Supplementary Material (ESI) for Chemical Communications

Chemical Communications

Unprecedented Thermal Rearrangement of Push-Pull-Chromophore –[60]Fullerene Conjugates: Formation of Chiral 1,2,9,12-Tetrakis-Adducts†

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Electronic Supplementary Information (ESI)

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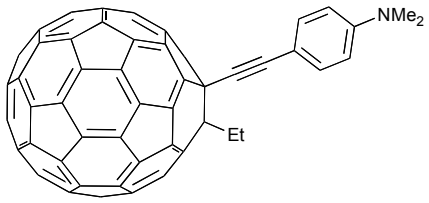
Materials and General Methods (ESI)

Reagents and solvents were purchased reagent grade from Acros, ABCR, Aldrich and Fluka, and used as received. Tetrahydrofuran (THF) was freshly distilled from Na/benzophenone and CH_2Cl_2 from CaH_2 under N_2. All reactions were performed under an inert atmosphere by applying a positive pressure of N_2. Flash chromatography (FC) and plug filtrations were carried out with silica gel 60 (particle size 0.040–0.063 mm, 230–400 mesh; Fluka). Elution was done with distilled technical solvents. Thin-layer chromatography (TLC) was conducted on aluminum sheets coated with silica gel 60 F254 obtained from Macherey-Nagel; visualisation with a UV lamp (254 or 366 nm). ^{1}H and ^{13}C NMR spectra were measured on a Varian Gemini 300, on a Bruker DRX400 spectrometer. Residual solvent signals in the ^{1}H and ^{13}C NMR spectra were used as an internal reference. Coupling constants (J) are given in Hz. The apparent resonance multiplicity is described as s (singlet), brs (broad singlet), d (doublet), dd (double doublet), t (triplet). Infrared spectra (IR) were recorded on a Perkin-Elmer FT1600. UV/Vis absorption spectra were recorded on a Varian Cary-5 spectrophotometer. The spectra were measured for samples in CH_2Cl_2 in a quartz cuvette (1 cm) at 293 K. The absorption maxima (λ_{max}) are reported in nm with the molar extinction coefficient (ε) in dm^3 mol^{-1} cm^{-1} in brackets; shoulders are indicated as sh. High-resolution (HR) FT-ICR-MALDI spectra were measured on an IonSpec Ultima Fourier transform (FT) instrument with 3-hydroxypicolinic acid (3-HPA) as the matrix. The most important peaks are reported in m/z units with M as the molecular ion.

Synthesis (ESI)

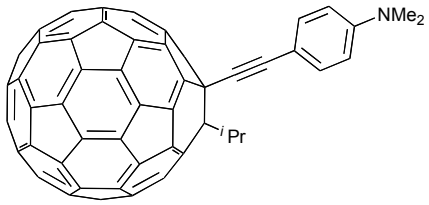
Synthesis of **1a**:



A solution of {[(4-dimethylamino)phenyl]ethynyl}lithium was prepared by adding a 1.30 mL (2.08 mmol) aliquot of 1.6 N *n*-BuLi in *n*-hexane to a stirred solution of 1-ethynyl-4-dimethylaniline (302 mg, 2.08 mmol) in THF (10 mL) at –78 °C and stirring the mixture at 0 °C for 0.5 h. To a vigorously stirred suspension of C_{60} (500 mg, 0.694 mmol) in THF (250 mL), obtained by irradiation in a ultasonic bath for 1 h, the solution of {[(4-dimethylamino)phenyl]ethynyl}lithium was added at 20 °C dropwise by the use of a syringe over 15 min. The mixture was stirred for 0.5 h, during which time the color changed into dark green. To the mixture, 5 mL aliquot of iodoethane was added. The mixture was heated to reflux for 12 h. The solvent was removed under reduced pressure. Evaporation and FC (SiO_2; toluene/cyclohexane 1:5, then 1:2) afforded unchanged C_{60} (87 mg. 17%) and **1a** (151 mg, 24%). Black solid. R_f = 0.42 (SiO_2; toluene/cyclohexane 1:2); $\lambda_{max}(CH_2Cl_2)$/nm 432 (ε/dm^3 mol^{-1} cm^{-1} 4200), 703 (400); ν_{max}(neat)/cm^{-1} 2954, 2920, 2853, 2803, 2327, 2210, 2161, 2083, 1871, 1738, 1604, 1506, 1462, 1440, 1428, 1355, 1323, 1267, 1224, 1188, 1164, 1127, 1100, 1086, 1062, 1033, 1002, 945, 883, 810, 778, 763, 744, 716, 699; δ_H(400 MHz; $C_2D_2Cl_4$; 298 K) 7.66 (2H, d, J 8.8), 6.76 (2H, d, J 8.8), 3.87 (2H, q, J 7.6), 3.06 (6H, s), 2.10 (3H, t, J 7.6); δ_C(100 MHz; $C_2D_2Cl_4$; 298 K) 155.94,

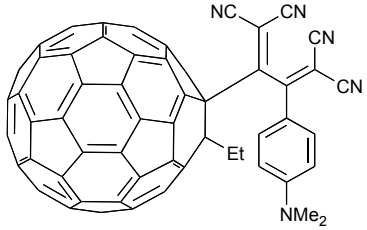
154.57, 150.47, 147.87, 147.73, 146.46, 146.43, 146.24, 146.22, 145.97, 145.46, 145.45, 145.39, 145.29, 144.76, 144.72, 143.16, 143.02, 142.57, 142.56, 142.18, 142.16, 142.06, 141.59, 141.35, 140.22, 139.71, 135.14, 134.34, 133.37, 112.00, 109.25, 86.60, 85.89, 66.55, 59.87, 40.39, 37.49, 15.06 (39 resonances out of 41 expected ones observed due to peak overlap); HR-FT-ICR-MALDI-MS (3-HPA) calcd for $C_{72}H_{15}N^-$ ([*M*]$^-$): 893.1204; found 893.1209.

Synthesis of **1b**:



A solution of {[(4-dimethylamino)phenyl]ethynyl}lithium was prepared by adding a 1.30 mL (2.08 mmol) aliquot of 1.6 N *n*-BuLi in *n*-hexane to a stirred solution of 1-ethynyl-4-dimethylaniline (302 mg, 2.08 mmol) in THF (10 mL) at –78 °C and stirring the mixture at 0 °C for 0.5 h. To a vigorously stirred suspension of C_{60} (500 mg, 0.69 mmol) in THF (250 mL), obtained by irradiation in a ultasonic bath for 1 h, the solution of {[(4-dimethylamino)phenyl]ethynyl}lithium was added at 20 °C dropwise by the use of a syringe over 15 min. The mixture was stirred for 0.5 h, during which time the color changed into dark green. To the mixture, 10 mL aliquot of 2-iodopropane was added. The mixture was heated to reflux for 12 h. The solvent was removed under reduced pressure. Evaporation and FC (SiO_2; toluene/cyclohexane 1:5, then 1:2) afforded unchanged C_{60} (13 mg. 3%) and **1b** (139 mg, 22%). Black solid. R_f = 0.52 (SiO_2; toluene/cyclohexane 1:2); $\lambda_{max}(CH_2Cl_2)$/nm 431 (ε/dm^3 mol^{-1} cm^{-1} 5000), 702 (500); ν_{max}(neat)/cm^{-1} 2952, 2920, 2851, 2798, 2326, 2205, 2161, 1870, 1740, 1604, 1512, 1459, 1440, 1428, 1385, 1355, 1261, 1219, 1188, 1162, 1118, 1061, 1031, 1003, 944, 865, 809, 777, 761, 744, 714; δ_H(400 MHz; $C_2D_2Cl_4$; 298 K) 7.66 (2H, d, *J* 8.8), 6.77 (2H, d, *J* 8.8), 4.53 (1H, sept, *J* 6.5), 3.06 (6H, s), 2.04 (6H, s); δ_C(100 MHz; $C_2D_2Cl_4$; 298 K) 155.15, 154.71, 150.50, 147.86, 147.77, 146.95, 146.51, 146.48, 146.27, 146.24, 146.02, 145.55, 145.49, 145.39, 145.34, 145.25, 144.76, 144.74, 143.20, 143.07, 142.64, 142.63, 142.33, 142.22, 142.19, 141.90, 141.60, 141.27, 140.28, 139.03, 135.44, 134.25, 133.34, 111.99, 87.32, 85.64, 63.10, 61.02, 40.36, 38.62, 23.97; HR-FT-ICR-MALDI-MS (3-HPA) calcd for $C_{73}H_{17}N^-$ ([*M*]$^-$): 907.1361; found 907.1359.

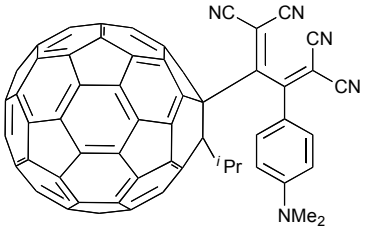
Synthesis of (±)-**2a**:



A mixture of ethynylated fullerene **1a** (44 mg, 0.049 mmol) and TCNE (11 mg, 0.084 mmol) in chlorobenzene (50 mL) was stirred for 6 d at 20 °C. The solvent was evaporated under reduced

pressure and the residue subjected to FC (SiO_2; CH_2Cl_2/cyclohexane 1:2, 1:1, then 2:1) to give (±)-**2a** (28 mg, 55%). Red solid. R_f = 0.55 (SiO_2; CH_2Cl_2); $\lambda_{max}(CH_2Cl_2)$/nm 316 (ε/dm^3 mol^{-1} cm^{-1} 42700), 405 (13500), 417 (13400), 431 (13100), 495 (9600, sh), 700 (500, sh); ν_{max}(neat)/cm^{-1} 2921, 2853, 2328, 2223, 1725, 1599, 1510, 1435, 1377, 1317, 1292, 1258, 1233, 1204, 1186, 1174, 1100, 1065, 1002, 945, 885, 844, 823, 799, 787, 762, 739, 706, 679, 661; δ_H(400 MHz; $C_2D_2Cl_4$; 298 K; 0.21:1.00 mixture of two atropisomers (±)-**2a-A** and (±)-**2a-B)** 7.65 (2H, d, *J* 9.2; (±)-**2a-B**), 7.55 (2H, d, *J* 9.0; (±)-**2a-A**), 6.95 (2H, d, *J* 9.2; (±)-**2a-B**), 6.60 (2H, d, *J* 9.0; (±)-**2a-A**), 3.88 (2H, dq, *J* 1.6 and 7.2; (±)-**2a-A**), 3.69 (2H, dq, *J* 12.0 and 7.2; (±)-**2a-B**), 3.21 (6H, s; (±)-**2a-B**), 3.03 (6H, s; (±)-**2a-A**), 1.87 (2H, t, *J* 7.2; (±)-**2a-A**), 1.73 (2H, t, *J* 7.2; (±)-**2a-B**) ; δ_C(100 MHz; $C_2D_2Cl_4$; 298 K; signals assigned only for (±)-**2a-B**) 172.74, 169.63, 154.39, 154.13, 153.48, 148.55, 147.97, 147.65, 147.44, 146.83, 146.74, 146.54, 146.42, 146.38, 146.29, 146.17, 146.11, 145.98, 145.85, 145.64, 145.60, 145.49, 145.35, 145.21, 145.12, 145.10, 144.83, 144.76, 144.35, 144.18, 143.83, 143.29, 143.22, 143.00, 142.94, 142.90, 142.80, 142.51, 142.44, 142.40, 142.29, 142.03, 141.79, 141.56, 141.54, 141.50, 141.24, 140.53, 140.04, 139.37, 139.29, 139.06, 138.75, 138.71, 135.93, 135.47, 132.94, 131.73, 113.67, 113.06, 112.59, 111.86, 111.63, 111.26, 98.96, 87.16, 72.40, 68.14, 53.91, 40.31, 34.82, 27.05, 14.4 (73 resonances out of 75 expected ones observed due to peak overlap); HR-FT-ICR-MALDI-MS (3-HPA) calcd for $C_{78}H_{15}N_5^-$ ([*M*]$^-$): 1021.1327; found 1021.1352.

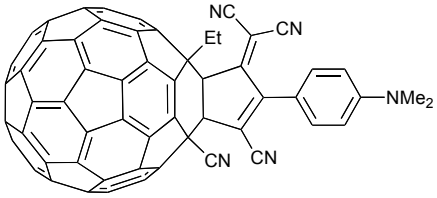
Synthesis of (±)-**2b**:



A mixture of ethynylated fullerene **1b** (9.4 mg, 0.010 mmol) and TCNE (2.3 mg, 0.018 mmol) in chlorobenzene (10 mL) was stirred for 4 d at 20 °C. The solvent was evaporated under reduced pressure and the residue subjected to FC (SiO_2; CH_2Cl_2/cyclohexane 1:2, 1:1, then 2:1) to give (±)-**2b** (2.2 mg, 21%) and unreacted **1b** (4.2 mg, 45%). Black solid. R_f = 0.51 (SiO_2; CH_2Cl_2); $\lambda_{max}(CH_2Cl_2)$/nm 404 (ε/dm^3 mol^{-1} cm^{-1} 11500), 416 (11000), 431 (10400), 490 (7600, sh); ν_{max}(neat)/cm^{-1} 2956, 2922, 2852, 2217, 1682, 1602, 1520, 1461, 1438, 1370, 1291, 1260, 1231, 1190, 1170, 1064, 1019, 945, 868, 805, 763, 727, 660, 640; δ_H(400 MHz; $C_2D_2Cl_4$; 298 K) 7.55 (2H, d, *J* 9.2), 6.91 (2H, d, *J* 9.2), 4.00 (1H, septet, *J* 6.6), 3.18 (6H, s), 1.96 (3H, d, *J* 6.6), 1.35 (3H, d, *J* 6.6); δ_C(100 MHz; $C_2D_2Cl_4$; 298 K) 172.93, 169.85, 155.15, 154.87, 153.87, 150.64, 149.68, 149.62, 149.43, 149.40, 149.12, 148.25, 146.38, 146.26, 146.07, 146.05, 145.84, 145.72, 145.57, 145.40, 145.31, 145.11, 144.90, 144.79, 144.73, 144.49, 144.40, 144.34, 144.11, 143.43, 143.36, 143.08, 143.05, 142.93, 142.90, 142.80, 142.61, 142.40, 142.37, 141.83, 141.68, 141.59, 141.54, 141.25, 141.11, 140.75, 140.30, 139.36, 139.27, 139.06, 137.75, 135.28, 135.27, 131.26, 120.40, 116.94, 115.24, 112.84, 112.42, 111.95, 72.67, 68.00, 40.24, 40.21, 36.68, 35.97, 25.75, 24.55 (68 resonances out of 76

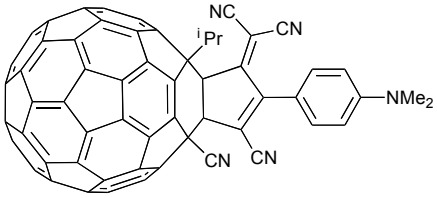
expected ones observed due to peak overlap); HR-FT-ICR-MALDI-MS (3-HPA) calcd for $C_{79}H_{17}N_5^-$ ([*M*]$^-$): 1035.1484; found 1035.1499.

Synthesis of (±)-**3a**:



A mixture of ethynylated fullerene **1a** (44 mg, 0.049 mmol) and TCNE (11 mg, 0.084 mmol) in chlorobenzene (50 mL) was heated to reflux for 6 d. The solvent was evaporated under reduced pressure and the residue subjected to FC (SiO_2; CH_2Cl_2/cyclohexane 1:2, 1:1, then 2:1) to give (±)-**3a** (29 mg, 58%). Dark green solid. R_f = 0.41 (SiO_2; CH_2Cl_2); λ_{max}(CH_2Cl_2)/nm 426 (ε/dm^3 mol^{-1} cm^{-1} 5100), 601 (3600); ν_{max}(neat)/cm^{-1} 2963, 2893, 2330, 2222, 1603, 1553, 1522, 1443, 1366, 1264, 1229, 1191, 1169, 1121, 1096, 1064, 946, 893, 839, 811, 787, 771, 763, 733, 700, 673, 660, 638, 603; δ_H(400 MHz; $C_2D_2Cl_4$; 298 K) 7.58 (2H, d, *J* 8.6), 6.95 (2H, d, *J* 8.6), 3.60 (1H, dq, *J* 7.2), 3.42 (1H, dq, *J* 7.2), 3.17 (6H, s), 1.93 (3H, t, *J* 7.2); δ_C(100 MHz; $C_2D_2Cl_4$; 298 K) 175.06, 155.31, 152.78, 150.61, 149.74, 149.65, 148.98, 148.97, 148.76, 147.75, 147.46, 147.31, 147.10, 147.00, 146.90, 146.82, 146.67, 146.13, 146.07, 145.32, 145.21, 145.20, 145.19, 145.14, 145.02, 144.98, 144.96, 144.94, 144.91, 144.88, 144.50, 144.20, 144.18, 143.54, 143.52, 143.48, 143.46, 143.02, 142.86, 142.79, 142.66, 142.06, 141.71, 141.65, 141.63, 141.44, 141.09, 139.60, 138.97, 138.86, 138.83, 138.30, 138.08, 137.69, 136.96, 136.38, 135.06, 130.30, 129.33, 117.50, 114.48, 113.90, 113.81, 112.09, 110.84, 90.47, 71.51, 71.48, 65.42, 54.17, 63.91, 40.26, 36.96, 27.05, 14.28; HR-FT-ICR-MALDI-MS (3-HPA) calcd for $C_{78}H_{15}N_5^-$ ([*M*]$^-$): 1021.1327; found 1021.1361.

Synthesis of (±)-**3b**:



A mixture of ethynylated fullerene **1b** (9.4 mg, 0.010 mmol) and TCNE (2.3 mg, 0.018 mmol) in chlorobenzene (10 mL) was heated to reflux for 4 d. The solvent was evaporated under reduced pressure and the residue subjected to FC (SiO_2; CH_2Cl_2/cyclohexane 1:2, 1:1, then 2:1) to give (±)-**3b** (4.1 mg, 38%). Dark green solid. R_f = 0.44 (SiO_2; CH_2Cl_2); λ_{max}(CH_2Cl_2)/nm 425 (ε/dm^3 mol^{-1} cm^{-1} 6200), 604 (4000, sh); ν_{max}(neat)/cm^{-1} 2947, 2341, 2216, 1605, 1521, 1461, 1442, 1368, 1298, 1270, 1230, 1191, 1169, 1118, 1065, 1003, 946, 886, 834, 816, 805, 787, 771, 763, 740, 727, 700, 683, 670, 662; δ_H(400 MHz; $C_2D_2Cl_4$; 298 K) 7.58 (2H, d, *J* 9.0), 6.94 (2H, d, *J* 9.0), 3.72 (1H, septet, *J* 6.6), 3.17 (6H, s), 1.91 (3H, d, *J* 6.6), 1.84 (3H, d, *J* 6.6); δ_C(100 MHz; $C_2D_2Cl_4$; 298 K) 175.45, 155.50, 152.79, 149.59, 149.57, 149.44, 148.87, 148.71, 148.34, 147.66, 147.43, 147.28, 147.08, 146.89,

146.82, 146.74, 146.34, 146.17, 145.99, 145.32, 145.24, 145.10, 145.06, 145.03, 144.98, 144.91, 144.88, 144.79, 144.46, 144.38, 144.23, 144.20, 143.60, 143.51, 143.31, 143.25, 143.07, 143.01, 142.72, 142.70, 142.03, 141.80, 141.55, 141.32, 141.05, 140.89, 140.40, 139.26, 139.11, 138.92, 138.53, 138.31, 137.10, 137.07, 136.19, 134.70, 130.28, 128.01, 117.45, 114.57, 114.01, 113.87, 112.07, 110.79, 91.47, 73.32, 71.76, 69.86, 54.35, 53.95, 40.28, 36.69, 23.71, 22.80 (74 resonances out of 76 expected ones observed due to peak overlap); HR-FT-ICR-MALDI-MS (3-HPA) calcd for $C_{79}H_{17}N_5^-$ ([*M*]$^-$): 1035.1484; found 1035.1482.

Thermal rearrangement of (±)-**2a** to (±)-**3a**:

A solution of (±)-**2a** (54 mg, 0.053 mmol) in chlorobenzene (30 mL) was heated to reflux for 2d. The solvent was evaporated under reduced pressure and the residue subjected to FC (SiO_2; CH_2Cl_2/cyclohexane 1:2, 1:1, then 2:1) to give (±)-**3a** (34 mg, 63%; 92% conversion) as a dark green solid and unreacted (±)-**2a** (15 mg, 29%).

Thermal rearrangement of (±)-**2b** to (±)-**3b**:

A solution of (±)-**2b** (2,2 mg, 2.1 μmol) in chlorobenzene (5 mL) was heated to reflux for 5d. The solvent was evaporated under reduced pressure and the residue subjected to FC (SiO_2; CH_2Cl_2/cyclohexane 1:2, 1:1, then 2:1) to give (±)-**3b** (1.3 mg, 59%; 87% conversion) as a dark green solid and unreacted **(±)-2b** (0.7 mg, 32%).

