

Supporting Information for:

A wide-range of redox states of core-modified expanded porphyrinoids

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General Experimental Methods

Column chromatography was performed on basic alumina in glass columns. ¹H-NMR spectra were recorded on a Bruker 400 MHz spectrometer. Chemical shifts were reported as the delta scale in ppm relative to CHCl₃ (7.28) or CD₂Cl₂ (δ = 5.51). Electronic spectra were recorded on a Perkin-Elmer λ - 35 UV-Vis spectro-photometer and Shimadzu UV3600 UV/Vis/NIR spectrophotometer in an optical quartz cuvette (10 mm path length). High Resolution Mass spectrum (HRMS) was obtained using WATERS G2 Synapt Mass Spectrometer. Single-crystal diffraction analysis data were collected at 100K with a BRUKER KAPPA APEX II CCD Duo diffractometer (operated at 1500 W power: 50 kV, 30 mA) using graphite monochromatic Mo K α radiation (λ = 0.71073 Å). In case of disordered solvent molecules, the contributions to the scattering arising from the disordered solvents in the crystal were removed by use of the utility SQUEEZE in the PLATON software package. More information on crystal structures can also be obtained from the Cambridge Crystallographic Data Centre (CCDC) with deposition number 1897560(**4a**), 1897561(**4b**), 1897874(**4c**), 1897562(**5a**), 1897563(**5d**), 1912149(**5b**). Cyclic voltammetry (CV) and Differential pulse voltammetry (DPV) measurements were carried out on a BAS electrochemical system using a conventional three-electrode cell in dry

CH_2Cl_2 containing tetrabutylammonium perchlorate as the supporting electrolyte. Measurements were carried out under an Argon atmosphere. A glassy carbon (working electrode), a platinum wire (counter electrode), and saturated calomel (reference electrode) were used. The final results were calibrated with the ferrocene/ferrocenium couple. Quantum mechanical calculations were performed with the Gaussian09 rev D program suite using a High Performance Computing Cluster facility of IISER PUNE. All calculations were carried out by Density functional theory (DFT) with Becke's three-parameter hybrid exchange functional and the Lee-Yang-Parr correlation functional (B3LYP) and 6-31G(d, p) basis set for all the atoms were employed in the calculations. The molecular structures obtained from single crystal analysis were used to obtain the geometry optimized structures. To simulate the steady-state absorption spectra, the time-dependent TD-DFT calculations were employed on the optimized structures. Molecular orbital contributions were determined using GaussSum 2.2. Program package. The global ring centres for the NICS (0) values were designated at the non-weighted mean centers of the macrocycles. The NICS (0) value was obtained with gauge independent atomic orbital (GIAO) method based on the optimized geometries.

Materials:

Dichloromethane (CH_2Cl_2) was dried by refluxing and distillation over P_2O_5 . Commercially available pyrrole and thiophene were freshly distilled prior to use. Other reagents and solvents were of commercial reagent grade and were used without further purification.

Synthesis

Experimental Procedures:

4b: A flame-dried 500-mL two neck round-bottomed flask was charged with ((phenylmethylene)bis(thiophene-5,2-diyl))bis((perfluorophenyl)methanol (0.37mmol), 6⁵, and pyrrole (0.37mmol), in 200 mL of anhydrous dichloromethane under nitrogen atmosphere and degassed with nitrogen for further ten minutes. BF₃.OEt₂ (0.37mmol) was added under dark using a syringe, and the resulting solution was stirred for one hour under inert atmosphere. After adding DDQ (1.16 mmol), the reaction mixture was opened to air and stirred for one more hour. A few drops of triethylamine were added and passed through a short pad of basic alumina. This mixture was concentrated and further purified by basic alumina column chromatography using CH₂Cl₂/Hexane as eluent. **2b** obtained in 12% yield as orange colored band.

HR-MS (ESI-TOF): m/z =1351.0403 (found), Calculated for (C₆₆H₂₂F₂₀N₂S₄); (1350.0346+H).

UV-Vis (CH₂Cl₂): λ_{max} nm (ϵ , Lmol⁻¹cm⁻¹): 471 (13000). 551 (8000).

¹H NMR (400 MHz, CDCl₃, 298K) δ : 16.82 (d, J =4.4 Hz, 2H), 15.66 (d, J =4.4 Hz, 2H), 7.08 (m, 6H), 6.64 (m, 4H), 5.16 (d, J =4.8 Hz, 2H), 4.83 (d, J =4.8 Hz, 2H), 4.70 (d, J =6 Hz, 2H), 4.53 (d, J =6 Hz, 2H).

Selected Crystal data: C₆₆ H₂₂ F₂₀ N₂ S₄ (M_r = 1351.10), triclinic, space group $P -1$, a = 6.2671(13), b = 12.536(3), c = 18.175(4) Å, α = 77.166(5), β = 89.244(6), γ = 77.342(6), V = 1357.5(5) Å³, Z = 1, T = 100(2) K, D_{calcd} = 1.653cm⁻³, R_1 = 0.0507 ($I > 2\sigma(I)$), R_w (all data) = 0.1584(6715), GOF = 0.889.

4a: The dication **4a**, was synthesized by the addition of triethyloxonium hexachloroantimonate (10 mg) to a solution of **4b** (2.5 mg) in dry dichloromethane and the resulting solution was stirred for ten minutes under nitrogen atmosphere. Evaporation of the solution gave green colored compound.

HRMS: m/z = 676.0233(found) calculated for (C₆₆H₂₂F₂₀N₂S₄)⁺² (675.0173+H).

¹H NMR (400 MHz, CDCl₃, 298K) δ : 8.96 (d, J =4.4 Hz 2H), 8.75 (d, J =4.8 Hz, 2H), 8.57 (d, J =4 Hz, 2H), 8.43 (br s, 2H), 7.45 (br s, 4H), 7.33 (br s, 6H), -0.14 (br s, 4H).

UV-Vis (CH₂Cl₂): λ_{max} nm (ϵ , Lmol⁻¹cm⁻¹): 676 (32000), 893 (2500), 990 (2100).

Crystal data C₆₆H₂₂F₂₀N₂S₄, 2(Cl₆, Sb), (M_r = 4164.0(9)), monoclinic, space group *P* 21/*c*, $a = 11.5683(14)$, $b = 16.3145(19)$, $c = 22.437(3)$ Å, $\alpha = 90$, $\beta = 100.478(2)$, $\gamma = 90$; $V = 4164.0(9)$ Å³, $Z = 2$, $T = 100(2)$ K, $D_{\text{calcd}} = 1.611\text{g cm}^{-3}$, $R_1 = 0.0547$ ($I > 2\sigma(I)$), R_w (all data) = 0.1551(10334), GOF = 1.050.

4c: To a solution of **4a** or **4b** (2 mg) in dichloromethane, zinc dust was added in excess, followed by addition of aqueous NH₄Cl, reaction was stirred for 5 minutes. The solution was filtered through Whatman filter paper to remove excess zinc powder. Resulting solution was extracted with DCM (20 mL x 2) and dried over anhydrous Na₂SO₄. Solvent was evaporated under reduced pressure to obtain **4c** quantitatively.

HRMS: (ESI-TOF): m/z = 1352.0455 (found), (Calculated For: C₆₆H₂₄F₂₀N₂S₄. 1352.0503).

UV-Vis (CH₂Cl₂): λ_{max} nm (ϵ , Lmol⁻¹cm⁻¹): 552 (36000), 683(3600), 742 (1500).

¹H NMR: (400 MHz, CDCl₃, 253K) δ : 9.0 (d, J =4.8 Hz, 2H), 8.94 (d, J =4 Hz, 2H), 8.36 (br s, 2H), 8.25 (br s, 2H), 8.23 (m, 4H), 7.91 (m, 6H), -1.40 (d, J =4.4 Hz, 2H), -1.60 (d, J =4.4 Hz, 2H), -2.07 (s, 2H, Exchangeable with D₂O).

Selected Crystal data C₆₆H₂₄F₂₀N₂S₄, (M_r = 1353.11), triclinic, space group *-1*, $a = 6.102(7)$, $b = 12.262(14)$, $c = 17.76(2)$ Å, $\alpha = 77.22(3)$, $\beta = 89.22(3)$, $\gamma = 78.68(3)$; $V = 1270(3)$ Å³, $Z = 1$, $T = 100(2)$ K, $D_{\text{calcd}} = 1.769\text{g cm}^{-3}$, $R_1 = 0.0920(1257)$ R_w (all data) = 0.3114(5954), GOF = 0.837.

Note for Alert A: Ratio Observed / Unique Reflections (too) Low. Explanation: The quality of the crystal was degrading during data collection hence only a few runs were collected successfully and subsequently used for solving the structure. Therefore this alert has been raised due to limited reflections in the diffraction data set.

5b and 5c: They were synthesized by a reported procedure.¹

5b: **HRMS**: (ESI-TOF): m/z = 1633.7279 (found), (Calculated For: C₁₁₂H₁₀₄N₄S₄. 1632.7144 + H).

UV-Vis (CH₂Cl₂): λ_{max} nm (ϵ , Lmol⁻¹cm⁻¹): 419 (9000), 622(5000), 742.

¹H NMR: (400 MHz, CD₂Cl₂, 213K) δ : 10.04 (d, J =4.4 Hz, 2H), 7.45 (d, J =4.4 Hz, 2H), 7.33 (d, J =4Hz, 2H), 7.18 (br s, 2H), 7.05 (br s, 2H), 7.02(br s, 2H), 6.85 (br s, 4H), 6.82 (br s, 2H), 6.78(br s, 4H), 6.19 (d, J =4.8 Hz, 2H), 6.08 (br s, 2H), 6.07(d, J =4.4 Hz, 2H), 5.90(d, J =4.8 Hz, 2H), 5.82(d, J =4.8 Hz, 2H), 2.93(br s, 6H), 2.66(br s, 6H), 2.40(br s, 6H), 2.35(br s, 6H), 2.30(br s, 6H), 2.26(br s, 6H), 2.21(br s, 6H), 2.14(br s, 6H), 1.86(br s, 6H), 1.63 (br s, 6H), 1.62(br s, 6H), 1.48(br s, 6H).

Selected Crystal data C₁₁₂H₁₀₄N₄S₄, (M_r = 1634.24), monoclinic, space group $C 2/c$, $a = 50.346(15)$, $b = 16.533(5)$, $c = 29.033(8)$ Å, $\alpha = 90$, $\beta = 112.241(9)$, $\gamma = 90$; $V = 22368(11)$ Å³, $Z = 8$, $T = 100(2)$ K, $D_{\text{calcd}} = 0.971\text{g cm}^{-3}$, $R_1 = 0.0692(13419)$ R_w (all data) = 0.2017(20809), GOF = 1.105.

5c: HRMS: (ESI-TOF): m/z =1634.7246 (found), (Calculated For: C₁₁₂H₁₀₆N₄S₄. 1634.7300).

UV-Vis (CH₂Cl₂): λ_{max} nm (ϵ , Lmol⁻¹cm⁻¹): 708 (15000), 916(1300), 1040(1600), 429(6300), 510(2400).

¹H NMR: (400 MHz, CD₂Cl₂, 193K) 11.24(br s, 2H, exchangeable with D₂O), 9.69(d, J =4.4 Hz, 2H), 9.65(d, J =4 Hz, 2H), 8.52 (d, J =3.6 Hz, 2H), 8.49(d, J =4 Hz, 2H), 7.56(br s, 4H), 7.48(br s, 4H), 7.43(br s 4H), 7.37(br s, 4H), 2.85(br s, 4H), 2.76(br s, 4H), 2.71(br s, 4H), 2.62(br s, 4H), 2.07(br s, 11H), 2.08-1.95(br s, 30H), 1.86(br s, 16H), -2.55(br s, 2H), -2.89(br s, 2H), -3.17(br s, 2H), -3.35(br s, 2H).

5a: The dication **5a** was synthesized by the addition of triethyloxonium hexachloroantimonate (20 mg) to a solution of **5b** or **5d** (2 mg) in dry dichloromethane and the resulting solution was stirred for 10 minutes under nitrogen atmosphere. Evaporation of the solution gave light blue colored compound which was further washed with diethyl ether and hexane to remove ethyl chloride produced in the course of reaction.

HRMS: m/z = 818.3687(found) calculated for (C₁₁₂H₁₀₄N₄S₄)⁺² (816.3572+2H).

UV-Vis (CH₂Cl₂): λ_{max} nm (ϵ , Lmol⁻¹cm⁻¹): 767 nm (38000), 1110 (2700), 1291 (3300).

¹H NMR (400 MHz, CD₂Cl₂, 213K) δ : 24.23 (br s, 8H), 0.20 (br s, 8H).

Crystal data: C₁₁₂ H₁₀₃ N₄ S₄, 2(Cl₆ Sb) [+ solvent], M_r = 2303.16, monoclinic, space group *P* 21/*n*, a = 23.877(5), b = 21.397(5), c = 24.554(6) Å, α = 90, β = 108.515(4), γ = 90; V = 11894(5) Å³, Z = 4, T = 100(2) K, D_{calcd} = 1.286 g cm⁻³, R_1 = 0.1469(8208), R_w (all data) = 0.4181(22134), GOF = 1.077.

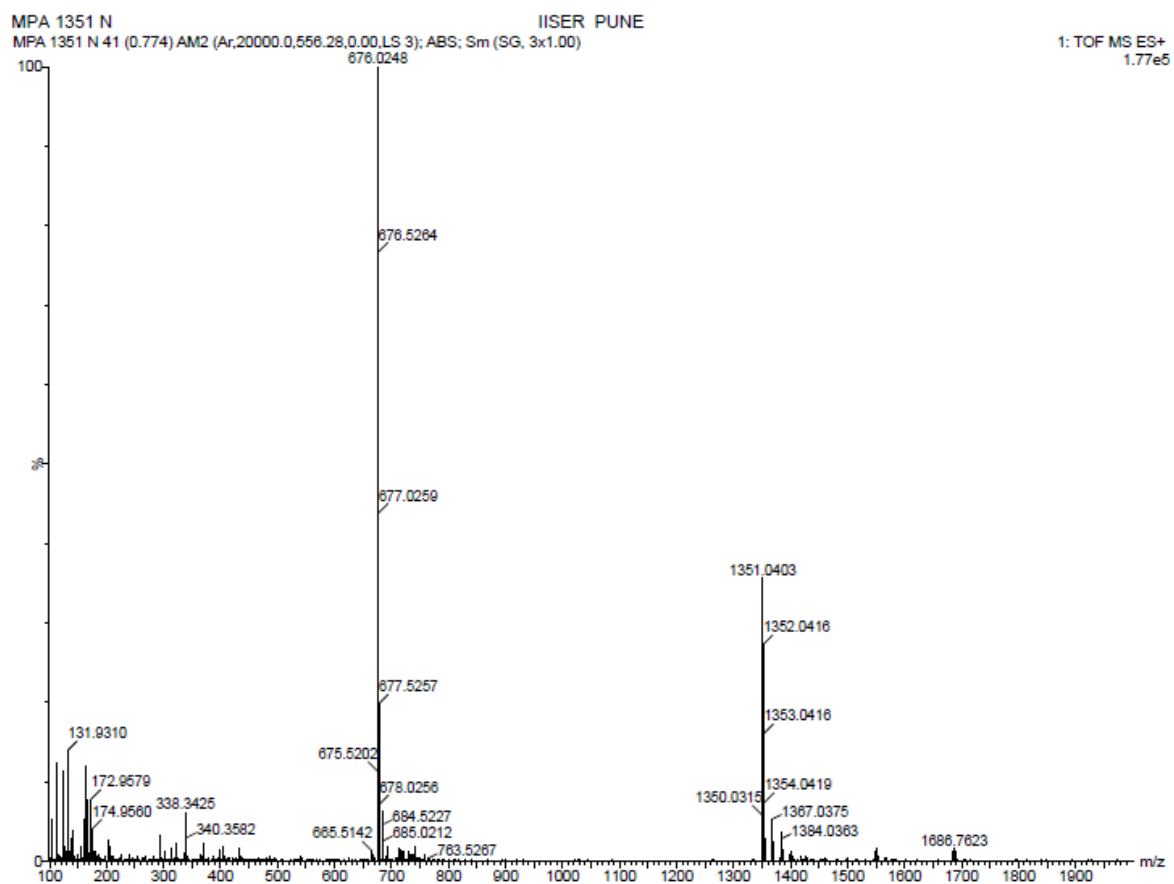
5d: To a solution of **5a**, **5b** or **5c** (2 mg) in dichloromethane, zinc dust was added in excess, followed by addition of aqueous NH₄Cl, reaction was stirred for 5 minutes. The solution was filtered through Whatman filter paper to remove excess zinc powder. Resulting solution was extracted with DCM (20 mL X 2) and dried over anhydrous Na₂SO₄. Solvent was evaporated under reduced pressure to obtain **4c** quantitatively.

