52251
C	4.71108	-0.07913	0.00954
H	3.71837	3.01699	-0.74768
C	5.66809	2.13129	-0.47224
S	6.27173	0.58108	-0.08924
H	6.34554	2.95341	-0.64033
H	4.56283	-1.12024	0.24692

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.33792247404908E+03 0.87420662058126E+00
0.29224922771837E+03 0.44970269408763E+00
0.28483531703901E+03 0.43673788171054E-02
0.27109137758250E+03 0.83365047428346E-01

0.26102904210213E+03	0.19692668505458E-01
0.25109895197329E+03	0.20369220283863E-02
0.25053896980727E+03	0.15590914998367E-02
0.24957244277517E+03	0.11599895957899E-01
0.24491122809806E+03	0.43263629676183E-01
0.24426715052668E+03	0.31633430181821E-02
0.23827501415133E+03	0.10551349886582E-01
0.23726240176749E+03	0.20109138437097E-01
0.23208988534885E+03	0.48133154197441E-02
0.22952736283528E+03	0.10195630880310E-01
0.22910851427291E+03	0.25045785971374E-02
0.22617325747924E+03	0.68517958133868E-01
0.22528101428896E+03	0.76213831753476E-01
0.21487916672949E+03	0.15695921668521E-01
0.21304144993992E+03	0.52432908955405E-01
0.21148567246617E+03	0.80405785486588E-01
0.20990628834462E+03	0.27667599968803E-01
0.20841777080398E+03	0.28068139187310E-02
0.20518628351231E+03	0.32181102667169E-02
0.20377651300143E+03	0.16996241780586E-01
0.20329633419515E+03	0.89480551275433E-01
0.20204333893562E+03	0.29575169382862E-03
0.20147984600215E+03	0.12480914826320E-01
0.20089195298959E+03	0.97620494243324E-03
0.19873700847826E+03	0.45870201282071E-01
0.19843043834524E+03	0.63353829894082E-02
0.19816574983203E+03	0.12432666083629E-01
0.19710691609982E+03	0.57823550530247E-02
0.19675605925476E+03	0.77016178357724E-01
0.19649636826381E+03	0.10770353558468E+00
0.19614858409509E+03	0.25168867959682E-01
0.19555968898383E+03	0.83152556714645E-01
0.19473326971187E+03	0.12214260707785E+00
0.19415718051362E+03	0.24514009605511E-02
0.19356794559323E+03	0.28023981533467E-01
0.19192789658862E+03	0.97349337467050E-02
0.19113661844806E+03	0.17918403276749E-02
0.19017323869774E+03	0.38761532407352E-01
0.18918212287105E+03	0.45300460100333E-01
0.18771907699930E+03	0.48235602438836E-02
0.18744197236698E+03	0.26767216936943E-01
0.18626469764590E+03	0.88316187628237E-01
0.18388860052283E+03	0.48840833336565E-01
0.18206842589788E+03	0.75068630505602E-01
0.18186407444527E+03	0.26508707457934E+00
0.18044451772484E+03	0.61330353509385E-02

6d/iso2

pbe0_def2-tzvpp energy (au): -1348.7349388970

XYZ coordinates:

38

C	-5.75710	1.30523	0.98402
C	-5.54532	0.12165	0.24923
C	-6.72013	-0.58426	-0.05679
N	-7.96726	-0.20912	0.21956
C	-8.01619	0.94458	0.86009
N	-6.99820	1.70402	1.26129
N	-4.75153	2.09607	1.42927
C	-4.44198	-0.66846	-0.22372
N	-6.37207	-1.74592	-0.67829
H	-9.00570	1.31937	1.10445
C	-3.00778	-0.38248	-0.20352
C	-5.00669	-1.79277	-0.77197
C	-7.30085	-2.73127	-1.16776
H	-4.52108	-2.61880	-1.26776
H	-3.81413	1.74031	1.46299
H	-5.01154	2.81366	2.08243
H	-7.20555	-2.85187	-2.24839
H	-8.30528	-2.38470	-0.93436
H	-7.13383	-3.69534	-0.68425
C	-0.23208	0.13248	-0.22972
C	-0.72462	-1.13838	0.08979
C	-2.08299	-1.38447	0.10659
C	-2.51066	0.88363	-0.53020
C	-1.15284	1.13994	-0.53905
C	1.16133	0.39179	-0.24139
H	-0.02613	-1.92751	0.33805
H	-2.44420	-2.36754	0.38445
H	-3.20184	1.67065	-0.80734
H	-0.78857	2.12517	-0.80158
C	2.34944	0.61537	-0.25683
C	3.74027	0.86552	-0.27003
C	4.73575	-0.11678	0.01975
C	4.30504	2.08544	-0.56289
H	4.50104	-1.14049	0.27410
C	5.99856	0.37875	-0.05988
S	5.99983	2.03190	-0.48551
H	6.92829	-0.14093	0.10916
H	3.78956	2.99754	-0.81701

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.33787622218244E+03 0.87388394317744E+00
 0.29222975889640E+03 0.44447019043640E+00
 0.28482479673007E+03 0.43326068235159E-02
 0.27105504318709E+03 0.51586620792540E-01
 0.26101296284322E+03 0.36781664119730E-01
 0.25092983930601E+03 0.27224899436389E-02
 0.25050664396647E+03 0.97470233410604E-03

0.24969329451436E+03	0.34616198909289E-01
0.24487582022227E+03	0.44352125583405E-01
0.24426554543831E+03	0.50837779001687E-02
0.23827111605015E+03	0.30121534792707E-02
0.23721409476772E+03	0.57946310787975E-01
0.23209667409187E+03	0.19717693710505E-02
0.22949023799981E+03	0.36277163076914E-01
0.22916283047849E+03	0.15904483517768E-02
0.22623248556264E+03	0.35957358693699E-01
0.22522801975677E+03	0.60579707145058E-01
0.21484858429498E+03	0.97549902187212E-02
0.21286682793007E+03	0.42484490892305E-01
0.21164653907627E+03	0.49174050921407E-01
0.20990062091001E+03	0.42767327202069E-01
0.20842423063419E+03	0.28199275393036E-02
0.20518437212784E+03	0.51834959064625E-02
0.20386489631582E+03	0.15257744792903E-01
0.20324111544183E+03	0.89872896808064E-01
0.20196407957486E+03	0.11782212716847E-02
0.20147323164639E+03	0.14557082569268E-01
0.20083413940594E+03	0.30668978240866E-02
0.19868141880987E+03	0.52766234039615E-01
0.19847034014311E+03	0.73869628475670E-03
0.19815352961804E+03	0.27108532149224E-01
0.19694204669782E+03	0.24226514356635E-02
0.19681130061919E+03	0.52149415599998E-02
0.19655285994205E+03	0.17787326077398E+00
0.19619931734983E+03	0.25134337298554E-01
0.19542592831761E+03	0.77679727913528E-01
0.19481969979134E+03	0.13427814143699E+00
0.19410863876645E+03	0.18875688377524E-02
0.19356995589330E+03	0.25850941634540E-01
0.19193392582897E+03	0.91719749904769E-02
0.19112891700956E+03	0.28562392469708E-02
0.19008381301544E+03	0.39495228514995E-01
0.18912806515018E+03	0.43964898947411E-01
0.18783809444165E+03	0.68516376513435E-02
0.18750051120278E+03	0.22434068668501E-01
0.18623686055782E+03	0.69658810788449E-01
0.18387913387969E+03	0.67751697503790E-01
0.18209933144674E+03	0.78006517252385E-01
0.18181662046209E+03	0.26841151209734E+00
0.18072131341480E+03	0.77936091381231E-02

6d/iso3

pbe0_def2-tzvpp energy (au): -1348.7349492030

XYZ coordinates:

38

C	-5.76871	1.29992	1.01680
C	-5.54443	0.08791	0.33407
C	-6.71148	-0.64345	0.06010
N	-7.95027	-0.33263	0.43583
C	-8.00193	0.79842	1.11532
N	-6.99964	1.62393	1.41178
N	-4.78312	2.17843	1.31903
C	-4.45100	-0.61530	-0.27827
N	-6.36909	-1.73347	-0.68248
H	-8.98228	1.10568	1.46719
C	-3.01930	-0.31631	-0.26274
C	-5.01495	-1.70948	-0.88520
C	-7.28871	-2.74083	-1.14354
H	-4.52875	-2.50834	-1.42308
H	-3.89608	2.11375	0.85473
H	-5.08115	3.07799	1.65222
H	-7.27531	-2.80823	-2.23263
H	-8.28577	-2.45424	-0.81595
H	-7.03995	-3.71654	-0.72200
C	-0.24267	0.19347	-0.23336
C	-0.88454	-0.22550	-1.40485
C	-2.24366	-0.46838	-1.41630
C	-2.37185	0.09275	0.90790
C	-1.01382	0.34758	0.92429
C	1.15040	0.45456	-0.22087
H	-0.30341	-0.34470	-2.31057
H	-2.72560	-0.76368	-2.34079
H	-2.94149	0.18677	1.82482
H	-0.53102	0.65615	1.84302
C	2.33910	0.67550	-0.21494
C	3.72796	0.93626	-0.19545
C	4.45013	1.35665	0.96287
C	4.55362	0.81797	-1.28970
H	3.98628	1.50914	1.92687
C	5.77364	1.54081	0.71599
S	6.16181	1.20923	-0.91301
H	6.54107	1.85381	1.40602
H	4.27395	0.51937	-2.28714

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.33792912721736E+03 0.87127499512396E+00
 0.29231394174006E+03 0.45214373330788E+00
 0.28480320982740E+03 0.42989605749412E-02
 0.27096942591279E+03 0.82176614820696E-01
 0.26096765586971E+03 0.19899768956577E-01
 0.25096772395248E+03 0.46847682356367E-03
 0.25063136312870E+03 0.11553791938349E-02

0.24984040739691E+03	0.14439216289635E-01
0.24490681487902E+03	0.43074472615413E-01
0.24427180352341E+03	0.30880144041385E-02
0.23824007398483E+03	0.10267328024399E-01
0.23725022065238E+03	0.21109874593506E-01
0.23208345668506E+03	0.49709391054016E-02
0.22949239527849E+03	0.13315902094503E-01
0.22922675107439E+03	0.26627827858815E-03
0.22617906781102E+03	0.67816279635793E-01
0.22527219246197E+03	0.76519837438566E-01
0.21484910064710E+03	0.16213700087269E-01
0.21307939134225E+03	0.46899853894505E-01
0.21144625146585E+03	0.82896257041342E-01
0.20994284560339E+03	0.28701424053944E-01
0.20841256190065E+03	0.29550903567281E-02
0.20515997971436E+03	0.32936977650338E-02
0.20389914459847E+03	0.15249052870441E-01
0.20329227347195E+03	0.90600692754500E-01
0.20205821061889E+03	0.24975381721889E-02
0.20153188073548E+03	0.13557381412076E-01
0.20086760425151E+03	0.12401576296014E-02
0.19879163628654E+03	0.41737736924748E-01
0.19844300547672E+03	0.14885368636160E-02
0.19818591079546E+03	0.24200584225370E-01
0.19714471126661E+03	0.11820519971335E-02
0.19686577479062E+03	0.75424438924094E-01
0.19662881596220E+03	0.10451009233127E+00
0.19605608337045E+03	0.30488107018446E-01
0.19555212547112E+03	0.85091825849595E-01
0.19465729602093E+03	0.11452026938513E+00
0.19418800437626E+03	0.58893654403788E-03
0.19356918992370E+03	0.31636116337031E-01
0.19192491999238E+03	0.97970461492475E-02
0.19114993925058E+03	0.17372235538378E-02
0.19025740488173E+03	0.36575686946807E-01
0.18916995691112E+03	0.45429311665302E-01
0.18773533145874E+03	0.49845092882459E-02
0.18746902073277E+03	0.27311516973035E-01
0.18626739226032E+03	0.88614641189278E-01
0.18387531830838E+03	0.48659554331006E-01
0.18216280455583E+03	0.54189228730137E-01
0.18186073363650E+03	0.28778504725873E+00
0.18050552999492E+03	0.56417813090042E-02

6d/iso4

pbe0_def2-tzvpp energy (au): -1348.7349490410

XYZ coordinates:

38

C	-5.77633	1.30106	1.00929
C	-5.54684	0.08817	0.32985
C	-6.71051	-0.64982	0.05947
N	-7.95027	-0.34459	0.43660
C	-8.00673	0.78819	1.11283
N	-7.00836	1.61998	1.40499
N	-4.79478	2.18535	1.30759
C	-4.45066	-0.61139	-0.28178
N	-6.36362	-1.74015	-0.68056
H	-8.98804	1.09117	1.46573
C	-3.02025	-0.30635	-0.26565
C	-5.00981	-1.71009	-0.88489
C	-7.27887	-2.75285	-1.13859
H	-4.52030	-2.50815	-1.42098
H	-3.90742	2.12302	0.84364
H	-5.09641	3.08425	1.63926
H	-7.27013	-2.81893	-2.22784
H	-8.27624	-2.47301	-0.80614
H	-7.02185	-3.72738	-0.71936
C	-0.24523	0.21081	-0.23185
C	-0.88382	-0.21072	-1.40413
C	-2.24221	-0.45761	-1.41769
C	-2.37613	0.10600	0.90569
C	-1.01896	0.36509	0.92404
C	1.14760	0.47273	-0.21549
H	-0.30066	-0.32973	-2.30858
H	-2.72166	-0.75570	-2.34259
H	-2.94777	0.19936	1.82143
H	-0.53857	0.67641	1.84308
C	2.33600	0.69459	-0.19790
C	3.72598	0.95028	-0.18982
C	4.56706	0.85388	-1.34001
C	4.43848	1.32260	0.92664
H	4.20267	0.57555	-2.31848
C	5.86465	1.14951	-1.06555
S	6.08476	1.54665	0.57985
H	6.70283	1.15475	-1.74410
H	4.05640	1.46907	1.92400

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.33785041068519E+03 0.87040963628331E+00
 0.29226702786492E+03 0.44704162326096E+00
 0.28480317409592E+03 0.42752213385946E-02
 0.27091317864208E+03 0.51973269062271E-01
 0.26099153531996E+03 0.36028686763798E-01
 0.25100043195528E+03 0.34214343110912E-02
 0.25059695707651E+03 0.85119567227117E-03

0.24976944335831E+03	0.34023826817091E-01
0.24483302708467E+03	0.43622833392746E-01
0.24426218144754E+03	0.49611266847529E-02
0.23821434860343E+03	0.34106904602425E-02
0.23718988108416E+03	0.55498371397217E-01
0.23206775132332E+03	0.20594506891760E-02
0.22955456420058E+03	0.32769259802865E-01
0.22915690354803E+03	0.64635117071364E-02
0.22622006485909E+03	0.38519892891011E-01
0.22520043483533E+03	0.60394099822982E-01
0.21481619544878E+03	0.10053867533084E-01
0.21290224891125E+03	0.37109400333586E-01
0.21164178883445E+03	0.54235513399043E-01
0.20991335593638E+03	0.42864530153589E-01
0.20840546427410E+03	0.28950804995906E-02
0.20521958080438E+03	0.51731466716029E-02
0.20389109184046E+03	0.13028310121252E-01
0.20326891822796E+03	0.90176457230884E-01
0.20201895682911E+03	0.47688373957883E-02
0.20154250933593E+03	0.16010175376238E-01
0.20081340161202E+03	0.33009957376422E-02
0.19880379513126E+03	0.46766580954946E-01
0.19851431088556E+03	0.82928931224297E-03
0.19831130341910E+03	0.22501743148144E-01
0.19697608023246E+03	0.49331496506224E-02
0.19681129604712E+03	0.63374323137338E-01
0.19666722813066E+03	0.98054421586850E-01
0.19612726602035E+03	0.46696330692308E-01
0.19541103686430E+03	0.88454853655784E-01
0.19473261721669E+03	0.12828331272834E+00
0.19411832358476E+03	0.49207583680673E-03
0.19357697408464E+03	0.27670867422682E-01
0.19192121108541E+03	0.92320136023713E-02
0.19115833843709E+03	0.29201568923733E-02
0.19007131957340E+03	0.34907949329953E-01
0.18909653922512E+03	0.45716893112544E-01
0.18789530426246E+03	0.73380342760529E-02
0.18751958144300E+03	0.22231632813038E-01
0.18621585507356E+03	0.70083128771589E-01
0.18386092919740E+03	0.66644020976339E-01
0.18218401550841E+03	0.70566037938578E-01
0.18180685528769E+03	0.27861052688926E+00
0.18084503917795E+03	0.87303471165467E-02

6e/iso1

pbe0_def2-tzvpp energy (au): -1364.9051970200

XYZ coordinates:

44

C	-5.46631	1.78870	0.32241
C	-5.43788	0.40576	0.05193
C	-6.70677	-0.19023	-0.03143
N	-7.88242	0.42854	0.04891
C	-7.75540	1.72860	0.24306
N	-6.63276	2.42903	0.39380
N	-4.35221	2.53701	0.50801
C	-4.46801	-0.64753	-0.07477
N	-6.53947	-1.53327	-0.19411
H	-8.67670	2.30027	0.30281
C	-3.00842	-0.57457	-0.09876
C	-5.19770	-1.80183	-0.21470
C	-7.60930	-2.48709	-0.33475
H	-4.84475	-2.80909	-0.37181
H	-3.47834	2.08832	0.71149
H	-4.50142	3.46486	0.86349
H	-7.54659	-3.00206	-1.29489
H	-8.54865	-1.94091	-0.28248
H	-7.57916	-3.22433	0.46951
C	-0.19048	-0.45987	-0.15363
C	-0.85379	-1.47823	0.54103
C	-2.23285	-1.52696	0.57048
C	-2.34000	0.42738	-0.81094
C	-0.96029	0.48963	-0.83474
C	1.22425	-0.38020	-0.15186
H	-0.27179	-2.21928	1.07425
H	-2.72762	-2.30160	1.14415
H	-2.91507	1.15536	-1.37036
H	-0.46165	1.27312	-1.39136
C	2.43002	-0.29486	-0.13087
C	3.84240	-0.18261	-0.09069
C	6.61700	0.06285	0.02407
C	5.86445	1.00811	-0.66066
C	4.48958	0.88811	-0.71837
C	4.61406	-1.13252	0.58853
C	5.98878	-1.00974	0.64361
C	8.11212	0.17853	0.06111
H	6.35498	1.84542	-1.13984
H	3.90008	1.62650	-1.24583
H	4.12147	-1.96360	1.07598
H	6.57642	-1.74430	1.17883
F	8.62851	-0.35303	1.17604
F	8.51819	1.45283	0.00127
F	8.68590	-0.45924	-0.97306