NMR data (ESI)

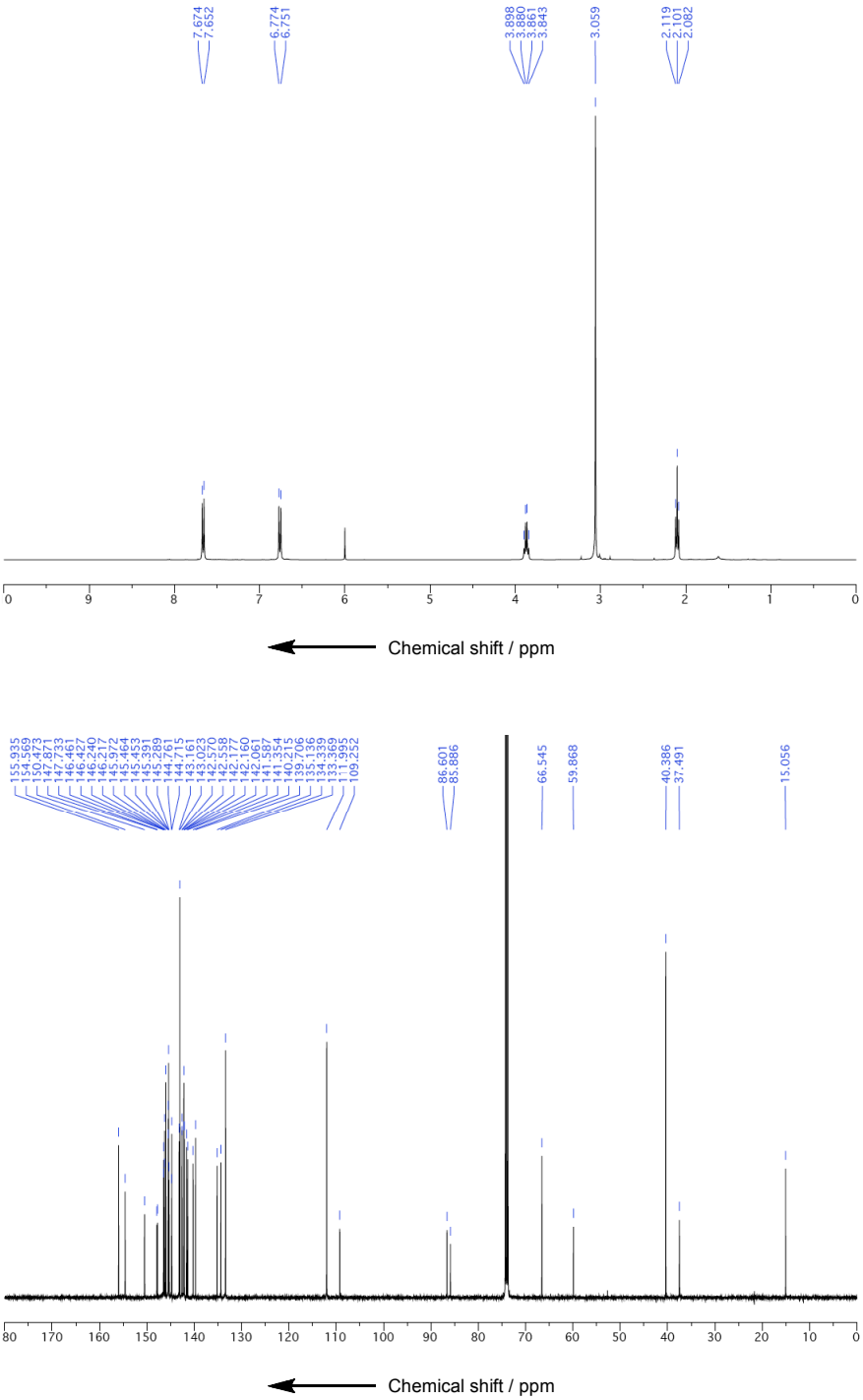


Fig. 1 (ESI). 400 MHz ^{1}H NMR and 100 MHz ^{13}C NMR spectra of **1a** recorded at 298 K in $C_2D_2Cl_4$.

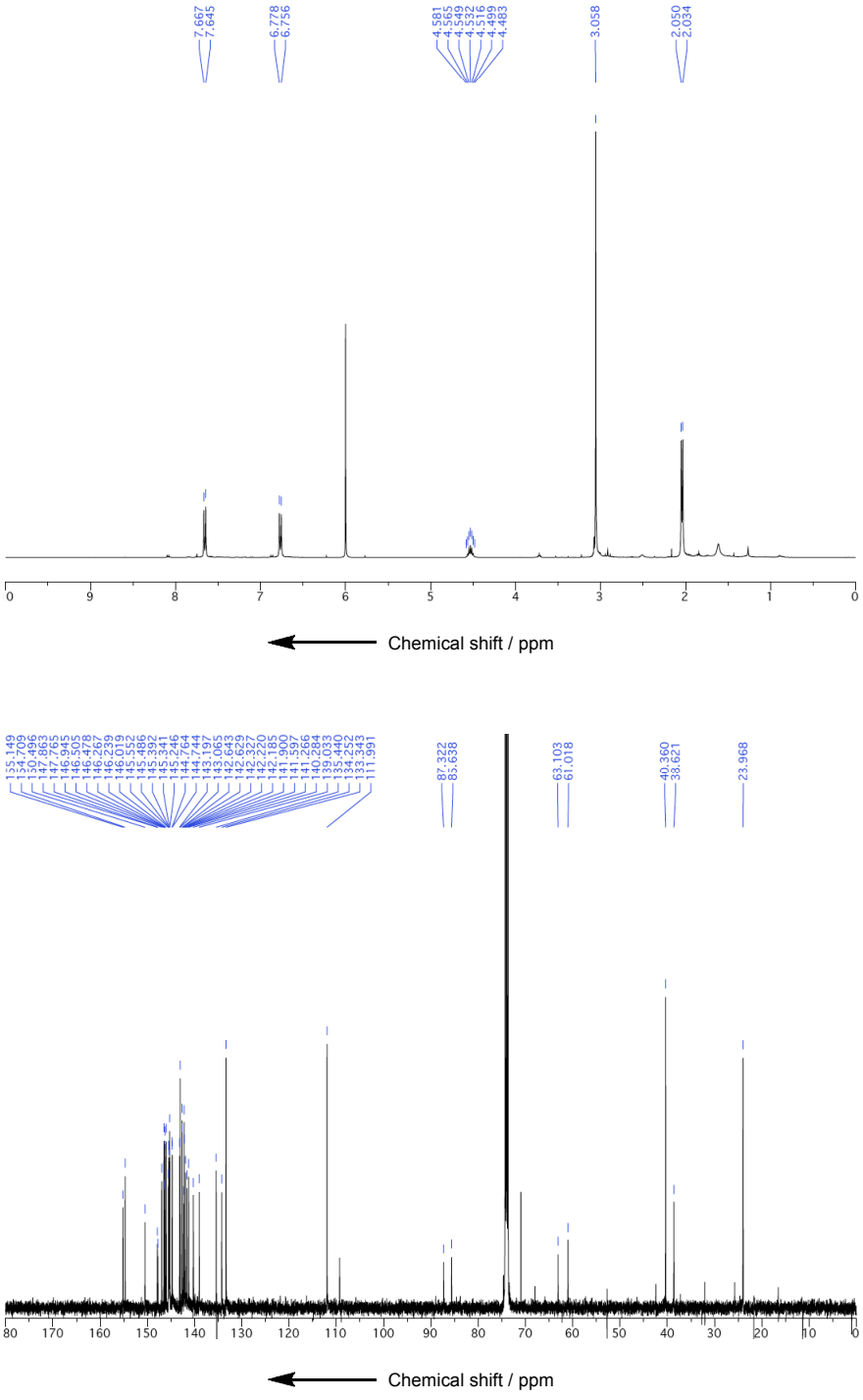


Fig. 2 (ESI). 400 MHz ^{1}H NMR and 100 MHz ^{13}C NMR spectra of **1b** recorded at 298 K in $C_2D_2Cl_4$.

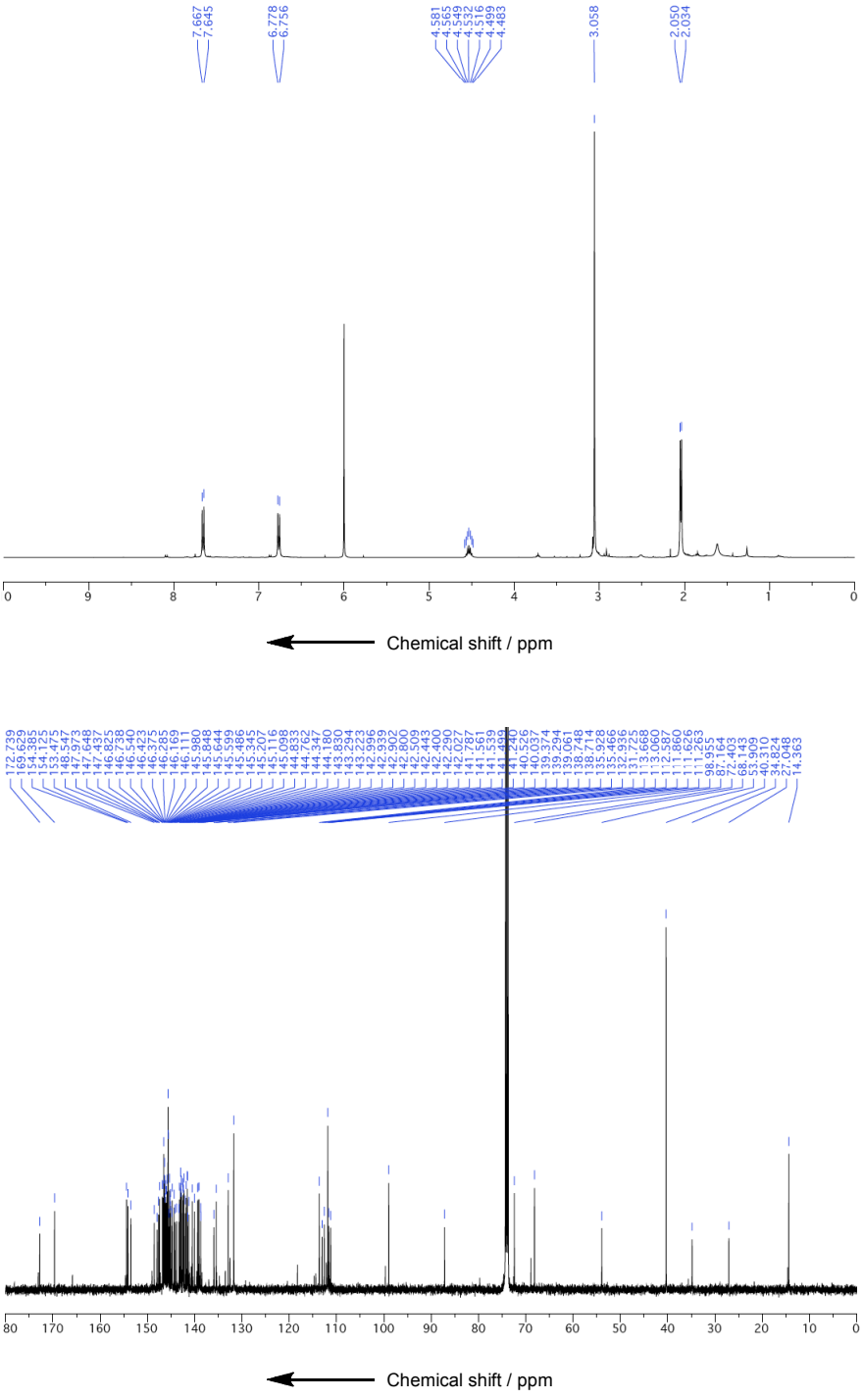


Fig. 3 (ESI). 400 MHz ^{1}H NMR and 100 MHz ^{13}C NMR spectra of (±)-**2a** recorded at 298 K in $C_2D_2Cl_4$.

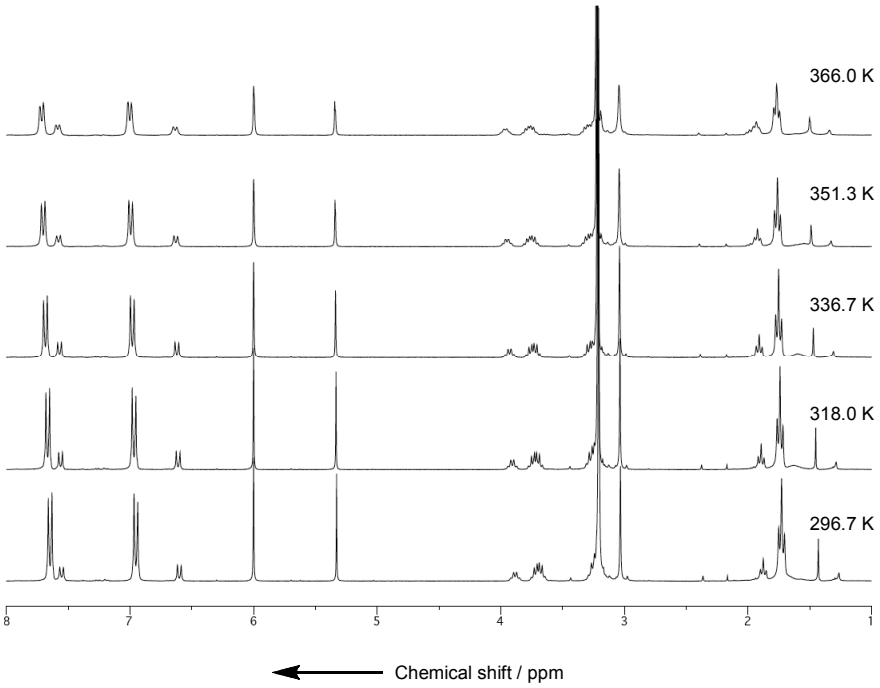


Fig. 4 (ESI). Variable-temperature (VT)-^{1}H NMR (300 MHz) spectra of (±)-**2a** recorded in $C_2D_2Cl_4$.

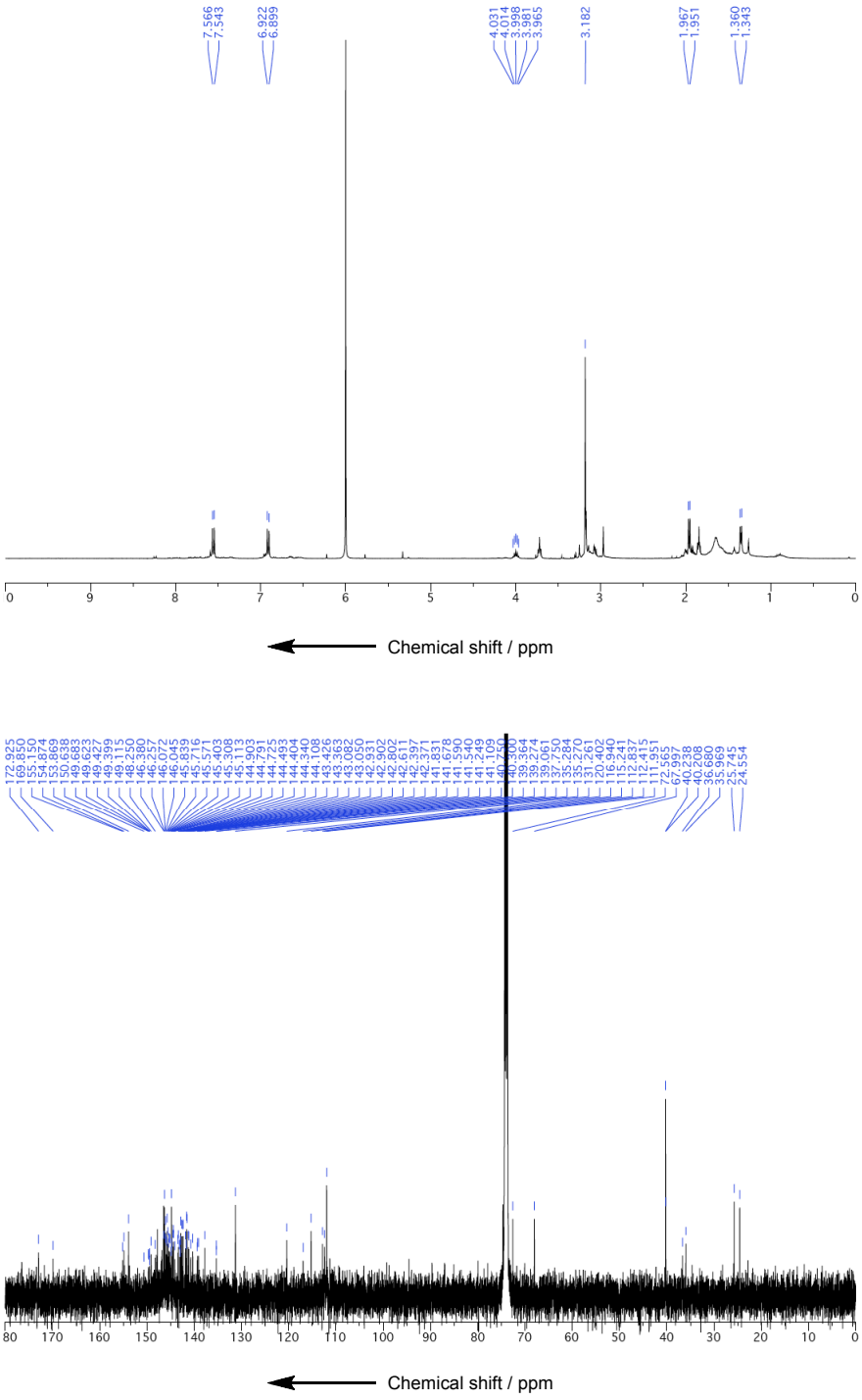


Fig. 5 (ESI). 400 MHz ^{1}H NMR and 100 MHz ^{13}C NMR spectra of (±)-**2b** recorded at 298 K in $C_2D_2Cl_4$.

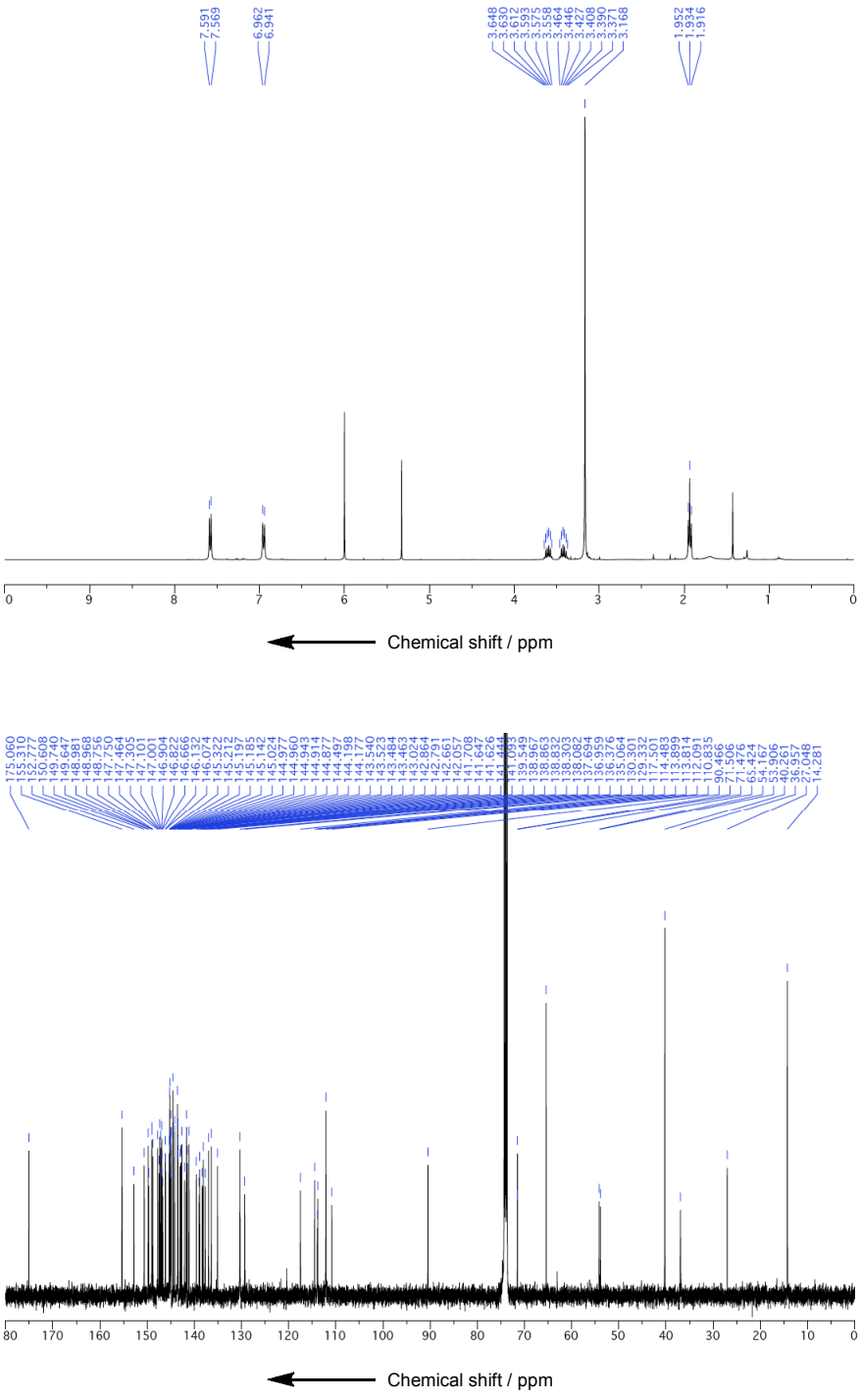


Fig. 6 (ESI). 400 MHz ^{1}H NMR and 100 MHz ^{13}C NMR spectra of (±)-**3a** recorded at 298 K in $C_2D_2Cl_4$.