HRMS Data: (ESI-TOF): m/z = 1637.7415 (found), Calcd. For: C₁₁₂H₁₀₈N₄S₄; (1636.7457+H).

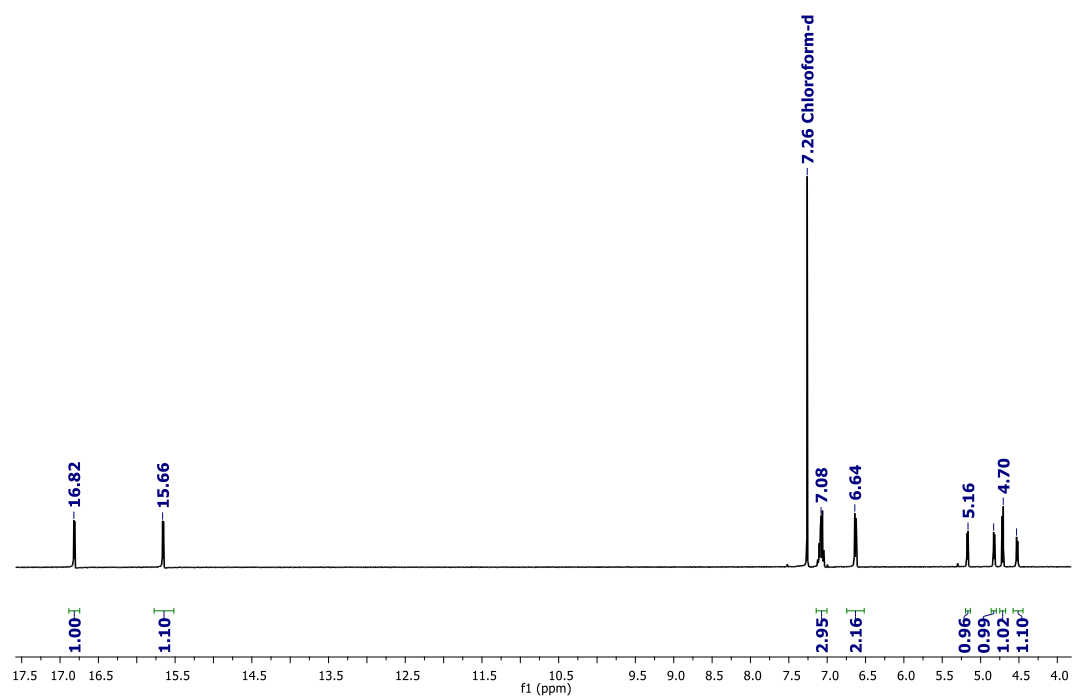
UV-Vis (CH₂Cl₂): λ_{max} nm (ϵ , Lmol⁻¹cm⁻¹): 553 (18000), 516(9000) 707 (5000), 1050(570).

¹H NMR (400 MHz, CD₂Cl₂, 253K) δ : 10.88 (s, 2H exchangeable with D₂O), 9.73 (br s, 2H), 9.45 (br s, 2H), 9.32 (br s, 2H), 8.70 (s, 2H), 6.83 (s, 2H), 6.43(s, 6H), 5.94 (br s, 2H), 5.52 (s, 3H), 2.2 to 2.5 (multiple signals, 74H), 0.35 (br s, 2H exchangeable with D₂O), 0.01 (br s, 2H), -1.45 (br s, 2H), -1.74 (br s, 2H), -1.94 (br s, 2H).

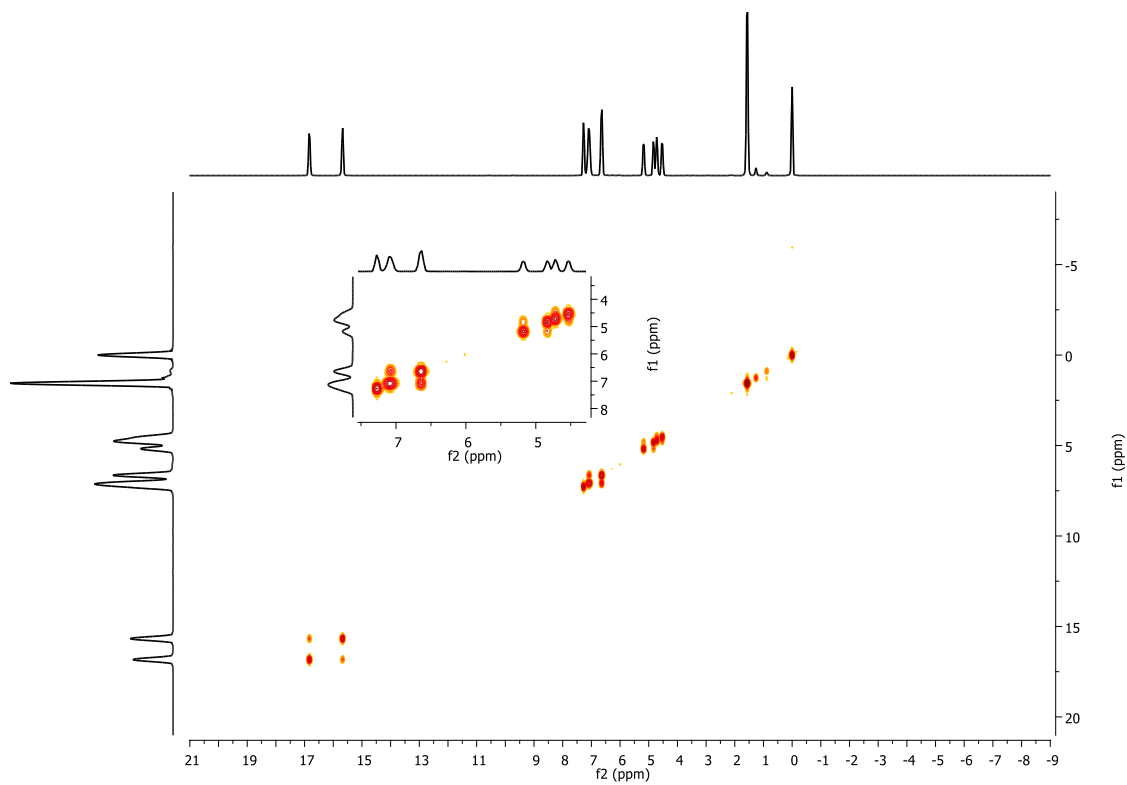
Selected Crystal data: C₁₁₂ H₁₀₈ N₄ S₄, 4(C H Cl₃) (M_r = 2115.74), monoclinic, space group *P* 21/*n*, a = 18.330(12), b = 14.715(9), c = 19.877(12), Å, α = 90, β = 96.404(14), γ = 90, V = 5328(6) Å³, Z = 2, T = 100 K, ρ_{calcd} = 1.319 g/cm³, R_{int} (all data) = 0.0762, R_1 (all data) = 0.1586, R_w (all data) = 0.2273, GOF = 1.075.



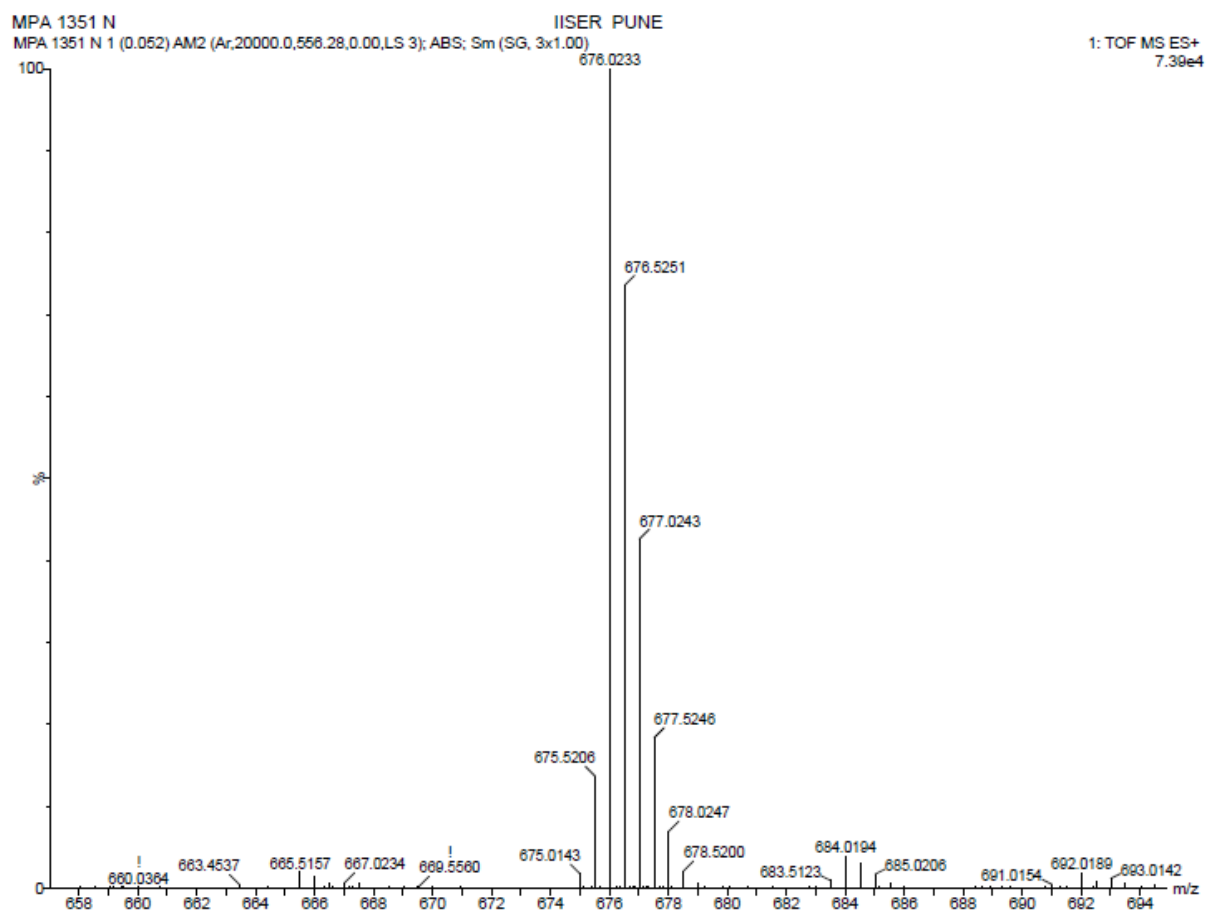
S1: High resolution mass spectrum of **4b**