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.36324874790519E+03 0.76904783363404E+00

0.30241278877579E+03	0.70972589197061E+00
0.28517147965027E+03	0.26588929418885E-02
0.27193148694583E+03	0.66312718996165E-01
0.27027167006034E+03	0.74370485814760E-03
0.26271295948309E+03	0.37059723481891E-01
0.26110783615046E+03	0.14353041211394E-01
0.25573012177131E+03	0.41369328479598E-02
0.25448400541529E+03	0.39737221845137E-01
0.25139965257019E+03	0.59139493092529E-02
0.24613429420173E+03	0.51745372341764E-02
0.24176589290988E+03	0.82580934045403E-02
0.23901871538723E+03	0.17947397462912E-01
0.23656874961018E+03	0.38704514976852E-02
0.23516988197277E+03	0.25816274098651E-01
0.22814648017356E+03	0.65420114981835E-01
0.22417457696641E+03	0.52132035843315E-01
0.21989459133224E+03	0.30918895744282E-01
0.21381214723323E+03	0.11866685754152E-01
0.21201432430011E+03	0.61569872149628E-01
0.21126005346701E+03	0.60560459464976E-01
0.21111746477538E+03	0.13441344621503E-01
0.20900908976842E+03	0.25055941109529E-02
0.20669910421909E+03	0.24615185817272E-02
0.20377226343574E+03	0.45661213551702E-02
0.20277024597864E+03	0.19301705886053E-01
0.20229149021252E+03	0.42249628383843E-01
0.20073357719988E+03	0.13125213578818E-01
0.19975446861710E+03	0.28673481790595E-02
0.19910163709330E+03	0.37728704583134E-02
0.19804450934241E+03	0.12243780772336E+00
0.19703963866744E+03	0.11306807804449E-02
0.19640887700256E+03	0.13676691296925E-01
0.19636676292068E+03	0.13921331617190E-02
0.19602712705244E+03	0.28266082972033E-02
0.19585144857865E+03	0.11110798396750E+00
0.19491489154467E+03	0.18171262771637E-01
0.19412685674025E+03	0.37227904663131E-02
0.19372003343755E+03	0.37779441640201E-02
0.19330185330479E+03	0.10033256504123E+00
0.19247046056243E+03	0.46500289670431E-03
0.19078559021369E+03	0.15956187760843E+00
0.18986351480934E+03	0.12602037359429E-01
0.18918316243307E+03	0.58174376326055E-02
0.18682945968785E+03	0.44778344943395E-01
0.18639818485812E+03	0.35595125119114E-01
0.18533079466396E+03	0.20060675359326E+00
0.18300836001307E+03	0.46512591268099E-02
0.18270778737093E+03	0.64602901354115E-03
0.18125037133909E+03	0.34696752618506E+00

6e/iso2

pbe0_def2-tzvpp energy (au): -1364.9052723000

XYZ coordinates:

44

C	-5.44087	1.79957	0.37888
C	-5.42852	0.40924	0.14918
C	-6.70405	-0.17110	0.05901
N	-7.87108	0.44466	0.23377
C	-7.72777	1.73056	0.49850
N	-6.59810	2.43265	0.56778
N	-4.31865	2.55624	0.43593
C	-4.47278	-0.62767	-0.12705
N	-6.55413	-1.48781	-0.26011
H	-8.64089	2.29312	0.66849
C	-3.01179	-0.58106	-0.11923
C	-5.21669	-1.75446	-0.37448
C	-7.63402	-2.42706	-0.42018
H	-4.87515	-2.75550	-0.58696
H	-3.45647	2.19845	0.06866
H	-4.45867	3.55110	0.43225
H	-7.62904	-2.85518	-1.42384
H	-8.56673	-1.88865	-0.26617
H	-7.56003	-3.23262	0.31273
C	-0.19211	-0.55657	-0.08296
C	-0.89076	-1.23650	-1.08753
C	-2.27072	-1.24150	-1.10456
C	-2.30858	0.08871	0.88806
C	-0.92733	0.10650	0.90582
C	1.22458	-0.53968	-0.07138
H	-0.33493	-1.74923	-1.86238
H	-2.79354	-1.74857	-1.90662
H	-2.85733	0.58000	1.68254
H	-0.40098	0.62370	1.69819
C	2.43337	-0.52595	-0.06832
C	3.85036	-0.50857	-0.07556
C	6.63689	-0.46946	-0.10092
C	5.94329	0.18948	0.90536
C	4.56195	0.16952	0.92051
C	4.56287	-1.17134	-1.08190
C	5.94347	-1.15001	-1.09353
C	8.13420	-0.40384	-0.15126
H	6.48567	0.71363	1.68140
H	4.01849	0.67904	1.70532
H	4.01953	-1.70235	-1.85237
H	6.48632	-1.66833	-1.87338
F	8.66746	-1.51472	-0.67519
F	8.67294	-0.23602	1.06219
F	8.55734	0.62259	-0.90869

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.36307206156463E+03 0.76352030029939E+00

0.30237996582569E+03	0.71947484418719E+00
0.28513148763871E+03	0.26095502139676E-02
0.27164206775099E+03	0.68300213700011E-01
0.27020384382771E+03	0.15484106814350E-02
0.26230652030706E+03	0.41764623953791E-01
0.26142764139996E+03	0.95712248976751E-02
0.25566357784768E+03	0.39124643313094E-02
0.25438049792135E+03	0.36284119042411E-01
0.25150676157391E+03	0.55449217683026E-02
0.24613611214783E+03	0.49345514692798E-02
0.24164372351393E+03	0.88177637224609E-02
0.23891206951917E+03	0.16402223212533E-01
0.23650352036326E+03	0.35656537692461E-02
0.23509810465844E+03	0.24997892206279E-01
0.22811292007750E+03	0.66002821313938E-01
0.22418570365436E+03	0.51645326525707E-01
0.21992684195882E+03	0.30530193148194E-01
0.21383853163480E+03	0.12855547902316E-01
0.21212210274427E+03	0.48827015780365E-01
0.21120028538383E+03	0.82608728118735E-01
0.21107788067989E+03	0.50463991857816E-02
0.20896418240732E+03	0.19689358915148E-02
0.20666772256316E+03	0.23807637379067E-02
0.20383383511855E+03	0.47863758930034E-02
0.20278641592100E+03	0.13951650508021E-01
0.20222363875156E+03	0.49660873200499E-01
0.20069041827013E+03	0.12906449447239E-01
0.19976530891128E+03	0.44097997825481E-02
0.19907582928956E+03	0.36062031591622E-02
0.19792514952150E+03	0.12777856964160E+00
0.19710594532301E+03	0.68342856732564E-03
0.19638807108047E+03	0.19205478594875E-02
0.19632052927375E+03	0.30670493253351E-02
0.19594990089490E+03	0.27489509945435E-02
0.19578843284960E+03	0.10882942456925E+00
0.19480208010927E+03	0.30359059869750E-01
0.19408828658515E+03	0.48379965673792E-02
0.19373496476200E+03	0.86770421653446E-03
0.19335477103582E+03	0.97547757931865E-01
0.19243633867702E+03	0.47853594476178E-03
0.19081026178466E+03	0.16125123342675E+00
0.18986274876989E+03	0.11556907403494E-01
0.18919850344831E+03	0.43244402107383E-02
0.18684519268686E+03	0.43580291606212E-01
0.18633310710451E+03	0.34527273363980E-01
0.18529321936913E+03	0.19517665472652E+00
0.18296756050263E+03	0.72681408824022E-03
0.18273530769423E+03	0.75895956177869E-03
0.18124650583987E+03	0.35846294986024E+00

6b/iso1

pbe0_def2-tzvpp energy (au): -1142.4724831170

XYZ coordinates:

45

C	-4.65725	1.75219	0.16964
C	-4.54583	0.35879	-0.00852
C	-5.77713	-0.31039	-0.10115
N	-6.98620	0.24710	-0.10302
C	-6.93490	1.56140	0.01343
N	-5.85772	2.33113	0.15877
N	-3.59117	2.56880	0.34374
C	-3.51643	-0.64388	-0.03199
N	-5.53237	-1.64894	-0.17195
H	-7.88678	2.08417	0.00351
C	-2.06182	-0.49285	-0.00760
C	-4.17713	-1.84289	-0.12672
C	-6.54215	-2.66773	-0.29427
H	-3.76450	-2.83645	-0.20714
H	-2.69906	2.18146	0.58975
H	-3.79725	3.50996	0.62789
H	-6.41630	-3.23041	-1.22100
H	-7.51146	-2.17393	-0.30490
H	-6.50126	-3.35733	0.55073
C	0.75251	-0.25613	0.00239
C	0.11034	-1.24362	0.75944
C	-1.26599	-1.35191	0.75642
C	-1.41589	0.48504	-0.77129
C	-0.03945	0.60667	-0.76418
C	2.16434	-0.13358	0.01194
H	0.70704	-1.91607	1.36282
H	-1.74387	-2.10395	1.37313
H	-2.00415	1.14277	-1.40015
H	0.44095	1.36674	-1.36749
C	3.36933	-0.02955	0.02020
C	4.78119	0.09363	0.02608
C	7.57372	0.33651	0.03503
C	6.78945	1.23527	-0.68978
C	5.41858	1.11530	-0.69380
C	5.57809	-0.79691	0.74658
C	6.95867	-0.68343	0.75593
O	8.90744	0.53379	-0.02243
H	7.28303	2.02318	-1.24450
H	4.81745	1.81652	-1.25848
H	5.10438	-1.59203	1.30830
H	7.54278	-1.39259	1.32571
C	9.73934	-0.34643	0.69455
H	9.53209	-0.30829	1.76842
H	10.75934	-0.01407	0.51515
H	9.62999	-1.37706	0.34282

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.34107033477777E+03	0.12264041091346E+01
0.29928490266169E+03	0.32149232529457E+00
0.28633752597325E+03	0.46244111870729E-02
0.27481545764905E+03	0.29199717084092E-01
0.27202448129570E+03	0.67822359439876E-01
0.25460382255181E+03	0.11192159790649E-01
0.25286518882047E+03	0.14039584121007E-02
0.25140401324631E+03	0.74297665068953E-03
0.24436762513969E+03	0.24155376681308E-01
0.24267298549660E+03	0.18325284515652E-01
0.24078227020439E+03	0.36592374684993E-01
0.23939846830417E+03	0.34343067754519E-01
0.23745312104081E+03	0.18325420119906E-02
0.23134317509371E+03	0.14590027715752E-01
0.22912367902360E+03	0.47637695580991E-01
0.22829530404947E+03	0.98510815117651E-02
0.22184870908225E+03	0.53524057245180E-01
0.21999340901898E+03	0.87473479058936E-02
0.21644211866438E+03	0.89764191924570E-02
0.21434503196849E+03	0.48480911011849E-02
0.21363195703289E+03	0.80021409893922E-01
0.21185170173777E+03	0.93158059137688E-01
0.20982548608198E+03	0.12415700242880E-02
0.20768995582693E+03	0.29557320563439E-02
0.20510088942436E+03	0.99913724466907E-02
0.20429002210148E+03	0.19545912034974E-01
0.20246653681382E+03	0.52213999520229E-02
0.20056345652211E+03	0.54013882809918E-02
0.19960425890972E+03	0.62007836767648E-02
0.19829292053979E+03	0.57104283150778E-02
0.19813995459733E+03	0.44397033418497E-02
0.19755492198162E+03	0.79915260547706E-01
0.19717076493633E+03	0.21801752600588E-03
0.19676734355556E+03	0.55523866291265E-01
0.19523154808044E+03	0.89195861316013E-01
0.19456091172909E+03	0.15829194344675E+00
0.19368955326588E+03	0.15481410680912E+00
0.19172913646889E+03	0.61705502079097E-02
0.19131709040272E+03	0.31636945588075E-01
0.19046408304264E+03	0.26691137893927E-01
0.19027475001395E+03	0.19255643644458E-01
0.18977432165910E+03	0.39587121025245E-02
0.18924310211758E+03	0.97325538165367E-02
0.18859438854776E+03	0.86676790640610E-02
0.18652969367246E+03	0.18607818527752E-02
0.18582507446379E+03	0.51679882195508E-02
0.18523540095925E+03	0.79261678020369E-01
0.18483304905364E+03	0.20277707327201E-01
0.18463241049176E+03	0.12174720369489E+00
0.18323083280819E+03	0.53709571085861E-01

6b/iso2

pbe0_def2-tzvpp energy (au): -1142.4724938050

XYZ coordinates:

45

C	-4.67621	1.74486	0.16632
C	-4.56482	0.35070	-0.00599
C	-5.79612	-0.31995	-0.08686
N	-7.00563	0.23663	-0.08393
C	-6.95466	1.55148	0.02606
N	-5.87721	2.32276	0.16080
N	-3.60967	2.56321	0.32952
C	-3.53476	-0.65135	-0.02996
N	-5.55073	-1.65875	-0.15048
H	-7.90701	2.07344	0.02013
C	-2.08036	-0.49685	-0.01640
C	-4.19503	-1.85145	-0.11295
C	-6.56053	-2.67895	-0.26058
H	-3.78227	-2.84528	-0.18959
H	-2.71570	2.17748	0.57141
H	-3.81476	3.50515	0.61182
H	-6.43963	-3.24736	-1.18445
H	-7.53020	-2.18581	-0.26871
H	-6.51434	-3.36316	0.58851
C	0.73275	-0.24739	-0.02425
C	0.09975	-1.23348	0.74202
C	-1.27615	-1.34818	0.74752
C	-1.44316	0.47782	-0.79151
C	-0.06742	0.60583	-0.79282
C	2.14354	-0.11472	-0.02222
H	0.70292	-1.89946	1.34601
H	-1.74692	-2.09861	1.37168
H	-2.03814	1.12836	-1.42156
H	0.40616	1.36351	-1.40436
C	3.34723	0.00389	-0.02145
C	4.75770	0.14358	-0.02167
C	7.54704	0.42102	-0.02416
C	6.75481	1.32006	-0.73287
C	5.37708	1.17635	-0.72697
C	5.57217	-0.75223	0.68720
C	6.94170	-0.61695	0.68604
O	8.89423	0.47234	0.03409
H	7.19830	2.13299	-1.29074
H	4.76515	1.87813	-1.27949
H	5.11039	-1.56003	1.24066
H	7.57184	-1.30758	1.23199
C	9.54918	1.50495	-0.66282
H	9.35450	1.44893	-1.73825
H	10.61292	1.36461	-0.48414
H	9.24911	2.49043	-0.29361

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.34100191927430E+03	0.12256244063065E+01
0.29929652753352E+03	0.31697118734598E+00
0.28626755468399E+03	0.47751800014021E-02
0.27478832354207E+03	0.74695265259199E-02
0.27205917501683E+03	0.82394971286770E-01
0.25484488816360E+03	0.13094907358582E-01
0.25283562950978E+03	0.13338344309622E-02
0.25119700515101E+03	0.90520528263234E-03
0.24439408118441E+03	0.34940059227997E-01
0.24266647241702E+03	0.22931352363765E-01
0.24083238191122E+03	0.43559351263961E-01
0.23939130349724E+03	0.33469022103619E-01
0.23746727037226E+03	0.19858137863702E-02
0.23132340688503E+03	0.12719366990102E-01
0.22910600490256E+03	0.47646869896561E-01
0.22826646191228E+03	0.63899726322697E-02
0.22185665292262E+03	0.53114962013137E-01
0.22000695644970E+03	0.11626251423653E-01
0.21647822384944E+03	0.30844294114364E-02
0.21431518025167E+03	0.11256340534753E-01
0.21354536885923E+03	0.68008727695101E-01
0.21188312626872E+03	0.79918283429097E-01
0.20984519482184E+03	0.11663798912316E-02
0.20768708970437E+03	0.29676440150861E-02
0.20505081451671E+03	0.13662508833741E-01
0.20436242701055E+03	0.26640719692264E-01
0.20248497477435E+03	0.36996906531903E-02
0.20052673971540E+03	0.55502352534435E-02
0.19965183305947E+03	0.70130328691958E-02
0.19818431685242E+03	0.10448499941735E-01
0.19812349400854E+03	0.20841347503395E-02
0.19749933342917E+03	0.73536540302987E-01
0.19720928464918E+03	0.35285910506821E-02
0.19675001844635E+03	0.66298654744938E-01
0.19523115836527E+03	0.76178866218452E-01
0.19458669508295E+03	0.17076872737012E+00
0.19371945871581E+03	0.14161904069206E+00
0.19179054088264E+03	0.72384884474832E-02
0.19136391446628E+03	0.24591727457372E-01
0.19049416168300E+03	0.22482403155688E-01
0.19024693900894E+03	0.36575883320042E-01
0.18982790309511E+03	0.24353291196351E-02
0.18918284066916E+03	0.12232647270344E-01
0.18852009751157E+03	0.11415381491094E-01
0.18653794353270E+03	0.21065143065149E-02
0.18583030214754E+03	0.55128618334326E-02
0.18523891364935E+03	0.51813163996016E-01
0.18485984767027E+03	0.26816991154551E-01
0.18465058354226E+03	0.15313451141198E+00
0.18324830447536E+03	0.23853568979835E-01

6b/iso3

pbe0_def2-tzvpp energy (au): -1142.4724875070

XYZ coordinates:

45

C	-4.69220	1.75624	0.21447
C	-4.56055	0.35855	0.09269
C	-5.78155	-0.33245	0.03189
N	-6.99913	0.19503	0.14223
C	-6.96748	1.50489	0.30633
N	-5.90155	2.30296	0.33700
N	-3.63763	2.60513	0.22864
C	-3.51598	-0.61084	-0.09137
N	-5.51622	-1.65190	-0.18066
H	-7.92739	2.00045	0.41784
C	-2.06401	-0.43359	-0.07815
C	-4.15788	-1.81206	-0.25789
C	-6.51043	-2.68841	-0.27907
H	-3.72991	-2.79354	-0.39027
H	-2.73659	2.29018	-0.07983
H	-3.85476	3.58278	0.15175
H	-6.45000	-3.19303	-1.24481
H	-7.48770	-2.22036	-0.18154
H	-6.38474	-3.42454	0.51711
C	0.74482	-0.14471	-0.03313
C	0.11916	-0.94949	-0.99298
C	-1.25479	-1.08370	-1.01476
C	-1.43439	0.35986	0.88650
C	-0.06058	0.50717	0.90798
C	2.15368	0.00809	-0.01707
H	0.72645	-1.45580	-1.73271
H	-1.72059	-1.68639	-1.78548
H	-2.03340	0.84902	1.64562
H	0.40724	1.12233	1.66643
C	3.35597	0.13937	-0.00565
C	4.76453	0.29484	0.01019
C	7.55020	0.60483	0.04036
C	6.75816	1.24766	0.99305
C	5.39065	1.09489	0.97771
C	5.56913	-0.34168	-0.93566
C	6.94638	-0.19325	-0.92747
O	8.87975	0.81484	0.13589
H	7.24314	1.86482	1.73875
H	4.78348	1.59719	1.72000
H	5.10405	-0.96281	-1.69068
H	7.53655	-0.70193	-1.67697
C	9.71912	0.18876	-0.80448
H	9.64034	-0.90133	-0.74883
H	10.73405	0.48737	-0.55178
H	9.49159	0.51453	-1.82424

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.34098150149368E+03	0.12144109892208E+01
0.29948892954806E+03	0.33277931416863E+00
0.28627883423209E+03	0.50786194683862E-02
0.27465467406972E+03	0.26382063660058E-01
0.27166375138036E+03	0.68944608600381E-01
0.25427343987453E+03	0.12116946145458E-01
0.25321868492087E+03	0.16497132230636E-02
0.25168577693970E+03	0.16473210199419E-03
0.24429556311807E+03	0.23744706159303E-01
0.24260053295691E+03	0.19175595760712E-01
0.24074738682116E+03	0.34650360447758E-01
0.23935578661179E+03	0.36379261732579E-01
0.23739998019064E+03	0.21919491643435E-02
0.23139766790214E+03	0.13820287859772E-01
0.22908848275662E+03	0.50926077092697E-01
0.22832898173538E+03	0.65270823447756E-02
0.22188453686887E+03	0.53766312948312E-01
0.22003631478044E+03	0.83815883831517E-02
0.21645786795609E+03	0.97194407814103E-02
0.21445914517047E+03	0.56884788085978E-02
0.21373239165570E+03	0.64186841578755E-01
0.21182973859129E+03	0.10394188888291E+00
0.20973137282318E+03	0.14614791467750E-02
0.20770130809433E+03	0.27702207458255E-02
0.20497420931611E+03	0.10332341205039E-01
0.20426088606238E+03	0.20380946905832E-01
0.20247287638325E+03	0.51473931618606E-02
0.20076269306948E+03	0.66947354094760E-02
0.19958990175428E+03	0.59201329153268E-02
0.19855983533475E+03	0.18049917667213E-01
0.19803414649846E+03	0.67462018368974E-02
0.19755920591108E+03	0.62216562234845E-01
0.19706547834079E+03	0.16668020705417E-01
0.19673058033807E+03	0.42846440613435E-01
0.19513444556697E+03	0.14958765591998E+00
0.19445009289276E+03	0.77610306103159E-01
0.19362395572262E+03	0.18296993957522E+00
0.19168269592863E+03	0.72956711856923E-02
0.19127565525147E+03	0.31215768095689E-01
0.19046154715348E+03	0.24454551671212E-01
0.19015781413125E+03	0.10584875818359E-02
0.18985768555030E+03	0.33689258855716E-02
0.18929044878668E+03	0.12884663638420E-01
0.18879048623306E+03	0.91297365675951E-02
0.18651997864531E+03	0.20152544973124E-02
0.18585199985128E+03	0.51287541292210E-02
0.18515621699706E+03	0.76975024256297E-01
0.18482136597737E+03	0.21030329691580E-01
0.18462710773088E+03	0.12810088204681E+00
0.18308133029562E+03	0.10031321123383E+00

6b/iso4

pbe0_def2-tzvpp energy (au): -1142.4725013720

XYZ coordinates:

45

C	-4.72221	1.75067	0.20111
C	-4.58275	0.35362	0.08127
C	-5.79985	-0.34414	0.01925
N	-7.02036	0.17668	0.12882
C	-6.99605	1.48681	0.29201
N	-5.93461	2.29087	0.32207
N	-3.67223	2.60544	0.21462
C	-3.53256	-0.61009	-0.10082
N	-5.52700	-1.66192	-0.19410
H	-7.95872	1.97709	0.40300
C	-2.08172	-0.42497	-0.07938
C	-4.16765	-1.81475	-0.26890
C	-6.51532	-2.70396	-0.29378
H	-3.73422	-2.79409	-0.39957
H	-2.76994	2.29493	-0.09479
H	-3.89509	3.58154	0.13428
H	-6.45221	-3.20686	-1.26024
H	-7.49522	-2.24162	-0.19548
H	-6.38524	-3.44048	0.50129
C	0.72540	-0.12477	-0.01110
C	0.11129	-0.93423	-0.97432
C	-1.26190	-1.07412	-1.00746
C	-1.46346	0.37372	0.88834
C	-0.09061	0.52649	0.92107
C	2.13339	0.03170	0.01978
H	0.72696	-1.44153	-1.70629
H	-1.71843	-1.68240	-1.77940
H	-2.07082	0.86102	1.64202
H	0.36830	1.14426	1.68272
C	3.33494	0.16749	0.04806
C	4.74287	0.32811	0.07772
C	7.52662	0.65201	0.13136
C	6.73025	1.29273	1.07659
C	5.35525	1.12777	1.04371
C	5.56168	-0.31113	-0.86530
C	6.92841	-0.15258	-0.83968
O	8.87140	0.74822	0.07490
H	7.16833	1.92082	1.83969
H	4.74010	1.62855	1.78064
H	5.10522	-0.93625	-1.62228
H	7.56171	-0.64438	-1.56712
C	9.51955	1.54859	1.03424
H	9.19770	2.59242	0.96847
H	10.58263	1.48746	0.81255
H	9.34217	1.18022	2.04943

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.34098720797457E+03	0.12211797061605E+01
0.29935820076865E+03	0.32314839846126E+00
0.28623257928031E+03	0.49937377706473E-02
0.27471793674236E+03	0.85419571578540E-02
0.27183417687701E+03	0.81677775263793E-01
0.25428729686511E+03	0.14170059855039E-01
0.25300514665964E+03	0.13500338619870E-02
0.25171687475594E+03	0.16406046832586E-03
0.24430926683910E+03	0.32786075549278E-01
0.24260677599669E+03	0.23213440821069E-01
0.24076866580036E+03	0.42412825966883E-01
0.23930787038288E+03	0.33463562732213E-01
0.23740055373602E+03	0.22699022806363E-02
0.23135023407694E+03	0.12267294477810E-01
0.22908227825383E+03	0.48149329044781E-01
0.22826824692513E+03	0.71535148280560E-02
0.22188367784343E+03	0.52804969349407E-01
0.21999308614072E+03	0.11144101680376E-01
0.21643596271273E+03	0.42921157647461E-02
0.21447931525064E+03	0.54259479140491E-02
0.21362542101569E+03	0.64906254970788E-01
0.21185273585402E+03	0.86214354847629E-01
0.20977420910614E+03	0.13559522503820E-02
0.20768869174043E+03	0.27537582707831E-02
0.20496706857971E+03	0.13309713768375E-01
0.20425590119483E+03	0.27462540907982E-01
0.20247403634320E+03	0.38671128717145E-02
0.20063674862544E+03	0.66606265436480E-02
0.19959504262337E+03	0.65363194436911E-02
0.19847137549245E+03	0.17648200753623E-01
0.19795018869738E+03	0.74196702885714E-02
0.19749837919432E+03	0.51476308359681E-01
0.19712722754903E+03	0.16974982307039E-01
0.19670570864759E+03	0.62021415735976E-01
0.19514886877437E+03	0.11561291047389E+00
0.19451073318324E+03	0.11444336006588E+00
0.19363691766377E+03	0.17923716045937E+00
0.19176116224088E+03	0.66769492331129E-02
0.19125806557011E+03	0.23563501863518E-01
0.19046324956957E+03	0.19741553465496E-01
0.19020914626829E+03	0.13695740158145E-02
0.18983460703563E+03	0.22503757630300E-02
0.18919787276813E+03	0.13965293514188E-01
0.18866555654008E+03	0.12593007659220E-01
0.18652201709862E+03	0.25348707060198E-02
0.18585803244829E+03	0.51828341639087E-02
0.18516095805690E+03	0.59487950197524E-01
0.18484724751280E+03	0.25293624111618E-01
0.18463664846291E+03	0.15078733124272E+00
0.18316262253666E+03	0.79335193822881E-01

6c/iso1

pbe0_def2-tzvpp energy (au): -1465.3745435430

XYZ coordinates:

45

C	-5.01160	1.79928	0.26841
C	-4.96033	0.40938	0.04176
C	-6.21953	-0.20434	-0.05939
N	-7.40403	0.40278	-0.03045
C	-7.29664	1.70926	0.12883
N	-6.18675	2.42774	0.28952
N	-3.91076	2.56479	0.45947
C	-3.97442	-0.63421	-0.02607
N	-6.03210	-1.54905	-0.17593
H	-8.22570	2.27133	0.14565
C	-2.51472	-0.54512	-0.01847
C	-4.68615	-1.80092	-0.15178
C	-7.08527	-2.52019	-0.31958
H	-4.31679	-2.80761	-0.26993
H	-3.03485	2.13234	0.68803
H	-4.07604	3.50251	0.77965
H	-6.98917	-3.06063	-1.26294
H	-8.03265	-1.98555	-0.30878
H	-7.06877	-3.23500	0.50515
C	0.30655	-0.42873	-0.05023
C	-0.36475	-1.41619	0.68107
C	-1.74429	-1.46628	0.69813
C	-1.83979	0.43419	-0.75498
C	-0.45964	0.49685	-0.76810
C	1.72209	-0.36775	-0.06556
H	0.21227	-2.13649	1.24715
H	-2.24387	-2.22113	1.29383
H	-2.40933	1.14029	-1.34747
H	0.04317	1.25846	-1.35075
C	2.93044	-0.31527	-0.08388
C	4.34524	-0.24777	-0.10646
C	7.15365	-0.11071	-0.14972
C	6.38142	0.84029	-0.82455
C	5.00596	0.77325	-0.80403
C	5.12309	-1.19430	0.56477
C	6.50497	-1.12909	0.54563
S	8.89064	0.07878	-0.24800
H	6.87190	1.63854	-1.36966
H	4.42157	1.51693	-1.33079
H	4.63167	-1.99098	1.10907
H	7.07030	-1.88135	1.07846
C	9.51897	-1.29592	0.71287
H	9.20262	-1.23659	1.75421
H	10.60422	-1.21007	0.67109
H	9.22618	-2.25373	0.28275

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.35319007979918E+03	0.14365705946838E+01
0.31211243081547E+03	0.20772877380451E+00
0.28740915296657E+03	0.57826573679554E-02
0.28444102936991E+03	0.10160692023475E-01
0.27408556971294E+03	0.61166033335327E-01
0.26634806310503E+03	0.64103566795296E-01
0.25530183673138E+03	0.14504099007218E-02
0.25525949465114E+03	0.25582735246340E-03
0.25212445581648E+03	0.33105472004925E-01
0.24623161041100E+03	0.39909946688414E-01
0.24515170785522E+03	0.36152202593225E-02
0.24419927874790E+03	0.44487193886535E-01
0.24392298306324E+03	0.64828709735913E-02
0.23753463630490E+03	0.43958056215918E-03
0.23668966736700E+03	0.13805111457054E-01
0.23534788507362E+03	0.39731858656455E-01
0.23288094362106E+03	0.14297306632532E-02
0.22992978097180E+03	0.78578715329162E-02
0.22741072106821E+03	0.22810437757758E-01
0.22630861137068E+03	0.46590050749331E-01
0.21904372254978E+03	0.67260339577461E-01
0.21634359911542E+03	0.23766956443094E-01
0.21472954653360E+03	0.55735540212014E-01
0.21436945272565E+03	0.10257009096419E-02
0.21321644787534E+03	0.14447249266022E-01
0.20881012452110E+03	0.41427381622256E-02
0.20645604967166E+03	0.21312415365471E-01
0.20512782692950E+03	0.64069584328486E-02
0.20392668275478E+03	0.20057834658023E-01
0.20330896035964E+03	0.31048249313224E-02
0.20209695546395E+03	0.22183365372735E-01
0.20083529830316E+03	0.10495215514548E-01
0.20040211520557E+03	0.92121384547657E-03
0.19870615651174E+03	0.61675029324199E-01
0.19832573208769E+03	0.80042450278585E-01
0.19762617631668E+03	0.62615023355139E-03
0.19723018396642E+03	0.95723570848302E-02
0.19680115338685E+03	0.21752355185728E-02
0.19625978145567E+03	0.12524836790711E+00
0.19610071259728E+03	0.74541756159070E-02
0.19438226261762E+03	0.17816703952969E-01
0.19384600806337E+03	0.63448548260951E-03
0.19367611047678E+03	0.17463864507404E-02
0.19318833929271E+03	0.59410489241779E-01
0.19164694554308E+03	0.11241645583955E+00
0.19054947896701E+03	0.34204486975199E-02
0.19047148993468E+03	0.45561092291915E-03
0.18893432880063E+03	0.13577725685101E-01
0.18872287705539E+03	0.71429180833612E+00
0.18800192273468E+03	0.36866070675175E-01

6c/iso2

pbe0_def2-tzvpp energy (au): -1465.3745547940

XYZ coordinates:

45

C	-3.78365	1.68085	0.48682
C	-3.67135	0.35003	0.03738
C	-4.90077	-0.27041	-0.23820
N	-6.10584	0.29234	-0.17801
C	-6.05355	1.55561	0.20283
N	-4.97985	2.26592	0.54429
N	-2.72159	2.43255	0.86292
C	-2.64700	-0.64170	-0.14349
N	-4.65986	-1.57108	-0.56530
H	-7.00158	2.08232	0.25925
C	-1.19416	-0.51923	-0.02682
C	-3.30906	-1.78854	-0.50366
C	-5.66827	-2.53001	-0.93522
H	-2.89842	-2.75169	-0.76362
H	-1.84427	1.99053	1.06679
H	-2.93632	3.29799	1.32556
H	-5.51154	-2.88547	-1.95531
H	-6.63484	-2.03428	-0.87464
H	-5.65977	-3.38290	-0.25446
C	1.61757	-0.32945	0.15312
C	0.93657	-1.43878	0.66887
C	-0.43854	-1.52511	0.58365
C	-0.50878	0.58179	-0.55132
C	0.86656	0.67997	-0.45995
C	3.02786	-0.23322	0.25059
H	1.50179	-2.22658	1.15064
H	-0.94771	-2.37858	1.01561
H	-1.06455	1.36007	-1.06064
H	1.37792	1.53758	-0.87874
C	4.23184	-0.15470	0.33722
C	5.64205	-0.06904	0.44186
C	8.44145	0.09843	0.65071
C	7.71136	1.13410	0.07141
C	6.33411	1.04895	-0.03010
C	6.38438	-1.10645	1.02359
C	7.75536	-1.02406	1.12546
S	10.18154	0.08806	0.83598
H	8.20874	2.01705	-0.30614
H	5.77895	1.86108	-0.48263
H	5.86730	-1.98204	1.39527
H	8.30993	-1.83809	1.57799
C	10.69097	1.64899	0.12038
H	10.43258	1.70967	-0.93681
H	11.77572	1.67523	0.21826
H	10.26974	2.49626	0.66162

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.35308855839119E+03	0.14322575305158E+01
0.31223574025832E+03	0.20844342381228E+00
0.28739691759545E+03	0.59636633263285E-02
0.28433089664794E+03	0.77845712919310E-02
0.27391609110376E+03	0.58603050970932E-01
0.26629519697965E+03	0.65766143715001E-01
0.25549725808499E+03	0.17775187374420E-02
0.25531285860061E+03	0.39326949374410E-03
0.25202465544458E+03	0.47004467250214E-01
0.24617111158394E+03	0.41222433985531E-01
0.24513425074060E+03	0.35815473364210E-02
0.24410206453493E+03	0.46078831141805E-01
0.24399859022860E+03	0.42173433263901E-02
0.23750338919549E+03	0.13194586892227E-03
0.23666582614602E+03	0.77818052700219E-02
0.23533684692395E+03	0.38245559863500E-01
0.23289606135056E+03	0.13566579719546E-02
0.22995098349039E+03	0.59257817615006E-02
0.22744546761491E+03	0.13391034467651E-01
0.22630451152011E+03	0.55892505757997E-01
0.21896812462054E+03	0.72521446187410E-01
0.21649663211319E+03	0.75588880947873E-02
0.21462474523650E+03	0.61383464352022E-01
0.21436019789211E+03	0.58915629302679E-03
0.21321473781706E+03	0.14266635882305E-01
0.20882102025633E+03	0.39331713779418E-02
0.20644908144868E+03	0.20994340240444E-01
0.20504308869714E+03	0.66078737255747E-02
0.20391891652448E+03	0.28002389442274E-01
0.20324388033694E+03	0.27399601215958E-02
0.20216824975065E+03	0.23135997964653E-01
0.20095039911718E+03	0.86243270769552E-02
0.20035242753115E+03	0.10850045612604E-02
0.19870489678672E+03	0.64079486519195E-01
0.19828320288970E+03	0.72797979803842E-01
0.19758223286924E+03	0.26667122259005E-02
0.19716434398188E+03	0.15121645150163E-01
0.19687816360952E+03	0.16205046743473E-02
0.19627497481160E+03	0.12567978372735E+00
0.19597567650403E+03	0.56827813845778E-02
0.19445656545516E+03	0.22496677221242E-01
0.19381145707360E+03	0.43159442983724E-04
0.19370708966036E+03	0.15924316209614E-02
0.19315976732225E+03	0.54136668035502E-01
0.19162148156896E+03	0.10408676602225E+00
0.19060759799183E+03	0.32222885287048E-02
0.19046380251657E+03	0.39175180992918E-03
0.18891252709019E+03	0.30859709991647E-01
0.18864910157810E+03	0.73244511399672E+00
0.18802694029142E+03	0.11895082005077E-01