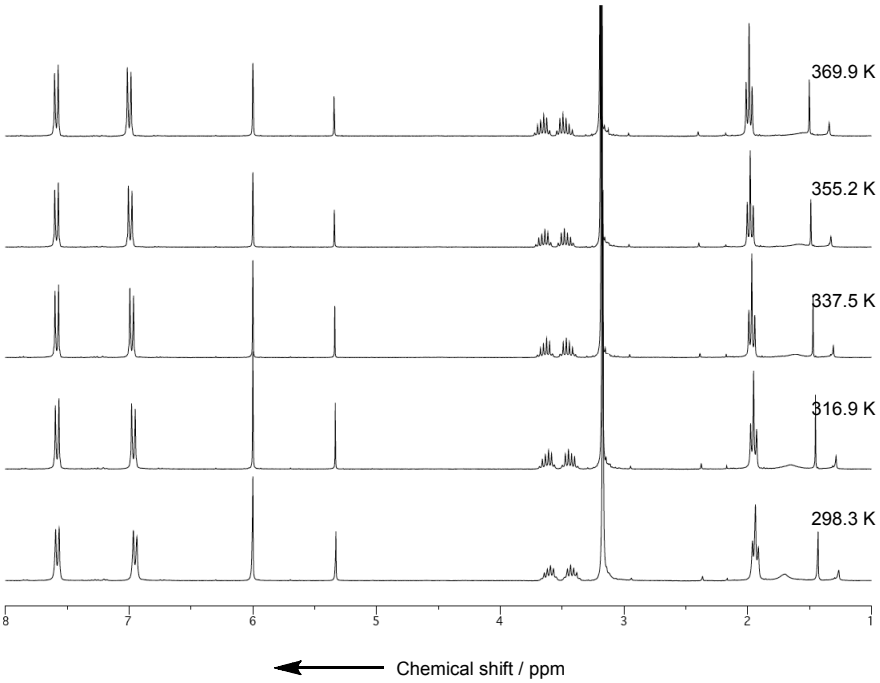


Fig. 7 (ESI). VT-^{1}H NMR (300 MHz) spectra of (±)-**3a** recorded in $C_2D_2Cl_4$.

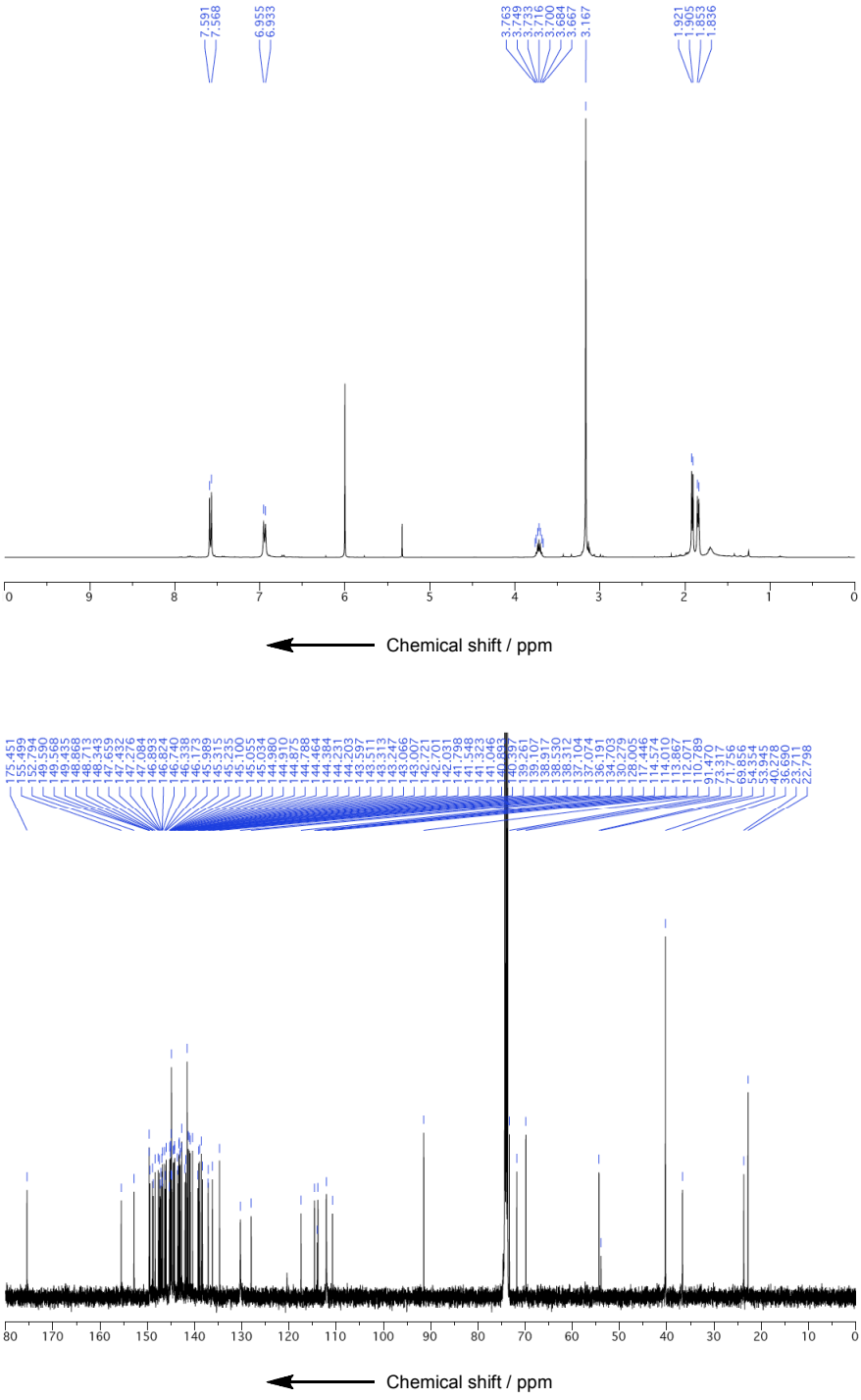


Fig. 8 (ESI). 400 MHz ^{1}H NMR and 100 MHz ^{13}C NMR spectra of (±)-**3b** recorded at 298 K in $C_2D_2Cl_4$.

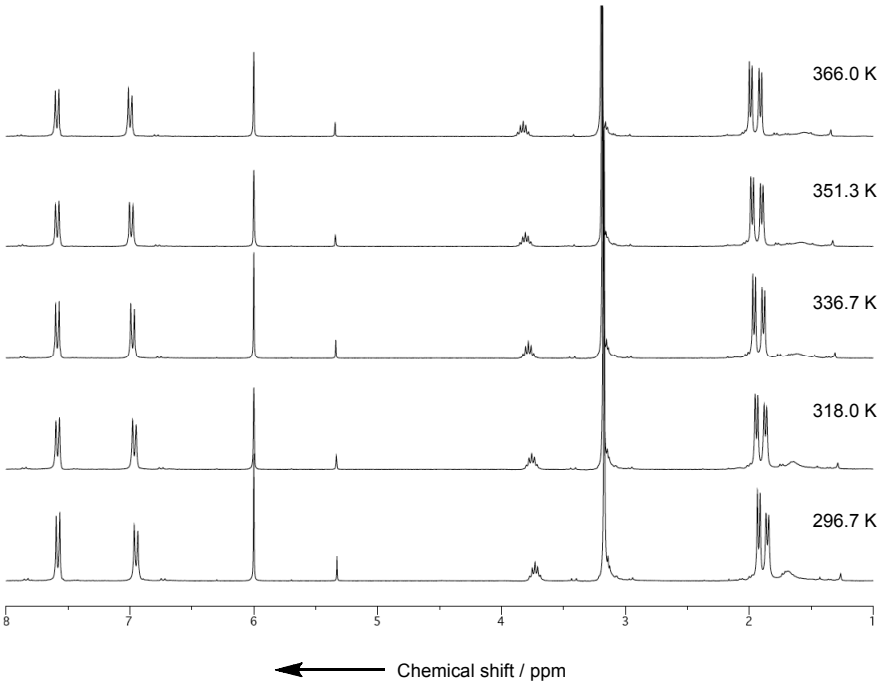


Fig. 9 (ESI). VT-^{1}H NMR (300 MHz) spectra of (±)-**3b** recorded in $C_2D_2Cl_4$.

UV/Vis data (ESI)

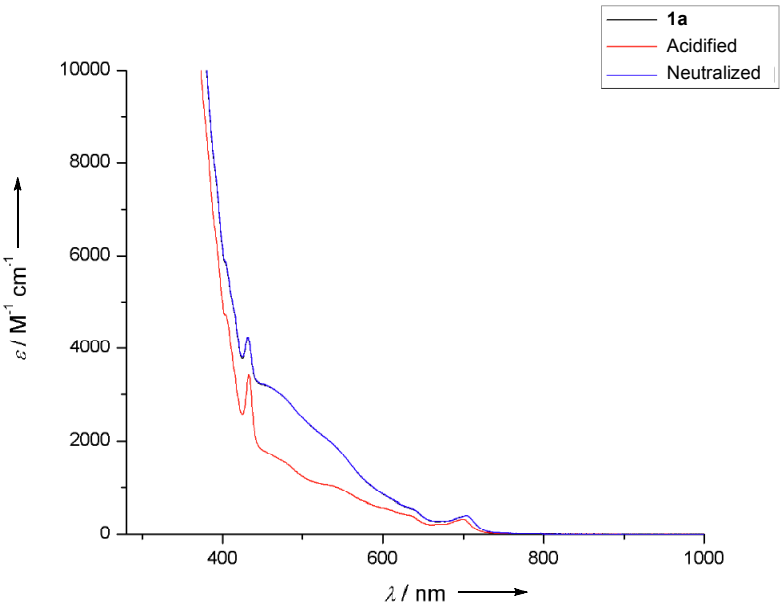


Fig. 10 (ESI). UV/Vis absorption spectra of **1a** in CH_2Cl_2 at 293 K recorded neat, after acidification with trifluoroacetic acid, and after neutralisation with triethylamine.

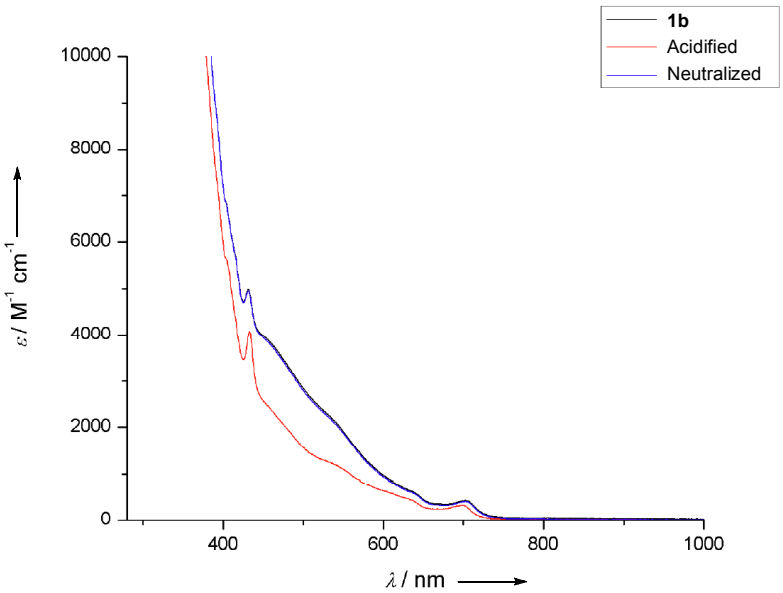


Fig. 11 (ESI). UV/Vis absorption spectra of **1b** in CH_2Cl_2 at 293 K recorded neat, after acidification with trifluoroacetic acid, and after neutralisation with triethylamine.

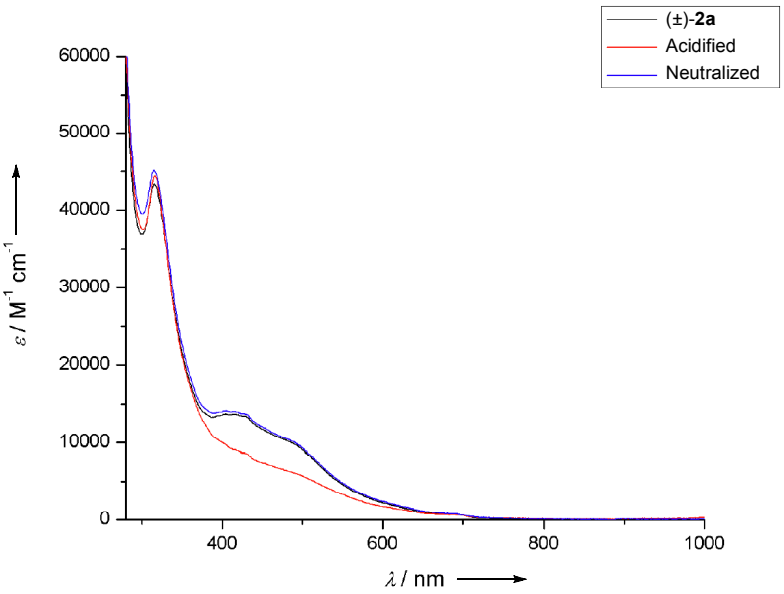


Fig. 12 (ESI). UV/Vis absorption spectra of (±)-**2a** in CH_2Cl_2 at 293 K recorded neat, after acidification with trifluoroacetic acid, and after neutralisation with triethylamine.

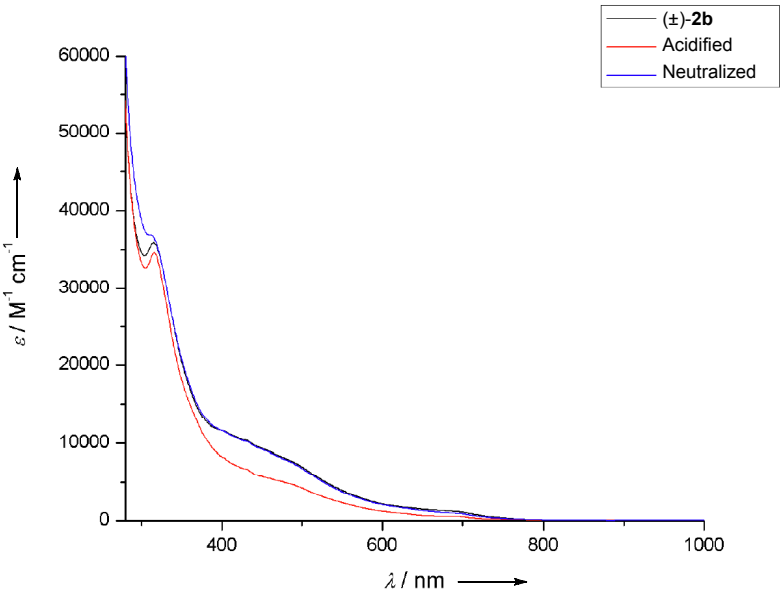


Fig. 13 (ESI). UV/Vis absorption spectra of (±)-**2b** in CH_2Cl_2 at 293 K recorded neat, after acidification with trifluoroacetic acid, and after neutralisation with triethylamine.

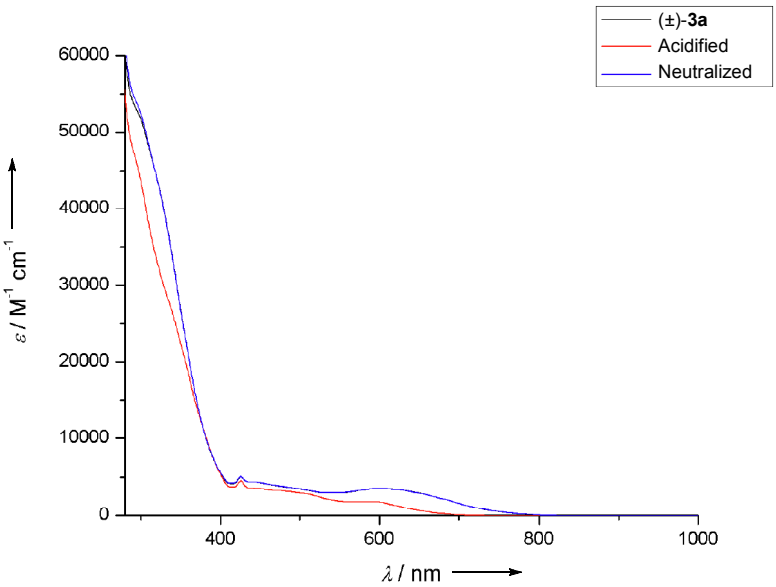


Fig. 14 (ESI). UV/Vis absorption spectra of (±)-**3a** in CH_2Cl_2 at 293 K recorded neat, after acidification with trifluoroacetic acid, and after neutralisation with triethylamine.

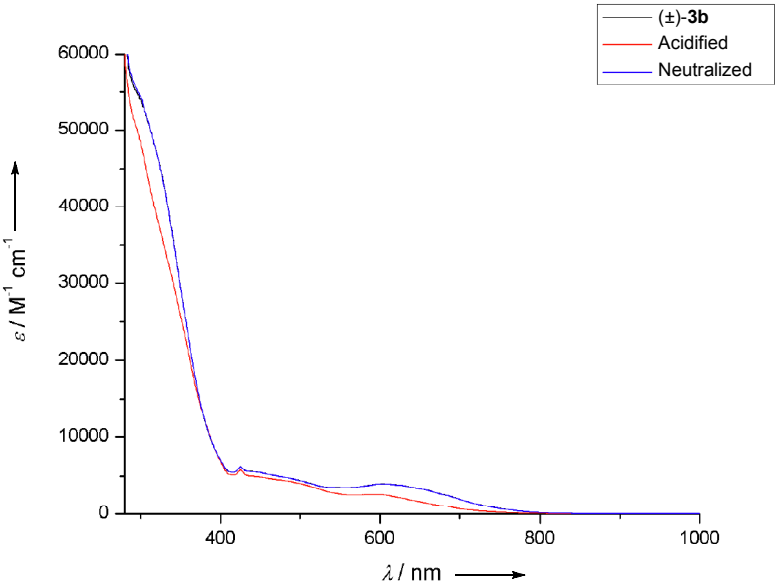


Fig. 15 (ESI). UV/Vis absorption spectra of (±)-**3b** in CH_2Cl_2 at 293 K recorded neat, after acidification with trifluoroacetic acid, and after neutralization with triethylamine.

IR data (ESI)

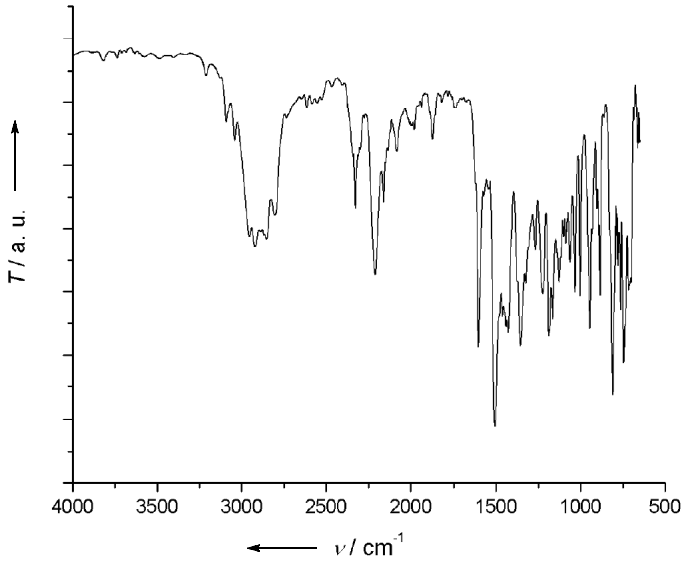


Fig. 16 (ESI). IR spectrum of **1a**.