S2: ¹H NMR spectrum of **4b** recorded in CDCl₃ at 298K

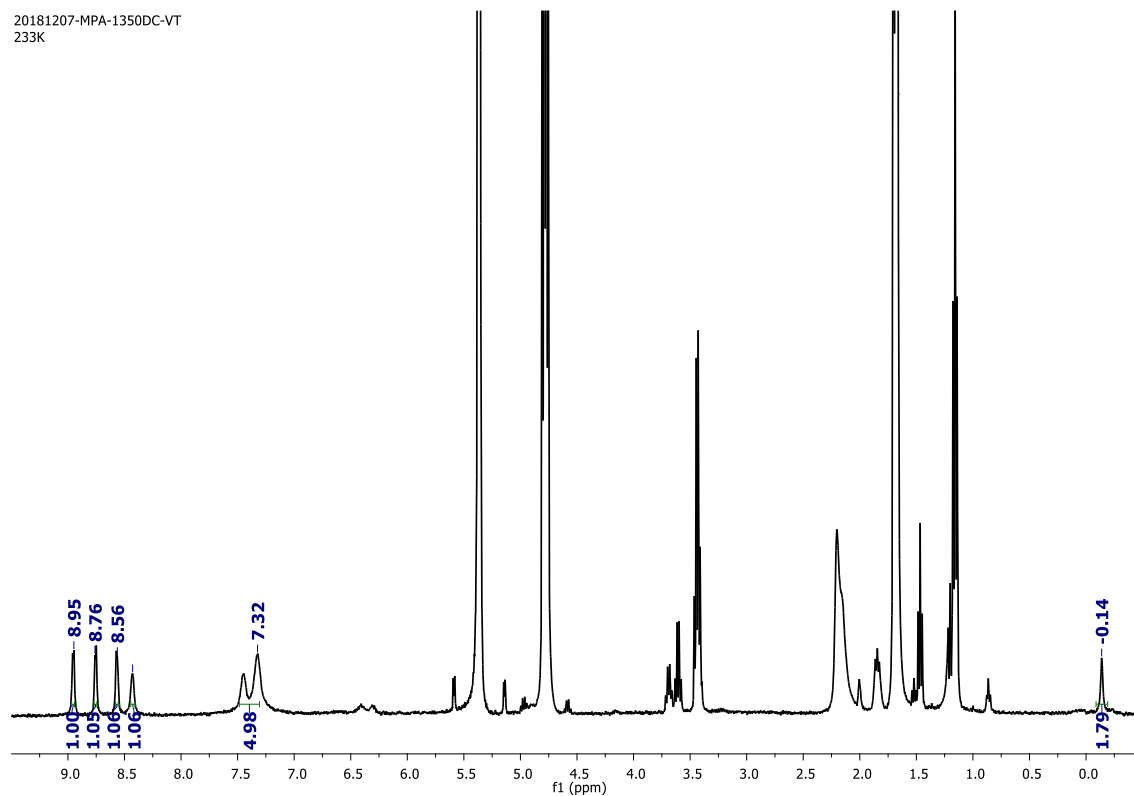


S3: ¹H-¹H COSY spectrum of **4b** at 298K

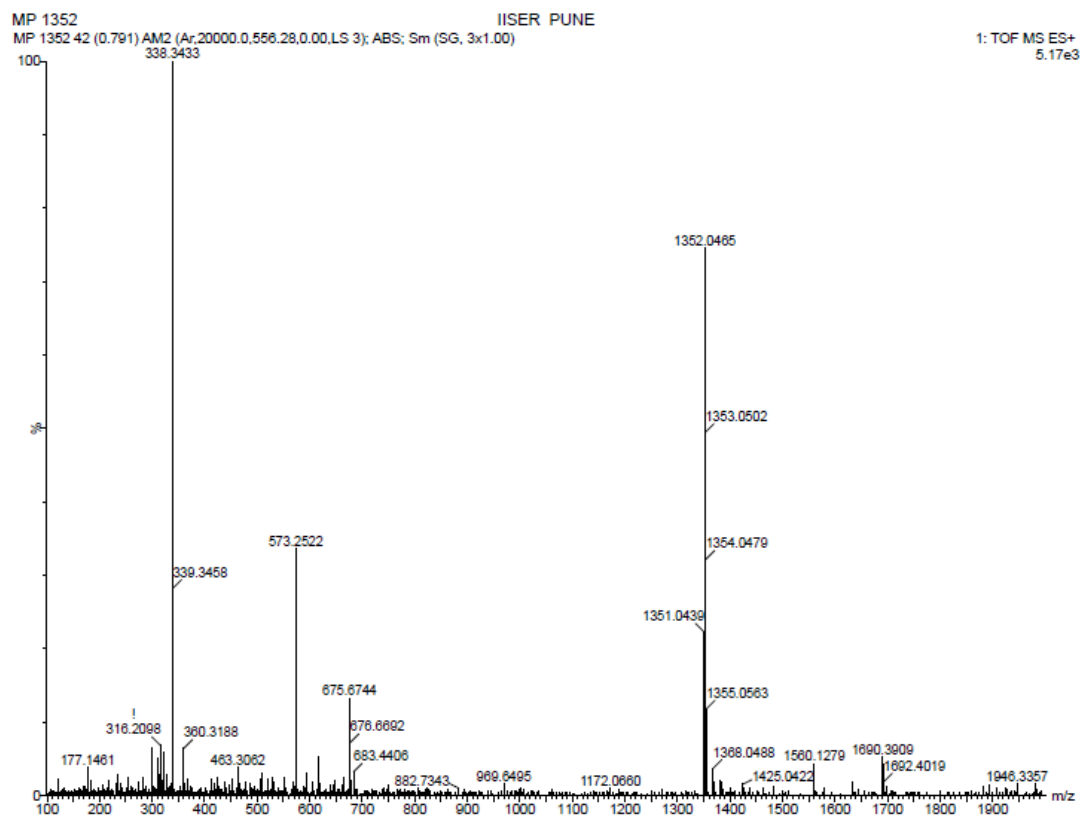


S4: High resolution mass spectrum of **4a**

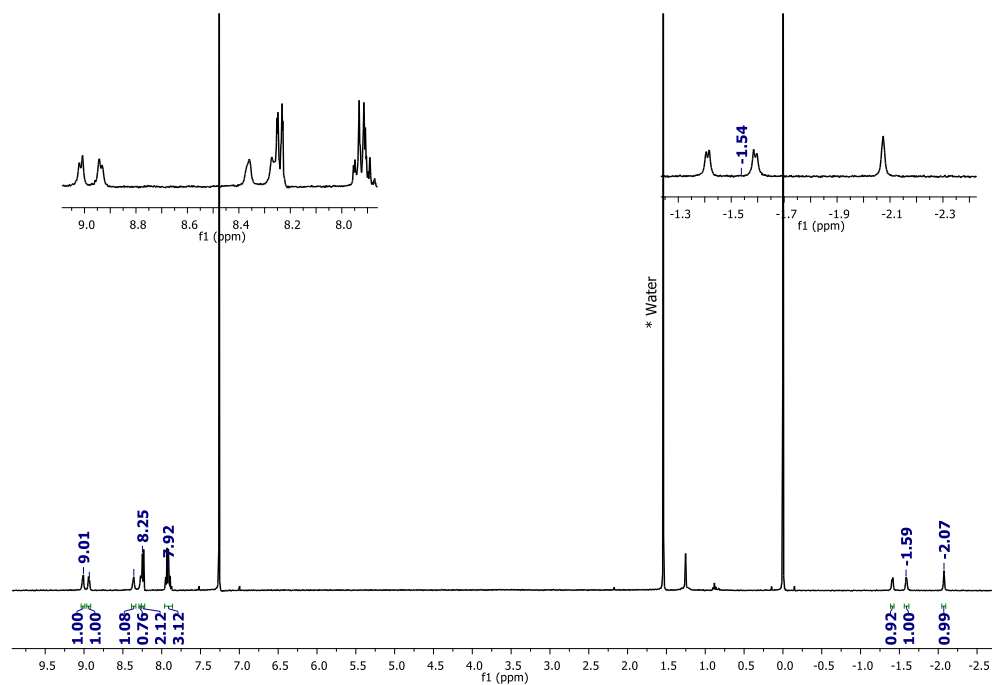
20181207-MPA-1350DC-VT
233K



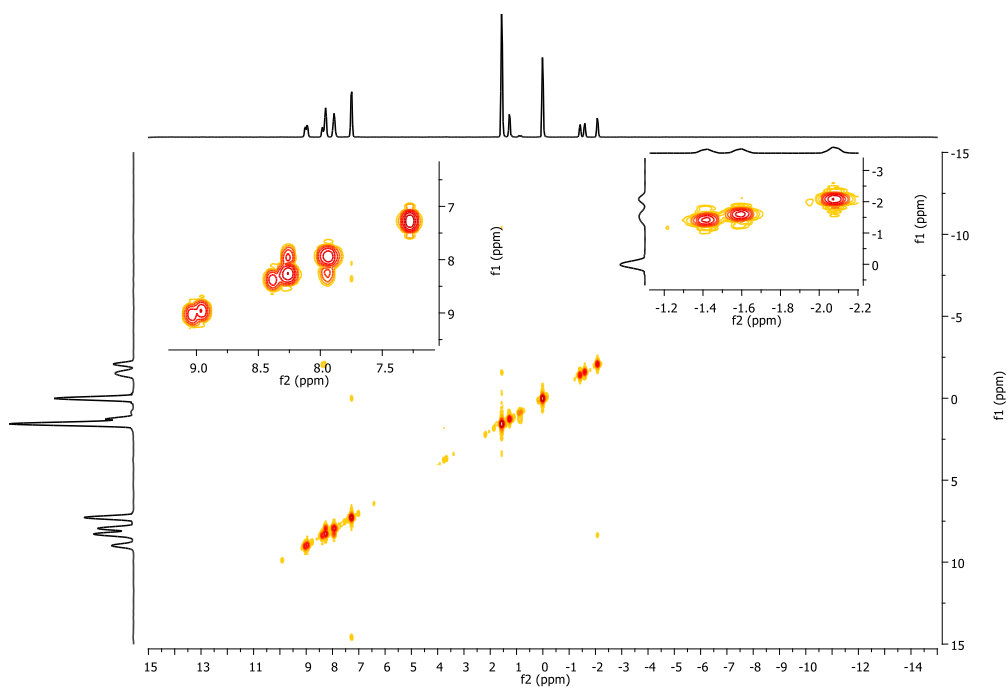
S5: ^1H NMR spectrum of **4a** at 233K in CD_2Cl_2 . (Signals observed in the range between 1- 5.5 ppm corresponds to ethyl group of ethyl chloride and diethyl ether from Meerwein salt)



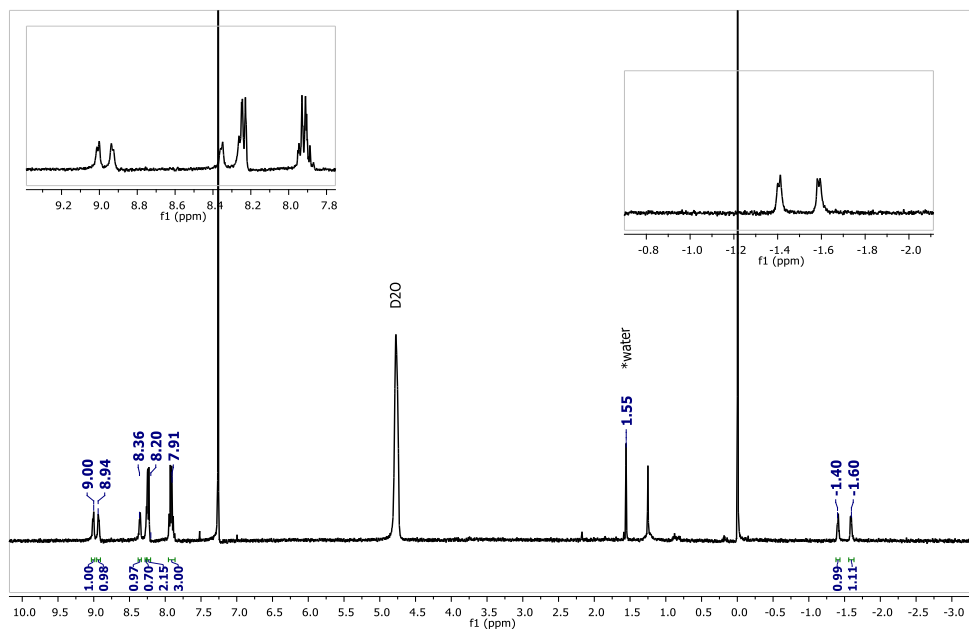
S6: High resolution mass spectrum of **4c**



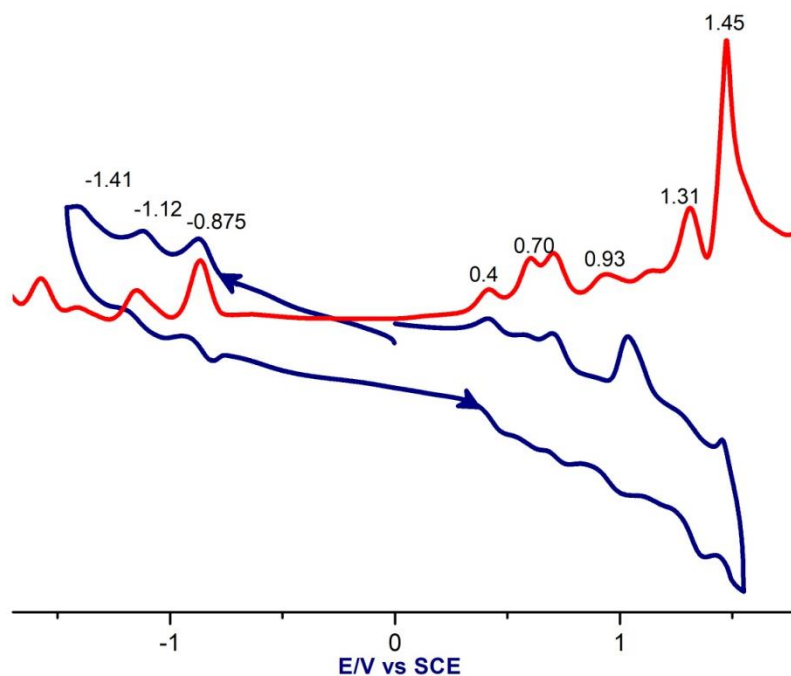
S7: ^1H NMR spectrum of **4c** in CDCl_3 at 298K



S8: ^1H - ^1H COSY spectrum of **4c** in CDCl_3



S9: ^1H NMR spectrum of **4c** upon addition of D_2O at 298K in CDCl_3

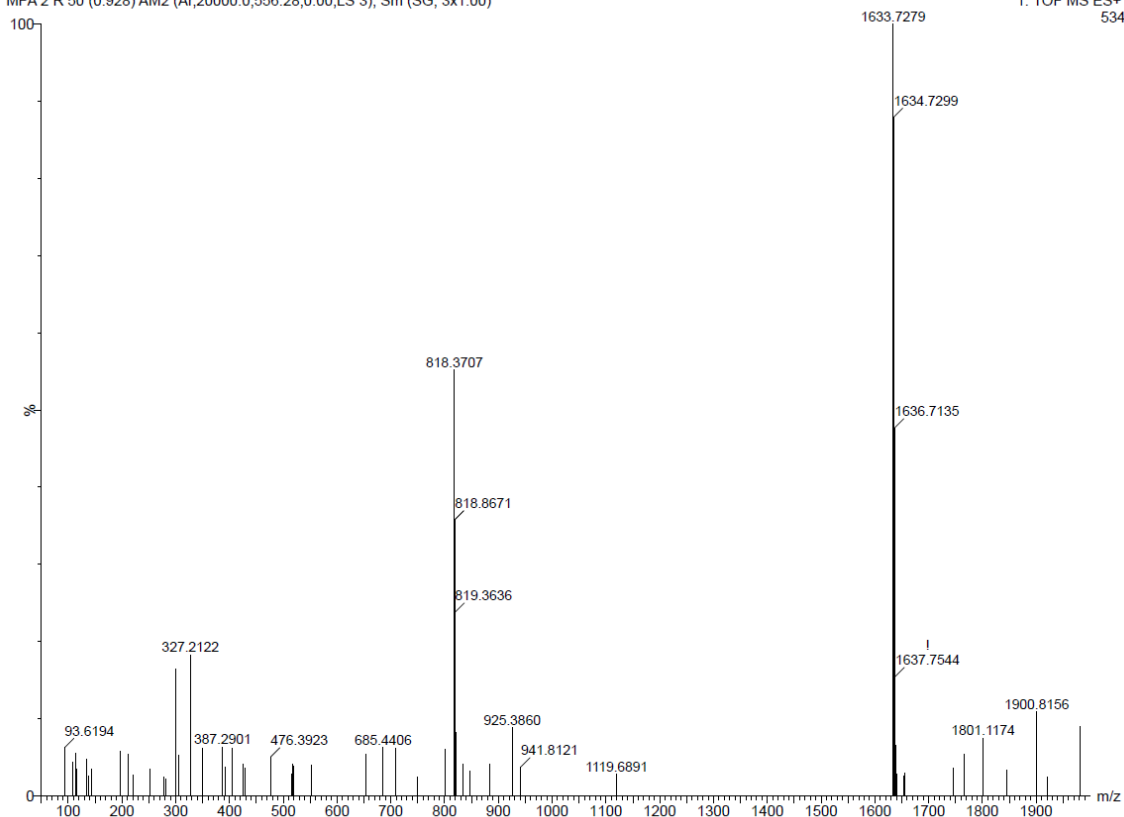


S10: Cyclic (blue) and differential pulse (red) Voltamogram of **4c** in dichloromethane containing 0.1M tetra butyl ammonium perchlorate as the supporting electrolyte recorded at a scan rate of 50 Mv s^{-1}