6c/iso3

pbe0_def2-tzvpp energy (au): -1465.3745552730

XYZ coordinates:

45

C	-5.04087	1.79781	0.28015
C	-4.97064	0.39691	0.14585
C	-6.22011	-0.24375	0.12609
N	-7.41042	0.33179	0.28324
C	-7.31976	1.63822	0.45301
N	-6.22174	2.39217	0.44941
N	-3.95242	2.60316	0.26152
C	-3.97381	-0.61280	-0.08110
N	-6.01665	-1.57140	-0.10329
H	-8.25408	2.17141	0.60174
C	-2.51615	-0.49677	-0.11958
C	-4.66991	-1.78598	-0.23052
C	-7.05503	-2.56642	-0.16949
H	-4.28737	-2.78318	-0.38278
H	-3.07819	2.25465	-0.08571
H	-4.13312	3.58904	0.19526
H	-7.04659	-3.07121	-1.13692
H	-8.00869	-2.05919	-0.03973
H	-6.93361	-3.30845	0.62190
C	0.30217	-0.33458	-0.17145
C	-0.43940	0.34676	0.80060
C	-1.81836	0.26153	0.82648
C	-1.77021	-1.17506	-1.08849
C	-0.39185	-1.10274	-1.11415
C	1.71618	-0.24982	-0.20302
H	0.08188	0.93353	1.54646
H	-2.36801	0.77059	1.60942
H	-2.28925	-1.75169	-1.84491
H	0.16619	-1.63169	-1.87636
C	2.92341	-0.18025	-0.23403
C	4.33742	-0.10471	-0.27368
C	7.14467	0.03884	-0.35077
C	6.44039	-0.69689	-1.30932
C	5.06548	-0.76754	-1.27186
C	5.04759	0.62911	0.67961
C	6.42880	0.70136	0.64421
S	8.88821	0.05248	-0.50021
H	6.98364	-1.21677	-2.09002
H	4.53395	-1.34090	-2.02072
H	4.50361	1.14827	1.45871
H	6.94066	1.27963	1.40116
C	9.42007	1.07375	0.87158
H	9.03524	2.09014	0.78876
H	10.50724	1.10467	0.80896
H	9.13643	0.63895	1.83000

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.35286889699557E+03	0.14210350341815E+01
0.31240583023684E+03	0.21680402834762E+00
0.28725750917422E+03	0.66710408665814E-02
0.28431715181188E+03	0.76841676513762E-02
0.27351131793620E+03	0.59459339120415E-01
0.26618947822091E+03	0.67456282095422E-01
0.25577521455357E+03	0.21687524843903E-02
0.25529637162159E+03	0.68505541517707E-04
0.25185362038708E+03	0.45513749201938E-01
0.24611673024096E+03	0.37613947451929E-01
0.24513261208243E+03	0.29872963767251E-02
0.24405468344790E+03	0.52104216865502E-01
0.24402122467195E+03	0.12145398583048E-02
0.23747949649984E+03	0.69121752988850E-03
0.23661871279194E+03	0.78623549771833E-02
0.23533120459415E+03	0.38012804210647E-01
0.23293002558900E+03	0.14123048911525E-02
0.22998351866097E+03	0.55999865691158E-02
0.22746988005813E+03	0.13239654183942E-01
0.22629969552083E+03	0.55694088945198E-01
0.21893557899914E+03	0.68127346917720E-01
0.21665379360552E+03	0.77980462642152E-02
0.21457120235447E+03	0.58271465487497E-01
0.21446126174580E+03	0.10390939104009E-01
0.21295114371453E+03	0.10736094863266E-01
0.20881042981830E+03	0.36197119504990E-02
0.20648646949172E+03	0.20189589258887E-01
0.20498814221150E+03	0.63574237211529E-02
0.20394492735975E+03	0.30374473075712E-01
0.20321054000703E+03	0.24660136656610E-02
0.20231182132414E+03	0.24338428769715E-01
0.20110129288374E+03	0.72718101659621E-02
0.20032963855782E+03	0.10629270063637E-02
0.19867161591855E+03	0.66338048467804E-01
0.19825130804623E+03	0.64844904621769E-01
0.19753031431862E+03	0.18040539978547E-02
0.19714050934808E+03	0.18481930933687E-01
0.19685494015283E+03	0.62602020338967E-04
0.19631987923473E+03	0.14159490372104E+00
0.19580501150250E+03	0.38640736512649E-02
0.19463451164666E+03	0.21857942979502E-01
0.19381755067366E+03	0.66178865723643E-03
0.19361648799387E+03	0.32504732270072E-02
0.19316524611013E+03	0.48205760787031E-01
0.19153435660184E+03	0.10327491166124E+00
0.19060814714413E+03	0.21557027684419E-02
0.19059028019686E+03	0.12361220532135E-02
0.18887397055060E+03	0.25187479199936E-01
0.18863705479161E+03	0.73846239344505E+00
0.18800441120693E+03	0.93741721574806E-02

6c/iso4

pbe0_def2-tzvpp energy (au): -1465.3745612790

XYZ coordinates:

45

C	-3.79085	1.65381	0.56493
C	-3.67873	0.31075	0.15296
C	-4.90685	-0.31091	-0.12522
N	-6.11847	0.21953	0.02744
C	-6.07203	1.46194	0.47264
N	-4.99481	2.20006	0.73457
N	-2.72339	2.44667	0.82036
C	-2.64395	-0.63072	-0.17612
N	-4.65477	-1.56155	-0.60390
H	-7.02727	1.95247	0.63468
C	-1.19285	-0.51171	-0.03741
C	-3.29804	-1.74622	-0.63563
C	-5.66100	-2.51906	-0.98332
H	-2.88244	-2.69063	-0.95069
H	-1.81234	2.17879	0.49710
H	-2.91824	3.42471	0.94054
H	-5.55773	-2.79436	-2.03437
H	-6.63356	-2.05599	-0.83016
H	-5.59191	-3.41892	-0.36954
C	1.61199	-0.34099	0.24130
C	0.75942	0.13587	1.24365
C	-0.61254	0.04569	1.10701
C	-0.33622	-0.98899	-1.03433
C	1.03560	-0.91251	-0.89948
C	3.01905	-0.24611	0.37799
H	1.18804	0.56584	2.14013
H	-1.25072	0.39053	1.91190
H	-0.76136	-1.40759	-1.93892
H	1.68048	-1.28260	-1.68650
C	4.22000	-0.16161	0.49544
C	5.62567	-0.05892	0.63833
C	8.41567	0.14781	0.92300
C	7.86181	-0.46737	-0.19781
C	6.48876	-0.56759	-0.33531
C	6.19135	0.55827	1.76303
C	7.55781	0.65951	1.90195
S	10.13161	0.33593	1.21022
H	8.49516	-0.87449	-0.97403
H	6.07156	-1.04845	-1.21122
H	5.53984	0.95914	2.52920
H	7.97399	1.14119	2.77925
C	10.88485	-0.42321	-0.22638
H	10.63950	-1.48291	-0.29628
H	11.95975	-0.32135	-0.08122
H	10.60517	0.09126	-1.14579

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.35324468902366E+03	0.14286074552067E+01
0.31243106927100E+03	0.21390697263172E+00
0.28735392335598E+03	0.60051029576291E-02
0.28429027559025E+03	0.99931924383028E-02
0.27381697495627E+03	0.60228516634272E-01
0.26642173579270E+03	0.64326626045788E-01
0.25551420082703E+03	0.17369826457390E-02
0.25530632260484E+03	0.35018283806328E-03
0.25208305228082E+03	0.33831805238094E-01
0.24620983286577E+03	0.38359369183473E-01
0.24519868781671E+03	0.53864293173811E-02
0.24418915426219E+03	0.47063238642158E-01
0.24402085549599E+03	0.44641831579488E-02
0.23751092379389E+03	0.27183560951552E-03
0.23666561695784E+03	0.14141127914001E-01
0.23535044615932E+03	0.39006895132647E-01
0.23291513636539E+03	0.13961183485766E-02
0.23006116610962E+03	0.73405006659551E-02
0.22750511078479E+03	0.23490686472455E-01
0.22635307197456E+03	0.46539985270086E-01
0.21905445415932E+03	0.63951891609606E-01
0.21634051198595E+03	0.22221467263925E-01
0.21473326010456E+03	0.60896432820386E-01
0.21435244863580E+03	0.55502811723049E-03
0.21313307454780E+03	0.13216103717626E-01
0.20881135673934E+03	0.38945822436496E-02
0.20650598481198E+03	0.19955204029115E-01
0.20513115087115E+03	0.67481119696133E-02
0.20397453833114E+03	0.21690395456088E-01
0.20325814965402E+03	0.27656532649342E-02
0.20218273269661E+03	0.23202448863437E-01
0.20097054080862E+03	0.96458960829490E-02
0.20040115417793E+03	0.93158694008213E-03
0.19869690389620E+03	0.60634666411663E-01
0.19832754863600E+03	0.79594948594792E-01
0.19760789465659E+03	0.97413860244376E-03
0.19726104258097E+03	0.98324936302313E-02
0.19674547605817E+03	0.43249311302908E-02
0.19629598906238E+03	0.12778781216880E+00
0.19594099281997E+03	0.78650682637970E-02
0.19452264322122E+03	0.17360627301535E-01
0.19381402232499E+03	0.71259613168548E-03
0.19368523275330E+03	0.16865182815675E-02
0.19318848025136E+03	0.56857563108280E-01
0.19161937260568E+03	0.11013241351372E+00
0.19051659066564E+03	0.44955975722186E-03
0.19050009242236E+03	0.33699082863324E-02
0.18893845685448E+03	0.15443443191412E-01
0.18868926480942E+03	0.70314725228520E+00
0.18799267865939E+03	0.41497866673231E-01

6a/iso1

pbe0_def2-tzvpp energy (au): -1028.0264851000

XYZ coordinates:

41

C	-3.76574	1.72941	0.33269
C	-3.66391	0.35439	0.04173
C	-4.89986	-0.29745	-0.09844
N	-6.10508	0.26638	-0.05165
C	-6.04489	1.56674	0.17046
N	-4.96219	2.31553	0.37271
N	-2.69306	2.52247	0.56774
C	-2.64142	-0.65011	-0.06620
N	-4.66442	-1.62813	-0.27561
H	-6.99316	2.09487	0.20527
C	-1.18595	-0.51174	-0.04174
C	-3.31084	-1.83377	-0.25165
C	-5.68200	-2.62809	-0.46978
H	-2.90535	-2.82050	-0.41284
H	-1.80635	2.10916	0.79035
H	-2.89284	3.43642	0.93414
H	-5.56048	-3.12421	-1.43438
H	-6.64739	-2.12707	-0.44441
H	-5.64657	-3.37679	0.32380
C	1.62869	-0.29662	-0.03814
C	0.98671	-1.34309	0.63472
C	-0.39026	-1.44135	0.63541
C	-0.53958	0.52538	-0.72288
C	0.83771	0.63617	-0.71840
C	3.04175	-0.18519	-0.03049
H	1.58390	-2.07094	1.16950
H	-0.86816	-2.24227	1.18719
H	-1.12841	1.24000	-1.28541
H	1.31854	1.44303	-1.25711
C	4.24682	-0.08934	-0.02340
C	5.66129	0.02238	-0.01549
C	8.44478	0.24190	-0.00062
C	7.67639	1.16730	-0.69382
C	6.29699	1.06238	-0.70373
C	6.44483	-0.90557	0.68051
C	7.82367	-0.79300	0.68530
H	9.52457	0.32678	0.00474
H	8.15556	1.97681	-1.23104
H	5.69508	1.78232	-1.24357
H	5.95755	-1.71170	1.21419
H	8.41819	-1.51805	1.22796

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.34472634503986E+03 0.89754625503403E+00
 0.29487376708381E+03 0.53485449489194E+00
 0.28425515569033E+03 0.37203359797541E-02
 0.27043592027184E+03 0.75179678104320E-01

0.26292548186125E+03	0.86043445271828E-03
0.25687486302296E+03	0.12861830555359E-03
0.25443298909959E+03	0.87667623343045E-02
0.25000245910913E+03	0.18018470381132E-02
0.24641772450523E+03	0.72816619077914E-02
0.24548798209421E+03	0.25661111346652E-01
0.23889355728517E+03	0.14721436799854E-01
0.23764311808470E+03	0.14565160413369E-01
0.23611256237012E+03	0.35713732189370E-01
0.23355138003458E+03	0.41116596263241E-02
0.23082597379986E+03	0.30961723763591E-01
0.22587458319472E+03	0.71935298095781E-01
0.22066211157192E+03	0.45590228943088E-01
0.21797432556629E+03	0.29329245191947E-02
0.21188149452016E+03	0.64786311324790E-01
0.21104620681841E+03	0.10200278624330E+00
0.21043838656050E+03	0.12883738375358E-02
0.20924510926328E+03	0.31443060906245E-03
0.20897913130716E+03	0.26876214071637E-02
0.20447124989154E+03	0.11644586944587E-01
0.20369893530799E+03	0.89407854330537E-02
0.20269315438125E+03	0.23863273528673E-02
0.20142801925288E+03	0.78204357473668E-02
0.19803265831352E+03	0.12427247664347E-01
0.19735198508563E+03	0.50096627627421E-04
0.19697072089391E+03	0.50883164911986E-02
0.19652727443109E+03	0.45546845025684E-01
0.19601965382224E+03	0.98436977457756E-01
0.19542577575468E+03	0.61739300529975E-02
0.19404382884027E+03	0.12142591068491E-01
0.19361207222448E+03	0.58875880859050E-03
0.19310481866530E+03	0.26779384306599E+00
0.19308690695832E+03	0.12977065016489E+00
0.19092503576710E+03	0.32703496063429E-01
0.19064656668197E+03	0.15695020877845E-01
0.19036119019384E+03	0.22395231171938E-01
0.18990319997599E+03	0.13297825424650E+00
0.18827822559090E+03	0.34762492651124E-01
0.18714354744986E+03	0.17647967700487E-02
0.18708737724690E+03	0.11691600500288E-02
0.18529809542215E+03	0.13222975179926E-02
0.18360421573244E+03	0.36121371720746E-01
0.18333334612605E+03	0.25066325641072E-02
0.18327441668442E+03	0.33978204360541E-02
0.18227724558568E+03	0.10976437102493E-01
0.18080719878991E+03	0.51989509509953E-01

6a/iso2

pbe0_def2-tzvpp energy (au): -1028.0265025820

XYZ coordinates:

41

C	-3.79652	1.73514	0.36443
C	-3.67490	0.34965	0.13777
C	-4.90075	-0.32874	0.04311
N	-6.11340	0.19494	0.21040
C	-6.07168	1.48887	0.47124
N	-5.00061	2.27709	0.54475
N	-2.73679	2.57563	0.42621
C	-2.63926	-0.60896	-0.13260
N	-4.64666	-1.63001	-0.27190
H	-7.02685	1.97931	0.63388
C	-1.18626	-0.44297	-0.12101
C	-3.29095	-1.79102	-0.38014
C	-5.64861	-2.65132	-0.43362
H	-2.87100	-2.76240	-0.59023
H	-1.84377	2.28138	0.07691
H	-2.95026	3.55714	0.42280
H	-5.61198	-3.07487	-1.43875
H	-6.62104	-2.18923	-0.27664
H	-5.50949	-3.45081	0.29645
C	1.62384	-0.18322	-0.07727
C	0.98484	-0.91067	-1.08822
C	-0.39033	-1.03110	-1.10880
C	-0.54265	0.27326	0.89368
C	0.83246	0.40638	0.91489
C	3.03472	-0.04848	-0.05872
H	1.58258	-1.36901	-1.86599
H	-0.86729	-1.57408	-1.91616
H	-1.13182	0.71014	1.69120
H	1.31190	0.95917	1.71294
C	4.23839	0.06463	-0.04323
C	5.65088	0.19832	-0.02533
C	8.43033	0.46223	0.00928
C	7.66319	1.03636	1.01377
C	6.28577	0.90813	1.00043
C	6.43315	-0.37684	-1.03352
C	7.80997	-0.24361	-1.01249
H	9.50846	0.56501	0.02248
H	8.14169	1.58839	1.81368
H	5.68484	1.35444	1.78255
H	5.94644	-0.92663	-1.82903
H	8.40342	-0.69360	-1.79917

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.34477856165810E+03 0.87190036275083E+00
 0.29518837810997E+03 0.55817915335363E+00
 0.28412915526193E+03 0.35967000423543E-02
 0.26985384420174E+03 0.75985709635253E-01