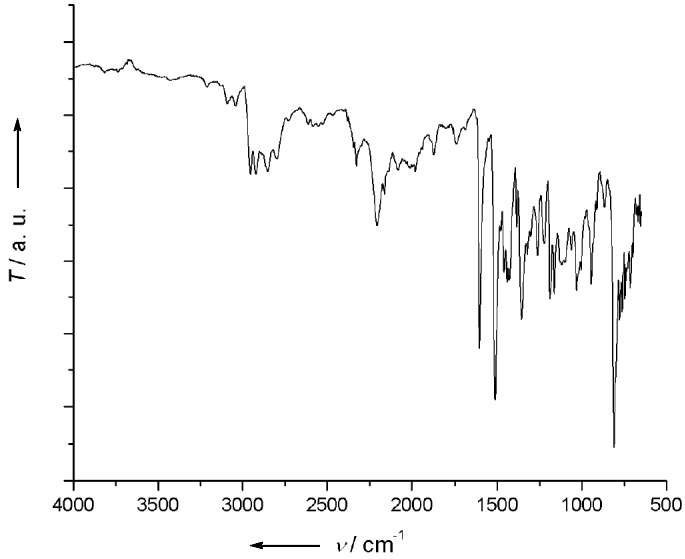


Fig. 17 (ESI). IR spectrum of **1b**.

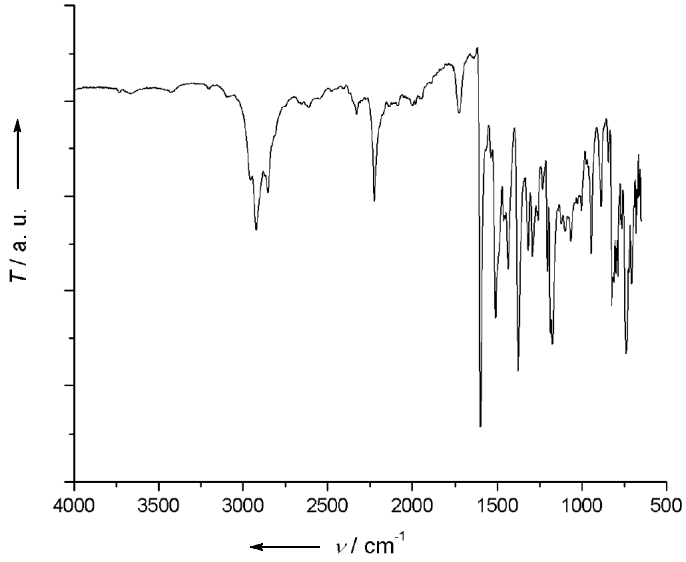


Fig. 18 (ESI). IR spectrum of (±)-**2a**.

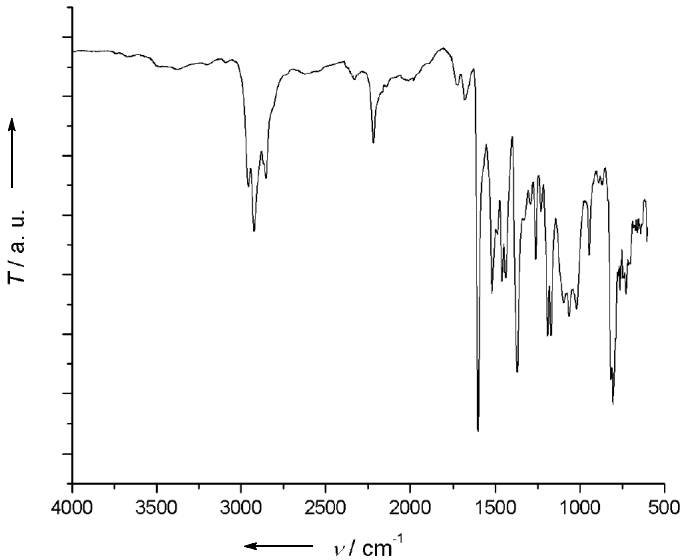


Fig. 19 (ESI). IR spectrum of (±)-**2b**.

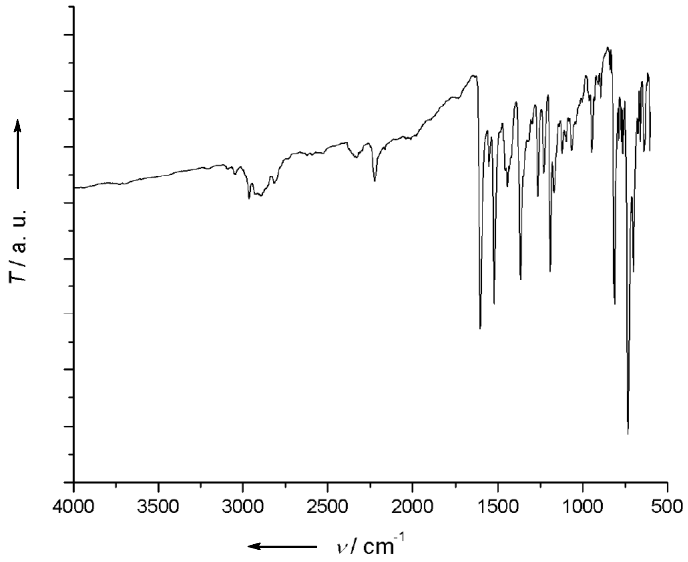


Fig. 20 (ESI). IR spectrum of (±)-**3a**.

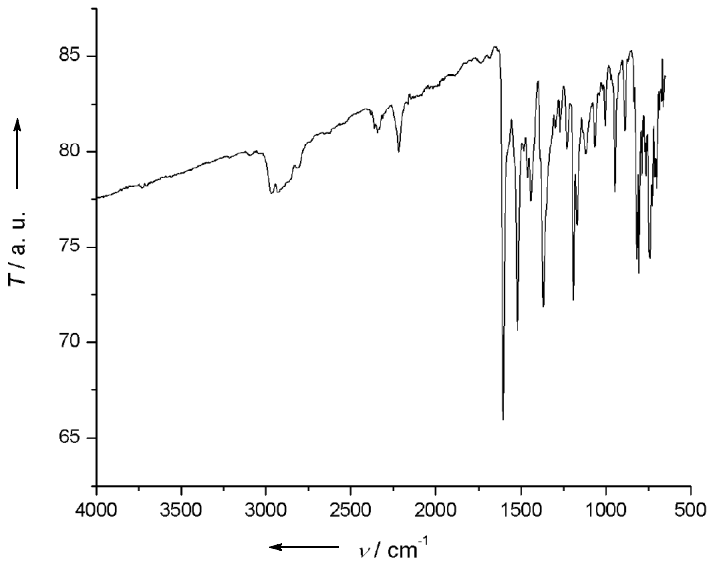


Fig. 21 (ESI). IR spectrum of (±)-**3b**.

X-ray data (ESI)

Suitable crystals were measured on a Bruker-Nonius Kappa-CCD diffractometer, MoKα radiation, λ = 0.71073 Å, with a graphite monochromator. All diagrams and calculations were performed using maXus (Bruker Nonius, Delft & MacScience, Japan). Structures were solved by direct methods (SIR97)[1] and refined by full-matrix least-squares analysis (SHELXL-97).[2] All heavy atoms were refined anisotropically; H-positions are based on stereochemical considerations and were included in the structure factor calculation with constrained isotropic thermal parameters. CCDC-770343 ((±)-**2a**), CCDC-770342 ((±)-**3a**) and CCDC-770541 ((±)-**3b**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Crystal data of (±)-**2a** at 123 K: $C_{78}H_{15}N_5 \cdot 3\ CS_2$, M_r = 1250.430, triclinic, space group P $\bar{1}$ (no. 2), ρ_{calcd} = 1.596 Mg cm^{-3}, Z = 2, a = 13.0651(3), b = 13.5710(3), c = 15.9971(5) Å, α = 74.0161(11), β = 77.3303(12), γ = 75.1841(12)°, V = 2602.02(12) Å^3, μ = 0.325 cm^{-1}. A dark brown crystal of (±)-**2a** (linear dimensons ca. 0.57 × 0.3 × 0.012 mm) was obtained by slow diffusion of *n*-hexane into a solution of compound (±)-**2a** in CS_2 at –15 °C. Numbers of measured and unique reflections were 19258 and 11674, respectively (R_{int} = 0.061). Two disordered CS_2 molecules refined over two positions with restraints. Final $R(F)$ = 0.0748, $wR(F^2)$ = 0.2109 for 893 parameters and 8566 reflections with $I > 2\sigma(I)$ and 3.27 < θ < 27.46° (corresponding *R*-values based on all 11674 reflections are 0.1008 and 0.2294, respectively).

Crystal data of (±)-**3a** at 123 K: $C_{78}H_{15}N_5 \cdot 1.5\ C_6H_5Cl$, M_r = 1190.851, monoclinic, space group $P2_1/c$ (no. 14), ρ_{calcd} = 1.578 Mg cm^{-3}, Z = 4, a = 15.9413(3), b = 18.6916(3), c = 17.0131(3) Å, β = 98.6182(6)°, V = 5012.1(2) Å^3, μ = 0.170 cm^{-1}. A brown crystal of (±)-**3a** (linear dimensons ca. 0.27 × 0.18 × 0.042 mm) was obtained by slow diffusion of *n*-hexane into a solution of compound (±)-**3a** in chlorobenzene at –15 °C. Numbers of measured and unique reflections were 19793 and 10912, respectively (R_{int} = 0.057). The structure contains 1.5 chlorobenzene molecules. One of them refined with constrained geometry and two-fold disorder at a symmetry center. No H-atoms included for the disordered chlorobenzene. Final $R(F)$ = 0.0664, $wR(F^2)$ = 0.1874 for 902 parameters and 8574 reflections with $I > 2\sigma(I)$ and 5.91 < θ < 27.48° (corresponding *R*-values based on all 10912 reflections are 0.0864 and 0.2032, respectively).

Crystal data of (±)-**3b** at 123 K: $C_{79}H_{17}N_5 \cdot 3\ C_6H_5Cl$, M_r = 1373.717, Triclinic, space group P $\bar{1}$ (no. 2), ρ_{calcd} = 1.552 Mg cm^{-3}, Z = 2, a = 9.9620(7), b = 17.8492(9), c = 18.4538(12) Å, α = 64.282(3), β = 84.813(2), γ = 85.112(2)°, V = 2940.3(3) Å^3, μ = 0.222 cm^{-1}. A black crystal of (±)-**3b** (linear dimensons ca. 0.27 × 0.075 × 0.012 mm) was obtained by slow diffusion of *n*-hexane into a solution of compound (±)-**3b** in chlorobenzene at –15 °C. Numbers of measured and unique reflections were 9701 and 5697, respectively (R_{int} = 0.145). The structure contains three chlorobenzene molecules, two of them are disordered and refined with contraints. Final $R(F)$ = 0.1200, $wR(F^2)$ = 0.2542 for 882 parameters and 3469 reflections with $I > 2\sigma(I)$ and 4.92 < θ < 20.68° (corresponding *R*-values based on all 5697 reflections are 0.1841 and 0.2873, respectively).

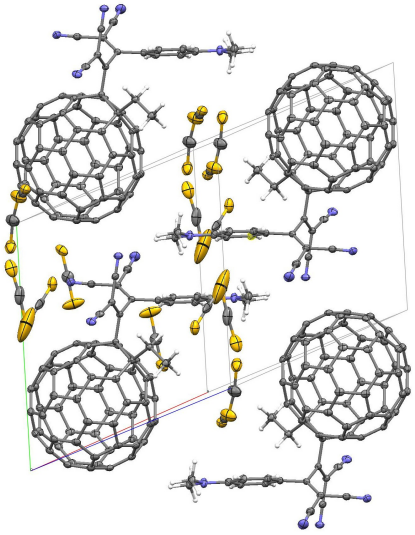


Fig. 22 (ESI). Crystal packing of (±)**-2a**.

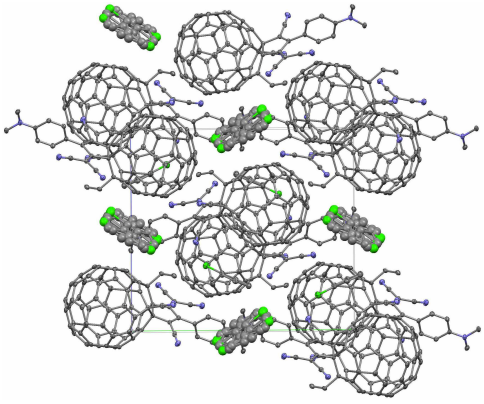


Fig. 23 (ESI). Crystal packing of (±)**-3a**.

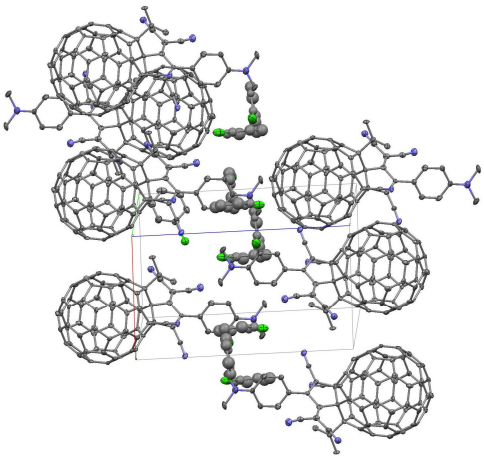


Fig. 24 (ESI). Crystal packing of (±)**-3b**.

Computational Details

All calculations were performed with the Gaussian 03 and 09 suite of programs. Geometry optimizations in the gas-phase were carried out using the ONIOM method with high-layer: B3LYP/6-31G(d) and low-layer: AM1 or SVWN/STO-3G and on selected structures with B3LYP/6-31G(d). Frequency calculations were performed on all optimised geometries to verify the nature of all stationary points as either minima or transition states and to provide zero point energy corrections. Orbital energies and shapes were calculated with HF/6-31G(d).

Full reference 7 (main text) for Gaussian 09 and Gaussian03

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

7(*b*) Gaussian 03. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian, Inc., Revision C.02, Wallingford CT, 2004.

XYZ coordinates and energies:

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C	0.13992100	0.75155100	-2.99285600
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Zero-point correction= 0.693948 (Hartree/Particle)
Thermal correction to Energy= 0.737927
Thermal correction to Enthalpy= 0.738871
Thermal correction to Gibbs Free Energy= 0.621556
Sum of electronic and zero-point Energies= -2344.880505
Sum of electronic and thermal Energies= -2344.836527
Sum of electronic and thermal Enthalpies= -2344.835582
Sum of electronic and thermal Free Energies= -2344.952898

TS1 [oniom(b3lyp/6-31g(d):AM1)]

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C	-0.36057900	2.86329800	-0.47298700
C	-1.73001800	3.39124500	-0.56529400
C	-2.52784400	3.49337700	0.57749100
C	-1.98977100	3.03348900	1.86590900
C	-0.69703600	2.49248100	1.90441800
C	-0.42507700	1.31477700	2.68614700
C	0.64806200	0.92552300	-1.64434400
C	0.23300100	-0.24489500	-2.37947700
C	0.50514100	-1.41461800	-1.58464300
C	1.27947100	-1.03897700	-0.37370000
C	0.74710400	-1.61423600	0.83138100
C	-0.15930100	-2.72140400	0.81799300
C	-0.70955300	-3.18236300	-0.38075300
C	-0.37090300	-2.49820700	-1.61177300
C	-1.57159300	-2.45532200	-2.43732700
C	-2.65975100	-3.15170400	-1.72233200
C	-2.12509000	-3.56670300	-0.43659500
C	-2.90667400	-3.51306600	0.72248200
C	-4.24454500	-2.96396900	0.63711400
C	-4.76114500	-2.53954800	-0.57733400
C	-3.93635800	-2.61497900	-1.77956700
C	-4.21202600	-1.42872600	-2.59171800
C	-5.26761500	-1.03427400	1.78441000
C	-5.55563700	-1.31162000	-0.64731500
C	-5.80381300	-0.57950000	0.50021500
C	-5.72433700	0.88185300	0.46929600
C	-5.39892300	1.53286000	-0.70862900
C	-5.13589200	0.75814800	-1.92228100
C	-4.04747600	1.41204100	-2.64754900
C	-3.63626100	2.59035800	-1.88241500
C	-4.47445400	2.66709200	-0.68822600
C	-3.92215500	3.09358900	0.50851200
C	-4.26323000	2.39951800	1.75170900
C	-5.13862900	1.32872200	1.73390800
C	-4.85835000	0.14320500	2.54565700

C	-5.21432400	-0.62432000	-1.89353100
C	-4.50642300	-2.19059000	1.84938300
C	-3.32946000	-2.25585800	2.69086200
C	-2.93994600	-1.12930400	3.42623500
C	-3.71367500	0.09186000	3.32428800
C	-2.78501600	1.22033600	3.33399000
C	-3.05209400	2.34683500	2.57325900
C	-1.44011700	0.69648700	3.43745300
C	-1.52321000	-0.75344400	3.46640600
C	-0.56864200	-1.50972100	2.77968300
C	0.49413000	-0.84077000	2.02999600
C	0.58079600	0.53439600	2.00691900
C	-0.10407700	2.07112800	-1.69885600
C	-1.30445200	2.12768700	-2.51458900
C	-2.30356600	2.96700700	-1.82921700
C	-1.69451400	1.02277100	-3.25524700
C	-0.90734800	-0.20315100	-3.18313600
C	-1.83145100	-1.33971000	-3.21415900
C	-3.18061700	-0.80756200	-3.27574300
C	-3.09638400	0.64919600	-3.30315400
C	-2.31876000	-3.04846300	1.98642900
C	-0.97364900	-2.67117100	2.03180900
C	2.56151400	2.01178100	1.48149800
C	2.44182500	2.76530700	2.81132300
C	3.05120600	0.65068800	-0.94502900
C	3.88180400	-0.46723100	-0.58860800
C	5.25470100	-0.38061500	-0.18766300
C	5.83738000	0.80059200	0.35922700
C	7.15223800	0.85722500	0.74954600
C	8.01106900	-0.27620400	0.62077800
C	7.44334700	-1.46150600	0.06950500
C	6.12402700	-1.50451000	-0.31430100
C	3.54317800	1.72363600	-1.68387700
C	4.78008400	1.64765900	-2.40183900
C	2.90517600	2.99392100	-1.80773600
C	3.17584500	-1.76140600	-0.56632200
C	3.07995600	-2.44136800	-1.83660700
C	3.48169900	-2.66179700	0.52735400
C	10.16764100	-1.40434400	0.88817900
C	9.89480900	1.02662900	1.48974300
H	3.28876200	1.20305300	1.60460000
H	2.95698200	2.70637500	0.73649300
H	1.74276600	3.60414500	2.74636700
H	3.42383000	3.17304900	3.07607000
H	2.12025500	2.11581700	3.63113100
H	5.22399300	1.68385100	0.49305100
H	7.53028400	1.78113300	1.16981200
H	8.05801800	-2.33943000	-0.08689100
H	5.75354700	-2.41264500	-0.77769900
H	9.74771300	-2.24752500	1.44929800
H	11.14998700	-1.17627300	1.30247900
H	10.29782200	-1.71117400	-0.15781600
H	9.79289600	1.83038800	0.75040700
H	10.95700200	0.87522900	1.68318600
H	9.41934400	1.34986800	2.42472900

Zero-point correction= 0.691832 (Hartree/Particle)
Thermal correction to Energy= 0.735117
Thermal correction to Enthalpy= 0.736061
Thermal correction to Gibbs Free Energy= 0.621682

Sum of electronic and zero-point Energies= -2344.837626
Sum of electronic and thermal Energies= -2344.794341
Sum of electronic and thermal Enthalpies= -2344.793397
Sum of electronic and thermal Free Energies= -2344.907776

Int [oniom(b3lyp/6-31g(d):AM1)]

N	5.66052200	2.04667100	-2.79757400
N	2.38885700	4.34565400	-1.28347300
N	3.33980000	-3.20701400	-2.27503100
N	3.65183000	-2.75705400	1.96437900
N	9.42116100	-0.45570600	0.57338900
C	1.57891600	0.65675500	-0.24997500
C	1.14375000	1.40638500	1.15156100
C	0.02396200	2.46624200	0.96032100
C	-0.43390100	2.91982200	-0.24506700
C	-1.81148400	3.41086900	-0.40042000
C	-2.68293400	3.42746100	0.69319600
C	-2.21014100	2.91334500	1.98603800
C	-0.90202800	2.41361600	2.08079400
C	-0.64025500	1.19913300	2.80769000
C	0.69873200	1.06977900	-1.43345600
C	0.38280500	-0.06726200	-2.25626200
C	0.66965100	-1.27482600	-1.53450600
C	1.45085000	-0.96932600	-0.24724300
C	0.74416600	-1.59820700	0.90931100
C	-0.12653400	-2.72179100	0.76903600
C	-0.57733400	-3.13930100	-0.48497300
C	-0.17782400	-2.36549600	-1.66205700
C	-1.32720300	-2.31446700	-2.55331100
C	-2.43452600	-3.08473400	-1.94904100
C	-1.96997600	-3.55252900	-0.65499700
C	-2.83234500	-3.59361300	0.45181100
C	-4.17676800	-3.07760300	0.30367500
C	-4.62784900	-2.60276000	-0.91846500
C	-3.72247000	-2.58590100	-2.06334200
C	-3.98825500	-1.36721300	-2.83096100
C	-5.33804300	-1.24360800	1.47937600
C	-5.45706900	-1.39796200	-0.97655500
C	-5.80513000	-0.73634800	0.18799600
C	-5.77343200	0.72608700	0.23861900
C	-5.39673600	1.45009400	-0.88006800
C	-5.02971900	0.75044100	-2.11196600
C	-3.92115500	1.47640600	-2.72977600
C	-3.60115400	2.62417100	-1.87866200
C	-4.51545500	2.60970100	-0.73947900
C	-4.05494500	2.98798100	0.51146300
C	-4.44926800	2.21627800	1.69159300
C	-5.28554000	1.12203300	1.56026300
C	-5.01791400	-0.09658900	2.32575200
C	-5.06065300	-0.63370900	-2.16004900
C	-4.54528600	-2.37884100	1.53438900
C	-3.42369200	-2.45430200	2.44735000
C	-3.11932500	-1.35683700	3.26229100
C	-3.92394700	-0.15504200	3.17328600
C	-3.03304500	0.99783300	3.29932800
C	-3.29121200	2.15682300	2.58529200
C	-1.68210300	0.50926200	3.45938100
C	-1.72073100	-0.94081400	3.41099700