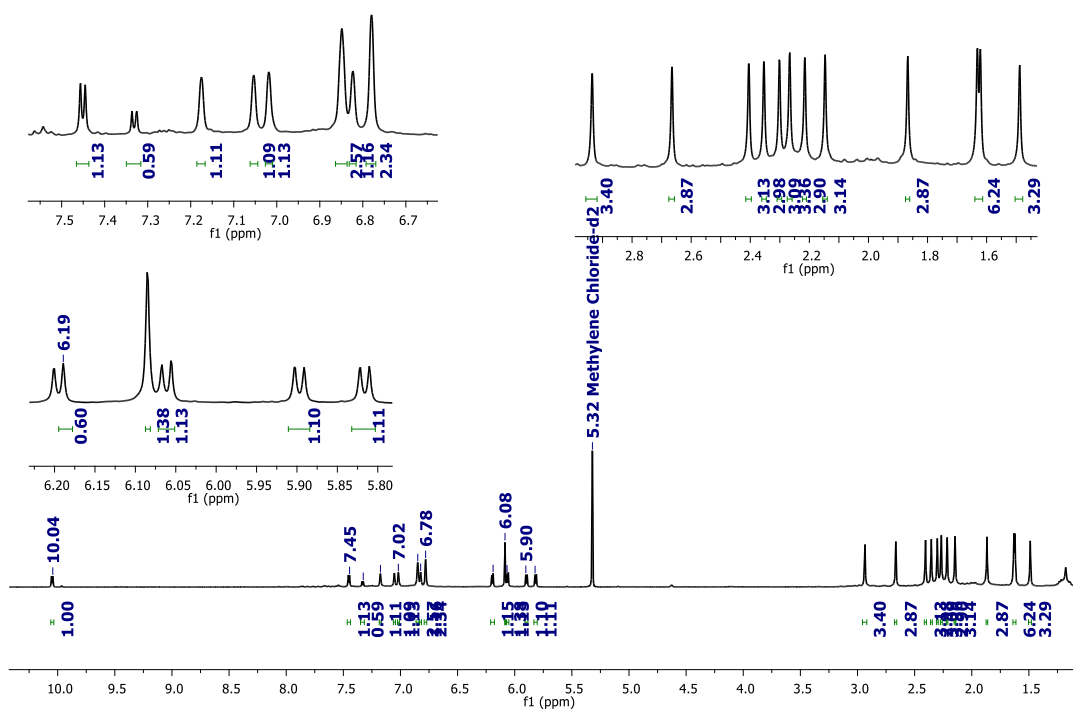
MPA 2 R
MPA 2 R 50 (0.928) AM2 (Ar,20000.0,556.28,0.00,LS 3); Sm (SG, 3x1.00)

IISER PUNE

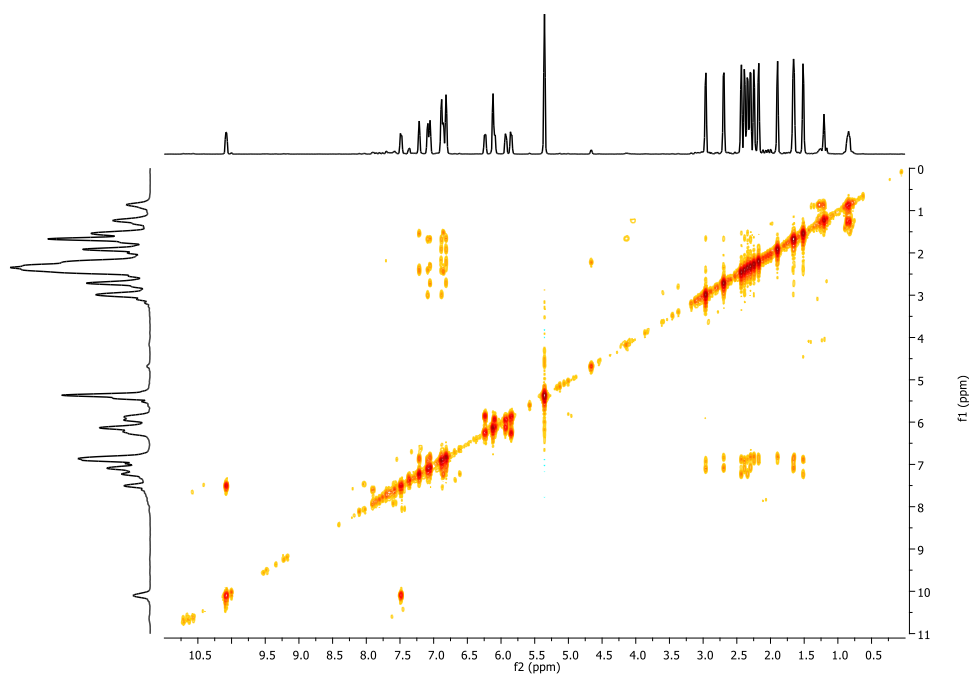
1: TOF MS ES+
534



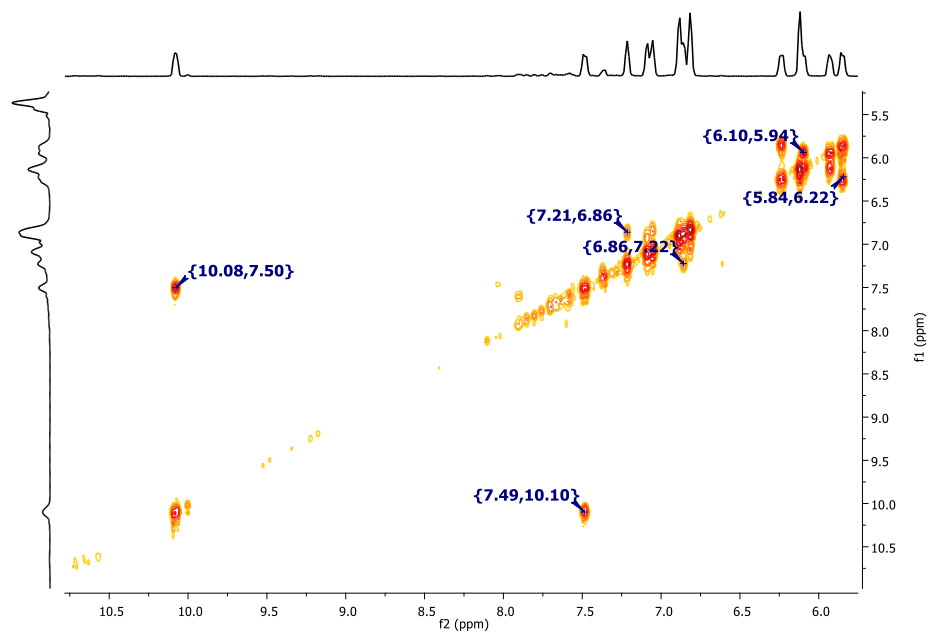
S11: High Resolution mass spectrum of **5b**



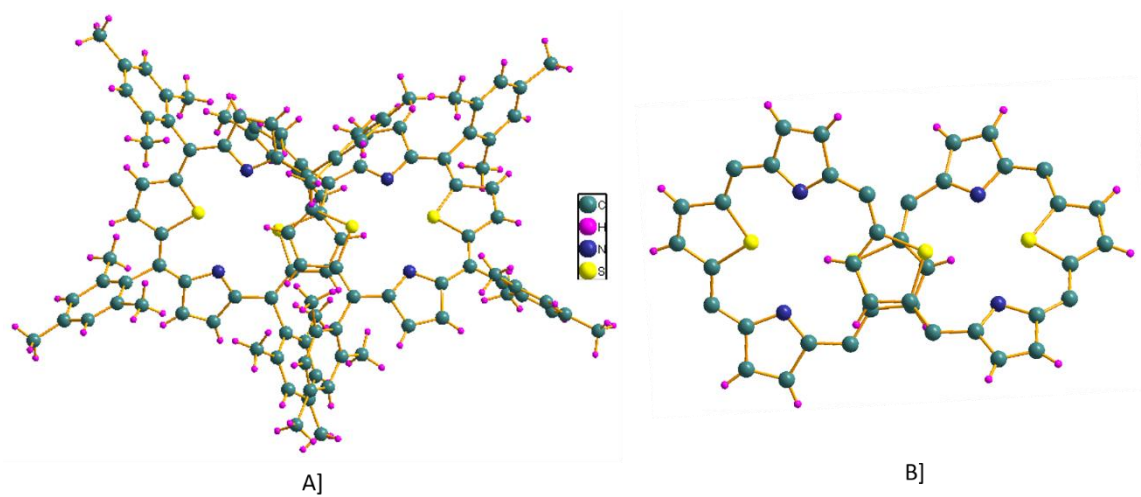
S12: ¹H NMR spectrum of **5b** at 213K in CD₂Cl₂



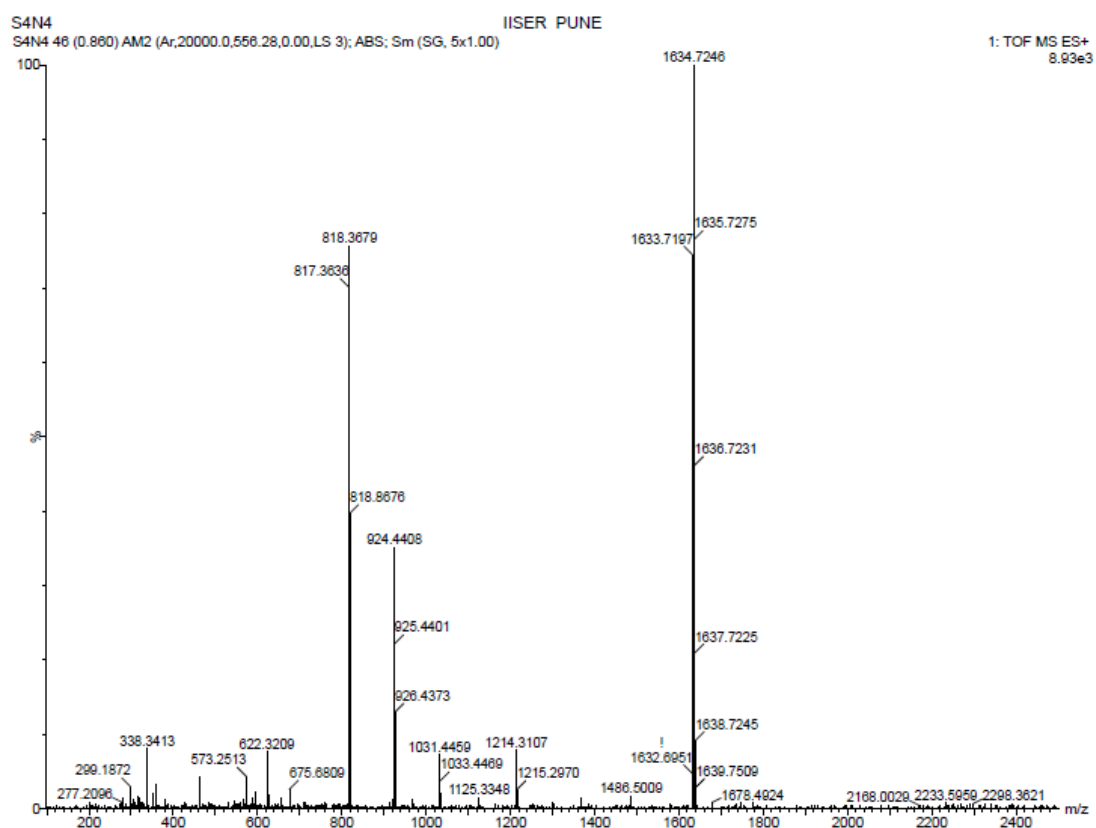
S13: Full ¹H-¹H COSY spectra of **5b** in CD₂Cl₂ at 213K



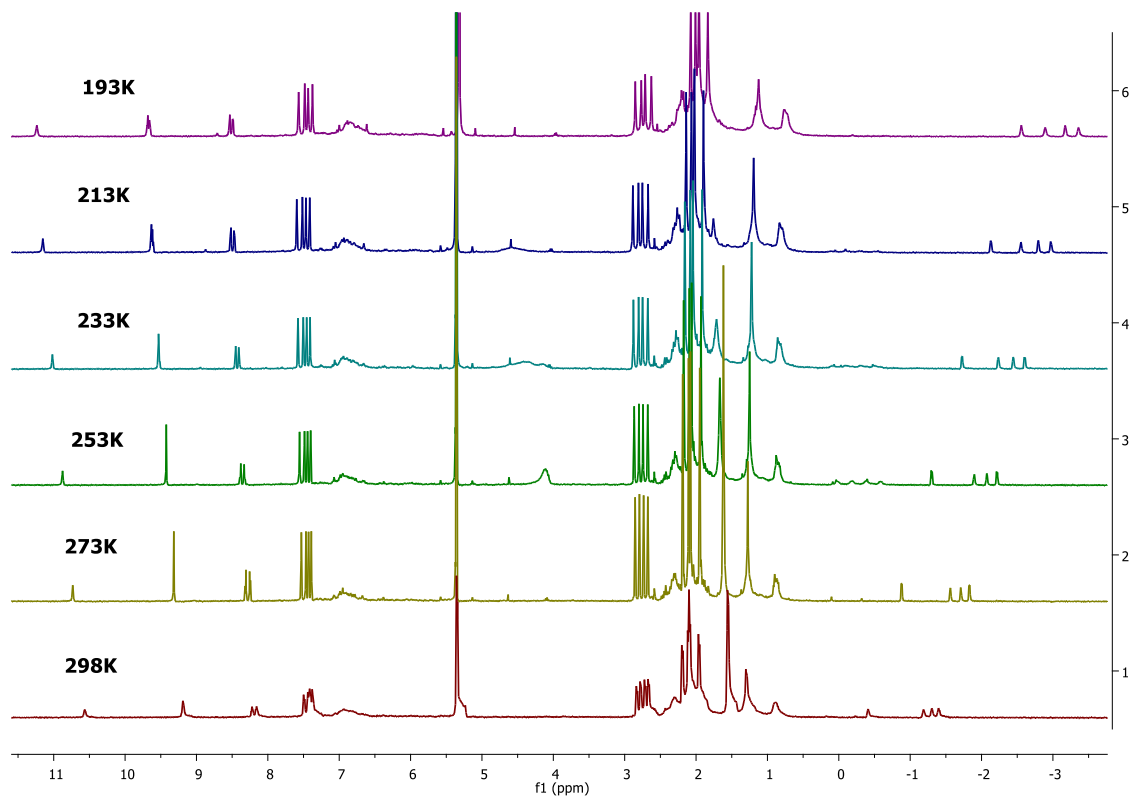
S14: Partial ^1H - ^1H COSY **5b** in CD_2Cl_2 at 213K