0.26276068660416E+03	0.84786517753413E-03
0.25688381000247E+03	0.12094414450452E-03
0.25441924485958E+03	0.90284374720690E-02
0.25045507606413E+03	0.19316964110312E-02
0.24646678457986E+03	0.60395698011681E-02
0.24548407513219E+03	0.26121934398168E-01
0.23896190537084E+03	0.14221075717525E-01
0.23747303048194E+03	0.16085519310319E-01
0.23610916805779E+03	0.31513714583334E-01
0.23363061959468E+03	0.41253914030364E-02
0.23106555217633E+03	0.31137921542860E-01
0.22573535164699E+03	0.73127746061551E-01
0.22085707443424E+03	0.46302750447138E-01
0.21811132524043E+03	0.37435542314300E-02
0.21218750790244E+03	0.41330925452260E-01
0.21090836649666E+03	0.12101153076981E+00
0.21056448756595E+03	0.33444605191540E-02
0.20920319709620E+03	0.34136400296968E-03
0.20894682783642E+03	0.27678444791838E-02
0.20433744371462E+03	0.12284543843249E-01
0.20359126724519E+03	0.90491842193754E-02
0.20270682657893E+03	0.27860432313758E-02
0.20168632693149E+03	0.82097596061044E-02
0.19828716901046E+03	0.21193248539024E-01
0.19728653401723E+03	0.68765679313240E-04
0.19699809775721E+03	0.14311001029120E-02
0.19644017112229E+03	0.70269455139850E-01
0.19592823238912E+03	0.75855333927794E-01
0.19530702085456E+03	0.27900371705297E-01
0.19407713300844E+03	0.97646375080754E-02
0.19343075631975E+03	0.48947905726308E-03
0.19305552036495E+03	0.96398338868679E-03
0.19300396945387E+03	0.36080380956445E+00
0.19081963004622E+03	0.31882302996552E-01
0.19063017212402E+03	0.23042732067007E-01
0.19039007288095E+03	0.18344823923359E-01
0.18991498545690E+03	0.13712425478382E+00
0.18832127266040E+03	0.32886227572147E-01
0.18734036978460E+03	0.12153157508366E-02
0.18714264754486E+03	0.99368674400711E-03
0.18538191754714E+03	0.14980424384391E-02
0.18359494683275E+03	0.36320321001180E-01
0.18333894741875E+03	0.45450274108119E-02
0.18310086828616E+03	0.21995418267912E-02
0.18220455586649E+03	0.12121209475272E-01
0.18077618829557E+03	0.41052224604661E-01

4a/iso1

pbe0_def2-tzvpp energy (au): -1484.6451167270

XYZ coordinates:

55

C	-3.74109	1.78278	0.58814
C	-3.68416	0.43448	0.18079
C	-4.93368	-0.17247	-0.01856
N	-6.11912	0.43614	0.07252
C	-6.02034	1.71273	0.40988
N	-4.91963	2.40225	0.68173
N	-2.64886	2.51188	0.89543
C	-2.68023	-0.57654	-0.00556
N	-4.72405	-1.49149	-0.30380
H	-6.95447	2.26183	0.47985
C	-1.22149	-0.46193	0.02980
C	-3.37001	-1.72301	-0.29164
C	-5.71409	-2.52160	-0.52597
H	-2.98812	-2.70218	-0.53388
H	-1.75545	2.07178	1.01357
H	-2.80591	3.41675	1.30126
C	1.59429	-0.28942	0.04867
C	0.93507	-1.35099	0.67939
C	-0.44354	-1.42909	0.67250
C	-0.55883	0.59148	-0.60850
C	0.82008	0.68105	-0.59713
C	3.00888	-0.20042	0.06155
H	1.51984	-2.10811	1.18623
H	-0.93565	-2.24485	1.18877
H	-1.13559	1.33473	-1.14625
H	1.31511	1.49985	-1.10380
C	4.21535	-0.12329	0.07193
C	5.63149	-0.03400	0.08392
C	8.41742	0.14123	0.10738
C	7.66311	1.12027	-0.52472
C	6.28227	1.03715	-0.53902
C	6.40078	-1.01619	0.71838
C	7.78115	-0.92512	0.72798
H	9.49835	0.20905	0.11629
H	8.15434	1.95461	-1.01054
H	5.69106	1.79891	-1.03113
H	5.90153	-1.84686	1.20082
H	8.36492	-1.69212	1.22235
C	-6.54448	-2.92236	0.70645
C	-7.94965	-2.40880	0.36711
C	-7.95160	-2.37844	-1.15651
C	-8.84036	-1.31565	-1.76505
O	-6.54357	-4.32203	0.80685
O	-8.95771	-3.27913	0.84305
O	-6.60431	-2.10628	-1.52424
O	-8.69657	-0.05760	-1.16937
H	-5.15611	-3.40759	-0.84522
H	-6.13739	-2.46811	1.61590
H	-8.08743	-1.39614	0.74732
H	-8.25295	-3.36561	-1.53139

H	-9.88224	-1.62629	-1.64217
H	-8.63272	-1.27944	-2.84315
H	-7.44734	-4.57335	1.03629
H	-9.35472	-2.89925	1.62679
H	-7.76396	0.07961	-0.92561

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.33573605364362E+03	0.10779733479593E+01
0.29145081014506E+03	0.42140038943612E+00
0.27986652090194E+03	0.45994076016673E-02
0.27211613640761E+03	0.70016334305632E-01
0.26068322168121E+03	0.23694604999642E-03
0.25744557918123E+03	0.99543121113298E-04
0.25162088364032E+03	0.48523728748615E-02
0.24767863374692E+03	0.52515014787598E-02
0.24597112530660E+03	0.16923956620312E-01
0.24309939266187E+03	0.17091380499268E-01
0.23970620869049E+03	0.31168737009816E-01
0.23634285945365E+03	0.44323794935184E-01
0.23508273594791E+03	0.27646166679883E-01
0.23487590748481E+03	0.25439018901451E-02
0.22911609379032E+03	0.19163820490702E-02
0.22612391715986E+03	0.79714383123116E-01
0.22454499069138E+03	0.66657991387339E-02
0.21906974632669E+03	0.13086494509811E-01
0.21810082857219E+03	0.33187427506979E-01
0.21568769652668E+03	0.12579331365216E-01
0.21312870120366E+03	0.77826337120555E-01
0.21179799580277E+03	0.22283325902212E-02
0.21033254675239E+03	0.90036585272572E-03
0.20976942149881E+03	0.80840580923146E-02
0.20932092914837E+03	0.19162055243639E-02
0.20832116650024E+03	0.44185484329466E-02
0.20807699320368E+03	0.40258270992748E-02
0.20794882777580E+03	0.21447800832746E-01
0.20478181461137E+03	0.10840219069363E-02
0.20077322888451E+03	0.16175356075127E-02
0.19921300314571E+03	0.37314103628789E-01
0.19853728892551E+03	0.66763619064901E-02
0.19845385956112E+03	0.11962115433741E-02
0.19838739222289E+03	0.41485149186272E-01
0.19659958660671E+03	0.76295698546598E-02
0.19638796542733E+03	0.29128595413929E-01
0.19490607690610E+03	0.24517280753231E+00
0.19411202500965E+03	0.55813707727888E-03
0.19403527928609E+03	0.65639479718999E-01
0.19272833249250E+03	0.44066934386258E-01
0.19253342147028E+03	0.53096246642885E-01
0.19233783321732E+03	0.24848800189523E-01
0.19230668618837E+03	0.52558264287038E-03
0.19170565139159E+03	0.10379275312910E+00
0.19076256688755E+03	0.91007839369499E-01
0.18953052055744E+03	0.33292639037337E-01
0.18879441768327E+03	0.17809289461726E-02
0.18847155040452E+03	0.12555748327947E-01
0.18773094853025E+03	0.11350811020780E+00
0.18711912400164E+03	0.24721801832138E-02

4a/iso2

pbe0_def2-tzvpp energy (au): -1484.6451274060

XYZ coordinates:

55

C	-1.37029	2.62309	0.69240
C	-1.46370	1.27154	0.30323
C	-2.77417	0.79538	0.14343
N	-3.89026	1.48854	0.38223
C	-3.65308	2.72303	0.79801
N	-2.47806	3.31893	0.95641
N	-0.19820	3.27741	0.82903
C	-0.57201	0.21360	-0.08515
N	-2.70666	-0.48784	-0.31926
H	-4.52667	3.32893	1.01911
C	0.89121	0.17339	-0.08198
C	-1.38217	-0.82383	-0.45849
C	-3.79874	-1.40703	-0.54618
H	-1.10807	-1.81410	-0.78658
H	0.65170	2.88071	0.47336
H	-0.24936	4.27015	0.97163
C	3.70830	0.02233	-0.06426
C	2.96988	-0.45358	-1.15397
C	1.59155	-0.37326	-1.16109
C	1.63200	0.64084	1.00832
C	3.01228	0.57260	1.01779
C	5.12356	-0.05463	-0.05665
H	3.49395	-0.87723	-2.00127
H	1.03972	-0.72272	-2.02563
H	1.11340	1.03714	1.87357
H	3.56773	0.93143	1.87507
C	6.33045	-0.12574	-0.05141
C	7.74678	-0.21281	-0.04567
C	10.53274	-0.38976	-0.03327
C	9.86495	0.16372	1.05060
C	8.48443	0.25354	1.04861
C	8.42928	-0.76843	-1.13403
C	9.80999	-0.85419	-1.12369
H	11.61358	-0.45897	-0.02820
H	10.42394	0.52771	1.90414
H	7.96060	0.68406	1.89262
H	7.86260	-1.12999	-1.98268
H	10.32591	-1.28674	-1.97233
C	-4.55897	-1.86125	0.71298
C	-5.94038	-1.21420	0.54516
C	-6.05842	-1.02370	-0.96248
C	-6.89533	0.16501	-1.38316
O	-4.66389	-3.26014	0.69120
O	-6.97746	-2.05432	1.01375
O	-4.72621	-0.82160	-1.41826
O	-6.59429	1.33698	-0.67979
H	-3.35066	-2.29849	-0.99565
H	-4.04464	-1.52641	1.62002
H	-5.96621	-0.24069	1.03477
H	-6.47435	-1.93878	-1.40488

H	-7.94766	-0.07248	-1.20105
H	-6.77031	0.29936	-2.46624
H	-5.57069	-3.46365	0.95411
H	-7.27144	-1.74152	1.86941
H	-5.63722	1.37167	-0.50567

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.33553050772840E+03	0.10794538838112E+01
0.29119322671462E+03	0.42017152900737E+00
0.27983561731412E+03	0.51070181702466E-02
0.27216718343052E+03	0.70702094463043E-01
0.26067478864393E+03	0.22809198956287E-03
0.25741937251161E+03	0.87934055374954E-04
0.25144691501966E+03	0.60699083509342E-02
0.24753997868689E+03	0.42928558267543E-02
0.24604879668536E+03	0.15233375193374E-01
0.24219906588487E+03	0.15862453730166E-01
0.23982426591189E+03	0.32443192116575E-01
0.23677053323824E+03	0.45163973464886E-01
0.23503103011089E+03	0.27855493796541E-01
0.23463755407991E+03	0.42650306100068E-02
0.22905975272352E+03	0.10854598133404E-01
0.22587416424509E+03	0.74427825530337E-01
0.22443141367405E+03	0.41105375862440E-02
0.21885946793412E+03	0.13232736715732E-01
0.21796675596981E+03	0.33269828754985E-01
0.21461852199077E+03	0.21661075459288E-01
0.21273975294793E+03	0.55256916557033E-01
0.21174436892793E+03	0.88138538780740E-02
0.21043181660929E+03	0.41019521843313E-02
0.21008654513461E+03	0.16173421443717E-02
0.20957040387081E+03	0.64595439518206E-02
0.20869852054514E+03	0.19620419990859E-02
0.20803981461411E+03	0.32386796885315E-02
0.20759937940975E+03	0.29067891976145E-01
0.20685331784409E+03	0.11391438726751E-02
0.20030844535895E+03	0.14698820079220E-02
0.19942913379439E+03	0.24748889068122E-01
0.19860588841049E+03	0.65989676904259E-01
0.19848304397954E+03	0.14292993833556E-01
0.19802017280468E+03	0.21316515231164E-01
0.19653177410297E+03	0.72399623271644E-02
0.19535806685173E+03	0.11281343467177E-01
0.19449314776251E+03	0.40085547342384E-01
0.19404395111382E+03	0.25672513092898E+00
0.19395850475854E+03	0.16174862296369E-02
0.19322566222007E+03	0.24908343342441E-01
0.19237612093996E+03	0.12620331410945E-02
0.19225710101558E+03	0.53798447468527E-03
0.19156721897400E+03	0.91872252556830E-02
0.19128119135180E+03	0.14111549348540E+00
0.19003944054993E+03	0.16227723026463E+00
0.18967873540245E+03	0.64668840924611E-01
0.18878246304907E+03	0.11532583232250E-01
0.18862977984391E+03	0.14229479583012E-01
0.18829250239660E+03	0.62657490719179E-02
0.18726081908622E+03	0.10830693306952E+00

4a/iso3

pbe0_def2-tzvpp energy (au): -1484.6478367610

XYZ coordinates:

55

C	-1.30436	2.61012	0.61118
C	-1.43774	1.25575	0.24492
C	-2.76088	0.80731	0.11748
N	-3.85259	1.56664	0.24463
C	-3.57914	2.82870	0.53481
N	-2.38872	3.37925	0.73110
N	-0.11572	3.20094	0.85049
C	-0.57802	0.12206	0.04198
N	-2.73153	-0.53380	-0.14380
H	-4.43308	3.49164	0.63488
C	0.88352	0.04785	0.02748
C	-1.41822	-0.93234	-0.18685
C	-3.85113	-1.41498	-0.35640
H	-1.17386	-1.95756	-0.41471
H	0.71874	2.65322	0.94751
H	-0.13873	4.12992	1.23062
C	3.69763	-0.14251	-0.03728
C	2.92818	-1.09642	0.63893
C	1.55136	-0.99681	0.67297
C	1.65509	0.99156	-0.65840
C	3.03388	0.90414	-0.68716
C	5.11198	-0.23314	-0.06336
H	3.42693	-1.91013	1.15004
H	0.97513	-1.72886	1.22618
H	1.16150	1.79029	-1.19953
H	3.61355	1.64099	-1.22869
C	6.31848	-0.30778	-0.08447
C	7.73456	-0.39453	-0.10953
C	10.52077	-0.56363	-0.15765
C	9.87445	0.47652	-0.81146
C	8.49400	0.56414	-0.79020
C	8.39544	-1.43959	0.54629
C	9.77630	-1.51961	0.51983
H	11.60174	-0.62899	-0.17597
H	10.45033	1.22515	-1.34191
H	7.98696	1.37419	-1.29883
H	7.81193	-2.18349	1.07362
H	10.27531	-2.33371	1.03139
C	-4.80162	-1.56515	0.84132
C	-6.10412	-1.94936	0.14366
C	-6.01965	-1.20285	-1.18736
C	-6.78633	0.10648	-1.20956
O	-4.36444	-2.48446	1.79254
O	-6.06059	-3.36099	-0.02144
O	-4.62886	-0.94409	-1.41944
O	-6.56115	0.89747	-0.08054
H	-3.41593	-2.39667	-0.58449
H	-4.92713	-0.59585	1.32339
H	-6.97690	-1.64767	0.72571
H	-6.38189	-1.84991	-1.99460

H	-7.85745	-0.11868	-1.24451
H	-6.53199	0.63145	-2.14047
H	-4.68675	-3.34537	1.50243
H	-6.94901	-3.69545	-0.13960
H	-5.61223	1.14357	-0.04317

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.33753830245608E+03	0.10478735268822E+01
0.29146846602584E+03	0.45444044576862E+00
0.28065397827178E+03	0.55605329124632E-02
0.27266202454529E+03	0.70798273910955E-01
0.26122610810410E+03	0.44098827510918E-03
0.25709408741549E+03	0.11468142755525E-03
0.25349429171059E+03	0.44275794282944E-02
0.24805374288988E+03	0.65162207515762E-02
0.24720021909585E+03	0.22088038198523E-01
0.24327419054968E+03	0.10352968939773E-01
0.24010686900028E+03	0.13811007460681E-01
0.23650915864289E+03	0.44013588237284E-01
0.23596920873727E+03	0.23459470741921E-01
0.23529442378839E+03	0.17538489918573E-01
0.22949727054630E+03	0.55037836030213E-02
0.22583738299742E+03	0.50293257979777E-01
0.22519547496122E+03	0.28352582837971E-01
0.21906740259423E+03	0.12168536806346E-01
0.21873237676630E+03	0.38187900532624E-01
0.21654752317239E+03	0.24869760581816E-01
0.21501359709809E+03	0.60936832351649E-01
0.21152998522635E+03	0.14431011413019E-01
0.21075511391612E+03	0.34209750432684E-02
0.21001250796883E+03	0.21849888780545E-01
0.20962209092743E+03	0.61475773371178E-03
0.20934017932651E+03	0.54926221966958E-02
0.20829113757599E+03	0.20694825481897E-02
0.20599799289732E+03	0.54729806542219E-02
0.20151363435440E+03	0.39563709595840E-02
0.20099360367498E+03	0.14475484089336E-02
0.19893024283062E+03	0.32924854542721E-01
0.19809015089948E+03	0.21829305072765E-01
0.19798612468380E+03	0.33846853200111E-01
0.19652377879751E+03	0.24934571008292E-02
0.19635699162275E+03	0.37425361641803E-01
0.19525066322699E+03	0.10975123055847E+00
0.19456038703736E+03	0.18124137866483E+00
0.19377485271818E+03	0.65504648847835E-03
0.19356721787415E+03	0.53906556809377E-03
0.19266068447968E+03	0.52999327982989E-03
0.19252591579232E+03	0.11149358936865E-02
0.19196881750873E+03	0.13628441426710E+00
0.19165907876783E+03	0.36542142941887E-02
0.19107832631810E+03	0.46319019534423E-01
0.19074005916026E+03	0.10455874047203E+00
0.19062075299033E+03	0.10423565260069E+00
0.19006987471914E+03	0.89021188956415E-02
0.18966157683861E+03	0.23640785126755E-01
0.18904406147698E+03	0.34106771037903E-01
0.18854325503693E+03	0.13235710555990E-01

5/iso1

pbe0_def2-tzvpp energy (au): -797.1668591064

XYZ coordinates:

31

C	-1.90309	1.67359	-0.06472
C	-1.84771	0.27109	-0.00661
C	-3.08612	-0.37339	0.01504
N	-4.28020	0.21602	-0.00667
C	-4.18733	1.53423	-0.05669
N	-3.08691	2.28564	-0.08916
N	-0.79313	2.43764	-0.08229
C	-0.83510	-0.74443	0.02626
N	-2.86329	-1.72199	0.05865
H	-5.12581	2.07974	-0.07679
C	0.55976	-0.56493	0.02275
C	-1.51479	-1.94240	0.06490
C	-3.89670	-2.72528	0.09152
H	-1.11740	-2.94419	0.09970
H	0.10854	2.01204	-0.19446
H	-0.90182	3.42239	-0.23922
H	-3.82753	-3.38070	-0.77835
H	-4.85542	-2.21100	0.07690
H	-3.82465	-3.32529	1.00019
C	1.75670	-0.38216	0.02159
C	3.16362	-0.19964	0.01552
C	5.93667	0.14942	-0.00623
C	5.38902	-1.10481	-0.23964
C	4.01706	-1.28210	-0.23086
C	3.72640	1.05960	0.25373
C	5.09932	1.22866	0.24049
H	7.01119	0.28477	-0.01537
H	6.03617	-1.95219	-0.43146
H	3.58869	-2.25898	-0.41546
H	3.07631	1.90140	0.45599
H	5.51906	2.20973	0.42654

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.31755543689716E+03 0.64751969289571E+00
 0.27257017821899E+03 0.33867815760842E-01
 0.27107306549207E+03 0.29611283558912E-01
 0.26173895580976E+03 0.25263796829567E+00
 0.24440447603878E+03 0.25739345935378E-01
 0.24245266597737E+03 0.98909112187287E-02
 0.24023376613158E+03 0.33827884902403E-02
 0.23312409489901E+03 0.12925127012992E-01
 0.23085994834964E+03 0.77373580456107E-02
 0.22528519602863E+03 0.61450463510544E-03
 0.22188902722050E+03 0.24624522218594E-01
 0.21809328256382E+03 0.10342025512314E+00
 0.21269712719045E+03 0.17357572375272E-01
 0.21024728644032E+03 0.66365998608455E-01

0.20983458325496E+03	0.10402559712020E-01
0.20515213315790E+03	0.76030601791480E-01
0.20431400332170E+03	0.62425257408930E-03
0.20297212908272E+03	0.31661736656697E-01
0.20091746976488E+03	0.10974247396555E-01
0.20077459986397E+03	0.91775581639409E-02
0.19438947756573E+03	0.96355692653756E-02
0.19341228018489E+03	0.42577254088848E-01
0.19140405931911E+03	0.11727539886624E-01
0.19121678034270E+03	0.69003095351343E-03
0.18934011878080E+03	0.23244773564916E-01
0.18860111300126E+03	0.54818507237655E-02
0.18776588868400E+03	0.23955969821950E+00
0.18725016814754E+03	0.92707167501365E-01
0.18665859516435E+03	0.16004061083267E-01
0.18290016607219E+03	0.83600323553790E-01
0.18211215724539E+03	0.44821591464331E-01
0.18047570502225E+03	0.10506517414776E-02
0.17950912540165E+03	0.25487993781045E-02
0.17744855062107E+03	0.29521758803503E+00
0.17672800038159E+03	0.13164328930253E+00
0.17582948582376E+03	0.14302419038990E+00
0.17329290142110E+03	0.33738218508548E+00
0.17245426839960E+03	0.46842320479682E-01
0.17201060578604E+03	0.15089184694044E-01
0.17136570225609E+03	0.80598480707852E-01
0.17089367464776E+03	0.12390276947094E-01
0.16967169635468E+03	0.19626402694380E-02
0.16941297580097E+03	0.55678037663524E-02
0.16831985442044E+03	0.28667025759670E-01
0.16822328330318E+03	0.33269625717432E-01
0.16669253565377E+03	0.43696992371792E-01
0.16619759165831E+03	0.45779806975893E-03
0.16526014084695E+03	0.53193359683658E-02
0.16431546088535E+03	0.12497033737853E-01
0.16382745184640E+03	0.96928931361433E-02

5/iso2

pbe0_def2-tzvpp energy (au): -797.1668638610

XYZ coordinates:

31

C	-1.90140	1.65883	-0.20062
C	-1.84545	0.26210	-0.05984
C	-3.08330	-0.38227	-0.01071
N	-4.27726	0.20151	-0.09229
C	-4.18539	1.51378	-0.22635
N	-3.08564	2.26548	-0.28144
N	-0.79164	2.42063	-0.27350
C	-0.83215	-0.74600	0.06670
N	-2.85967	-1.72287	0.13960
H	-5.12414	2.05487	-0.29856
C	0.56286	-0.56468	0.06370
C	-1.51130	-1.93885	0.18685
C	-3.89198	-2.72380	0.22740
H	-1.11338	-2.93418	0.30143
H	0.10704	2.01705	-0.08211
H	-0.90536	3.41725	-0.25636
H	-3.81154	-3.43651	-0.59510
H	-4.85156	-2.21479	0.16647
H	-3.83038	-3.26116	1.17501
C	1.75989	-0.38201	0.05094
C	3.16679	-0.19797	0.04104
C	5.93928	0.15480	0.02718
C	5.10352	1.18012	-0.39326
C	3.73065	1.00885	-0.38938
C	4.01883	-1.22601	0.46256
C	5.39050	-1.04720	0.45293
H	7.01366	0.29140	0.02196
H	5.52425	2.11997	-0.72976
H	3.08101	1.80681	-0.72684
H	3.58958	-2.16191	0.79678
H	6.03668	-1.85223	0.78157

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.31750722362210E+03 0.64382651384603E+00
 0.27250082274191E+03 0.36561051333876E-01
 0.27104176649365E+03 0.27203559980527E-01
 0.26170778436139E+03 0.25023400047666E+00
 0.24462680163165E+03 0.29501737768101E-01
 0.24242769223359E+03 0.89679055298070E-02
 0.24025812242750E+03 0.34812055678607E-02
 0.23314074235082E+03 0.12917936006109E-01
 0.23082865113437E+03 0.85980645628204E-02
 0.22526011228136E+03 0.67813415020595E-03
 0.22189357756146E+03 0.24000547777635E-01
 0.21811058447726E+03 0.10540607463871E+00
 0.21251018214875E+03 0.16364287362271E-01
 0.21019950893533E+03 0.70481128695187E-01

0.20964899880984E+03	0.54848164728638E-02
0.20517501180815E+03	0.78362914898096E-01
0.20432907599169E+03	0.83584685880785E-03
0.20294667646598E+03	0.28467522378522E-01
0.20087755010674E+03	0.16046988286122E-01
0.20083891563788E+03	0.60011799219051E-02
0.19459681952301E+03	0.10371207641865E-01
0.19368533470988E+03	0.44068110647954E-01
0.19148609682669E+03	0.10592628759608E-01
0.19119126657619E+03	0.50528769111273E-03
0.18929037278398E+03	0.26583100492267E-01
0.18850669550172E+03	0.58596165150086E-02
0.18780930774922E+03	0.24654576332276E+00
0.18734610447070E+03	0.75939100754226E-01
0.18668127192513E+03	0.16088234714106E-01
0.18283669489156E+03	0.99234618194598E-01
0.18207625069071E+03	0.38890113301493E-01
0.18036248034304E+03	0.11952351580883E-02
0.17941478620675E+03	0.25985517631312E-02
0.17749392036508E+03	0.30214739988886E+00
0.17668499890489E+03	0.12580450070015E+00
0.17593291821808E+03	0.15146201915760E+00
0.17322438011895E+03	0.34118508101954E+00
0.17267820633197E+03	0.30498061124228E-01
0.17192075126025E+03	0.25286900790839E-01
0.17141373371160E+03	0.76514462432480E-01
0.17080931920897E+03	0.92626028670860E-02
0.16966921255053E+03	0.21034768241015E-02
0.16946350999437E+03	0.87226899801944E-02
0.16857339618723E+03	0.16748723253232E-01
0.16836552437009E+03	0.43485183575174E-01
0.16688326900742E+03	0.44108675286853E-01
0.16618577083234E+03	0.34827272703235E-03
0.16514916312161E+03	0.56519149031378E-02
0.16429723123134E+03	0.21199301171534E-01
0.16378450431026E+03	0.59535907022614E-02

3/iso1

pbe0_def2-tzvpp energy (au): -1253.7853954490

XYZ coordinates:

45

C	-1.24848	2.45678	0.58356
C	-1.44296	1.11856	0.20118
C	-2.77055	0.71523	0.04885
N	-3.83741	1.50013	0.22522
C	-3.51572	2.73560	0.58158
N	-2.30558	3.24912	0.77290
N	-0.02413	2.98140	0.76213
C	-0.60832	-0.01505	-0.07517
N	-2.77063	-0.60869	-0.30487
H	-4.34751	3.41683	0.73382
C	-1.47141	-1.03929	-0.37805
C	-3.91193	-1.47599	-0.50712
H	-1.24752	-2.05775	-0.65038
H	0.79078	2.39684	0.71745
H	0.04471	3.91935	1.11122
C	0.79881	-0.06325	-0.05658
C	2.00901	-0.06914	-0.03746
C	3.42910	-0.09657	-0.02407
C	6.22102	-0.15527	-0.00120
C	5.55154	0.99931	-0.38226
C	4.16832	1.03177	-0.39705
C	4.11343	-1.25551	0.35960
C	5.49673	-1.28059	0.36755
H	7.30376	-0.17851	0.00682
H	6.11080	1.87973	-0.67477
H	3.64575	1.92834	-0.70679
H	3.54641	-2.13064	0.65038
H	6.01346	-2.18485	0.66551
C	-4.70470	-1.83484	0.76183
C	-6.03727	-1.10188	0.56271
C	-6.14173	-0.97467	-0.95242
C	-6.90636	0.24035	-1.43192
O	-4.90477	-3.22326	0.78001
O	-7.12641	-1.84631	1.07203
O	-4.79716	-0.87470	-1.40904
O	-6.54850	1.42262	-0.77479
H	-3.50953	-2.40777	-0.91655
H	-4.17211	-1.50744	1.66132
H	-5.99482	-0.10620	1.00497
H	-6.60887	-1.88324	-1.35494
H	-7.97175	0.06843	-1.25201
H	-6.76480	0.32072	-2.51836
H	-5.81327	-3.35840	1.07818
H	-7.42387	-1.44836	1.89013
H	-5.58857	1.42206	-0.60816

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.31079560088509E+03	0.59195288893752E+00
0.27366360060210E+03	0.69039203873003E-01
0.26512122630869E+03	0.19095521160030E-02
0.25643554006481E+03	0.19022801930213E+00
0.25018670887625E+03	0.10390803141014E+00
0.24244564530509E+03	0.91519576747949E-02
0.24045259938806E+03	0.34853052428089E-02
0.23278392110996E+03	0.12580246907783E-01
0.23114089670205E+03	0.28403035197321E-01
0.22638129736701E+03	0.52337364719271E-03
0.22207021985705E+03	0.93931680993099E-01
0.22121247264290E+03	0.24241123523343E-02
0.21436498490803E+03	0.95063517604715E-01
0.21157753364502E+03	0.27339455206448E-02
0.21024417956551E+03	0.32323190857763E-02
0.20887353311740E+03	0.39135918854951E-01
0.20771764397847E+03	0.31997668974395E-01
0.20741782718589E+03	0.82457217353788E-01
0.20579150341111E+03	0.93300511859954E-02
0.20437526284953E+03	0.13497766137896E-01
0.20374858164929E+03	0.27760345821773E-01
0.20228695894651E+03	0.79535173335487E-02
0.19942621775255E+03	0.16179340223618E-01
0.19826877245827E+03	0.46851018750869E-01
0.19815976338114E+03	0.35243903356789E-02
0.19578933915668E+03	0.10210506045904E-01
0.19246830735580E+03	0.11294843091914E-01
0.19165956355406E+03	0.85842429113934E-02
0.19110831034835E+03	0.12238434630273E-01
0.19095480517526E+03	0.67383540816069E-01
0.19045060413824E+03	0.17053810865958E+00
0.18820824532042E+03	0.58549189284429E-01
0.18798464631194E+03	0.13542555251082E-01
0.18544649566942E+03	0.29462427273297E-02
0.18527457721109E+03	0.49617194233100E-01
0.18492626565119E+03	0.21790764646265E-03
0.18398771325335E+03	0.57404568725773E-02
0.18245158728020E+03	0.81762178200744E-02
0.18206880876545E+03	0.15427851423553E+00
0.18178800674121E+03	0.19042625885606E+00
0.18100251066440E+03	0.54141781826599E-01
0.18081785202017E+03	0.12599943094401E-01
0.18042796829035E+03	0.36728538035884E+00
0.17985400072039E+03	0.22703422616870E-02
0.17918637750896E+03	0.16847168805788E+00
0.17798839772381E+03	0.42157066406073E-01
0.17706148229833E+03	0.36532874108120E-01
0.17675900266886E+03	0.24716968463399E-02
0.17631522550785E+03	0.10150621314059E+00
0.17501804066764E+03	0.94617939833233E-01

3/iso2

pbe0_def2-tzvpp energy (au): -1253.7853439280

XYZ coordinates:

45

C	-1.27983	2.46440	0.70846
C	-1.45875	1.15195	0.23939
C	-2.78200	0.73628	0.08047
N	-3.85824	1.48284	0.34401
C	-3.55116	2.69359	0.78732
N	-2.34633	3.21867	0.98079
N	-0.06076	2.99457	0.91181
C	-0.60979	0.06501	-0.15546
N	-2.76573	-0.55060	-0.39061
H	-4.39159	3.34269	1.01408
C	-1.46038	-0.94517	-0.53175
C	-3.89278	-1.42970	-0.62339
H	-1.22385	-1.93296	-0.89234
H	0.76011	2.50303	0.60686
H	-0.00364	3.96896	1.14463
C	0.79838	0.04166	-0.15826
C	2.00850	0.05461	-0.13917
C	3.42903	0.05199	-0.12358
C	6.22116	0.04500	-0.09477
C	5.51594	0.70696	0.90068
C	4.13226	0.71091	0.89118
C	4.14912	-0.61153	-1.12338
C	5.53256	-0.61407	-1.10394
H	7.30417	0.04170	-0.08350
H	6.04735	1.22009	1.69301
H	3.58118	1.21687	1.67415
H	3.60975	-1.12095	-1.91167
H	6.07745	-1.13228	-1.88370
C	-4.62037	-1.91759	0.64138
C	-5.97250	-1.19710	0.56648
C	-6.15126	-0.95136	-0.92667
C	-6.96485	0.27704	-1.27243
O	-4.79751	-3.30569	0.54335
O	-7.02573	-2.00059	1.06096
O	-4.83152	-0.78104	-1.43343
O	-6.60452	1.41257	-0.53948
H	-3.48399	-2.31074	-1.12776
H	-4.05203	-1.66165	1.54225
H	-5.92548	-0.23926	1.08536
H	-6.61610	-1.83677	-1.38018
H	-8.01636	0.06267	-1.05968
H	-6.87581	0.44624	-2.35430
H	-5.69288	-3.48366	0.85845
H	-7.26322	-1.70124	1.93873
H	-5.63800	1.42466	-0.41635

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.31011002961290E+03	0.55806478506785E+00
0.27394809555796E+03	0.75188246658989E-01
0.26456816100094E+03	0.19015089635111E-02
0.25598224995499E+03	0.16440986192110E+00
0.25109976446110E+03	0.13608046728699E+00
0.24164816648938E+03	0.10366416740961E-01
0.24135785088557E+03	0.21171351688123E-02
0.23303004517905E+03	0.10957110626448E-01
0.23089652584209E+03	0.23311946823582E-01
0.22671205713375E+03	0.43754480490256E-02
0.22244284928694E+03	0.10552520915246E+00
0.22097519733509E+03	0.83655257437464E-02
0.21406255813695E+03	0.10307589330709E+00
0.21109877015420E+03	0.67065084241021E-02
0.21054774894652E+03	0.19450123635587E-01
0.20880735025324E+03	0.79222130894181E-02
0.20784118109698E+03	0.52978598336381E-01
0.20734457383215E+03	0.76249149513254E-01
0.20662744813113E+03	0.44542576286957E-01
0.20447458076497E+03	0.26036356788514E-01
0.20399164520857E+03	0.88673281749520E-02
0.20109245932218E+03	0.64538489139828E-02
0.19951447872162E+03	0.11936875179225E-01
0.19855940890435E+03	0.52954214131811E-02
0.19689308268841E+03	0.34713418514610E-01
0.19521717576354E+03	0.10692559449717E-01
0.19305175751280E+03	0.35683188219486E-02
0.19260677636876E+03	0.52364741909542E-01
0.19154961964613E+03	0.21282789437580E-01
0.19147495034203E+03	0.47155069392607E-01
0.19027573069019E+03	0.12956433375883E+00
0.18991216881924E+03	0.78028608714267E-03
0.18775525246981E+03	0.38357211311075E-01
0.18728550653839E+03	0.10375560207896E+00
0.18521181507432E+03	0.39791240110467E-02
0.18479131857312E+03	0.61185489159023E-02
0.18375919981040E+03	0.34212464206347E-01
0.18233037885682E+03	0.12129105104761E-01
0.18209212362089E+03	0.10227832769851E+00
0.18166725747257E+03	0.21878601740917E-02
0.18093855745142E+03	0.38485118511838E-01
0.18050498015171E+03	0.29853150324819E+00
0.17990538125318E+03	0.46482813839119E+00
0.17942672505390E+03	0.68154881206763E-02
0.17879728737449E+03	0.88883264680450E-01
0.17829515856397E+03	0.11028439388167E-01
0.17723281465087E+03	0.20435477838674E-02
0.17720121745868E+03	0.89363391292793E-03
0.17639726175147E+03	0.15098384091548E-02
0.17518017683649E+03	0.57629950568156E-01

3/iso3

pbe0_def2-tzvpp energy (au): -1253.7880346890

XYZ coordinates:

45

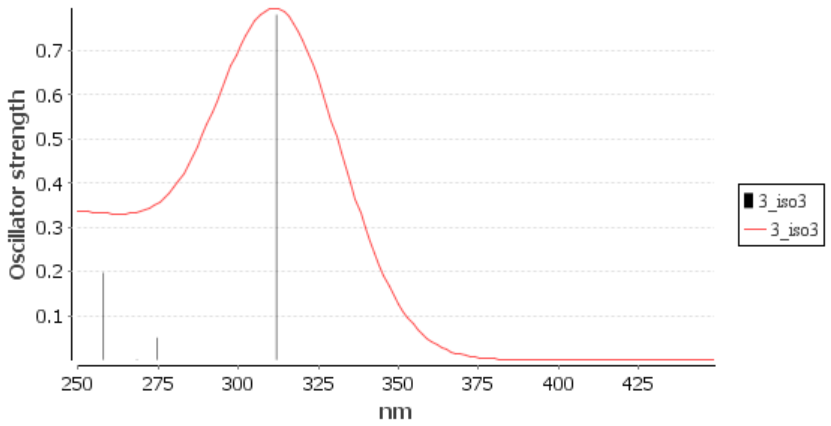
C	-1.28295	2.52437	0.73172
C	-1.46445	1.19520	0.31424
C	-2.78767	0.76908	0.19709
N	-3.86123	1.52201	0.45436
C	-3.55277	2.74956	0.84667
N	-2.34723	3.28544	0.99553
N	-0.06370	3.06765	0.88531
C	-0.61839	0.09798	-0.05988
N	-2.77556	-0.53412	-0.22942
H	-4.39189	3.40087	1.07110
C	-1.47260	-0.92686	-0.38617
C	-3.91177	-1.38289	-0.48794
H	-1.23977	-1.92535	-0.71741
H	0.75806	2.55384	0.62459
H	-0.00139	4.04059	1.12105
C	0.78816	0.07228	-0.08908
C	1.99883	0.07377	-0.10326
C	3.41719	0.04121	-0.13457
C	6.20974	-0.03421	-0.20701
C	5.55604	1.04007	0.38023
C	4.17371	1.08027	0.41958
C	4.08638	-1.03828	-0.72374
C	5.46889	-1.07177	-0.75622
H	7.29195	-0.06321	-0.23552
H	6.12726	1.85244	0.81298
H	3.66721	1.91615	0.88588
H	3.50753	-1.84581	-1.15348
H	5.97223	-1.91429	-1.21489
C	-4.80625	-1.66351	0.72932
C	-6.14237	-1.96141	0.05388
C	-6.11372	-1.06625	-1.18452
C	-6.87058	0.23842	-1.02064
O	-4.33290	-2.68421	1.55026
O	-6.11295	-3.34449	-0.27296
O	-4.73272	-0.78596	-1.44966
O	-6.58962	0.89344	0.18063
H	-3.49719	-2.33293	-0.84830
H	-4.90133	-0.75369	1.32145
H	-6.98557	-1.72780	0.70630
H	-6.51710	-1.61432	-2.04408
H	-7.94382	0.02096	-1.03250
H	-6.65460	0.86640	-1.89549
H	-4.67396	-3.50781	1.18382
H	-7.00239	-3.64955	-0.44982
H	-5.63976	1.13672	0.20255

Electronic excitation spectrum of , IRREP a
singlet excitations
excitation energy / nm oscillator strength (length rep.)

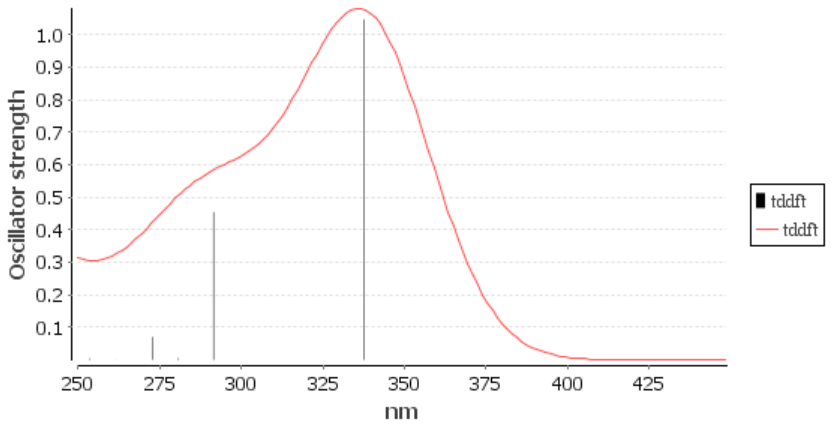
0.31188122094753E+03	0.78123179014921E+00
0.27463406791127E+03	0.50442159481790E-01
0.26831197317113E+03	0.17876807268206E-02
0.25789505907419E+03	0.19748453392241E+00
0.24848142265310E+03	0.40419152784778E-01
0.24107848862978E+03	0.12215447157945E-02
0.23987924897782E+03	0.50817978748848E-02
0.23086007086843E+03	0.15852395994881E-01
0.23020227001369E+03	0.10121070779134E-01
0.22904320881783E+03	0.12787160339040E-03
0.22260283785816E+03	0.41354245360399E-02
0.22056266833185E+03	0.53994716839898E-02
0.21912254831731E+03	0.65395555500382E-01
0.21165137667188E+03	0.28823999584667E-03
0.21092116715246E+03	0.68426729882817E-01
0.20950448009273E+03	0.39548006736477E-01
0.20917466581442E+03	0.37804452485720E-01
0.20742894429153E+03	0.67171895341059E-01
0.20709373509825E+03	0.19659823330766E-01
0.20629206239422E+03	0.10663015055209E-02
0.20355016672814E+03	0.12463178354342E-01
0.20075786477473E+03	0.54475892455346E-03
0.19988375449262E+03	0.29609916326977E-01
0.19640808452976E+03	0.77254701819903E-01
0.19435008665229E+03	0.12206526909396E-02
0.19255658731421E+03	0.30814694468878E-03
0.19205869573254E+03	0.38926499048276E-02
0.19082910840770E+03	0.12356864133862E-02
0.19050630373703E+03	0.47106820888667E-03
0.18997742833977E+03	0.19931097379215E-01
0.18832166496334E+03	0.12799155633233E-01
0.18725900591810E+03	0.47799454728434E+00
0.18618844856031E+03	0.12759234548655E-01
0.18504223333992E+03	0.16292609931246E-01
0.18499498048053E+03	0.56396303328974E-01
0.18449698490154E+03	0.89742185748680E-02
0.18356949916011E+03	0.17821868053222E-01
0.18334433954573E+03	0.33984957159055E-01
0.18318130422274E+03	0.84289364770598E-02
0.18296063595818E+03	0.60503963103336E-01
0.18199187289488E+03	0.34322683910673E-01
0.18050262215401E+03	0.20483369145017E-01
0.17981933321524E+03	0.37838833307002E-02
0.17951258290993E+03	0.42480216708203E-02
0.17823848596240E+03	0.36760869094317E-01
0.17786552162877E+03	0.13713676868628E-01
0.17767130116604E+03	0.27097803364208E-01
0.17652630009829E+03	0.11125322171054E+00
0.17509625912996E+03	0.63223835066396E-01
0.17448405365649E+03	0.38076122488430E-02

6 TDDFT data

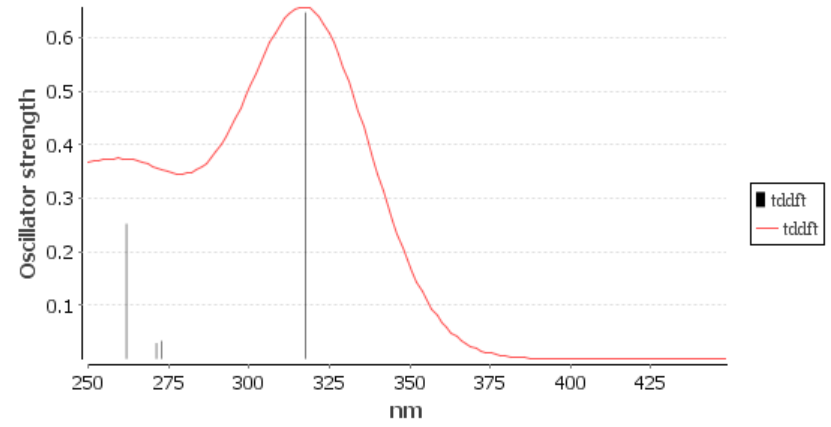
Examples of simulated absorption spectra (from 250 to 450 nm), excitation energies and oscillator strengths are given below for one isomer of each compound. Other isomers give rise to very similar data and so are not presented here.



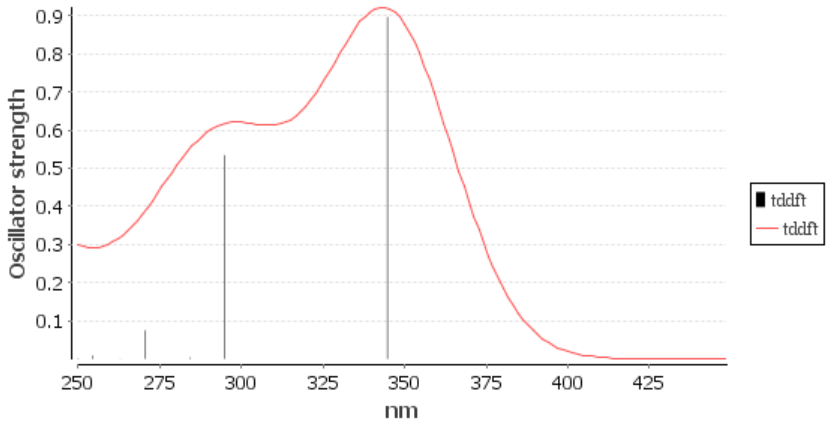
3_iso3 (C3'-endo)



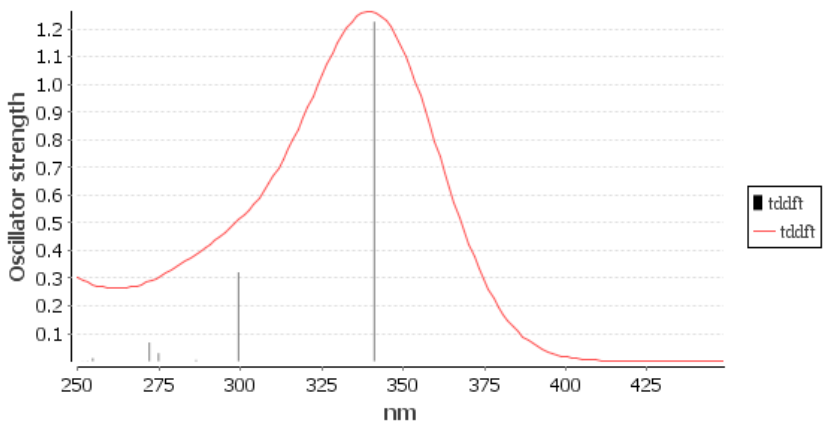
4a_iso3 (C3'-endo)



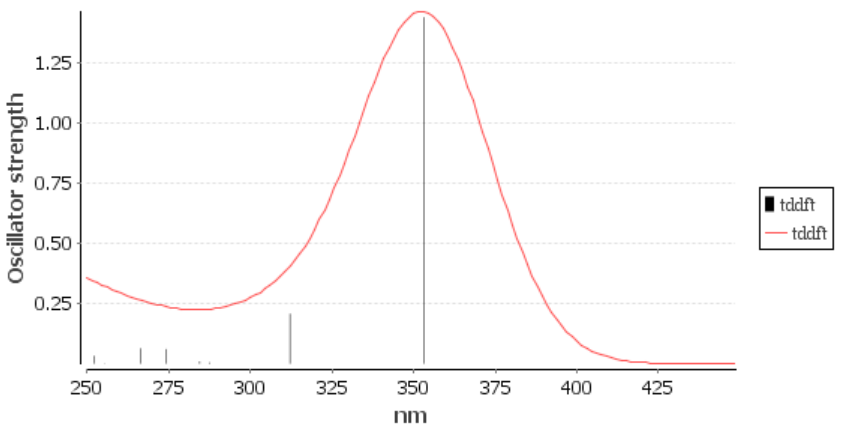
5_iso1



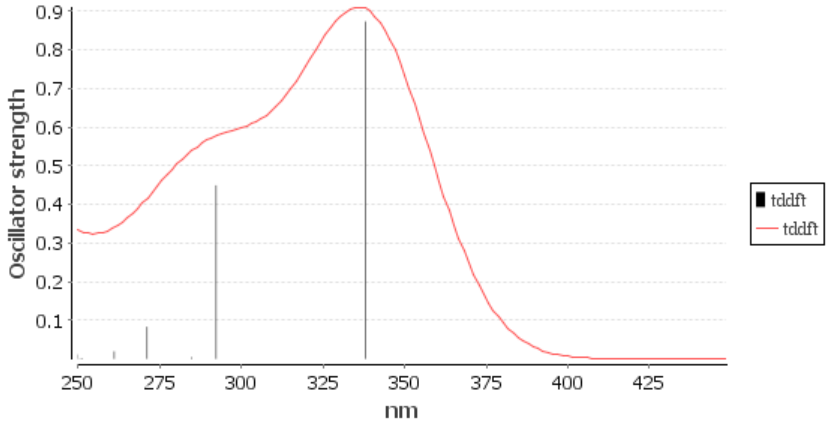
6a_iso1



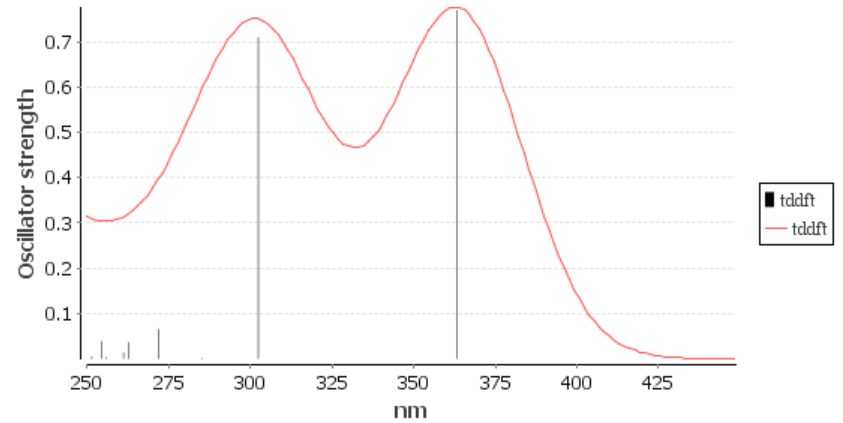
6b_iso1



6c_iso1



6d_iso1



6e_iso1

3_iso3 (C3'-endo)

excitation energy / nm	oscillator strength (length rep.)
0.31188122094753E+03	0.78123179014921E+00
0.27463406791127E+03	0.50442159481790E-01
0.26831197317113E+03	0.17876807268206E-02
0.25789505907419E+03	0.19748453392241E+00
0.24848142265310E+03	0.40419152784778E-01
0.24107848862978E+03	0.12215447157945E-02
0.23987924897782E+03	0.50817978748848E-02
0.23086007086843E+03	0.15852395994881E-01
0.23020227001369E+03	0.10121070779134E-01
0.22904320881783E+03	0.12787160339040E-03
0.22260283785816E+03	0.41354245360399E-02
0.22056266833185E+03	0.53994716839898E-02
0.21912254831731E+03	0.65395555500382E-01
0.21165137667188E+03	0.28823999584667E-03
0.21092116715246E+03	0.68426729882817E-01
0.20950448009273E+03	0.39548006736477E-01
0.20917466581442E+03	0.37804452485720E-01
0.20742894429153E+03	0.67171895341059E-01
0.20709373509825E+03	0.19659823330766E-01
0.20629206239422E+03	0.10663015055209E-02
0.20355016672814E+03	0.12463178354342E-01
0.20075786477473E+03	0.54475892455346E-03
0.19988375449262E+03	0.29609916326977E-01
0.19640808452976E+03	0.77254701819903E-01
0.19435008665229E+03	0.12206526909396E-02
0.19255658731421E+03	0.30814694468878E-03
0.19205869573254E+03	0.38926499048276E-02
0.19082910840770E+03	0.12356864133862E-02
0.19050630373703E+03	0.47106820888667E-03
0.18997742833977E+03	0.19931097379215E-01
0.18832166496334E+03	0.12799155633233E-01
0.18725900591810E+03	0.47799454728434E+00
0.18618844856031E+03	0.12759234548655E-01
0.18504223333992E+03	0.16292609931246E-01
0.18499498048053E+03	0.56396303328974E-01
0.18449698490154E+03	0.89742185748680E-02
0.18356949916011E+03	0.17821868053222E-01
0.18334433954573E+03	0.33984957159055E-01
0.18318130422274E+03	0.84289364770598E-02
0.18296063595818E+03	0.60503963103336E-01
0.18199187289488E+03	0.34322683910673E-01
0.18050262215401E+03	0.20483369145017E-01
0.17981933321524E+03	0.37838833307002E-02
0.17951258290993E+03	0.42480216708203E-02
0.17823848596240E+03	0.36760869094317E-01
0.17786552162877E+03	0.13713676868628E-01
0.17767130116604E+03	0.27097803364208E-01
0.17652630009829E+03	0.11125322171054E+00
0.17509625912996E+03	0.63223835066396E-01
0.17448405365649E+03	0.38076122488430E-02

4a_iso3 (C3'-endo)

excitation energy / nm	oscillator strength (length rep.)
0.33753830245608E+03	0.10478735268822E+01
0.29146846602584E+03	0.45444044576862E+00
0.28065397827178E+03	0.55605329124632E-02