C	-0.70480200	-1.63240200	2.74964600
C	0.37611000	-0.89124900	2.09123800
C	0.43055900	0.49237400	2.15652500
C	-0.07914200	2.19837900	-1.48628200
C	-1.21972200	2.26607400	-2.37831400
C	-2.28908500	3.04007400	-1.71785200
C	-1.52265900	1.19241600	-3.19862200
C	-0.70166200	-0.01259200	-3.13570700
C	-1.57792800	-1.16975500	-3.29123900
C	-2.93917900	-0.67833700	-3.41492200
C	-2.90484200	0.77963500	-3.36094400
C	-2.34468600	-3.17961200	1.77053900
C	-1.01814800	-2.76683700	1.92767400
C	2.40945000	2.04384900	1.82988800
C	2.20558300	2.67456200	3.21146400
C	3.05199400	0.87105000	-0.66645900
C	3.85917700	-0.27339800	-0.43504400
C	5.26172500	-0.31658500	-0.20275900
C	5.98387600	0.81956300	0.28566700
C	7.32678400	0.77861800	0.54983700
C	8.08698800	-0.41656500	0.34046200
C	7.37425900	-1.56683100	-0.11931300
C	6.02610500	-1.51606400	-0.36885300
C	3.51712400	2.01564400	-1.33539100
C	4.70735100	2.00869700	-2.12699600
C	2.85899900	3.27788800	-1.32187000
C	2.98952000	-1.52330500	-0.28080600
C	3.16473100	-2.46272300	-1.40108900
C	3.33761900	-2.23419900	0.97702500
C	10.16781400	-1.70247900	0.40308600
C	10.13842000	0.74846600	0.99337400
H	3.16799000	1.25730100	1.91174100
H	2.80210600	2.81257900	1.16037300
H	1.47171700	3.48595300	3.18754200
H	3.15634100	3.09858500	3.55275100
H	1.87980700	1.94294000	3.95760800
H	5.44398600	1.73712400	0.49323200
H	7.80853900	1.66739900	0.93985500
H	7.89933800	-2.49760800	-0.29780300
H	5.54762500	-2.41027900	-0.75358600
H	9.76714100	-2.49555300	1.04613500
H	11.20917200	-1.53355700	0.67837200
H	10.13819700	-2.04722000	-0.63843800
H	9.99701100	1.56279400	0.27295900
H	11.20413600	0.52515600	1.05116200
H	9.80500400	1.09179700	1.98142200

Zero-point correction= 0.694031 (Hartree/Particle)
Thermal correction to Energy= 0.737471
Thermal correction to Enthalpy= 0.738416
Thermal correction to Gibbs Free Energy= 0.624025
Sum of electronic and zero-point Energies= -2344.843757
Sum of electronic and thermal Energies= -2344.800316
Sum of electronic and thermal Enthalpies= -2344.799372
Sum of electronic and thermal Free Energies= -2344.913762

TS2 [oniom(b3lyp/6-31g(d):AM1)]

N	5.74617500	2.54342200	-2.57886100
N	2.29721700	4.59324200	-1.10141000

N	3.36050400	-2.74148100	-2.96663600
N	3.58388900	-2.85845900	1.14958400
N	9.22341000	-0.71986200	0.83769800
C	1.55846500	0.83750500	-0.38366300
C	1.21636300	1.28788500	1.16069900
C	0.05678100	2.31254300	1.26214000
C	-0.50541400	2.98012300	0.21089600
C	-1.90522300	3.43240800	0.26483900
C	-2.68028400	3.20333200	1.40566700
C	-2.08731300	2.47154800	2.53354800
C	-0.76715600	2.01087100	2.42167300
C	-0.41838700	0.69357100	2.87882300
C	0.58489400	1.45091000	-1.40357100
C	0.20784100	0.47241900	-2.39486800
C	0.56835700	-0.83353600	-1.93319400
C	1.44859500	-0.74607900	-0.70414300
C	1.01486100	-1.71365000	0.41687900
C	0.04446400	-2.77491000	0.10706100
C	-0.51320100	-2.92191300	-1.15229400
C	-0.24183900	-1.92238400	-2.19937200
C	-1.46038600	-1.75460900	-2.96997000
C	-2.49006900	-2.66703700	-2.43617800
C	-1.90674400	-3.35317200	-1.29503900
C	-2.67280000	-3.64285200	-0.15972200
C	-4.04107000	-3.16581900	-0.10131700
C	-4.60256900	-2.48528200	-1.16978100
C	-3.79653900	-2.21328700	-2.35698000
C	-4.15895400	-0.88469600	-2.85480300
C	-5.14279500	-1.63612700	1.49071800
C	-5.46526200	-1.32688900	-0.93226500
C	-5.72981800	-0.91299600	0.36146200
C	-5.73105400	0.51382100	0.68862400
C	-5.46857300	1.45103700	-0.29623800
C	-5.19055500	1.01335300	-1.66466400
C	-4.15847700	1.88928600	-2.21748200
C	-3.79491800	2.86689100	-1.19003500
C	-4.60792500	2.59884000	-0.00625800
C	-4.05190200	2.75128300	1.25334100
C	-4.32572000	1.75482300	2.29089500
C	-5.14227600	0.67167800	2.01921600
C	-4.78089000	-0.65790800	2.51321500
C	-5.18981500	-0.33696300	-1.97433000
C	-4.31980600	-2.72867500	1.26502800
C	-3.12306200	-2.93091700	2.05527400
C	-2.77861500	-1.99588600	3.03850100
C	-3.61727400	-0.83205600	3.24479800
C	-2.74951600	0.31184200	3.51934900
C	-3.09447100	1.57313300	3.06161400
C	-1.37680600	-0.14280100	3.47277000
C	-1.38407600	-1.55784500	3.15148300
C	-0.41034900	-2.06417600	2.28748500
C	0.59730800	-1.17938600	1.71690100
C	0.61310500	0.16038300	2.01458300
C	-0.23530200	2.52754200	-1.17190200
C	-1.45560500	2.71167800	-1.93772400
C	-2.48444900	3.29895400	-1.05782400
C	-1.80313100	1.80332000	-2.92437400
C	-0.94930300	0.64395900	-3.15958700
C	-1.80294200	-0.50039800	-3.45608700

C	-3.18237200	-0.05393100	-3.37682800
C	-3.18256900	1.36878800	-3.04984500
C	-2.08818900	-3.47394000	1.17050200
C	-0.76032400	-3.04361000	1.29146100
C	2.50227400	1.85733300	1.85912800
C	2.37803100	2.22821500	3.34094900
C	3.03169300	1.10251900	-0.78495300
C	3.82300300	-0.09489300	-0.69940800
C	5.18953900	-0.23414500	-0.35045300
C	5.93386700	0.82293100	0.26377300
C	7.23500600	0.66722900	0.65986000
C	7.92384700	-0.57351500	0.47059900
C	7.18804400	-1.64377700	-0.11269700
C	5.87789200	-1.48282900	-0.49585500
C	3.50108700	2.30751400	-1.29914700
C	4.74732100	2.41463200	-1.99315700
C	2.79581300	3.54486400	-1.20840200
C	2.91420200	-1.27307100	-0.83762400
C	3.15689800	-2.08839600	-2.02770600
C	2.90374600	-2.22258500	0.41800100
C	9.88928700	-2.01366000	0.69767600
C	9.97779200	0.41100700	1.37491800
H	3.29460300	1.10785400	1.75764300
H	2.81786200	2.74767600	1.30821600
H	1.62607300	3.00440300	3.51132200
H	3.34068500	2.61823300	3.68976200
H	2.12461600	1.36493200	3.96410400
H	5.44648900	1.77033800	0.46087900
H	7.73609300	1.49968000	1.13859600
H	7.65843400	-2.60554400	-0.27506600
H	5.37980200	-2.32093700	-0.96653600
H	9.35654000	-2.79512700	1.25247700
H	10.90010100	-1.93906700	1.09929200
H	9.95773700	-2.31739900	-0.35471400
H	9.95155800	1.26481400	0.68820100
H	11.01841500	0.11355600	1.50634500
H	9.58688500	0.73233000	2.34922400

Zero-point correction= 0.692603 (Hartree/Particle)
Thermal correction to Energy= 0.735351
Thermal correction to Enthalpy= 0.736295
Thermal correction to Gibbs Free Energy= 0.623967
Sum of electronic and zero-point Energies= -2344.830445
Sum of electronic and thermal Energies= -2344.787697
Sum of electronic and thermal Enthalpies= -2344.786753
Sum of electronic and thermal Free Energies= -2344.899081

(±)-3a [oniom(b3lyp/6-31g(d):AM1)]

N	6.09695500	3.11940400	0.11813600
N	2.25982600	4.61490700	-0.14051700
N	3.74520600	-3.59119600	-0.43349000
N	2.67065300	-2.75924700	3.03180900
N	9.44723300	-0.72667400	-0.81780200
C	1.56154500	0.81180700	0.33390900
C	0.84174700	1.49838400	1.62290100
C	-0.26152500	2.52927700	1.23344800
C	-0.50692800	2.99351200	-0.02673900
C	-1.85098200	3.43798200	-0.42895400
C	-2.90845900	3.41024100	0.48505000

C	-2.66372200	2.89011400	1.83661000
C	-1.37881000	2.42500800	2.16088900
C	-1.22637500	1.20370200	2.89625100
C	0.89066800	1.20135900	-0.99511200
C	0.75240500	0.06519100	-1.86355300
C	0.90799800	-1.13639200	-1.09815200
C	1.54767200	-0.83633000	0.25604900
C	0.85934900	-1.67298000	1.45151100
C	-0.18477900	-2.74019200	0.99816200
C	-0.40306800	-3.07922100	-0.30728100
C	0.17926200	-2.26230400	-1.39843800
C	-0.78295200	-2.23391300	-2.48451300
C	-1.95638300	-3.04288700	-2.09703300
C	-1.73029700	-3.52406300	-0.74779200
C	-2.78343000	-3.61421300	0.17008400
C	-4.09746900	-3.13949100	-0.22394300
C	-4.32173900	-2.65615900	-1.50243600
C	-3.21632100	-2.59156000	-2.45556000
C	-3.37731300	-1.37374400	-3.25219900
C	-5.51058700	-1.35544500	0.72980700
C	-5.16572500	-1.47751000	-1.70677600
C	-5.74536700	-0.84400000	-0.62153000
C	-5.77151800	0.61825600	-0.55469800
C	-5.21730900	1.36897200	-1.57747800
C	-4.60565300	0.69898800	-2.72579700
C	-3.42799900	1.46962400	-3.12258300
C	-3.30902700	2.61525000	-2.21828000
C	-4.41668000	2.55470900	-1.26778500
C	-4.20777100	2.92910900	0.04946500
C	-4.78748100	2.12785300	1.12915200
C	-5.54876200	1.01011400	0.83785100
C	-5.38931900	-0.21095700	1.62925100
C	-4.58080100	-0.68478700	-2.78882700
C	-4.70637000	-2.46855100	0.92223300
C	-3.76836900	-2.52240800	2.02430400
C	-3.65406000	-1.42753900	2.88537700
C	-4.46783000	-0.24881600	2.66306700
C	-3.65591000	0.92998100	2.96017700
C	-3.81069200	2.09022600	2.21949400
C	-2.33748100	0.47950000	3.35063200
C	-2.31875100	-0.96543600	3.27849900
C	-1.17569400	-1.60632500	2.79081600
C	-0.02314500	-0.83139700	2.38172200
C	-0.03606900	0.52383800	2.41978600
C	0.10119400	2.31081500	-1.18897800
C	-0.86537300	2.34440300	-2.27194000
C	-2.06427400	3.07337100	-1.81590600
C	-0.97542300	1.27312800	-3.14555200
C	-0.14437700	0.09564700	-2.93405800
C	-0.93301800	-1.08943300	-3.25251100
C	-2.26296000	-0.64277400	-3.62622900
C	-2.28930600	0.81563400	-3.56020000
C	-2.56184400	-3.21087400	1.55115700
C	-1.28829900	-2.75921000	1.93749100
C	1.81355200	2.15747800	2.66975300
C	2.78451600	1.21464100	3.38709000
C	3.06976800	1.14188900	0.17408100
C	3.85259100	-0.08628000	0.05752600
C	5.30822500	-0.20584600	-0.16517700

C	6.11745300	-0.83763700	0.79254400
C	7.47864100	-1.00421300	0.58902900
C	8.09687200	-0.56441600	-0.60751100
C	7.26696200	0.04290800	-1.58359300
C	5.91136500	0.21714100	-1.36028700
C	3.60458400	2.40408300	0.05772900
C	5.00758300	2.71198900	0.06665100
C	2.82397200	3.60119800	-0.04347100
C	3.02326200	-1.16585000	0.10509300
C	3.44599200	-2.49710400	-0.17069700
C	1.88857700	-2.30340400	2.30421500
C	10.06559700	-0.20352800	-2.02546200
C	10.27881600	-1.31929900	0.21736700
H	2.35348200	2.98775900	2.21317700
H	1.16064800	2.61644500	3.42084300
H	2.25941800	0.41050500	3.91174600
H	3.35349500	1.78098800	4.13246600
H	3.51075600	0.75311900	2.71175500
H	5.67362000	-1.19665900	1.71734800
H	8.06327700	-1.48259000	1.36506200
H	7.68492200	0.38332400	-2.52287800
H	5.30988000	0.68506500	-2.13510400
H	9.65330000	-0.67433600	-2.92834800
H	11.13585700	-0.41359700	-1.99882300
H	9.93366500	0.88398600	-2.11604400
H	10.26677600	-0.72791300	1.14434300
H	11.30918100	-1.37141600	-0.13755100
H	9.95441800	-2.34004500	0.45990600

Zero-point correction= 0.694614 (Hartree/Particle)
Thermal correction to Energy= 0.737927
Thermal correction to Enthalpy= 0.738872
Thermal correction to Gibbs Free Energy= 0.624220
Sum of electronic and zero-point Energies= -2344.894464
Sum of electronic and thermal Energies= -2344.851151
Sum of electronic and thermal Enthalpies= -2344.850206
Sum of electronic and thermal Free Energies= -2344.964858

oniom(b3lyp/6-31g(d):SVWN/STO-3G)

(±)-2a [oniom(b3lyp/6-31g(d):SVWN/STO-3G)]

N	-5.71986800	-3.96151300	1.00845800
N	-2.04320000	-3.90545900	3.18111300
N	-5.72756700	-1.59946200	-3.70019500
N	-2.73773500	-4.32138700	-2.20304100
N	-7.04937200	3.36521100	0.03539300
C	-1.59033300	-1.10127100	0.51411800
C	-1.35061900	-0.14269500	1.83785500
C	-0.10337400	-0.54262600	2.65408100
C	0.60029700	-1.71775400	2.51358500
C	2.00520900	-1.78172700	2.85026800
C	2.67766300	-0.65302000	3.33501800
C	1.94709000	0.59728500	3.46987100
C	0.59163300	0.63611700	3.09679100
C	0.07293200	1.76983700	2.36938600
C	-0.51467600	-2.21043500	0.35403700
C	-0.15444400	-2.35444400	-1.02995200
C	-0.66694400	-1.21026100	-1.75632600

C	-1.35817500	-0.35816400	-0.82894300
C	-1.24657200	1.00630700	-0.96499900
C	-0.49106300	1.57583600	-2.05997200
C	0.13957200	0.74572300	-2.99419400
C	0.04411700	-0.68624700	-2.84246500
C	1.31795100	-1.27071100	-3.22679700
C	2.20593500	-0.18594300	-3.61611100
C	1.46834700	1.06598700	-3.47322100
C	2.11929000	2.21460300	-3.00684100
C	3.52311700	2.16544400	-2.66713900
C	4.24209700	0.96110600	-2.80271900
C	3.55707100	-0.23843800	-3.28901100
C	4.09047300	-1.38977600	-2.55566900
C	4.66310600	2.62833300	-0.49858500
C	5.19300800	0.55247800	-1.76651000
C	5.39920600	1.36947500	-0.63696000
C	5.51732300	0.76700800	0.69265500
C	5.41979900	-0.63208200	0.84314100
C	5.20605500	-1.48247100	-0.33308800
C	4.31008400	-2.57034500	0.05320100
C	3.95733300	-2.38731000	1.46415300
C	4.65666400	-1.19593100	1.95416100
C	4.01518100	-0.34470400	2.87733200
C	4.12181400	1.10822400	2.72303200
C	4.85582500	1.65350900	1.65144000
C	4.32754100	2.80495400	0.91250700
C	5.09779500	-0.90068400	-1.61333300
C	3.73778300	3.01963600	-1.48941200
C	2.46714400	3.59113600	-1.11498800
C	2.14224600	3.76576300	0.24366700
C	3.08230300	3.36380300	1.26823100
C	2.31674600	2.79006100	2.38165400
C	2.82654000	1.68215100	3.09235500
C	0.91587600	2.84220300	2.02818300
C	0.80224900	3.43531700	0.71355400
C	-0.15483100	2.94160800	-0.17540000
C	-1.04289200	1.86706800	0.21917300
C	-0.94382100	1.29880800	1.46735400
C	0.38740400	-2.57461700	1.32823300
C	1.66313200	-3.14805900	0.96258200
C	2.66598300	-2.66342500	1.89748900
C	1.99929200	-3.33600300	-0.38411300
C	1.06469300	-2.92726500	-1.40766900
C	1.81885900	-2.36721500	-2.52142400
C	3.22293400	-2.43595200	-2.18279600
C	3.33521600	-3.04045100	-0.84953000
C	1.45834200	3.08749000	-2.04398700
C	0.18435800	2.76410800	-1.57661000
C	-2.61427400	-0.10248500	2.76201100
C	-2.54140900	0.80917700	3.99312300
C	-2.98808700	-1.80118500	0.43644100
C	-3.93494100	-1.35765700	-0.64815600
C	-4.69843700	-0.11465900	-0.46130000
C	-5.44133000	0.10641400	0.71590400
C	-6.22512300	1.23578800	0.87985300
C	-6.28986200	2.23392100	-0.12656600
C	-5.53556400	2.01251900	-1.30804200
C	-4.77680900	0.86738900	-1.46887000
C	-3.37652200	-2.85152700	1.21710500

C	-4.67093600	-3.46250300	1.06955000
C	-2.60331900	-3.42101300	2.28442200
C	-4.06218400	-2.12843800	-1.77827100
C	-4.98911300	-1.81192600	-2.82648500
C	-3.31575200	-3.33283000	-1.99699800
C	-7.15253300	4.33774600	-1.04382700
C	-7.83892600	3.54914900	1.24464500
H	-3.45982400	0.21636700	2.14826300
H	-2.82222800	-1.11590300	3.11186900
H	-1.73789400	0.51905200	4.67647400
H	-3.48594000	0.73056500	4.54283300
H	-2.39881700	1.86060800	3.72595700
H	-5.45475700	-0.64849300	1.49589900
H	-6.80498200	1.33570600	1.78890600
H	-5.54468400	2.74215100	-2.10801900
H	-4.20939900	0.74320000	-2.38471900
H	-6.17252400	4.76235000	-1.29744500
H	-7.80015900	5.15582500	-0.72636600
H	-7.58151600	3.89521400	-1.95314600
H	-8.60296300	2.76759700	1.35979800
H	-8.34541700	4.51390000	1.19745100
H	-7.20531400	3.54473700	2.14086200

Zero-point correction= 0.674497 (Hartree/Particle)
Thermal correction to Energy= 0.719647
Thermal correction to Enthalpy= 0.720591
Thermal correction to Gibbs Free Energy= 0.601484
Sum of electronic and zero-point Energies= -3237.873978
Sum of electronic and thermal Energies= -3237.828828
Sum of electronic and thermal Enthalpies= -3237.827884
Sum of electronic and thermal Free Energies= -3237.946991

TS1 [oniom(b3lyp/6-31g(d):SVWN/STO-3G)]