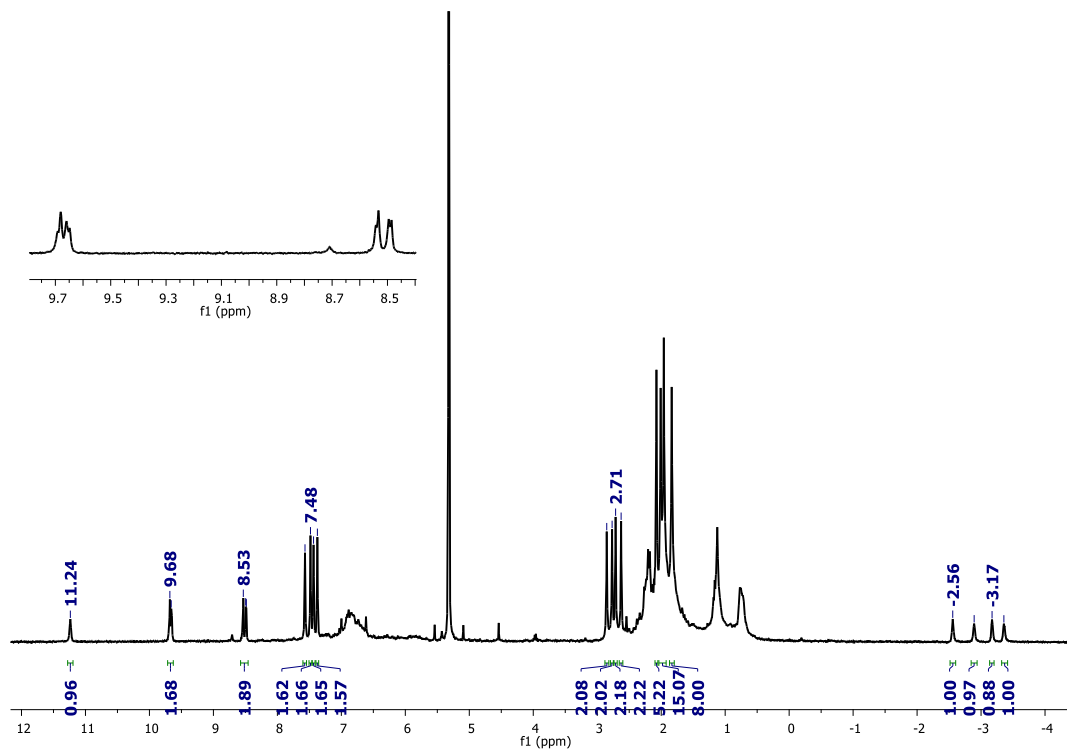
S15: Molecular Structure of **5b** A) with meso-mesityl substituents B) meso substituents are omitted for clarity



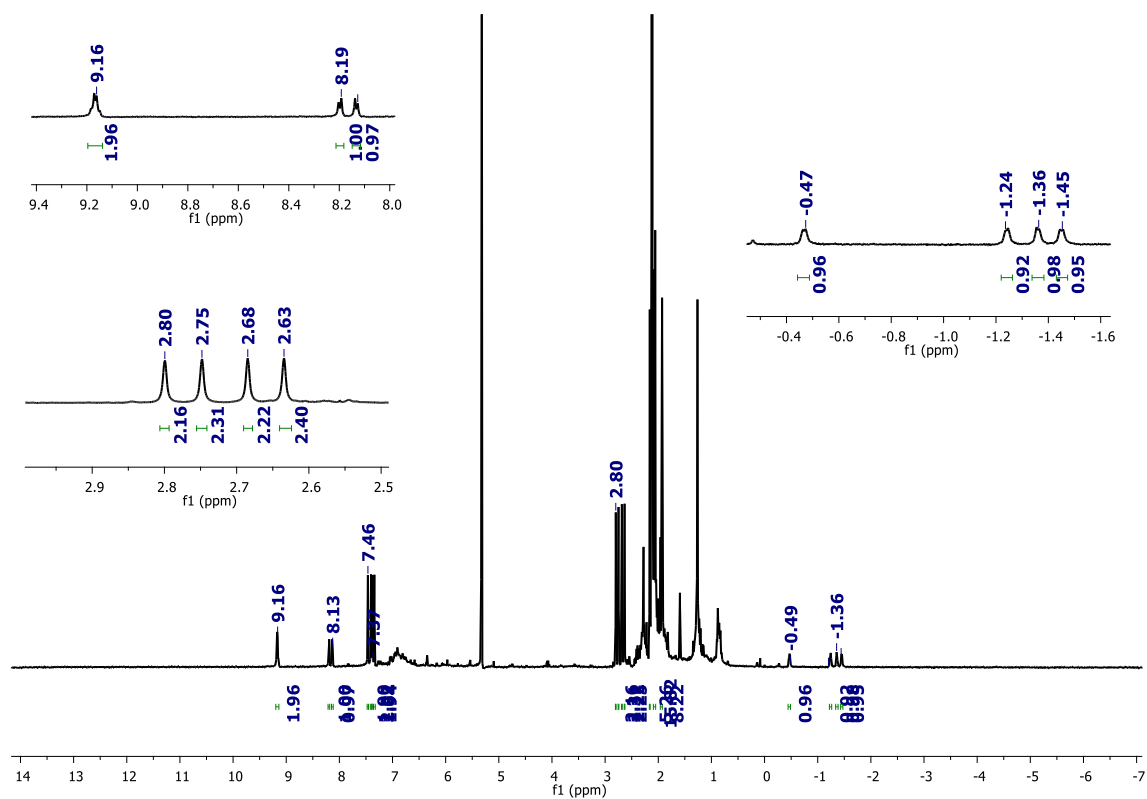
S16: HRMS Spectrum of **5c**



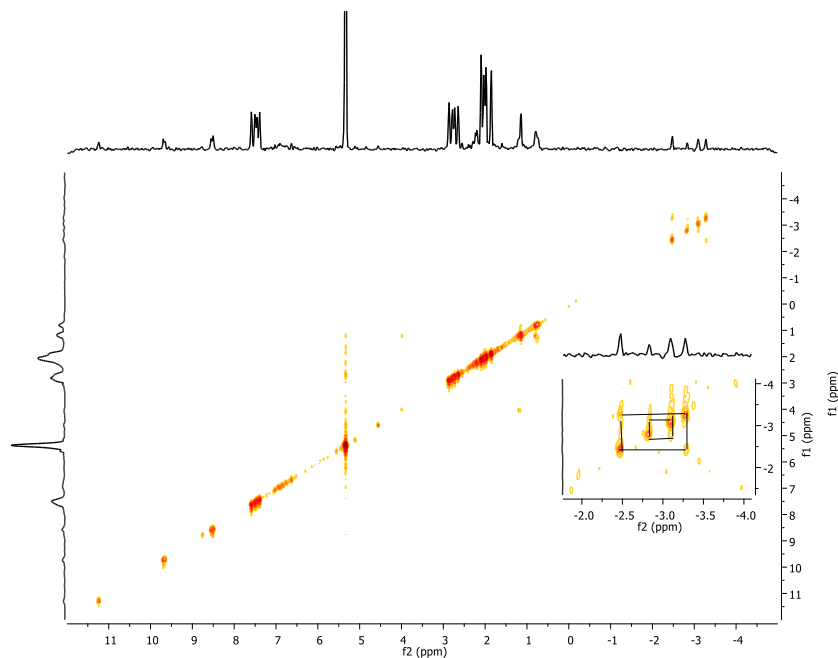
S17: Variable temperature ^1H NMR spectra of **5c** in CD_2Cl_2



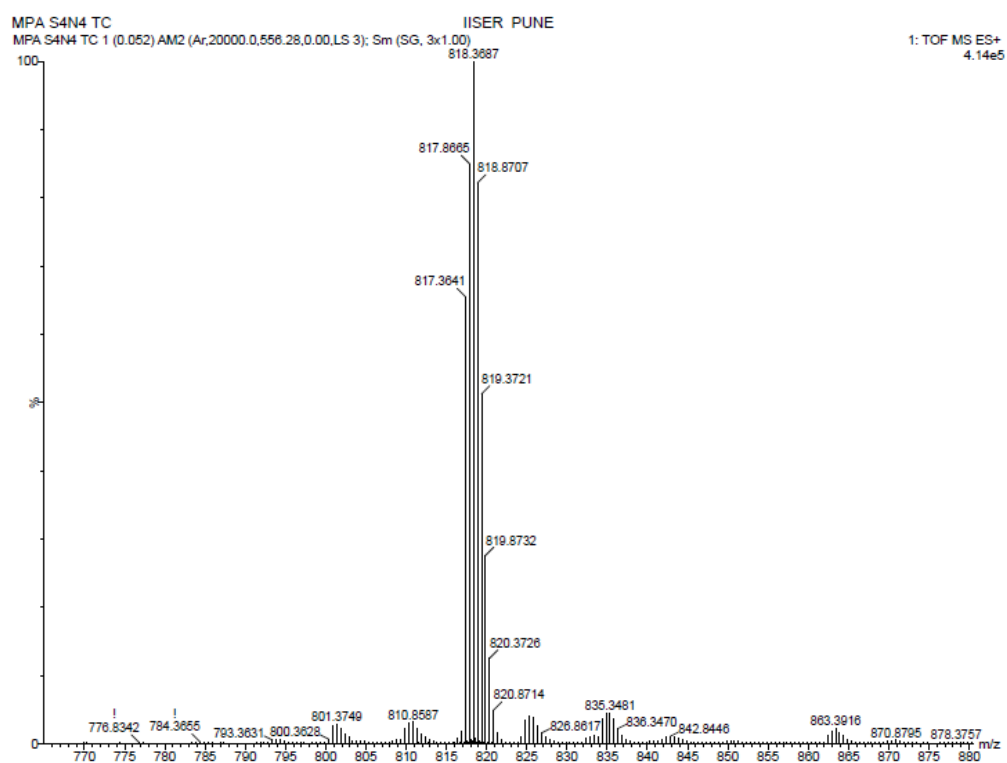
S18: ^1H NMR spectrum of **5c** at 193K in CD_2Cl_2



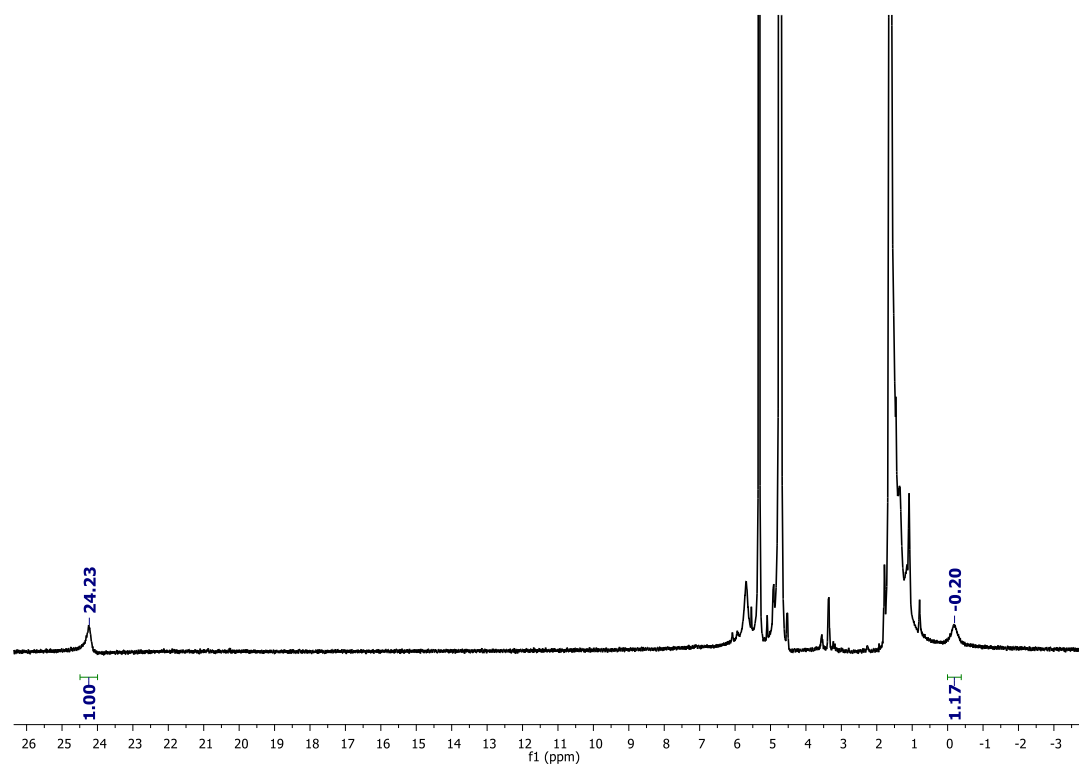
S19: ¹H NMR spectrum of **5c** at 298K in CD₂Cl₂ upon addition of D₂O



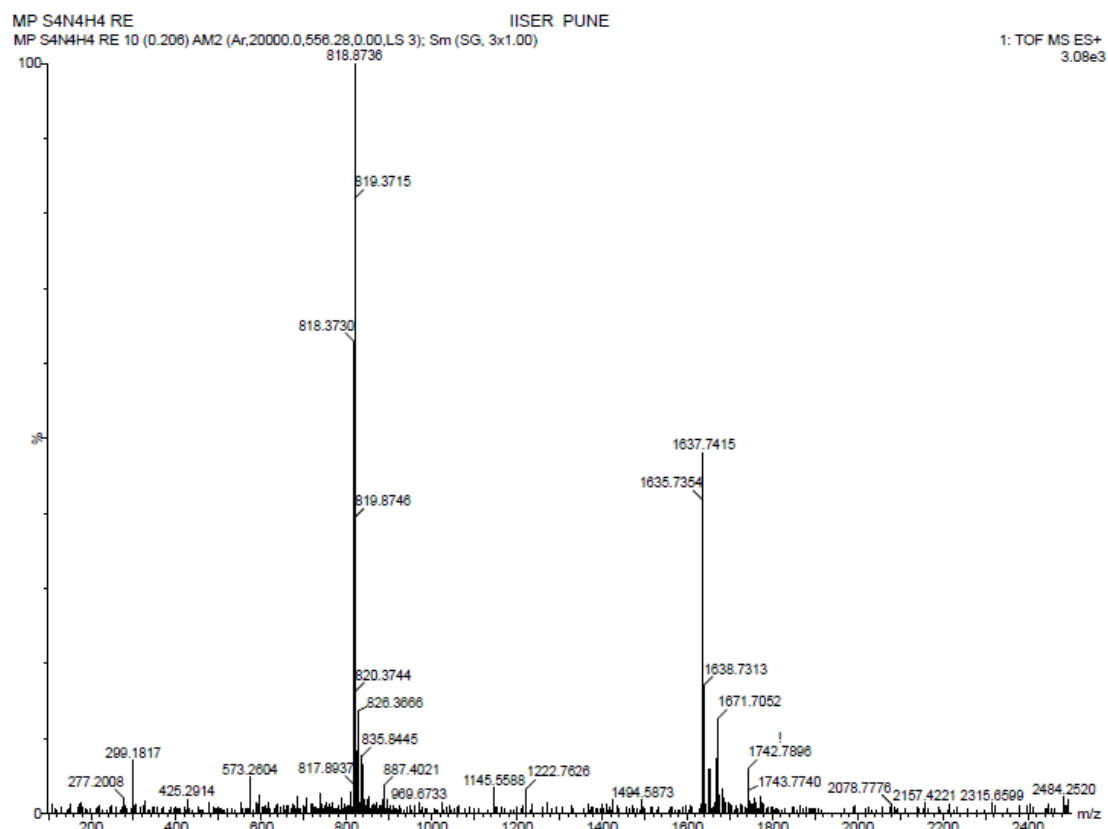
S20: ¹H-¹H COSY spectra of **5c** in CD₂Cl₂ at 193K