0.27266202454529E+03	0.70798273910955E-01
0.26122610810410E+03	0.44098827510918E-03
0.25709408741549E+03	0.11468142755525E-03
0.25349429171059E+03	0.44275794282944E-02
0.24805374288988E+03	0.65162207515762E-02
0.24720021909585E+03	0.22088038198523E-01
0.24327419054968E+03	0.10352968939773E-01
0.24010686900028E+03	0.13811007460681E-01
0.23650915864289E+03	0.44013588237284E-01
0.23596920873727E+03	0.23459470741921E-01
0.23529442378839E+03	0.17538489918573E-01
0.22949727054630E+03	0.55037836030213E-02
0.22583738299742E+03	0.50293257979777E-01
0.22519547496122E+03	0.28352582837971E-01
0.21906740259423E+03	0.12168536806346E-01
0.21873237676630E+03	0.38187900532624E-01
0.21654752317239E+03	0.24869760581816E-01
0.21501359709809E+03	0.60936832351649E-01
0.21152998522635E+03	0.14431011413019E-01
0.21075511391612E+03	0.34209750432684E-02
0.21001250796883E+03	0.21849888780545E-01
0.20962209092743E+03	0.61475773371178E-03
0.20934017932651E+03	0.54926221966958E-02
0.20829113757599E+03	0.20694825481897E-02
0.20599799289732E+03	0.54729806542219E-02
0.20151363435440E+03	0.39563709595840E-02
0.20099360367498E+03	0.14475484089336E-02
0.19893024283062E+03	0.32924854542721E-01
0.19809015089948E+03	0.21829305072765E-01
0.19798612468380E+03	0.33846853200111E-01
0.19652377879751E+03	0.24934571008292E-02
0.19635699162275E+03	0.37425361641803E-01
0.19525066322699E+03	0.10975123055847E+00
0.19456038703736E+03	0.18124137866483E+00
0.19377485271818E+03	0.65504648847835E-03
0.19356721787415E+03	0.53906556809377E-03
0.19266068447968E+03	0.52999327982989E-03
0.19252591579232E+03	0.11149358936865E-02
0.19196881750873E+03	0.13628441426710E+00
0.19165907876783E+03	0.36542142941887E-02
0.19107832631810E+03	0.46319019534423E-01
0.19074005916026E+03	0.10455874047203E+00
0.19062075299033E+03	0.10423565260069E+00
0.19006987471914E+03	0.89021188956415E-02
0.18966157683861E+03	0.23640785126755E-01
0.18904406147698E+03	0.34106771037903E-01
0.18854325503693E+03	0.13235710555990E-01

5_iso1

excitation energy / nm	**oscillator strength (length rep.)**
0.31755543689716E+03	0.64751969289571E+00
0.27257017821899E+03	0.33867815760842E-01
0.27107306549207E+03	0.29611283558912E-01
0.26173895580976E+03	0.25263796829567E+00
0.24440447603878E+03	0.25739345935378E-01
0.24245266597737E+03	0.98909112187287E-02
0.24023376613158E+03	0.33827884902403E-02
0.23312409489901E+03	0.12925127012992E-01
0.23085994834964E+03	0.77373580456107E-02

0.22528519602863E+03	0.61450463510544E-03
0.22188902722050E+03	0.24624522218594E-01
0.21809328256382E+03	0.10342025512314E+00
0.21269712719045E+03	0.17357572375272E-01
0.21024728644032E+03	0.66365998608455E-01
0.20983458325496E+03	0.10402559712020E-01
0.20515213315790E+03	0.76030601791480E-01
0.20431400332170E+03	0.62425257408930E-03
0.20297212908272E+03	0.31661736656697E-01
0.20091746976488E+03	0.10974247396555E-01
0.20077459986397E+03	0.91775581639409E-02
0.19438947756573E+03	0.96355692653756E-02
0.19341228018489E+03	0.42577254088848E-01
0.19140405931911E+03	0.11727539886624E-01
0.19121678034270E+03	0.69003095351343E-03
0.18934011878080E+03	0.23244773564916E-01
0.18860111300126E+03	0.54818507237655E-02
0.18776588868400E+03	0.23955969821950E+00
0.18725016814754E+03	0.92707167501365E-01
0.18665859516435E+03	0.16004061083267E-01
0.18290016607219E+03	0.83600323553790E-01
0.18211215724539E+03	0.44821591464331E-01
0.18047570502225E+03	0.10506517414776E-02
0.17950912540165E+03	0.25487993781045E-02
0.17744855062107E+03	0.29521758803503E+00
0.17672800038159E+03	0.13164328930253E+00
0.17582948582376E+03	0.14302419038990E+00
0.17329290142110E+03	0.33738218508548E+00
0.17245426839960E+03	0.46842320479682E-01
0.17201060578604E+03	0.15089184694044E-01
0.17136570225609E+03	0.80598480707852E-01
0.17089367464776E+03	0.12390276947094E-01
0.16967169635468E+03	0.19626402694380E-02
0.16941297580097E+03	0.55678037663524E-02
0.16831985442044E+03	0.28667025759670E-01
0.16822328330318E+03	0.33269625717432E-01
0.16669253565377E+03	0.43696992371792E-01
0.16619759165831E+03	0.45779806975893E-03
0.16526014084695E+03	0.53193359683658E-02
0.16431546088535E+03	0.12497033737853E-01
0.16382745184640E+03	0.96928931361433E-02

6a_iso1

excitation energy / nm	**oscillator strength (length rep.)**
0.34472634503986E+03	0.89754625503403E+00
0.29487376708381E+03	0.53485449489194E+00
0.28425515569033E+03	0.37203359797541E-02
0.27043592027184E+03	0.75179678104320E-01
0.26292548186125E+03	0.86043445271828E-03
0.25687486302296E+03	0.12861830555359E-03
0.25443298909959E+03	0.87667623343045E-02
0.25000245910913E+03	0.18018470381132E-02
0.24641772450523E+03	0.72816619077914E-02
0.24548798209421E+03	0.25661111346652E-01
0.23889355728517E+03	0.14721436799854E-01
0.23764311808470E+03	0.14565160413369E-01
0.23611256237012E+03	0.35713732189370E-01
0.23355138003458E+03	0.41116596263241E-02
0.23082597379986E+03	0.30961723763591E-01

0.22587458319472E+03	0.71935298095781E-01
0.22066211157192E+03	0.45590228943088E-01
0.21797432556629E+03	0.29329245191947E-02
0.21188149452016E+03	0.64786311324790E-01
0.21104620681841E+03	0.10200278624330E+00
0.21043838656050E+03	0.12883738375358E-02
0.20924510926328E+03	0.31443060906245E-03
0.20897913130716E+03	0.26876214071637E-02
0.20447124989154E+03	0.11644586944587E-01
0.20369893530799E+03	0.89407854330537E-02
0.20269315438125E+03	0.23863273528673E-02
0.20142801925288E+03	0.78204357473668E-02
0.19803265831352E+03	0.12427247664347E-01
0.19735198508563E+03	0.50096627627421E-04
0.19697072089391E+03	0.50883164911986E-02
0.19652727443109E+03	0.45546845025684E-01
0.19601965382224E+03	0.98436977457756E-01
0.19542577575468E+03	0.61739300529975E-02
0.19404382884027E+03	0.12142591068491E-01
0.19361207222448E+03	0.58875880859050E-03
0.19310481866530E+03	0.26779384306599E+00
0.19308690695832E+03	0.12977065016489E+00
0.19092503576710E+03	0.32703496063429E-01
0.19064656668197E+03	0.15695020877845E-01
0.19036119019384E+03	0.22395231171938E-01
0.18990319997599E+03	0.13297825424650E+00
0.18827822559090E+03	0.34762492651124E-01
0.18714354744986E+03	0.17647967700487E-02
0.18708737724690E+03	0.11691600500288E-02
0.18529809542215E+03	0.13222975179926E-02
0.18360421573244E+03	0.36121371720746E-01
0.18333334612605E+03	0.25066325641072E-02
0.18327441668442E+03	0.33978204360541E-02
0.18227724558568E+03	0.10976437102493E-01
0.18080719878991E+03	0.51989509509953E-01

6b_iso1

excitation energy / nm	**oscillator strength (length rep.)**
0.34107033477777E+03	0.12264041091346E+01
0.29928490266169E+03	0.32149232529457E+00
0.28633752597325E+03	0.46244111870729E-02
0.27481545764905E+03	0.29199717084092E-01
0.27202448129570E+03	0.67822359439876E-01
0.25460382255181E+03	0.11192159790649E-01
0.25286518882047E+03	0.14039584121007E-02
0.25140401324631E+03	0.74297665068953E-03
0.24436762513969E+03	0.24155376681308E-01
0.24267298549660E+03	0.18325284515652E-01
0.24078227020439E+03	0.36592374684993E-01
0.23939846830417E+03	0.34343067754519E-01
0.23745312104081E+03	0.18325420119906E-02
0.23134317509371E+03	0.14590027715752E-01
0.22912367902360E+03	0.47637695580991E-01
0.22829530404947E+03	0.98510815117651E-02
0.22184870908225E+03	0.53524057245180E-01
0.21999340901898E+03	0.87473479058936E-02
0.21644211866438E+03	0.89764191924570E-02
0.21434503196849E+03	0.48480911011849E-02
0.21363195703289E+03	0.80021409893922E-01

0.21185170173777E+03	0.93158059137688E-01
0.20982548608198E+03	0.12415700242880E-02
0.20768995582693E+03	0.29557320563439E-02
0.20510088942436E+03	0.99913724466907E-02
0.20429002210148E+03	0.19545912034974E-01
0.20246653681382E+03	0.52213999520229E-02
0.20056345652211E+03	0.54013882809918E-02
0.19960425890972E+03	0.62007836767648E-02
0.19829292053979E+03	0.57104283150778E-02
0.19813995459733E+03	0.44397033418497E-02
0.19755492198162E+03	0.79915260547706E-01
0.19717076493633E+03	0.21801752600588E-03
0.19676734355556E+03	0.55523866291265E-01
0.19523154808044E+03	0.89195861316013E-01
0.19456091172909E+03	0.15829194344675E+00
0.19368955326588E+03	0.15481410680912E+00
0.19172913646889E+03	0.61705502079097E-02
0.19131709040272E+03	0.31636945588075E-01
0.19046408304264E+03	0.26691137893927E-01
0.19027475001395E+03	0.19255643644458E-01
0.18977432165910E+03	0.39587121025245E-02
0.18924310211758E+03	0.97325538165367E-02
0.18859438854776E+03	0.86676790640610E-02
0.18652969367246E+03	0.18607818527752E-02
0.18582507446379E+03	0.51679882195508E-02
0.18523540095925E+03	0.79261678020369E-01
0.18483304905364E+03	0.20277707327201E-01
0.18463241049176E+03	0.12174720369489E+00
0.18323083280819E+03	0.53709571085861E-01

6c_iso1

excitation energy / nm	**oscillator strength (length rep.)**
0.35319007979918E+03	0.14365705946838E+01
0.31211243081547E+03	0.20772877380451E+00
0.28740915296657E+03	0.57826573679554E-02
0.28444102936991E+03	0.10160692023475E-01
0.27408556971294E+03	0.61166033335327E-01
0.26634806310503E+03	0.64103566795296E-01
0.25530183673138E+03	0.14504099007218E-02
0.25525949465114E+03	0.25582735246340E-03
0.25212445581648E+03	0.33105472004925E-01
0.24623161041100E+03	0.39909946688414E-01
0.24515170785522E+03	0.36152202593225E-02
0.24419927874790E+03	0.44487193886535E-01
0.24392298306324E+03	0.64828709735913E-02
0.23753463630490E+03	0.43958056215918E-03
0.23668966736700E+03	0.13805111457054E-01
0.23534788507362E+03	0.39731858656455E-01
0.23288094362106E+03	0.14297306632532E-02
0.22992978097180E+03	0.78578715329162E-02
0.22741072106821E+03	0.22810437757758E-01
0.22630861137068E+03	0.46590050749331E-01
0.21904372254978E+03	0.67260339577461E-01
0.21634359911542E+03	0.23766956443094E-01
0.21472954653360E+03	0.55735540212014E-01
0.21436945272565E+03	0.10257009096419E-02
0.21321644787534E+03	0.14447249266022E-01
0.20881012452110E+03	0.41427381622256E-02
0.20645604967166E+03	0.21312415365471E-01

0.20512782692950E+03	0.64069584328486E-02
0.20392668275478E+03	0.20057834658023E-01
0.20330896035964E+03	0.31048249313224E-02
0.20209695546395E+03	0.22183365372735E-01
0.20083529830316E+03	0.10495215514548E-01
0.20040211520557E+03	0.92121384547657E-03
0.19870615651174E+03	0.61675029324199E-01
0.19832573208769E+03	0.80042450278585E-01
0.19762617631668E+03	0.62615023355139E-03
0.19723018396642E+03	0.95723570848302E-02
0.19680115338685E+03	0.21752355185728E-02
0.19625978145567E+03	0.12524836790711E+00
0.19610071259728E+03	0.74541756159070E-02
0.19438226261762E+03	0.17816703952969E-01
0.19384600806337E+03	0.63448548260951E-03
0.19367611047678E+03	0.17463864507404E-02
0.19318833929271E+03	0.59410489241779E-01
0.19164694554308E+03	0.11241645583955E+00
0.19054947896701E+03	0.34204486975199E-02
0.19047148993468E+03	0.45561092291915E-03
0.18893432880063E+03	0.13577725685101E-01
0.18872287705539E+03	0.71429180833612E+00
0.18800192273468E+03	0.36866070675175E-01

6d_iso1

excitation energy / nm	**oscillator strength (length rep.)**
0.33792247404908E+03	0.87420662058126E+00
0.29224922771837E+03	0.44970269408763E+00
0.28483531703901E+03	0.43673788171054E-02
0.27109137758250E+03	0.83365047428346E-01
0.26102904210213E+03	0.19692668505458E-01
0.25109895197329E+03	0.20369220283863E-02
0.25053896980727E+03	0.15590914998367E-02
0.24957244277517E+03	0.11599895957899E-01
0.24491122809806E+03	0.43263629676183E-01
0.24426715052668E+03	0.31633430181821E-02
0.23827501415133E+03	0.10551349886582E-01
0.23726240176749E+03	0.20109138437097E-01
0.23208988534885E+03	0.48133154197441E-02
0.22952736283528E+03	0.10195630880310E-01
0.22910851427291E+03	0.25045785971374E-02
0.22617325747924E+03	0.68517958133868E-01
0.22528101428896E+03	0.76213831753476E-01
0.21487916672949E+03	0.15695921668521E-01
0.21304144993992E+03	0.52432908955405E-01
0.21148567246617E+03	0.80405785486588E-01
0.20990628834462E+03	0.27667599968803E-01
0.20841777080398E+03	0.28068139187310E-02
0.20518628351231E+03	0.32181102667169E-02
0.20377651300143E+03	0.16996241780586E-01
0.20329633419515E+03	0.89480551275433E-01
0.20204333893562E+03	0.29575169382862E-03
0.20147984600215E+03	0.12480914826320E-01
0.20089195298959E+03	0.97620494243324E-03
0.19873700847826E+03	0.45870201282071E-01
0.19843043834524E+03	0.63353829894082E-02
0.19816574983203E+03	0.12432666083629E-01
0.19710691609982E+03	0.57823550530247E-02
0.19675605925476E+03	0.77016178357724E-01

0.19649636826381E+03	0.10770353558468E+00
0.19614858409509E+03	0.25168867959682E-01
0.19555968898383E+03	0.83152556714645E-01
0.19473326971187E+03	0.12214260707785E+00
0.19415718051362E+03	0.24514009605511E-02
0.19356794559323E+03	0.28023981533467E-01
0.19192789658862E+03	0.97349337467050E-02
0.19113661844806E+03	0.17918403276749E-02
0.19017323869774E+03	0.38761532407352E-01
0.18918212287105E+03	0.45300460100333E-01
0.18771907699930E+03	0.48235602438836E-02
0.18744197236698E+03	0.26767216936943E-01
0.18626469764590E+03	0.88316187628237E-01
0.18388860052283E+03	0.48840833336565E-01
0.18206842589788E+03	0.75068630505602E-01
0.18186407444527E+03	0.26508707457934E+00
0.18044451772484E+03	0.61330353509385E-02

6e_iso1

excitation energy / nm	**oscillator strength (length rep.)**
0.36324874790519E+03	0.76904783363404E+00
0.30241278877579E+03	0.70972589197061E+00
0.28517147965027E+03	0.26588929418885E-02
0.27193148694583E+03	0.66312718996165E-01
0.27027167006034E+03	0.74370485814760E-03
0.26271295948309E+03	0.37059723481891E-01
0.26110783615046E+03	0.14353041211394E-01
0.25573012177131E+03	0.41369328479598E-02
0.25448400541529E+03	0.39737221845137E-01
0.25139965257019E+03	0.59139493092529E-02
0.24613429420173E+03	0.51745372341764E-02
0.24176589290988E+03	0.82580934045403E-02
0.23901871538723E+03	0.17947397462912E-01
0.23656874961018E+03	0.38704514976852E-02
0.23516988197277E+03	0.25816274098651E-01
0.22814648017356E+03	0.65420114981835E-01
0.22417457696641E+03	0.52132035843315E-01
0.21989459133224E+03	0.30918895744282E-01
0.21381214723323E+03	0.11866685754152E-01
0.21201432430011E+03	0.61569872149628E-01
0.21126005346701E+03	0.60560459464976E-01
0.21111746477538E+03	0.13441344621503E-01
0.20900908976842E+03	0.25055941109529E-02
0.20669910421909E+03	0.24615185817272E-02
0.20377226343574E+03	0.45661213551702E-02
0.20277024597864E+03	0.19301705886053E-01
0.20229149021252E+03	0.42249628383843E-01
0.20073357719988E+03	0.13125213578818E-01
0.19975446861710E+03	0.28673481790595E-02
0.19910163709330E+03	0.37728704583134E-02
0.19804450934241E+03	0.12243780772336E+00
0.19703963866744E+03	0.11306807804449E-02
0.19640887700256E+03	0.13676691296925E-01
0.19636676292068E+03	0.13921331617190E-02
0.19602712705244E+03	0.28266082972033E-02
0.19585144857865E+03	0.11110798396750E+00
0.19491489154467E+03	0.18171262771637E-01
0.19412685674025E+03	0.37227904663131E-02
0.19372003343755E+03	0.37779441640201E-02

0.19330185330479E+03	0.10033256504123E+00
0.19247046056243E+03	0.46500289670431E-03
0.19078559021369E+03	0.15956187760843E+00
0.18986351480934E+03	0.12602037359429E-01
0.18918316243307E+03	0.58174376326055E-02
0.18682945968785E+03	0.44778344943395E-01
0.18639818485812E+03	0.35595125119114E-01
0.18533079466396E+03	0.20060675359326E+00
0.18300836001307E+03	0.46512591268099E-02
0.18270778737093E+03	0.64602901354115E-03
0.18125037133909E+03	0.34696752618506E+00

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