N	5.75710900	1.61870300	-3.03382300
N	2.45145100	4.05655200	-1.88935000
N	3.04097200	-3.04219400	-2.79072200
N	3.62627500	-3.31864400	1.52267900
N	9.33373300	-0.21593300	0.97215100
C	1.57473100	0.51642700	-0.46884800
C	1.25110000	1.38296600	0.90259900
C	0.15459900	2.45679600	0.70909900
C	-0.36607900	2.84864000	-0.50351100
C	-1.71246400	3.36687200	-0.60417400
C	-2.52210000	3.48039100	0.53266200
C	-1.99467700	3.04282600	1.81558000
C	-0.69283400	2.51021900	1.86912800
C	-0.42390600	1.34549500	2.67848400
C	0.64488700	0.89550400	-1.63732300
C	0.22345300	-0.27302600	-2.35310800
C	0.50644700	-1.42951700	-1.55242000
C	1.29156800	-1.04407700	-0.34554000
C	0.74739200	-1.60167600	0.86266900
C	-0.16046000	-2.70965300	0.86149400
C	-0.71195000	-3.18718800	-0.33557500
C	-0.36960000	-2.51262200	-1.57419800
C	-1.55578700	-2.48499100	-2.40617200
C	-2.63484000	-3.13828900	-1.68053300
C	-2.10075300	-3.57340000	-0.39191000

C	-2.89951800	-3.49182100	0.75860500
C	-4.24571600	-2.98110600	0.67262000
C	-4.76847300	-2.56197400	-0.56822500
C	-3.93212300	-2.64704600	-1.76836700
C	-4.21885400	-1.47485300	-2.60178600
C	-5.28554000	-1.01416700	1.79909300
C	-5.56075600	-1.33466500	-0.65478900
C	-5.81535600	-0.57499400	0.50539400
C	-5.73664200	0.88526200	0.45739200
C	-5.40381700	1.53468300	-0.75129700
C	-5.14157400	0.74512500	-1.95886400
C	-4.05618500	1.39051200	-2.69466600
C	-3.63673900	2.57256600	-1.93564400
C	-4.48173500	2.66781600	-0.74168000
C	-3.92134300	3.11571300	0.47253700
C	-4.27159400	2.44379700	1.72683300
C	-5.15944100	1.34995000	1.71940500
C	-4.88067600	0.17317600	2.54930100
C	-5.22054900	-0.66299000	-1.91150300
C	-4.51255600	-2.19085900	1.88506400
C	-3.32912400	-2.22666900	2.71015600
C	-2.93844600	-1.08420200	3.43609200
C	-3.72106700	0.12992000	3.35031100
C	-2.79134800	1.26742900	3.34876300
C	-3.06287700	2.40267300	2.55083800
C	-1.45122600	0.74262600	3.42497600
C	-1.53244800	-0.70487200	3.47381100
C	-0.58083700	-1.46212300	2.79750500
C	0.49059700	-0.81536300	2.05320100
C	0.57787900	0.56114100	2.01081300
C	-0.10947000	2.04355500	-1.71131200
C	-1.29344400	2.09272800	-2.53794800
C	-2.28963300	2.90623400	-1.86028000
C	-1.68951100	0.97237200	-3.27603200
C	-0.91216500	-0.24227300	-3.18244600
C	-1.82259800	-1.36961500	-3.20447200
C	-3.17047000	-0.85452500	-3.30969800
C	-3.08624200	0.61037800	-3.35577100
C	-2.32285700	-3.02234600	2.01387200
C	-0.98569600	-2.63465800	2.05399800
C	2.56349600	2.02440500	1.47539500
C	2.43995700	2.79105300	2.79695500
C	3.05241700	0.64112800	-0.94329500
C	3.87789100	-0.46817000	-0.57610700
C	5.26264500	-0.38147200	-0.18470100
C	5.84218200	0.79653600	0.36065000
C	7.16251500	0.85584000	0.74147600
C	8.02049500	-0.27253000	0.60128000
C	7.45418100	-1.45495800	0.05050600
C	6.12919500	-1.50000000	-0.32380700
C	3.54000100	1.71470800	-1.68823600
C	4.77169900	1.63540000	-2.41238300
C	2.90078600	2.98335000	-1.80983700
C	3.17304800	-1.75871500	-0.52239100
C	3.06877600	-2.47344700	-1.77571000
C	3.48694000	-2.63810300	0.58955400
C	10.18753700	-1.39170500	0.84077000
C	9.90991600	1.03236600	1.46052200
H	3.28885500	1.21553400	1.60800700

H	2.96251600	2.71066300	0.72484600
H	1.74077700	3.62903600	2.72189500
H	3.42113100	3.20202400	3.05949500
H	2.11718300	2.15030400	3.62315800
H	5.22817700	1.67852200	0.49895000
H	7.54086800	1.77996000	1.16056700
H	8.06910300	-2.33111300	-0.11328400
H	5.75736800	-2.40820800	-0.78567100
H	9.77793600	-2.24275900	1.39772600
H	11.17337500	-1.16391800	1.24687200
H	10.30846900	-1.68871400	-0.20933800
H	9.80549900	1.83690900	0.72206200
H	10.97266700	0.88340200	1.65277100
H	9.43589500	1.35545100	2.39633000

Zero-point correction= 0.672262 (Hartree/Particle)
Thermal correction to Energy= 0.716749
Thermal correction to Enthalpy= 0.717693
Thermal correction to Gibbs Free Energy= 0.601422
Sum of electronic and zero-point Energies= -3237.831435
Sum of electronic and thermal Energies= -3237.786948
Sum of electronic and thermal Enthalpies= -3237.786004
Sum of electronic and thermal Free Energies= -3237.902275

(±)-3a [oniom(b3lyp/6-31g(d):SVWN/STO-3G)]

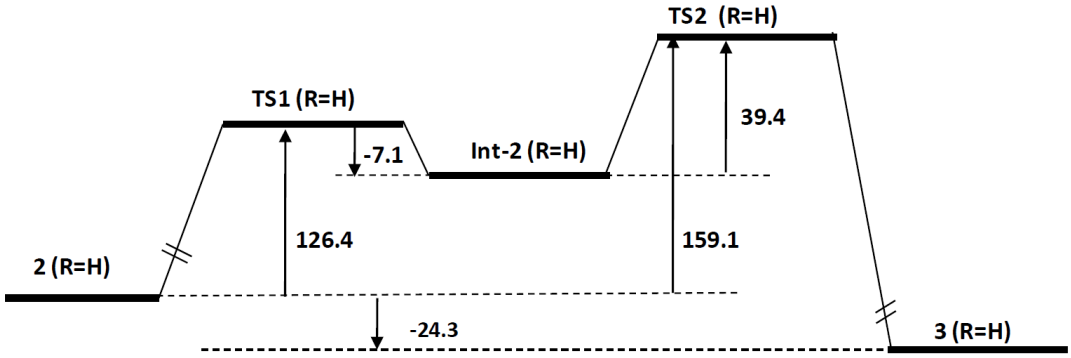
N	6.09098300	3.12297500	0.10747000
N	2.24754500	4.60475800	-0.14616300
N	3.73245300	-3.59705200	-0.47665300
N	2.68572400	-2.77708300	3.00750300
N	9.45220300	-0.73065100	-0.80722500
C	1.56311600	0.80343500	0.33009100
C	0.85437000	1.48954900	1.62473300
C	-0.25003900	2.51948000	1.24803000
C	-0.50688300	2.98682400	-0.02042600
C	-1.82887200	3.42699100	-0.40716900
C	-2.89078000	3.39194400	0.50500400
C	-2.64532000	2.87342900	1.84185400
C	-1.35400400	2.41343800	2.16501500
C	-1.20044700	1.19149500	2.90908400
C	0.88004400	1.19237200	-0.99215000
C	0.72141900	0.06665800	-1.85854300
C	0.89293500	-1.13082600	-1.10248800
C	1.54656400	-0.84133400	0.24735100
C	0.86561600	-1.68109500	1.44230100
C	-0.18321500	-2.74093200	0.99034400
C	-0.41188400	-3.07721700	-0.32319300
C	0.16102200	-2.25674400	-1.40842700
C	-0.79254300	-2.22753500	-2.49265600
C	-1.95747400	-3.00187700	-2.09548300
C	-1.71916300	-3.51973500	-0.75358300
C	-2.77850100	-3.60197200	0.16107500
C	-4.10272600	-3.15961600	-0.21859200
C	-4.33720000	-2.66046000	-1.51433800
C	-3.23055900	-2.58968100	-2.47286200
C	-3.40302400	-1.37278800	-3.27302700
C	-5.52449400	-1.35436500	0.75216600
C	-5.17881000	-1.47959500	-1.70962400
C	-5.76123000	-0.83742000	-0.59748200
C	-5.78516600	0.62447900	-0.52497600

C	-5.22577200	1.39198900	-1.56822100
C	-4.62412500	0.72559500	-2.72605800
C	-3.44979600	1.49574000	-3.13208700
C	-3.31522900	2.63267200	-2.21476500
C	-4.42316800	2.57445100	-1.25753600
C	-4.20182900	2.94902000	0.08332400
C	-4.78515200	2.15129000	1.16655000
C	-5.56072800	1.01250700	0.86881700
C	-5.39986600	-0.21250500	1.65666000
C	-4.60097000	-0.68437900	-2.79549100
C	-4.70841400	-2.49046900	0.94257700
C	-3.75111000	-2.52660800	2.02123300
C	-3.62944200	-1.42752700	2.89028700
C	-4.45993800	-0.25741800	2.70759800
C	-3.64507600	0.92752300	3.00713100
C	-3.80494600	2.10954500	2.25067400
C	-2.31945300	0.47355800	3.35307400
C	-2.30204200	-0.96830000	3.27814200
C	-1.16742400	-1.60165600	2.78057300
C	-0.01132800	-0.84139200	2.37909600
C	-0.02100000	0.51660300	2.42431200
C	0.09012800	2.30637900	-1.18194400
C	-0.86555600	2.34907900	-2.26411200
C	-2.05509200	3.04143500	-1.79336600
C	-0.98888000	1.27348100	-3.15083400
C	-0.17050100	0.10227600	-2.94697600
C	-0.95084200	-1.06964600	-3.26513400
C	-2.26963100	-0.63233300	-3.66322000
C	-2.29377000	0.83485600	-3.59184000
C	-2.55311800	-3.20823800	1.53466500
C	-1.28428000	-2.75305400	1.91382600
C	1.83478100	2.14271300	2.66695800
C	2.80792800	1.19455400	3.37401500
C	3.07005100	1.13456200	0.15779800
C	3.85113100	-0.09348400	0.03436200
C	5.30683300	-0.21450500	-0.18407500
C	6.10604300	-0.86685800	0.76872100
C	7.46904400	-1.03097200	0.57547900
C	8.09895600	-0.56935800	-0.60627800
C	7.27982800	0.05851200	-1.57799000
C	5.92213900	0.23080400	-1.36466100
C	3.60121600	2.39881000	0.04389100
C	5.00304100	2.71150400	0.05337200
C	2.81711300	3.59372800	-0.05250000
C	3.02042600	-1.17310500	0.08053600
C	3.43914700	-2.50333200	-0.20510900
C	1.90044800	-2.31656500	2.28599500
C	10.08810200	-0.14913800	-1.97870400
C	10.27675100	-1.31558500	0.23799800
H	2.37336500	2.97404600	2.21082000
H	1.18728600	2.59927000	3.42415300
H	2.28400500	0.38900800	3.89775300
H	3.38229900	1.75606300	4.11879700
H	3.52937400	0.73471200	2.69239000
H	5.65314000	-1.24152400	1.68290000
H	8.04559400	-1.52269400	1.34910700
H	7.70750900	0.41796000	-2.50563100
H	5.32937100	0.71530400	-2.13595500
H	9.68428900	-0.57315300	-2.90760100

H	11.15664200	-0.36776400	-1.95081700
H	9.96261200	0.94250800	-2.01756600
H	10.26118800	-0.71860700	1.16176400
H	11.30871600	-1.37419800	-0.11130300
H	9.94797300	-2.33350600	0.48391600

Zero-point correction= 0.675341 (Hartree/Particle)
Thermal correction to Energy= 0.719771
Thermal correction to Enthalpy= 0.720716
Thermal correction to Gibbs Free Energy= 0.604591
Sum of electronic and zero-point Energies= -3237.890424
Sum of electronic and thermal Energies= -3237.845993
Sum of electronic and thermal Enthalpies= -3237.845049
Sum of electronic and thermal Free Energies= -3237.961174

Fig. 25 (ESI). Reaction path for the rearrangement of **2** to (±)-**3** with R=H. Free energies in kJ/mol are given, calculated at the ONIOM(B3LYP/6-31G(d):AM1) level.



XYZ coordinates and energies:

2 (R=H) [oniom(b3lyp/6-31g(d):AM1)]

N	5.93543400	-3.66782800	-1.54580900
N	2.10614400	-3.62840500	-3.47372500
N	6.11945200	-1.76800900	3.39346900
N	3.09814300	-4.46797200	1.88816500
N	6.54187500	3.67165000	-0.43927800
C	1.66876300	-1.22567700	-0.49544500
C	1.40919200	-0.33196500	-1.81436800
C	0.19668700	-0.74141200	-2.65939400
C	-0.51753700	-1.89011600	-2.47095300
C	-1.94512100	-1.94082000	-2.81097400
C	-2.58249700	-0.81715100	-3.34666800
C	-1.81642600	0.42261200	-3.53909200
C	-0.46569200	0.45053000	-3.16274400
C	0.07936800	1.59642500	-2.48012800
C	0.60286500	-2.33573700	-0.29072700
C	0.25301500	-2.41554600	1.10973800
C	0.77997600	-1.23549500	1.78995100
C	1.46933100	-0.43650700	0.82148900
C	1.38660100	0.93772400	0.89338800

C	0.65211900	1.57042200	1.96593400
C	0.01197200	0.79546200	2.93129900
C	0.08175100	-0.64497300	2.84862900
C	-1.21671800	-1.18161200	3.25241600
C	-2.08746200	-0.04772300	3.62603900
C	-1.32992600	1.17067200	3.39931000
C	-1.94326700	2.32147800	2.89271300
C	-3.34535600	2.26304200	2.52990500
C	-4.07679300	1.10075800	2.71694100
C	-3.42257300	-0.08828800	3.25575600
C	-3.96947600	-1.25670600	2.56610200
C	-4.46464200	2.66028800	0.36819800
C	-5.04004200	0.66900400	1.70181300
C	-5.23025500	1.42705200	0.56016100
C	-5.36361000	0.77105500	-0.74170000
C	-5.29601100	-0.60897600	-0.83117800
C	-5.09351200	-1.41052500	0.37671600
C	-4.21685700	-2.52970000	0.03394200
C	-3.87714400	-2.42132200	-1.38564900
C	-4.54667500	-1.23753800	-1.91979400
C	-3.90243200	-0.45417500	-2.86320500
C	-3.97043400	1.00488000	-2.76321500
C	-4.68016200	1.59958700	-1.73612500
C	-4.12634200	2.76707200	-1.04845300
C	-4.97171900	-0.78985500	1.60845400
C	-3.54474800	3.06269600	1.32340400
C	-2.26670700	3.61999100	0.93164800
C	-1.94458800	3.72897600	-0.42509200
C	-2.89043600	3.26952100	-1.42219000
C	-2.13933900	2.63751000	-2.50463200
C	-2.66399800	1.53555600	-3.15983200
C	-0.72981200	2.70937900	-2.17907700
C	-0.60202100	3.34927800	-0.88400400
C	0.35112800	2.87876700	0.03203100
C	1.20025900	1.75256600	-0.32351700
C	1.08745600	1.14419900	-1.55051900
C	-0.31055300	-2.71012500	-1.24899400
C	-1.61151200	-3.22877700	-0.85703500
C	-2.61832200	-2.78106400	-1.83904400
C	-1.93862000	-3.34724400	0.48632900
C	-0.98140100	-2.92017500	1.50038400
C	-1.73264300	-2.28620400	2.60034300
C	-3.13689600	-2.31387900	2.23743600
C	-3.26459300	-2.96671500	0.93821300
C	-1.26019200	3.13931400	1.88418800
C	0.01328400	2.77219200	1.43360400
C	3.09205600	-1.83882000	-0.54060500
C	4.08575200	-1.37948800	0.48831200
C	4.69692200	-0.07129400	0.27057600
C	4.93148300	0.40391700	-1.03938300
C	5.54056300	1.62039700	-1.28174000
C	5.93912900	2.46426300	-0.21198300
C	5.67718700	2.00270900	1.10637600
C	5.08350600	0.77740800	1.33331300
C	3.50634900	-2.74102200	-1.47448600
C	4.85166000	-3.25096400	-1.48618700
C	2.69813700	-3.22534700	-2.55766900
C	4.34265600	-2.21344600	1.55499800
C	5.32694000	-1.94403200	2.55931100

C	3.64929700	-3.45561400	1.72590700
C	6.99048800	4.49109300	0.67980900
C	6.79717300	4.11840600	-1.80253500
H	4.67626500	-0.21636900	-1.89222300
H	5.72249400	1.91319900	-2.30827100
H	5.93666100	2.61475100	1.96124100
H	4.88838700	0.48563200	2.35795200
H	6.15082300	4.80299200	1.31460000
H	7.47246200	5.38955300	0.29304300
H	7.71695900	3.95696000	1.30594000
H	7.47851900	3.43965900	-2.33332100
H	7.25725600	5.10666200	-1.77446600
H	5.86717300	4.19486400	-2.38020000
H	2.31762400	-0.40497500	-2.42445500

Zero-point correction= 0.637646 (Hartree/Particle)
Thermal correction to Energy= 0.678666
Thermal correction to Enthalpy= 0.679610
Thermal correction to Gibbs Free Energy= 0.567194
Sum of electronic and zero-point Energies= -2266.326262
Sum of electronic and thermal Energies= -2266.285242
Sum of electronic and thermal Enthalpies= -2266.284298
Sum of electronic and thermal Free Energies= -2266.396714

TS1 (R=H) [oniom(b3lyp/6-31g(d):AM1)]

N	5.99750900	2.89891000	-1.80778300
N	2.37034100	4.60344100	-0.38574500
N	3.10309300	-1.26737600	-3.98204400
N	3.71007400	-3.59383100	-0.35641300
N	9.09855100	-0.56156600	1.43366900
C	1.62202800	0.79137800	-0.48803200
C	1.34899600	1.18072600	1.05882200
C	0.26823100	2.24201300	1.30364300
C	-0.33566200	2.96208100	0.31381400
C	-1.71266000	3.44344600	0.47612400
C	-2.41715100	3.17996400	1.65494400
C	-1.77214800	2.39218800	2.71644500
C	-0.47049100	1.91227500	2.50938000
C	-0.11176200	0.57277100	2.90257700
C	0.63158000	1.48846900	-1.44284700
C	0.16678600	0.55530300	-2.44491000
C	0.51339900	-0.78247200	-2.04356300
C	1.39480700	-0.74699900	-0.84203600
C	0.95313400	-1.65933600	0.19118600
C	0.06475800	-2.74726200	-0.07646500
C	-0.57062300	-2.86886600	-1.31526800
C	-0.34252900	-1.84576200	-2.31771900
C	-1.60434800	-1.61448000	-3.00856200
C	-2.62044700	-2.52794800	-2.44982900
C	-1.97859400	-3.27326800	-1.37921900
C	-2.66841300	-3.58510500	-0.20215600
C	-4.01699200	-3.08505500	-0.03049600
C	-4.63477500	-2.35073800	-1.03099700
C	-3.90601200	-2.04684000	-2.25901600
C	-4.26373500	-0.68881200	-2.67256300
C	-4.97741300	-1.60526900	1.69441700
C	-5.45196900	-1.18561100	-0.68714900
C	-5.62092500	-0.82288000	0.63741200