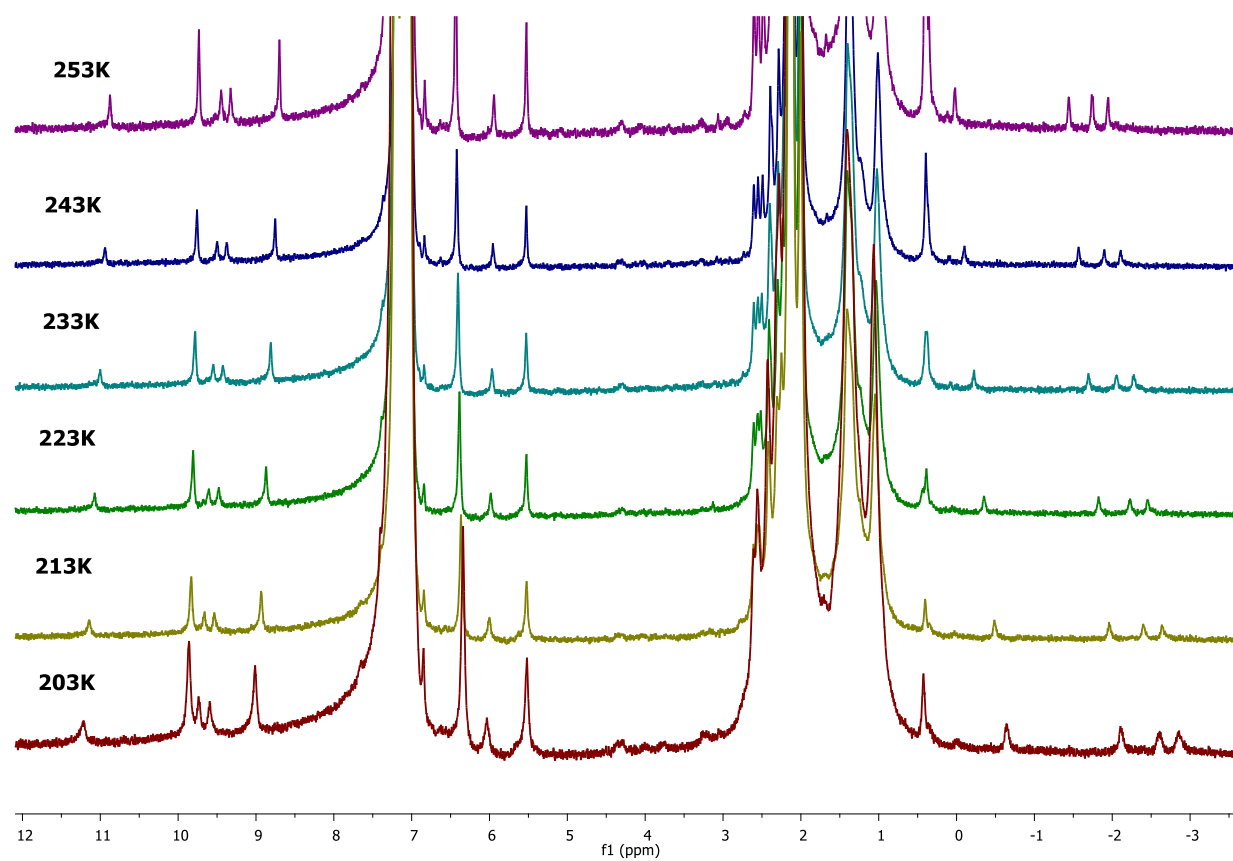
S21: High resolution mass spectrum of **5a**



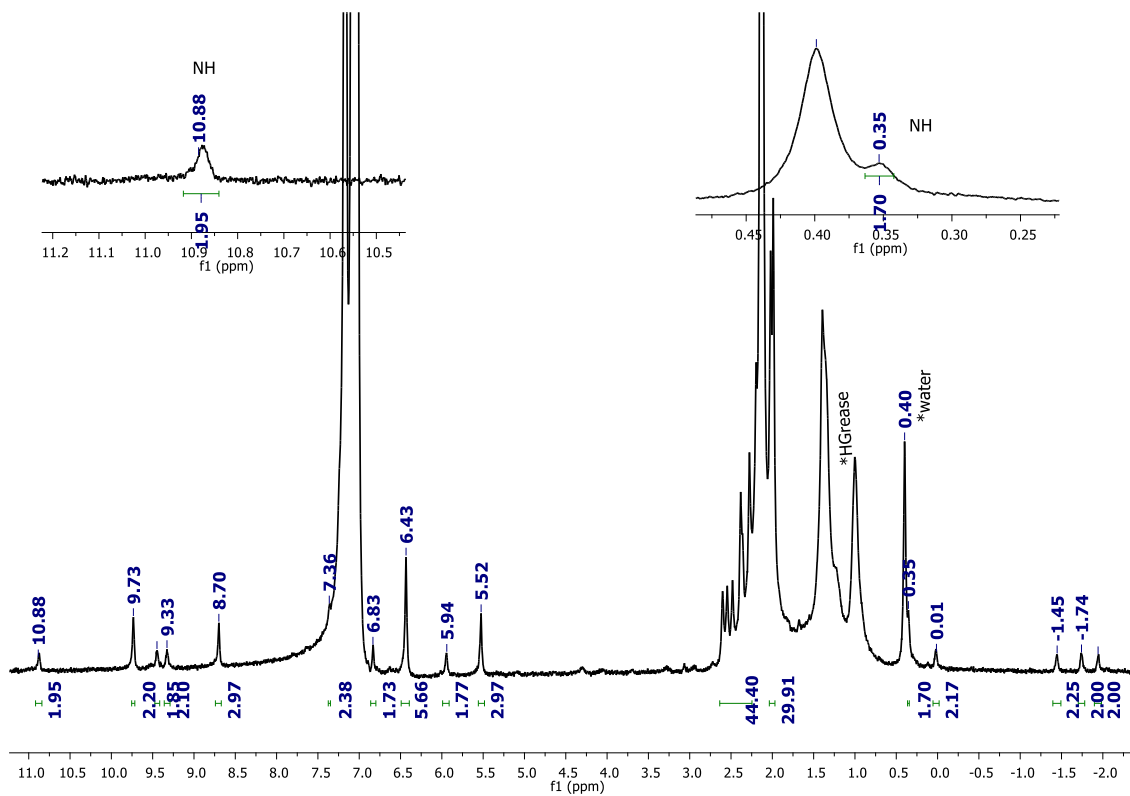
S22: ^1H NMR spectrum of **5a** recorded at 213K in CD_2Cl_2 (Signal observed in the range between 1 to 6 ppm corresponds to ethyl group of ethyl chloride and diethyl ether from Meerwein salt)



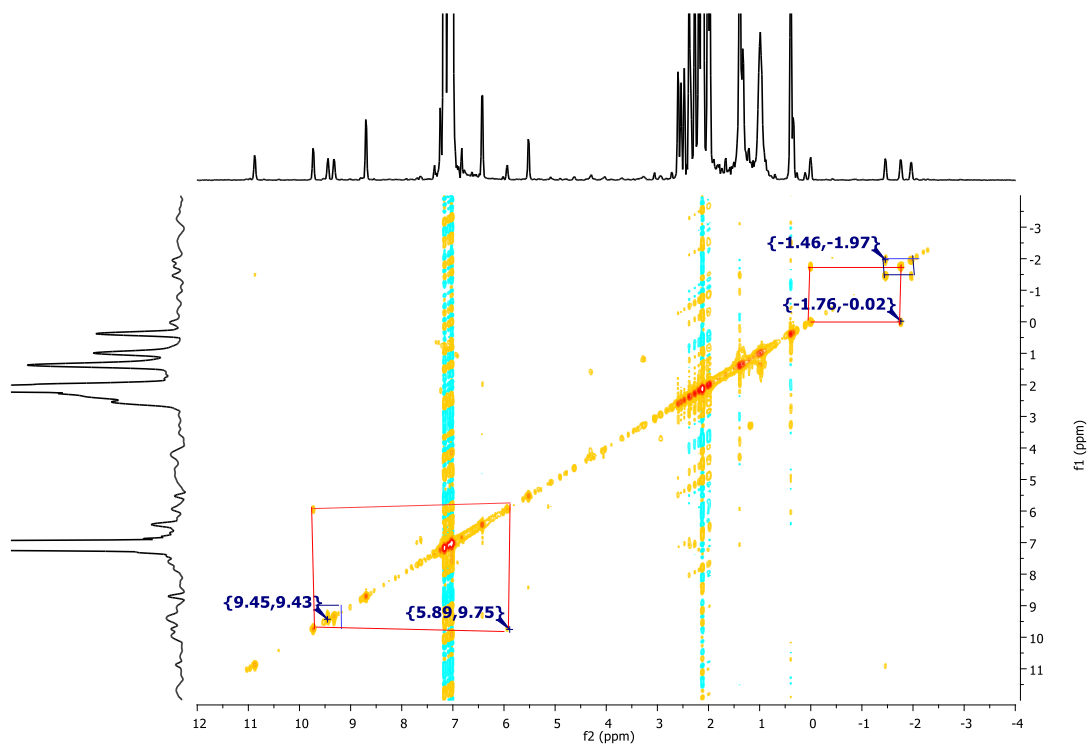
S23: High resolution mass spectrum of **5d**



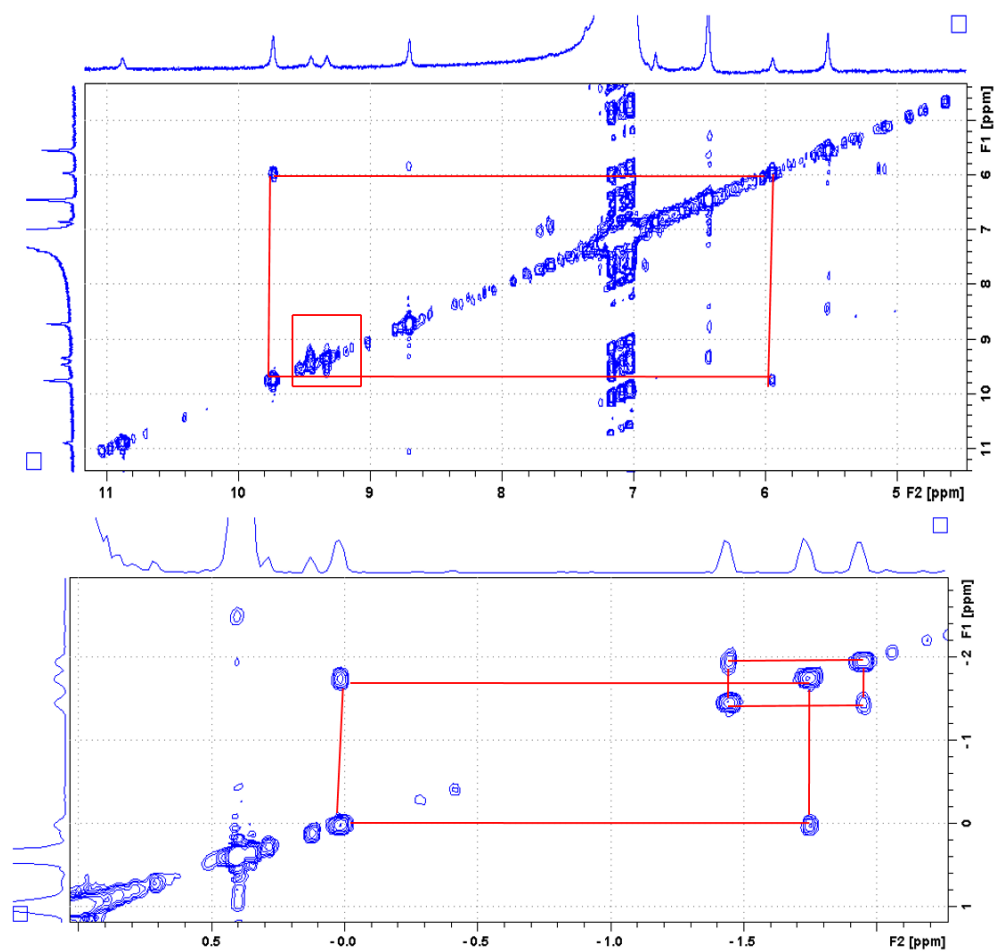
S24: Variable temperature ^1H NMR spectra of **5d** in $\text{toluene-}d_8$



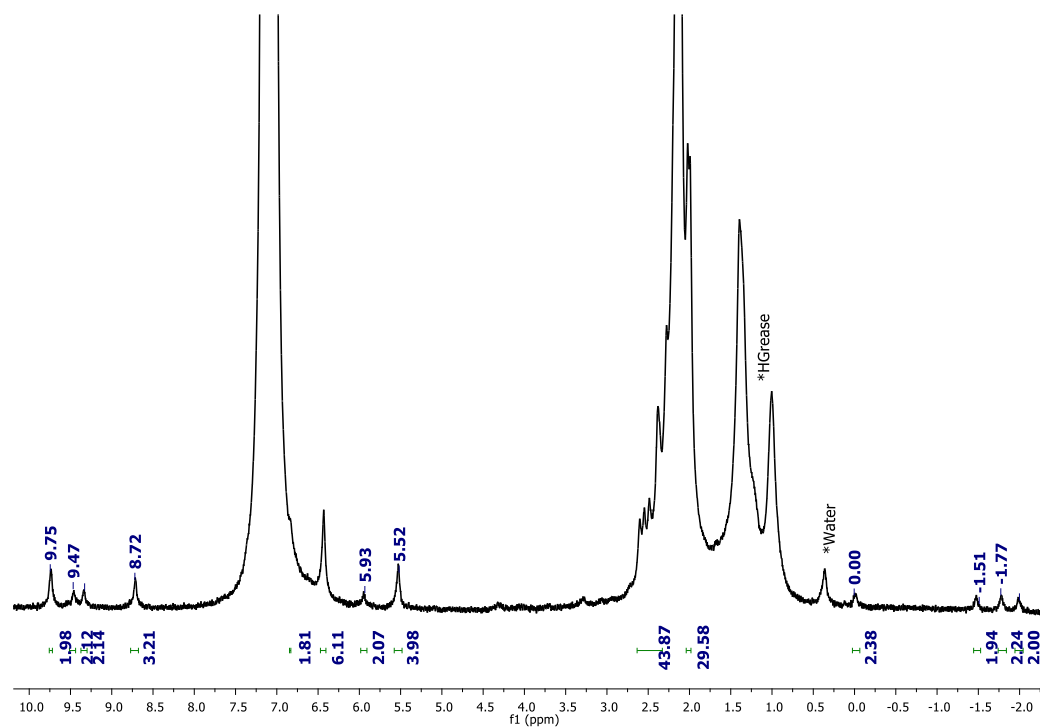
S25: ¹H NMR spectrum of **5d** at 253K in toluene-*d*₈



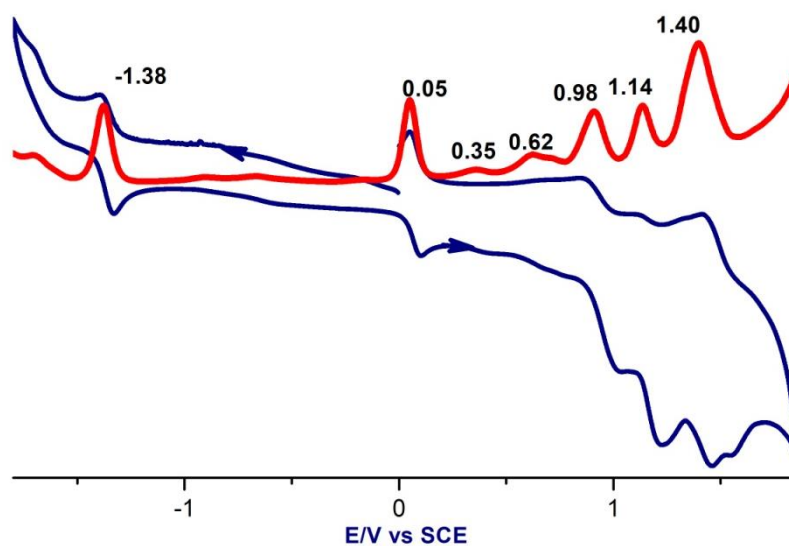
S26: ¹H-¹H COSY spectrum of **5d** at 253K in toluene-*d*₈



S27: Partial ^1H - ^1H COSY spectrum of **5d** at 253K in toluene- d_8



S28: ¹H NMR spectrum of **5d** upon addition of D₂O



S29: Cyclic (blue) and differential pulse (red) Voltamogram of **5d** in dichloromethane containing 0.1M tetra butyl ammonium perchlorate as the supporting electrolyte recorded at a scan rate of 50 Mvs⁻¹.

References

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S30: Coordinates for optimized structure **4a**.

Atomic no	X	Y	Z
16	-1.526280000	-3.401870000	0.123239000
16	-1.526457000	3.401901000	0.123468000
9	-6.067959000	1.353002000	-2.105063000
9	-6.067196000	-1.353024000	-2.106052000
9	-5.192004000	-3.921222000	1.794608000
9	-5.191553000	3.921064000	1.795440000
9	-9.604711000	2.966500000	0.515484000
7	-4.344594000	-0.000055000	-0.223951000
9	-7.840191000	4.163745000	2.209195000
9	-8.704680000	1.539566000	-1.623787000
9	-7.840795000	-4.163945000	2.207532000
9	-8.704116000	-1.539683000	-1.625647000
9	-9.604785000	-2.966687000	0.513298000
6	-5.529341000	-2.604446000	-0.158468000
6	-4.082646000	-2.400440000	-0.346573000
6	-3.599855000	-1.080756000	-0.554700000
6	-2.334104000	-0.676357000	-1.184726000
1	-1.608338000	-1.325047000	-1.651211000
6	-4.082819000	2.400383000	-0.346101000
6	-0.000076000	5.779052000	-0.000160000
6	1.252553000	5.121992000	0.135351000
6	-0.000096000	7.265630000	-0.000193000
6	-3.551826000	-4.875338000	-0.576102000
1	-4.549308000	-5.175618000	-0.871621000
6	-1.252691000	5.121959000	-0.135672000
6	-5.529458000	2.604335000	-0.157585000
6	-6.472862000	2.009804000	-1.017795000
6	-2.475296000	-5.738600000	-0.509660000
1	-2.532174000	-6.789980000	-0.757838000
6	-3.599959000	1.080804000	-0.554507000

6	-3.220604000	-3.528524000	-0.309086000
6	-6.033566000	3.347856000	0.926199000
6	-3.220796000	3.528528000	-0.308705000
6	-2.334162000	0.676644000	-1.184596000
1	-1.608451000	1.325489000	-1.650950000
6	-6.472472000	-2.009895000	-1.018962000
6	0.803647000	7.979848000	-0.910407000
1	1.406775000	7.441237000	-1.634577000
6	-0.803862000	7.979861000	0.909989000
1	-1.406976000	7.441261000	1.634179000
6	-2.475526000	5.738576000	-0.509531000
1	-2.532433000	6.789935000	-0.757799000
6	-7.397183000	3.472716000	1.162060000
6	-6.033766000	-3.348001000	0.925133000
6	-8.303586000	2.854386000	0.298089000
6	-7.839540000	2.121076000	-0.796200000
6	-7.397458000	-3.472883000	1.160559000
6	-3.552076000	4.875304000	-0.575759000
1	-4.549598000	5.175550000	-0.871178000
6	-0.000139000	10.070917000	-0.000251000
1	-0.000155000	11.156105000	-0.000273000
6	-0.793663000	9.372336000	0.913318000
1	-1.400726000	9.912492000	1.632494000
6	0.793407000	9.372322000	-0.913792000
1	1.400453000	9.912468000	-1.632990000
6	-8.303592000	-2.854546000	0.296313000
6	-7.839221000	-2.121188000	-0.797807000
16	1.526366000	3.401940000	-0.123773000
16	1.526382000	-3.401847000	-0.123019000
9	6.067707000	-1.352862000	2.105617000
9	6.067376000	1.353125000	2.105508000
9	5.191896000	3.921043000	-1.795275000
9	5.191737000	-3.921192000	-1.794811000
9	9.604749000	-2.966534000	-0.514433000
7	4.344589000	0.000054000	0.223948000
9	7.840415000	-4.163904000	-2.208248000
9	8.704482000	-1.539444000	1.624636000
9	7.840657000	4.163653000	-2.208466000
9	8.704252000	1.539654000	1.624835000
9	9.604767000	2.966470000	-0.514303000
6	5.529376000	2.604413000	0.157876000
6	4.082693000	2.400467000	0.346126000
6	3.599869000	1.080853000	0.554485000
6	2.334110000	0.676602000	1.184583000
1	1.608358000	1.325398000	1.650945000
6	4.082762000	-2.400353000	0.346524000

6	0.000071000	-5.779044000	0.000167000
6	-1.252511000	-5.121964000	-0.135629000
6	0.000090000	-7.265635000	0.000212000
6	3.551950000	4.875412000	0.575415000
1	4.549465000	5.175702000	0.870812000
6	1.252643000	-5.121933000	0.135945000
6	5.529421000	-2.604343000	0.158177000
6	6.472732000	-2.009741000	1.018440000
6	2.475399000	5.738669000	0.509088000
1	2.532300000	6.790053000	0.757246000
6	3.599924000	-1.080708000	0.554688000
6	3.220676000	3.528589000	0.308562000
6	6.033649000	-3.347937000	-0.925503000
6	3.220720000	-3.528467000	0.309202000
6	2.334129000	-0.676398000	1.184690000
1	1.608398000	-1.325139000	1.651159000
6	6.472568000	2.009901000	1.018329000
6	-0.803550000	-7.979847000	0.910517000
1	-1.406595000	-7.441234000	1.634756000
6	0.803754000	-7.979872000	-0.910053000
1	1.406783000	-7.441278000	-1.634318000
6	2.475417000	-5.738508000	0.510098000
1	2.532298000	-6.789858000	0.758403000
6	7.397293000	-3.472808000	-1.161206000
6	6.033723000	3.347866000	-0.925833000
6	8.303601000	-2.854411000	-0.297183000
6	7.839435000	-2.121022000	0.797000000
6	7.397396000	3.472687000	-1.161397000
6	3.551946000	-4.875229000	0.576437000
1	4.549432000	-5.175461000	0.871992000
6	0.000133000	-10.070924000	0.000287000
1	0.000149000	-11.156111000	0.000316000
6	0.793557000	-9.372348000	-0.913372000
1	1.400540000	-9.912509000	-1.632612000
6	-0.793312000	-9.372323000	0.913910000
1	-1.400278000	-9.912464000	1.633179000
6	8.303590000	2.854389000	-0.297186000
6	7.839299000	2.121131000	0.797036000

S31: Reaction co-ordinate for optimized geometry 4b

Atomic no	X	Y	Z
16	1.429621000	4.223477000	0.180119000
16	-2.922986000	2.035082000	-0.437213000
9	4.057430000	3.374370000	3.276229000

9	-11.006817000	3.415719000	-0.855304000
9	5.447372000	7.347827000	-0.186701000
9	4.542136000	4.988220000	-1.150319000
9	-10.076358000	1.472926000	-2.531308000
9	-7.532413000	0.596956000	-2.310448000
9	-6.824850000	3.599742000	1.289970000
9	5.659477000	7.731109000	2.507456000
9	-9.364237000	4.472523000	1.052484000
9	4.963988000	5.735307000	4.231027000
7	4.385218000	0.468652000	-0.018670000
6	0.038290000	3.447994000	-0.546053000
6	3.767226000	2.797029000	0.499775000
6	-2.441840000	3.715672000	-0.826861000
6	-8.908282000	3.522450000	0.227877000
6	2.394482000	2.762081000	0.069328000
6	0.333500000	2.116730000	-0.834150000
1	-0.370333000	1.457303000	-1.327168000
6	-7.084097000	2.068974000	-0.506672000
6	-9.272628000	1.989567000	-1.595222000
6	-1.164138000	4.230249000	-0.768049000
6	4.637619000	5.149431000	0.175665000
6	-4.642328000	2.417624000	-0.640037000
6	-4.781860000	3.783143000	-1.082365000
1	-5.750728000	4.205861000	-1.313506000
6	4.271496000	4.105998000	1.031843000
6	1.644024000	1.733894000	-0.498338000
1	2.074017000	0.757798000	-0.676340000
6	4.393200000	4.333865000	2.405955000
6	-9.749004000	2.982391000	-0.742071000
6	6.642414000	0.661347000	0.477749000
1	7.675063000	0.364272000	0.592547000
6	-7.598943000	3.060097000	0.338032000
6	-3.617956000	4.471440000	-1.179640000
1	-3.552461000	5.503070000	-1.498451000
6	5.544550000	-0.183320000	-0.007814000
6	4.668608000	1.750544000	0.436391000
6	-0.192356000	6.235880000	-1.947437000
1	0.282068000	5.558679000	-2.651018000
6	6.090201000	1.861278000	0.767952000
1	6.587433000	2.742273000	1.147438000
6	-5.687516000	1.556170000	-0.373519000
6	5.213416000	6.566042000	2.032686000
6	-0.632062000	8.486850000	-1.179654000

1	-0.495312000	9.559074000	-1.283542000
6	4.857790000	5.545882000	2.911642000
6	-0.024694000	7.612185000	-2.083722000
1	0.580951000	8.002123000	-2.896286000
6	-7.957343000	1.549912000	-1.470776000
6	-1.588087000	6.599921000	-0.007719000
1	-2.186303000	6.203621000	0.806958000
6	5.102606000	6.369781000	0.657953000
6	-0.983919000	5.710661000	-0.911565000
6	-1.410770000	7.977382000	-0.140049000
1	-1.877849000	8.650475000	0.572726000
16	-1.468611000	-4.245173000	0.086852000
16	2.932937000	-2.030649000	-0.429729000
9	-5.453985000	-4.542041000	-0.941482000
9	11.006820000	-3.424857000	-0.955813000
9	-4.033995000	-6.238249000	4.039601000
9	-3.140702000	-3.851259000	3.134807000
9	9.386048000	-4.473323000	0.975044000
9	6.850968000	-3.596718000	1.240368000
9	7.518252000	-0.607397000	-2.379222000
9	-5.635001000	-7.784265000	2.462487000
9	10.058251000	-1.486822000	-2.627303000
9	-6.341224000	-6.925188000	-0.028645000
7	-4.382261000	-0.476094000	0.022336000
6	-0.041538000	-3.424566000	-0.513691000
6	-3.766323000	-2.797747000	0.567046000
6	2.434319000	-3.701163000	-0.834903000
6	9.265390000	-1.999280000	-1.679627000
6	-2.387941000	-2.752218000	0.155745000
6	-0.299803000	-2.059948000	-0.640348000
1	0.427846000	-1.359808000	-1.029675000
6	7.090057000	-2.071967000	-0.564195000
6	8.921285000	-3.525528000	0.152861000
6	1.150345000	-4.203663000	-0.783020000
6	-3.926343000	-4.588597000	2.340609000
6	4.646085000	-2.421691000	-0.660218000
6	4.772497000	-3.786759000	-1.105701000
1	5.736297000	-4.216543000	-1.344985000
6	-4.271588000	-4.116438000	1.069531000
6	-1.602403000	-1.684312000	-0.273169000
1	-1.997502000	-0.679838000	-0.327109000
6	-5.093441000	-4.933965000	0.286712000
6	9.750924000	-2.989782000	-0.828937000

6	-6.629150000	-0.642996000	0.571828000
1	-7.655700000	-0.334362000	0.708720000
6	7.952209000	-1.557821000	-1.540897000
6	3.601411000	-4.464291000	-1.200510000
1	3.525601000	-5.493827000	-1.523765000
6	-5.535535000	0.185107000	0.049101000
6	-4.666604000	-1.750163000	0.499822000
6	1.516454000	-6.601517000	-0.083758000
1	2.086277000	-6.237879000	0.765810000
6	-6.080778000	-1.843674000	0.865551000
1	-6.573548000	-2.708564000	1.285461000
6	5.695741000	-1.558697000	-0.415755000
6	-5.196283000	-6.605929000	2.014622000
6	0.591251000	-8.438820000	-1.355063000
1	0.448894000	-9.505597000	-1.499686000
6	-5.557242000	-6.165109000	0.743818000
6	1.331417000	-7.971951000	-0.268253000
1	1.762901000	-8.673025000	0.439961000
6	7.613905000	-3.061239000	0.277363000
6	0.207047000	-6.159399000	-2.067046000
1	-0.229237000	-5.454319000	-2.767973000
6	-4.376858000	-5.816286000	2.818039000
6	0.958749000	-5.677625000	-0.982235000
6	0.030920000	-7.529058000	-2.254540000
1	-0.543535000	-7.886019000	-3.104102000

S32: Coordinates for optimized structure 4c.