C	-5.56811300	0.58794200	1.02389900
C	-5.34752200	1.56100200	0.06382100
C	-5.16835200	1.17710900	-1.33719700
C	-4.15149200	2.05258900	-1.91829400
C	-3.70107600	2.97746400	-0.87712800
C	-4.44299700	2.67639300	0.34520200
C	-3.80545400	2.76283100	1.57213500
C	-4.03579000	1.72945000	2.58347700
C	-4.89201400	0.67598800	2.31899000
C	-4.52833700	-0.68039700	2.73200800
C	-5.22125100	-0.15759900	-1.70301900
C	-4.19481200	-2.70152800	1.36875400
C	-2.95395400	-2.95928700	2.06975600
C	-2.52552300	-2.07603800	3.06873800
C	-3.32488900	-0.90812300	3.37942000
C	-2.41670100	0.20481200	3.65015100
C	-2.76344400	1.49082900	3.26834000
C	-1.05863600	-0.27489100	3.50713300
C	-1.11613600	-1.67387000	3.11697400
C	-0.20708500	-2.16754300	2.17585000
C	0.78038300	-1.27089900	1.57482800
C	0.85027800	0.05373200	1.95972200
C	-0.15305100	2.56545800	-1.10330900
C	-1.41743000	2.80616000	-1.77988800
C	-2.37521000	3.37502700	-0.81313500
C	-1.84670800	1.94484800	-2.77682100
C	-1.03571100	0.78116200	-3.11849300
C	-1.94121700	-0.33307300	-3.40974500
C	-3.29975400	0.14160400	-3.21926700
C	-3.24193300	1.54714100	-2.83127300
C	-1.98985600	-3.47849500	1.09691000
C	-0.65161100	-3.07991700	1.15485200
C	3.10482700	1.10526200	-0.78223200
C	3.92889300	-0.06735900	-0.82153000
C	5.23973200	-0.17301500	-0.25818300
C	5.67239100	0.64343300	0.82741200
C	6.92009000	0.51804400	1.38657800
C	7.85584300	-0.44124800	0.89354300
C	7.43424500	-1.26304000	-0.19306600
C	6.17859400	-1.13266000	-0.73674100
C	3.61018500	2.39186300	-0.92141400
C	4.93591000	2.63990100	-1.40501700
C	2.88683400	3.58942400	-0.63738300
C	3.21414300	-1.23695100	-1.37113900
C	3.13563300	-1.26212100	-2.81950000
C	3.54579300	-2.54203600	-0.82287800
C	10.02323300	-1.57983700	0.94126100
C	9.53090500	0.33319900	2.50416200
H	4.98769800	1.37150100	1.25069600
H	7.18223400	1.15516700	2.22252300
H	8.11377000	-1.98725100	-0.62550300
H	5.91847800	-1.75082400	-1.58973400
H	9.59001200	-2.58364100	1.02725600
H	10.93529100	-1.55097900	1.53788800
H	10.29320900	-1.40496500	-0.10828500
H	9.46149400	1.38335300	2.19582900
H	10.57158400	0.11898800	2.74855600
H	8.93009600	0.19508800	3.41255900
H	2.30561600	1.55664200	1.44524100

Zero-point correction= 0.635420 (Hartree/Particle)
Thermal correction to Energy= 0.675726
Thermal correction to Enthalpy= 0.676670
Thermal correction to Gibbs Free Energy= 0.567645
Sum of electronic and zero-point Energies= -2266.280718
Sum of electronic and thermal Energies= -2266.240412
Sum of electronic and thermal Enthalpies= -2266.239468
Sum of electronic and thermal Free Energies= -2266.348493

Int-2 (R=H) [oniom(b3lyp/6-31g(d):AM1)]

N	5.89012200	2.96063000	-1.75019600
N	2.31127400	4.60965200	-0.14730700
N	3.46046500	-2.13597900	-3.22307900
N	3.75199700	-3.24137400	0.89198200
N	9.38510600	-0.49656200	0.91301100
C	1.62731300	0.79209800	-0.23589300
C	1.21095600	1.26983700	1.24851400
C	0.10676200	2.33679500	1.32564000
C	-0.40748200	2.98574100	0.24064300
C	-1.79410200	3.46730600	0.24169100
C	-2.60543500	3.27472500	1.36545000
C	-2.06005600	2.55877800	2.52757300
C	-0.74211000	2.07790600	2.47404400
C	-0.41972300	0.76718100	2.97769600
C	0.71422200	1.40222800	-1.30933500
C	0.35539700	0.40846600	-2.29098800
C	0.68169600	-0.89881100	-1.79480500
C	1.52616500	-0.80127800	-0.52202300
C	0.89949000	-1.63517200	0.54832900
C	0.03630500	-2.73750700	0.26121700
C	-0.47555900	-2.94416200	-1.02096100
C	-0.15064000	-1.97302100	-2.06724100
C	-1.34372300	-1.79691400	-2.87997700
C	-2.40687400	-2.68314800	-2.36259300
C	-1.86851200	-3.35461100	-1.19184100
C	-2.67075900	-3.60180900	-0.06793000
C	-4.02851400	-3.09927500	-0.05894300
C	-4.54920300	-2.43350800	-1.15803100
C	-3.70554400	-2.20147600	-2.32662800
C	-4.02662000	-0.87568100	-2.85973100
C	-5.15085400	-1.51929100	1.46916300
C	-5.39667900	-1.25527200	-0.96825000
C	-5.69199400	-0.81005100	0.30829900
C	-5.67768200	0.62265000	0.60705800
C	-5.36966400	1.53482800	-0.38828500
C	-5.05808800	1.06406000	-1.73851300
C	-3.99330900	1.90927400	-2.27665900
C	-3.64520600	2.90219400	-1.25864600
C	-4.49806200	2.67291100	-0.09466800
C	-3.97868300	2.84200700	1.17876000
C	-4.30048800	1.87223600	2.22761100
C	-5.12700200	0.79804500	1.95156300
C	-4.80214200	-0.52665600	2.48277800
C	-5.07278300	-0.29190500	-2.02137300
C	-4.34083500	-2.62907100	1.28987900
C	-3.17182600	-2.83366100	2.12004700
C	-2.83964600	-1.88461500	3.09475600

C	-3.66440000	-0.70401600	3.25270000
C	-2.78435700	0.42986000	3.53274400
C	-3.09720100	1.68739300	3.04115300
C	-1.42000500	-0.04830900	3.54590200
C	-1.44064800	-1.46998400	3.24656000
C	-0.45058500	-2.01799600	2.42822200
C	0.58525700	-1.15190400	1.85522100
C	0.62609600	0.19989400	2.16597400
C	-0.09527100	2.49824600	-1.12149200
C	-1.28637600	2.68974300	-1.93020300
C	-2.33263500	3.31498000	-1.09521000
C	-1.61791100	1.76460800	-2.90518400
C	-0.77727800	0.58576700	-3.09125000
C	-1.64604500	-0.54786700	-3.39598000
C	-3.01848100	-0.07381800	-3.36703600
C	-3.00116700	1.35402200	-3.06656600
C	-2.11998500	-3.40890300	1.27731000
C	-0.79261200	-3.00033000	1.43790100
C	3.11022400	1.11693800	-0.47690200
C	3.92481700	-0.03936200	-0.49054600
C	5.30882700	-0.13836600	-0.16297500
C	5.93694000	0.77320300	0.74117400
C	7.25343700	0.65641800	1.10338400
C	8.07522400	-0.38959400	0.57683200
C	7.45481500	-1.31833800	-0.31397100
C	6.13025500	-1.19994500	-0.65513400
C	3.58637000	2.42044900	-0.68489900
C	4.86605300	2.68874900	-1.26370700
C	2.84632000	3.60425100	-0.40138000
C	3.08580600	-1.28701700	-0.75854600
C	3.26899200	-1.76326100	-2.13993800
C	3.45032000	-2.38912600	0.16463500
C	10.19274800	-1.60472000	0.40446400
C	10.00997200	0.49393200	1.78899200
H	5.34351500	1.56116300	1.19308100
H	7.66295400	1.36403800	1.81432500
H	8.03275100	-2.12470400	-0.74942200
H	5.71947000	-1.91088500	-1.36499800
H	9.76610300	-2.57253500	0.69498500
H	11.19674900	-1.53485500	0.82389800
H	10.27360100	-1.57198400	-0.68959800
H	9.90124100	1.50588800	1.38119100
H	11.07441300	0.27300300	1.87328500
H	9.57345500	0.47310800	2.79622200
H	2.12686500	1.67537900	1.69827000

Zero-point correction= 0.637338 (Hartree/Particle)
Thermal correction to Energy= 0.677774
Thermal correction to Enthalpy= 0.678718
Thermal correction to Gibbs Free Energy= 0.569795
Sum of electronic and zero-point Energies= -2266.283585
Sum of electronic and thermal Energies= -2266.243149
Sum of electronic and thermal Enthalpies= -2266.242204
Sum of electronic and thermal Free Energies= -2266.351128

TS2 (R=H) [oniom(b3lyp/6-31g(d):AM1)]

N	5.90070200	3.25899200	-1.54388300
N	2.23593800	4.77420900	0.01714000

N	3.51620600	-1.97342000	-3.43090000
N	3.71317900	-2.92324300	0.57760700
N	9.21650000	-0.76856900	1.00769400
C	1.60443000	0.97804500	-0.27442100
C	1.25811600	1.17491700	1.28413400
C	0.12623300	2.16715500	1.59981000
C	-0.46809600	2.97375600	0.67227400
C	-1.87047100	3.38481800	0.82631400
C	-2.61004000	2.96800100	1.93798800
C	-1.97644500	2.08936700	2.93176300
C	-0.65033500	1.67822800	2.72606900
C	-0.26349700	0.31550900	2.97793300
C	0.62134100	1.73305900	-1.18486500
C	0.23379100	0.90173200	-2.30099000
C	0.62640800	-0.45300000	-2.04581600
C	1.52996800	-0.52883400	-0.83255000
C	1.13765800	-1.66376800	0.13773100
C	0.17850900	-2.68548800	-0.30410800
C	-0.40421700	-2.65680200	-1.55894900
C	-0.17458000	-1.50574800	-2.45012400
C	-1.41500700	-1.25092200	-3.15911800
C	-2.41515600	-2.25455400	-2.74521500
C	-1.79213800	-3.09188200	-1.73382400
C	-2.52403600	-3.56465400	-0.63750800
C	-3.89828400	-3.13038800	-0.47739300
C	-4.49793700	-2.30940400	-1.41887400
C	-3.72691300	-1.84572700	-2.56945800
C	-4.12448300	-0.46550700	-2.85398500
C	-4.98508800	-1.87939800	1.35077100
C	-5.37425200	-1.21795200	-0.99075700
C	-5.61302300	-1.00804300	0.35610300
C	-5.63060500	0.35331900	0.89372900
C	-5.40956700	1.43250000	0.05486900
C	-5.15879100	1.21055500	-1.36974100
C	-4.15632600	2.18048000	-1.80812100
C	-3.78463200	3.00108900	-0.65417300
C	-4.56179100	2.54156000	0.49452200
C	-3.97669400	2.51490400	1.74996000
C	-4.20667100	1.36923600	2.63246500
C	-5.01098700	0.32245000	2.21938100
C	-4.61379000	-1.05799400	2.50004300
C	-5.14234300	-0.07780100	-1.87851200
C	-4.14962100	-2.90847200	0.94520900
C	-2.92984100	-3.20107500	1.66915400
C	-2.57636300	-2.41718600	2.77411500
C	-3.42913700	-1.31498100	3.17110800
C	-2.57457200	-0.20759800	3.59644800
C	-2.95376900	1.10042700	3.34062700
C	-1.19518900	-0.62198000	3.45614500
C	-1.18628000	-1.97255000	2.92301900
C	-0.22653700	-2.32534300	1.97035000
C	0.75134300	-1.34531500	1.51656100
C	0.75093200	-0.06659500	2.01905800
C	-0.21924200	2.73889800	-0.76895200
C	-1.46225600	3.01033000	-1.47020000
C	-2.47951900	3.43683500	-0.48871300
C	-1.81791300	2.25136800	-2.57335600
C	-0.94908100	1.15959800	-3.00110800
C	-1.79100600	0.05409200	-3.44446300

C	-3.17571600	0.45408400	-3.26733700
C	-3.19242000	1.81118400	-2.73055800
C	-1.90938300	-3.58413200	0.68958200
C	-0.58741900	-3.14842200	0.84468600
C	3.08841100	1.33194000	-0.50557500
C	3.89150500	0.15477300	-0.64479300
C	5.24405600	-0.04942900	-0.26254800
C	5.91145900	0.81009100	0.66546900
C	7.19232500	0.57496500	1.08890800
C	7.93569000	-0.55044800	0.61019400
C	7.27426600	-1.43196100	-0.29102200
C	5.98141500	-1.19837200	-0.69564500
C	3.55959200	2.63770100	-0.61295200
C	4.86016600	2.95318900	-1.11833000
C	2.78929000	3.79365100	-0.28466200
C	3.01181300	-0.98676300	-1.05246000
C	3.28830000	-1.53464300	-2.37965700
C	3.02282700	-2.15742400	-0.00473100
C	9.93963700	-1.95339300	0.54966200
C	9.89164100	0.17720100	1.89439000
H	5.37715700	1.65305800	1.08776600
H	7.63348600	1.24974300	1.81214100
H	7.78748800	-2.30344000	-0.67785800
H	5.53892100	-1.88350700	-1.40830000
H	9.41632000	-2.87321700	0.83738700
H	10.92907500	-1.96580500	1.00726100
H	10.06446900	-1.94916000	-0.54059200
H	9.90024700	1.18589900	1.46492200
H	10.92478400	-0.14183400	2.03376600
H	9.41028100	0.22026200	2.87994400
H	2.18212700	1.52985200	1.76008300

Zero-point correction= 0.636141 (Hartree/Particle)
Thermal correction to Energy= 0.675925
Thermal correction to Enthalpy= 0.676869
Thermal correction to Gibbs Free Energy= 0.569862
Sum of electronic and zero-point Energies= -2266.269828
Sum of electronic and thermal Energies= -2266.230044
Sum of electronic and thermal Enthalpies= -2266.229100
Sum of electronic and thermal Free Energies= -2266.336106

(±)-3 (R=H) [oniom(b3lyp/6-31g(d):AM1)]

N	-6.13808600	3.02246300	-1.16095400
N	-2.29281000	4.58319300	-0.91265400
N	-3.81387000	-3.51298800	0.60420200
N	-2.76753400	-2.82656400	-2.96334500
N	-9.53059900	-0.48047300	0.73594100
C	-1.62619900	0.81669000	-0.40827500
C	-0.87641200	1.45541600	-1.66296300
C	0.19203500	2.51616400	-1.34058200
C	0.41918900	3.02593800	-0.09519300
C	1.75917300	3.48702700	0.29391100
C	2.81694800	3.43465100	-0.62004400
C	2.57865400	2.87898200	-1.95895300
C	1.29810400	2.39678500	-2.27310600
C	1.14551700	1.16241600	-2.98877000
C	-0.99842400	1.26265000	0.92694900

C	-0.84194000	0.14690200	1.82183100
C	-0.98278800	-1.07571900	1.08572600
C	-1.61889800	-0.81632700	-0.27374400
C	-0.93252000	-1.67974700	-1.45489200
C	0.11603900	-2.72803600	-0.97283900
C	0.33418900	-3.03128800	0.34210100
C	-0.25086300	-2.19049500	1.41343300
C	0.70881600	-2.13211900	2.49928300
C	1.88482000	-2.94695300	2.13282600
C	1.66101400	-3.46217400	0.79555700
C	2.71461500	-3.57409300	-0.11915600
C	4.02703400	-3.08593900	0.26353800
C	4.24891700	-2.56861300	1.52915300
C	3.14287300	-2.48227800	2.47989800
C	3.29861700	-1.24302100	3.24386300
C	5.43574900	-1.32413900	-0.73583800
C	5.08896700	-1.38240200	1.70302500
C	5.66760300	-0.77629700	0.60173800
C	5.68900400	0.68367000	0.49616900
C	5.13096800	1.45940400	1.49805800
C	4.52051500	0.81847800	2.66340900
C	3.33973700	1.59529000	3.03850300
C	3.21733300	2.71570400	2.10406400
C	4.32613200	2.63338400	1.15613900
C	4.11774300	2.97090600	-0.17097400
C	4.70260000	2.14411400	-1.22876500
C	5.46698600	1.03722900	-0.90675000
C	5.31174100	-0.20466800	-1.66579200
C	4.50038800	-0.56310800	2.76319100
C	4.63492100	-2.44410600	-0.89958000
C	3.69817800	-2.52981400	-2.00087000
C	3.58151700	-1.45962300	-2.89151700
C	4.39160000	-0.27317300	-2.69944400
C	3.57727600	0.89458000	-3.03091700
C	3.72891300	2.07410000	-2.32019300
C	2.26177400	0.42956900	-3.41710900
C	2.24568000	-1.01295800	-3.30292400
C	1.10183300	-1.64527200	-2.80224800
C	-0.05652400	-0.86416200	-2.42116100
C	-0.04762800	0.49088600	-2.50758300
C	-0.19879900	2.37572000	1.08248500
C	0.77203800	2.44013600	2.16434300
C	1.97105400	3.15881900	1.69004800
C	0.88672300	1.39257100	3.06591200
C	0.05876600	0.20748600	2.88813300
C	0.85318400	-0.96646700	3.23581000
C	2.18145500	-0.50579600	3.59733800
C	2.20242100	0.95027400	3.49229000
C	2.49296600	-3.20823600	-1.51062000
C	1.21910500	-2.77020500	-1.91130500
C	-3.13689400	1.14993700	-0.43108400
C	-3.92726100	-0.04965300	-0.17253200
C	-5.38130900	-0.12045800	0.04135400
C	-6.17220400	-0.99059200	-0.72866500
C	-7.53554500	-1.10682400	-0.51277000
C	-8.17841700	-0.36910800	0.51297900
C	-7.37002600	0.48761100	1.30335200
C	-6.01213300	0.60814200	1.06421000
C	-3.66618400	2.39210000	-0.68861900

C	-5.05810500	2.66739500	-0.91137700
C	-2.87508100	3.57977800	-0.81610000
C	-3.09774100	-1.13229700	-0.10879300
C	-3.51686100	-2.43876600	0.26623400
C	-1.97139500	-2.33932600	-2.27247900
C	-10.17485800	0.34675100	1.74414900
C	-10.33906400	-1.35032700	-0.10407700
H	-5.71240800	-1.56876600	-1.52538800
H	-8.10492800	-1.77311500	-1.14894600
H	-7.80803100	1.06500600	2.10809000
H	-5.42754400	1.27159200	1.69603700
H	-9.78439500	0.13876900	2.74973800
H	-11.24480700	0.13393300	1.75041100
H	-10.04158500	1.41829700	1.53996400
H	-10.32192000	-1.03761100	-1.15794900
H	-11.37353300	-1.32042000	0.24121000
H	-9.99621200	-2.39196900	-0.05108500
H	-1.64842700	1.90643200	-2.29879800

Zero-point correction= 0.638340 (Hartree/Particle)
Thermal correction to Energy= 0.678715
Thermal correction to Enthalpy= 0.679659
Thermal correction to Gibbs Free Energy= 0.570332
Sum of electronic and zero-point Energies= -2266.337985
Sum of electronic and thermal Energies= -2266.297609
Sum of electronic and thermal Enthalpies= -2266.296665
Sum of electronic and thermal Free Energies= -2266.405993

2 (R=H) [oniom(b3lyp/6-31g(d):SVWN/STO-3G)]

N	5.91801900	-3.67657300	-1.57136100
N	2.09182600	-3.58121600	-3.50642100
N	6.09798100	-1.81593300	3.39395100
N	3.06554000	-4.47950300	1.85066700
N	6.60193500	3.64228100	-0.40405500
C	1.67276400	-1.20110400	-0.50819600
C	1.41341100	-0.30327300	-1.82195600
C	0.19949900	-0.70459400	-2.66589300
C	-0.52105100	-1.86129700	-2.47592800
C	-1.92458500	-1.91403500	-2.80984300
C	-2.57485100	-0.78957300	-3.33529500
C	-1.82210400	0.44175700	-3.52136000
C	-0.46312900	0.47180900	-3.15637200
C	0.08233900	1.62421100	-2.47631200
C	0.60312200	-2.30635000	-0.30204600
C	0.24443100	-2.38922800	1.08864900
C	0.77839700	-1.22570200	1.77090900
C	1.47838600	-0.41861700	0.81171600
C	1.38891700	0.95274900	0.89157800
C	0.64964400	1.57712000	1.96587600
C	0.00773600	0.79311900	2.93184600
C	0.07753900	-0.64544900	2.83583400
C	-1.20658200	-1.19055200	3.24363400
C	-2.07352500	-0.07559800	3.59359300
C	-1.31348200	1.15588300	3.40165700
C	-1.94422400	2.29859700	2.89446300
C	-3.34958500	2.26340900	2.56024100
C	-4.09036600	1.07856300	2.74269500
C	-3.42623200	-0.11472100	3.27159900

C	-3.98286600	-1.28253800	2.58300200
C	-4.48744100	2.66651900	0.37896700
C	-5.05202600	0.64940800	1.72488700
C	-5.24663800	1.42763000	0.56620200
C	-5.37981000	0.77898900	-0.73991300
C	-5.30837100	-0.62620100	-0.83835700
C	-5.10680100	-1.43636800	0.36825000
C	-4.23197100	-2.55397400	0.02099900
C	-3.88079600	-2.43001000	-1.39660800
C	-4.55877200	-1.24454700	-1.92952200
C	-3.90491800	-0.43997900	-2.88532700
C	-3.98458300	1.01927400	-2.78534800
C	-4.70466600	1.61690100	-1.73245000
C	-4.15250800	2.78447600	-1.03840300
C	-4.98413400	-0.81005100	1.62581900
C	-3.55195900	3.07697600	1.35203500
C	-2.27228700	3.61036000	0.95303500
C	-1.94848300	3.72883000	-0.41197000
C	-2.89849000	3.30668100	-1.41849600
C	-2.14705500	2.67970500	-2.51322500
C	-2.68036900	1.55551900	-3.18050200
C	-0.74318600	2.72184200	-2.16779400
C	-0.61575600	3.35775500	-0.87369200
C	0.33445900	2.88124100	0.03286200
C	1.19872600	1.77604400	-0.32314100
C	1.08968200	1.17162300	-1.55419500
C	-0.31349900	-2.68001600	-1.26161900
C	-1.59938100	-3.21574500	-0.87263800
C	-2.59698100	-2.74727300	-1.82241600
C	-1.93376500	-3.34670500	0.48101000
C	-0.98791900	-2.91958800	1.48755700
C	-1.72939300	-2.30341700	2.58088400
C	-3.13549700	-2.35762500	2.24744600
C	-3.26286800	-3.00862600	0.93791300
C	-1.27041000	3.12320600	1.89850800
C	-0.00436400	2.75992300	1.44073200
C	3.09123700	-1.82740600	-0.55669600
C	4.08547800	-1.38736200	0.47953300
C	4.71132000	-0.08408500	0.27376000
C	4.95335400	0.39859100	-1.03208300
C	5.57729600	1.60972800	-1.26381300
C	5.98296800	2.44036800	-0.18688300
C	5.71187100	1.97290700	1.12721900
C	5.10328100	0.75286900	1.34375900
C	3.49816600	-2.72520800	-1.49790200
C	4.83829500	-3.24900600	-1.51066900
C	2.68805100	-3.19263000	-2.58687400
C	4.32867700	-2.23203200	1.54124900
C	5.30940800	-1.97891900	2.55325300
C	3.62489000	-3.46998100	1.69901900
C	7.05130700	4.45122500	0.72191400
C	6.86029600	4.09837200	-1.76330900
H	4.69113100	-0.21118600	-1.89035000
H	5.76291800	1.90912800	-2.28770300
H	5.97376700	2.57681400	1.98704100
H	4.90027700	0.45682900	2.36564900
H	6.21087600	4.77045400	1.35214100
H	7.54733200	5.34540900	0.34314400
H	7.76661300	3.90546300	1.35070700

H	7.52994700	3.41432900	-2.30191700
H	7.33598200	5.07892100	-1.72715700
H	5.93038900	4.19465300	-2.33831700
H	2.32004900	-0.37296200	-2.43504100

Zero-point correction= 0.618171 (Hartree/Particle)
Thermal correction to Energy= 0.660367
Thermal correction to Enthalpy= 0.661312
Thermal correction to Gibbs Free Energy= 0.547131
Sum of electronic and zero-point Energies= -3159.319562
Sum of electronic and thermal Energies= -3159.277365
Sum of electronic and thermal Enthalpies= -3159.276421
Sum of electronic and thermal Free Energies= -3159.390602

TS1 (R=H) [oniom(b3lyp/6-31g(d):SVWN/STO-3G)]

N	5.98957700	2.81747400	-1.88333000
N	2.38094400	4.55928300	-0.45373000
N	3.11348500	-1.52386700	-3.84731700
N	3.72421500	-3.60150400	-0.07383300
N	9.17783800	-0.47217400	1.35804900
C	1.62676300	0.75025400	-0.46606200
C	1.34039600	1.19864000	1.05966700
C	0.26237400	2.27043900	1.25635200
C	-0.33470500	2.95462900	0.22372600
C	-1.68799600	3.44235100	0.34746600
C	-2.41872300	3.22393800	1.52279400
C	-1.80100300	2.48122000	2.61157000
C	-0.49050700	1.99274100	2.44603100
C	-0.14589500	0.66621500	2.90569700
C	0.64540900	1.40850300	-1.45518400
C	0.18049300	0.45155400	-2.41973800
C	0.52506800	-0.86715800	-1.97338000
C	1.40000500	-0.79630300	-0.76416200
C	0.93274700	-1.66492400	0.29300600
C	0.04049000	-2.75824500	0.05409000
C	-0.58357500	-2.92059700	-1.19082700
C	-0.33423900	-1.93246800	-2.22604900
C	-1.57371300	-1.72230700	-2.94662500
C	-2.59250000	-2.57608900	-2.35542500
C	-1.96713000	-3.31920700	-1.26303400
C	-2.68880800	-3.56892400	-0.08574500
C	-4.04398100	-3.09405700	0.04881200
C	-4.65424000	-2.37894200	-1.00238900
C	-3.89898000	-2.11879500	-2.23072200
C	-4.25559600	-0.77747500	-2.70481700
C	-5.03123000	-1.52588400	1.71759900
C	-5.46667300	-1.19714700	-0.71228400
C	-5.65247700	-0.77802600	0.62120200
C	-5.59556600	0.64464500	0.95719000
C	-5.35367100	1.59956900	-0.05413000
C	-5.16289300	1.16502900	-1.44128000
C	-4.13757300	2.01410100	-2.04417900
C	-3.68404800	2.96671000	-1.02627400
C	-4.44767100	2.71728600	0.19989100
C	-3.81331800	2.84492700	1.45297900
C	-4.06998900	1.85682000	2.50404700
C	-4.94161100	0.77755900	2.25991700
C	-4.59182200	-0.56698100	2.72936600
C	-5.22012500	-0.20749600	-1.76455700

C	-4.23951700	-2.65962700	1.44124700
C	-3.00261100	-2.87541500	2.15318700
C	-2.57839000	-1.95383000	3.13049000
C	-3.38077200	-0.78490000	3.41768100
C	-2.46784000	0.34029000	3.66342300
C	-2.80886100	1.63745900	3.21416100
C	-1.11802500	-0.14478300	3.52042400
C	-1.17738500	-1.55567000	3.18359100
C	-0.26390000	-2.08120900	2.27444300
C	0.74550600	-1.22843500	1.66200400
C	0.81920900	0.11135300	1.99599800
C	-0.13904100	2.50577500	-1.16740800
C	-1.37867100	2.73455100	-1.87656300
C	-2.33972000	3.31025000	-0.94859900
C	-1.80882500	1.83670700	-2.85847800
C	-1.01035600	0.66485400	-3.13884100
C	-1.90613000	-0.44372800	-3.40202400
C	-3.26458000	0.03927200	-3.28450800
C	-3.20343600	1.46609600	-2.94593900
C	-2.03538300	-3.42915800	1.21119000
C	-0.70333900	-3.02723400	1.27220300
C	3.11295200	1.05091300	-0.76885800
C	3.93025100	-0.11730100	-0.76554200
C	5.26293900	-0.19753700	-0.22422800
C	5.70439500	0.64443700	0.83095600
C	6.97301300	0.55560600	1.35638000
C	7.91052700	-0.39156000	0.85405500
C	7.47526100	-1.24503200	-0.19744500
C	6.19942100	-1.14882600	-0.70834400
C	3.61651400	2.33676800	-0.94825300
C	4.93393300	2.57078100	-1.45680400
C	2.89739300	3.53991900	-0.68480800
C	3.22041500	-1.31653900	-1.24286600
C	3.13787200	-1.44125800	-2.68736800
C	3.55431700	-2.58465900	-0.61070300
C	10.11070800	-1.47215000	0.85020100
C	9.62604700	0.46599400	2.38113700
H	5.01835000	1.36999800	1.25615500
H	7.24635200	1.21606900	2.17006300
H	8.15483900	-1.96657100	-0.63368700
H	5.92606700	-1.79140000	-1.53877000
H	9.70788600	-2.48554700	0.96580900
H	11.04142500	-1.41109500	1.41477200
H	10.34123900	-1.30848000	-0.21076300
H	9.52451600	1.50409500	2.04164500
H	10.67836000	0.28112700	2.59810900
H	9.05912500	0.34762400	3.31378500
H	2.29516600	1.57999800	1.44561800

Zero-point correction= 0.615758 (Hartree/Particle)
Thermal correction to Energy= 0.657276
Thermal correction to Enthalpy= 0.658220
Thermal correction to Gibbs Free Energy= 0.547267
Sum of electronic and zero-point Energies= -3159.274332
Sum of electronic and thermal Energies= -3159.232815
Sum of electronic and thermal Enthalpies= -3159.231871
Sum of electronic and thermal Free Energies= -3159.342824

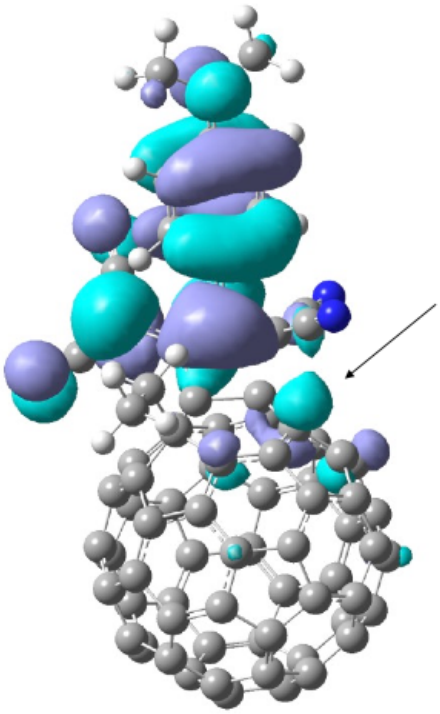
TS2 (R=H) [oniom(b3lyp/6-31g(d):SVWN/STO-3G)]

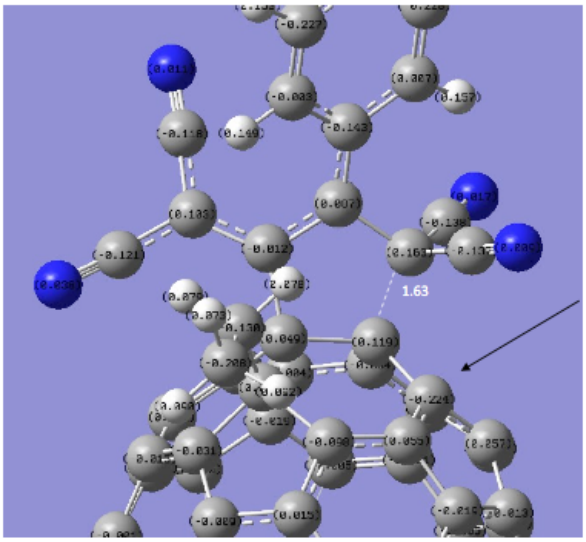
N	5.89727500	3.25151000	-1.54710000
N	2.22925100	4.75644300	0.02420900
N	3.50046400	-2.04738700	-3.37968700
N	3.72870000	-2.91394100	0.63960100
N	9.24264600	-0.74632700	0.98136600
C	1.60691400	0.96737100	-0.26469900
C	1.25784400	1.18136200	1.28958000
C	0.12598500	2.17315600	1.59594600
C	-0.47362000	2.97129100	0.64949900
C	-1.85284900	3.37765900	0.79207400
C	-2.60625900	2.96901900	1.90066100
C	-1.98603800	2.10882500	2.89723100
C	-0.65151400	1.70038300	2.70689800
C	-0.26602700	0.33765300	2.98551200
C	0.62099800	1.70688500	-1.18419400
C	0.22723000	0.87385000	-2.28438000
C	0.62764200	-0.47305400	-2.02167900
C	1.53367300	-0.54187600	-0.80764000
C	1.12963100	-1.66169600	0.16952200
C	0.17628600	-2.69005100	-0.26586700
C	-0.40672700	-2.67040400	-1.52792000
C	-0.17232000	-1.52664200	-2.42584200
C	-1.39815100	-1.27806700	-3.14843100
C	-2.39212000	-2.24615100	-2.70911900
C	-1.76947000	-3.10534500	-1.70618000
C	-2.52038400	-3.55571200	-0.60779500
C	-3.90051000	-3.15699600	-0.46163300
C	-4.50587900	-2.32734500	-1.42689300
C	-3.72287400	-1.86874000	-2.57779700
C	-4.13018900	-0.49320200	-2.88299200
C	-5.00698300	-1.86981300	1.36563500
C	-5.38059300	-1.23116200	-1.01148400
C	-5.62739600	-1.00537700	0.35841000
C	-5.64522500	0.35982900	0.88417100
C	-5.41728400	1.45239800	0.01983100
C	-5.16565400	1.21930100	-1.40485700
C	-4.16477100	2.18550700	-1.85291800
C	-3.78546000	3.00921800	-0.70035000
C	-4.57157700	2.56302800	0.45351100
C	-3.97956400	2.54566700	1.73300000
C	-4.22063900	1.41223000	2.63161400
C	-5.03596800	0.34118200	2.21505500
C	-4.64130500	-1.03927500	2.51133300
C	-5.14783600	-0.09839300	-1.91106000
C	-4.15808800	-2.92380300	0.96817200
C	-2.93477900	-3.18522900	1.68772600
C	-2.58153700	-2.38701200	2.79275600
C	-3.44163200	-1.29969800	3.20555500
C	-2.58659500	-0.18149100	3.62823200
C	-2.97177200	1.14991500	3.34598900
C	-1.21344500	-0.58648700	3.46136800
C	-1.20160700	-1.93989400	2.94354700
C	-0.24431000	-2.29557700	1.99913100
C	0.74361900	-1.33576600	1.54510300
C	0.74392500	-0.04955100	2.03654400
C	-0.22251700	2.72164400	-0.78153000
C	-1.44903400	2.99430000	-1.49546800
C	-2.46167300	3.39685300	-0.53039200

C	-1.80958800	2.22311200	-2.60523800
C	-0.95113500	1.13441300	-3.01170600
C	-1.78152200	0.03488000	-3.44852100
C	-3.16411300	0.43660200	-3.31592100
C	-3.18197100	1.80703200	-2.78889700
C	-1.91745400	-3.57063900	0.71307800
C	-0.60355500	-3.12680300	0.87048800
C	3.09215200	1.31792800	-0.50053100
C	3.89084500	0.14392700	-0.63943000
C	5.25693300	-0.05413800	-0.26594200
C	5.91391800	0.79849900	0.66790900
C	7.20243200	0.57303100	1.08367500
C	7.95309200	-0.53489000	0.58864300
C	7.30067100	-1.40966100	-0.32034100
C	6.00100900	-1.18389600	-0.71767700
C	3.56140600	2.62663800	-0.60787500
C	4.85850500	2.94414400	-1.11765200
C	2.78878200	3.77898600	-0.27723600
C	3.01509100	-1.00165700	-1.02196000
C	3.28111700	-1.58633800	-2.33615200
C	3.03500000	-2.16177500	0.04505500
C	9.97375600	-1.91701500	0.50679000
C	9.90841600	0.19493200	1.87651200
H	5.37328800	1.63221900	1.10019500
H	7.63880400	1.24540600	1.81167900
H	7.82133900	-2.26994000	-0.72135800
H	5.56372400	-1.86553100	-1.43656300
H	9.46061600	-2.84573800	0.78436700
H	10.96503300	-1.92661800	0.96039200
H	10.09521500	-1.89930000	-0.58381200
H	9.90454200	1.20921400	1.46011300
H	10.94559800	-0.11330100	2.00985100
H	9.42969700	0.22144700	2.86407300
H	2.18164300	1.53789500	1.76502000

Zero-point correction= 0.616570 (Hartree/Particle)
Thermal correction to Energy= 0.657604
Thermal correction to Enthalpy= 0.658548
Thermal correction to Gibbs Free Energy= 0.549468
Sum of electronic and zero-point Energies= -3159.263904
Sum of electronic and thermal Energies= -3159.222870
Sum of electronic and thermal Enthalpies= -3159.221926
Sum of electronic and thermal Free Energies= -3159.331006

Fig. 26 (ESI). HOMO and Mulliken charge distribution of **Int-2a** (the attacking carbon atom is highlighted with an arrow).





Example input for ONIOM partitioning:

0 1 0 1 0 1

N	0	-5.719868	-3.961513	1.008458 H
N	0	-2.043200	-3.905459	3.181113 H
N	0	-5.727567	-1.599462	-3.700195 H
N	0	-2.737735	-4.321387	-2.203041 H
N	0	-7.049372	3.365211	0.035393 H
C	0	-1.590333	-1.101271	0.514118 H
C	0	-1.350619	-0.142695	1.837855 H
C	0	-0.103374	-0.542626	2.654081 H
C	0	0.600297	-1.717754	2.513585 H
C	0	2.005209	-1.781727	2.850268 H
C	0	2.677663	-0.653020	3.335018 H
C	0	1.947090	0.597285	3.469871 H
C	0	0.591633	0.636117	3.096791 H
C	0	0.072932	1.769837	2.369386 H
C	0	-0.514676	-2.210435	0.354037 H
C	0	-0.154444	-2.354444	-1.029952 H
C	0	-0.666944	-1.210261	-1.756326 H
C	0	-1.358175	-0.358164	-0.828943 H
C	0	-1.246572	1.006307	-0.964999 H
C	0	-0.491063	1.575836	-2.059972 H
C	0	0.139572	0.745723	-2.994194 H
C	0	0.044117	-0.686247	-2.842465 H
C	0	1.317951	-1.270711	-3.226797 H
C	0	2.205935	-0.185943	-3.616111 H
C	0	1.468347	1.065987	-3.473221 H
C	0	2.119290	2.214603	-3.006841 H

C	0	3.523117	2.165444	-2.667139	L H	26	0.0000
C	0	4.242097	0.961106	-2.802719	L		
C	0	3.557071	-0.238438	-3.289011	L H	24	0.0000
C	0	4.090473	-1.389776	-2.555669	L		
C	0	4.663106	2.628333	-0.498585	L		
C	0	5.193008	0.552478	-1.766510	L		
C	0	5.399206	1.369475	-0.636960	L		
C	0	5.517323	0.767008	0.692655	L		
C	0	5.419799	-0.632082	0.843141	L		
C	0	5.206055	-1.482471	-0.333088	L		
C	0	4.310084	-2.570345	0.053201	L		
C	0	3.957333	-2.387310	1.464153	L H	58	0.0000
C	0	4.656664	-1.195931	1.954161	L		
C	0	4.015181	-0.344704	2.877332	L H	11	0.0000
C	0	4.121814	1.108224	2.723032	L		
C	0	4.855825	1.653509	1.651440	L		
C	0	4.327541	2.804954	0.912507	L		
C	0	5.097795	-0.900684	-1.613333	L		
C	0	3.737783	3.019636	-1.489412	L H	46	0.0000
C	0	2.467144	3.591136	-1.114988	H		
C	0	2.142246	3.765763	0.243667	H		
C	0	3.082303	3.363803	1.268231	L H	47	0.0000
C	0	2.316746	2.790061	2.381654	L H	51	0.0000
C	0	2.826540	1.682151	3.092355	L H	12	0.0000
C	0	0.915876	2.842203	2.028183	H		
C	0	0.802249	3.435317	0.713554	H		
C	0	-0.154831	2.941608	-0.175400	H		
C	0	-1.042892	1.867068	0.219173	H		
C	0	-0.943821	1.298808	1.467354	H		
C	0	0.387404	-2.574617	1.328233	H		
C	0	1.663132	-3.148059	0.962582	H		
C	0	2.665983	-2.663425	1.897489	H		
C	0	1.999292	-3.336003	-0.384113	H		
C	0	1.064693	-2.927265	-1.407669	H		
C	0	1.818859	-2.367215	-2.521424	H		
C	0	3.222934	-2.435952	-2.182796	L H	61	0.0000
C	0	3.335216	-3.040451	-0.849530	L H	59	0.0000
C	0	1.458342	3.087490	-2.043987	H		
C	0	0.184358	2.764108	-1.576610	H		
C	0	-2.614274	-0.102485	2.762011	H		
C	0	-2.541409	0.809177	3.993123	H		
C	0	-2.988087	-1.801185	0.436441	H		
C	0	-3.934941	-1.357657	-0.648156	H		
C	0	-4.698437	-0.114659	-0.461300	H		
C	0	-5.441330	0.106414	0.715904	H		
C	0	-6.225123	1.235788	0.879853	H		
C	0	-6.289862	2.233921	-0.126566	H		
C	0	-5.535564	2.012519	-1.308042	H		
C	0	-4.776809	0.867389	-1.468870	H		
C	0	-3.376522	-2.851527	1.217105	H		
C	0	-4.670936	-3.462503	1.069550	H		
C	0	-2.603319	-3.421013	2.284422	H		
C	0	-4.062184	-2.128438	-1.778271	H		
C	0	-4.989113	-1.811926	-2.826485	H		
C	0	-3.315752	-3.332830	-1.996998	H		
C	0	-7.152533	4.337746	-1.043827	H		
C	0	-7.838926	3.549149	1.244645	H		
H	0	-3.459824	0.216367	2.148263	H		
H	0	-2.822228	-1.115903	3.111869	H		

H	0	-1.737894	0.519052	4.676474	H
H	0	-3.485940	0.730565	4.542833	H
H	0	-2.398817	1.860608	3.725957	H
H	0	-5.454757	-0.648493	1.495899	H
H	0	-6.804982	1.335706	1.788906	H
H	0	-5.544684	2.742151	-2.108019	H
H	0	-4.209399	0.743200	-2.384719	H
H	0	-6.172524	4.762350	-1.297445	H
H	0	-7.800159	5.155825	-0.726366	H
H	0	-7.581516	3.895214	-1.953146	H
H	0	-8.602963	2.767597	1.359798	H
H	0	-8.345417	4.513900	1.197451	H
H	0	-7.205314	3.544737	2.140862	H

1 77 3.0
2 78 3.0
3 80 3.0
4 81 3.0
5 73 1.5 82 1.0 83 1.0
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