Atomic no	X	Y	Z
16	1.885012000	4.425329000	0.126147000
16	-2.801046000	2.264397000	0.053400000
9	5.594752000	3.676890000	2.126443000
9	-10.804261000	4.370518000	0.019181000
9	5.545058000	7.114297000	-2.195086000
9	4.235720000	4.715345000	-2.361143000
9	-9.945657000	2.925217000	-2.176750000
9	-7.469486000	1.754136000	-2.170609000
9	-6.690647000	3.452125000	2.253356000
9	6.891855000	7.805322000	0.117777000
9	-9.164169000	4.627650000	2.229414000
9	6.914158000	6.073554000	2.273578000
7	4.572103000	0.350326000	-0.079569000

6	0.256620000	3.646587000	-0.196570000
6	4.152306000	2.823026000	-0.199266000
6	-2.235868000	4.006620000	-0.158171000
6	-8.736499000	3.911173000	1.137072000
6	2.746751000	2.850228000	-0.216270000
6	0.460058000	2.281813000	-0.499885000
1	-0.355586000	1.626462000	-0.775783000
6	-7.012602000	2.567212000	0.042915000
6	-9.131434000	3.051799000	-1.076800000
6	-0.900335000	4.448272000	-0.140587000
6	4.890519000	5.032528000	-1.191807000
6	-4.562833000	2.782151000	-0.063973000
6	-4.603748000	4.181840000	-0.250568000
1	-5.541309000	4.709682000	-0.360516000
6	4.875165000	4.130147000	-0.120021000
6	1.785459000	1.855926000	-0.514998000
1	2.058451000	0.856470000	-0.830202000
6	5.571787000	4.514345000	1.032781000
6	-9.565048000	3.781300000	0.026271000
6	6.799983000	0.319659000	-0.425755000
1	7.803986000	-0.038935000	-0.582927000
6	-7.481926000	3.307119000	1.135165000
6	-3.380280000	4.824867000	-0.293476000
1	-3.282593000	5.892186000	-0.433619000
6	5.666775000	-0.513293000	-0.174401000
6	4.974425000	1.676507000	-0.243365000
6	-0.215432000	6.669252000	-1.145117000
1	0.038730000	6.146445000	-2.061264000
6	6.384943000	1.636024000	-0.462382000
1	7.001334000	2.498332000	-0.657722000
6	-5.661773000	1.918689000	0.049550000
6	6.232530000	6.604000000	0.040809000
6	-0.373547000	8.730414000	0.124236000
1	-0.241469000	9.805535000	0.190684000
6	6.244520000	5.729852000	1.123264000
6	-0.049588000	8.055135000	-1.058825000
1	0.330784000	8.605362000	-1.913357000
6	-7.870616000	2.460933000	-1.058637000
6	-1.041276000	6.629110000	1.134718000
1	-1.425822000	6.073593000	1.983953000
6	5.551015000	6.255116000	-1.121608000
6	-0.713084000	5.941335000	-0.048147000
6	-0.867831000	8.014573000	1.220977000
1	-1.117127000	8.531935000	2.141825000
16	-1.884990000	-4.425020000	-0.127074000
16	2.800982000	-2.264353000	-0.053571000

9	-5.595884000	-3.676906000	-2.126149000
9	10.804579000	-4.369882000	-0.018167000
9	-5.543660000	-7.114756000	2.194995000
9	-4.234642000	-4.715634000	2.360726000
9	9.945432000	-2.924349000	2.177432000
9	7.469063000	-1.753767000	2.170808000
9	6.691067000	-3.452654000	-2.252979000
9	-6.891447000	-7.805728000	-0.117311000
9	9.164746000	-4.627747000	-2.228510000
9	-6.915003000	-6.073714000	-2.272912000
7	-4.572122000	-0.350415000	0.079605000
6	-0.256711000	-3.646438000	0.196236000
6	-4.152469000	-2.823064000	0.199051000
6	2.235738000	-4.006627000	0.157816000
6	8.736847000	-3.911129000	-1.136348000
6	-2.746771000	-2.850146000	0.216047000
6	-0.460119000	-2.281884000	0.500050000
1	0.355500000	-1.626660000	0.776322000
6	7.012569000	-2.567261000	-0.042650000
6	9.131383000	-3.051264000	1.077391000
6	0.900338000	-4.448248000	0.140234000
6	-4.889916000	-5.032779000	1.191643000
6	4.562793000	-2.782178000	0.063790000
6	4.603633000	-4.181993000	0.250251000
1	5.541199000	-4.709827000	0.360188000
6	-4.875182000	-4.130257000	0.119958000
6	-1.785630000	-1.855982000	0.515205000
1	-2.058666000	-0.856671000	0.830832000
6	-5.572283000	-4.514451000	-1.032568000
6	9.565263000	-3.780891000	-0.025491000
6	-6.800147000	-0.319821000	0.425169000
1	-7.804191000	0.038777000	0.582073000
6	7.482168000	-3.307300000	-1.134699000
6	3.380238000	-4.824948000	0.293066000
1	3.282485000	-5.892279000	0.433074000
6	-5.666802000	0.513248000	0.174264000
6	-4.974502000	-1.676631000	0.243061000
6	0.214745000	-6.669141000	1.144520000
1	-0.039731000	-6.146308000	2.060567000
6	-6.385177000	-1.636117000	0.461697000
1	-7.001626000	-2.498458000	0.656705000
6	5.661709000	-1.918853000	-0.049536000
6	-6.232259000	-6.604319000	-0.040522000
6	0.373112000	-8.730324000	-0.124770000
1	0.240911000	-9.805427000	-0.191271000
6	-6.244884000	-5.730046000	-1.122868000

6	0.048759000	-8.054999000	1.058161000
1	-0.332031000	-8.605177000	1.912537000
6	7.870460000	-2.460633000	1.058977000
6	1.041530000	-6.629107000	-1.134974000
1	1.426492000	-6.073639000	-1.984053000
6	-5.550247000	-6.255462000	1.121611000
6	0.712952000	-5.941283000	0.047759000
6	0.867936000	-8.014549000	-1.221306000
1	1.117537000	-8.531938000	-2.142056000
1	-3.660501000	-0.078686000	-0.250883000
1	3.660608000	0.078587000	0.251254000

33: Coordinates for optimized structure 5a.

Atomic no	X	Y	Z
6	-5.938097000	2.459248000	-0.391346000
6	-6.685238000	3.661226000	-0.379150000
1	-7.767379000	3.652097000	-0.397954000
6	-5.914655000	4.807710000	-0.378077000
1	-6.315149000	5.813005000	-0.394866000
6	-4.519555000	4.570026000	-0.389158000
6	-3.523784000	5.580078000	-0.348868000
6	-2.156867000	5.357268000	-0.643833000
6	-1.522426000	4.217307000	-1.322408000
1	-2.021212000	3.385894000	-1.798090000
6	-0.193110000	4.474787000	-1.327569000
1	0.577021000	3.888976000	-1.807331000
6	-0.026285000	5.772491000	-0.656821000
6	1.160305000	6.496899000	-0.382004000
6	2.460538000	5.937580000	-0.409680000
6	3.664056000	6.683999000	-0.375330000
1	3.655222000	7.766283000	-0.383048000
6	4.809339000	5.913419000	-0.365151000
1	5.815025000	6.313285000	-0.363667000
6	4.571633000	4.517624000	-0.390508000
6	5.581229000	3.522452000	-0.342502000
6	5.362131000	2.156172000	-0.642710000
6	4.229085000	1.522356000	-1.334761000
1	3.402134000	2.021627000	-1.817547000
6	4.487504000	0.193471000	-1.340177000
1	3.907084000	-0.576163000	-1.827155000
6	5.778914000	0.026138000	-0.656209000
6	6.500890000	-1.160287000	-0.376079000
6	5.942261000	-2.460095000	-0.411467000
6	6.688749000	-3.663842000	-0.360600000
1	7.770939000	-3.654202000	-0.348102000
6	5.919269000	-4.808811000	-0.359636000

1	6.319634000	-5.814189000	-0.345849000
6	4.522551000	-4.572457000	-0.409518000
6	3.529697000	-5.580619000	-0.371223000
6	2.158246000	-5.360380000	-0.652787000
6	1.516054000	-4.227313000	-1.336414000
1	2.009658000	-3.400059000	-1.824789000
6	0.187653000	-4.487601000	-1.328209000
1	-0.587019000	-3.908698000	-1.808852000
6	0.027857000	-5.776411000	-0.637168000
6	-1.155014000	-6.494526000	-0.338295000
6	-2.457995000	-5.936088000	-0.386765000
6	-3.659640000	-6.684888000	-0.368542000
1	-3.648469000	-7.767140000	-0.372067000
6	-4.806775000	-5.916851000	-0.381804000
1	-5.811374000	-6.319273000	-0.396098000
6	-4.571758000	-4.520361000	-0.410666000
6	-5.581832000	-3.527940000	-0.384486000
6	-5.357874000	-2.155812000	-0.659965000
6	-4.215517000	-1.512000000	-1.325215000
1	-3.381279000	-2.004239000	-1.802775000
6	-4.476414000	-0.183380000	-1.318063000
1	-3.890846000	0.592529000	-1.788417000
6	-5.775087000	-0.025673000	-0.646719000
6	-6.497673000	1.156335000	-0.355428000
6	-3.968732000	6.951450000	0.043737000
6	-4.054609000	7.968362000	-0.933827000
6	-3.686443000	7.722591000	-2.379151000
1	-2.603445000	7.610891000	-2.495740000
1	-4.003063000	8.559290000	-3.005759000
1	-4.150816000	6.814326000	-2.777544000
6	-4.522664000	9.226784000	-0.549308000
1	-4.614558000	10.001984000	-1.305762000
6	-4.876874000	9.517809000	0.771638000
6	-5.342297000	10.897081000	1.166483000
1	-4.498400000	11.511161000	1.503899000
1	-6.062351000	10.857320000	1.988641000
1	-5.809574000	11.418700000	0.327009000
6	-4.763101000	8.498250000	1.722439000
1	-5.021462000	8.707436000	2.757467000
6	-4.324895000	7.216098000	1.386827000
6	-4.189072000	6.168928000	2.470185000
1	-3.190258000	5.720172000	2.468292000
1	-4.912620000	5.354261000	2.354847000
1	-4.352832000	6.612735000	3.454573000
6	1.053758000	7.947088000	-0.026835000
6	0.850876000	8.900763000	-1.048309000

6	0.727656000	8.497494000	-2.500218000
1	0.637734000	9.378160000	-3.139801000
1	-0.154310000	7.871147000	-2.670454000
1	1.597848000	7.926892000	-2.844212000
6	0.792289000	10.251775000	-0.698129000
1	0.651270000	10.988789000	-1.484751000
6	0.907697000	10.681947000	0.627385000
6	0.864992000	12.149579000	0.974362000
1	1.872802000	12.582501000	0.970186000
1	0.446594000	12.313230000	1.971288000
1	0.266631000	12.714687000	0.254537000
6	1.085363000	9.712937000	1.619890000
1	1.154720000	10.024276000	2.659125000
6	1.170693000	8.351364000	1.321082000
6	1.320620000	7.344984000	2.439217000
1	0.493698000	6.626655000	2.435276000
1	1.324875000	7.844608000	3.410366000
1	2.251082000	6.771840000	2.360126000
6	6.948515000	3.965956000	0.067087000
6	7.199568000	4.310580000	1.415269000
6	6.141209000	4.165362000	2.486473000
1	5.325075000	4.886347000	2.365536000
1	6.573398000	4.326101000	3.476514000
1	5.696276000	3.164868000	2.474759000
6	8.480411000	4.739802000	1.768968000
1	8.680762000	4.983001000	2.809321000
6	9.509761000	4.859584000	0.830137000
6	10.871064000	5.371856000	1.229526000
1	11.661719000	4.921951000	0.622642000
1	11.085380000	5.163531000	2.281143000
1	10.935538000	6.458277000	1.092567000
6	9.233865000	4.509877000	-0.495643000
1	10.020930000	4.594469000	-1.240755000
6	7.977781000	4.051674000	-0.897787000
6	7.749968000	3.682881000	-2.345859000
1	8.588378000	4.010691000	-2.964420000
1	6.839618000	4.136234000	-2.751860000
1	7.652894000	2.598590000	-2.464591000
6	7.946993000	-1.052840000	-0.003299000
6	8.334036000	-1.161701000	1.350230000
6	7.313147000	-1.305519000	2.455875000
1	6.601411000	-0.472927000	2.444112000
1	7.800735000	-1.314984000	3.433110000
1	6.733669000	-2.231306000	2.368280000
6	9.691756000	-1.075560000	1.665684000
1	9.989992000	-1.139462000	2.709114000

6	10.673304000	-0.904062000	0.684408000
6	12.136368000	-0.859970000	1.050179000
1	12.714057000	-0.281114000	0.324509000
1	12.564239000	-1.869606000	1.075832000
1	12.288455000	-0.418893000	2.039180000
6	10.260050000	-0.796853000	-0.647034000
1	11.006956000	-0.661374000	-1.425239000
6	8.913385000	-0.857406000	-1.013813000
6	8.528203000	-0.744183000	-2.471477000
1	7.962114000	-1.616981000	-2.816435000
1	9.416686000	-0.658598000	-3.100797000
1	7.903688000	0.136334000	-2.655909000
6	3.976198000	-6.957564000	0.009732000
6	4.242015000	-7.260422000	1.363404000
6	4.005957000	-6.249239000	2.462334000
1	4.647823000	-5.367184000	2.360923000
1	4.206226000	-6.689652000	3.441465000
1	2.968039000	-5.898992000	2.458365000
6	4.676864000	-8.547403000	1.687453000
1	4.862927000	-8.787860000	2.731137000
6	4.872987000	-9.532490000	0.714463000
6	5.387801000	-10.900714000	1.087209000
1	5.041568000	-11.663964000	0.385010000
1	5.067664000	-11.189299000	2.092154000
1	6.484406000	-10.922492000	1.076769000
6	4.598655000	-9.204883000	-0.617036000
1	4.743237000	-9.956719000	-1.388831000
6	4.143006000	-7.938810000	-0.991961000
6	3.870755000	-7.642854000	-2.449361000
1	4.136270000	-8.498704000	-3.073672000
1	4.443872000	-6.780743000	-2.808721000
1	2.812779000	-7.419833000	-2.623164000
6	-1.050856000	-7.929694000	0.066965000
6	-0.757592000	-8.913385000	-0.904339000
6	-0.521113000	-8.559231000	-2.354772000
1	-1.299538000	-7.900228000	-2.753736000
1	-0.499466000	-9.458998000	-2.973525000
1	0.436605000	-8.044126000	-2.483450000
6	-0.706526000	-10.250793000	-0.506508000
1	-0.499826000	-11.010146000	-1.256477000
6	-0.910245000	-10.640865000	0.821078000
6	-0.870911000	-12.095803000	1.217083000
1	-0.575239000	-12.218742000	2.262426000
1	-0.172883000	-12.662198000	0.594374000
1	-1.858316000	-12.559283000	1.101124000
6	-1.173171000	-9.644020000	1.765766000

1	-1.310123000	-9.923445000	2.807291000
6	-1.259806000	-8.294689000	1.416623000
6	-1.508008000	-7.261087000	2.492764000
1	-0.738055000	-6.482487000	2.481784000
1	-1.497881000	-7.726188000	3.480913000
1	-2.476957000	-6.763025000	2.375931000
6	-6.963365000	-3.977106000	-0.027012000
6	-7.935127000	-4.120873000	-1.042158000
6	-7.625034000	-3.818631000	-2.490689000
1	-7.419389000	-2.753780000	-2.642330000
1	-8.468164000	-4.087917000	-3.130508000
1	-6.748398000	-4.369891000	-2.848684000
6	-9.205557000	-4.581362000	-0.689804000
1	-9.949478000	-4.709129000	-1.472170000
6	-9.548109000	-4.880834000	0.632761000
6	-10.921808000	-5.398712000	0.979869000
1	-10.954614000	-6.493328000	0.917780000
1	-11.680437000	-5.012676000	0.293447000
1	-11.208795000	-5.122912000	1.998253000
6	-8.573179000	-4.706019000	1.619800000
1	-8.825661000	-4.911171000	2.657099000
6	-7.281555000	-4.268920000	1.318182000
6	-6.282491000	-4.057351000	2.433304000
1	-5.915235000	-3.025442000	2.443771000
1	-5.409656000	-4.712707000	2.339232000
1	-6.740144000	-4.258688000	3.404289000
6	-7.939414000	1.050963000	0.026469000
6	-8.908549000	0.782487000	-0.965766000
6	-10.253387000	0.737962000	-0.591165000
1	-11.002343000	0.557228000	-1.357830000
6	-10.663056000	0.919719000	0.733607000
6	-9.680823000	1.166179000	1.697572000
1	-9.977239000	1.299011000	2.735054000
6	-8.324902000	1.245228000	1.372508000
6	-8.532299000	0.576241000	-2.415320000
1	-9.424055000	0.543595000	-3.044988000
1	-7.993117000	-0.366733000	-2.553763000
1	-7.887378000	1.376322000	-2.794569000
6	-12.119401000	0.825123000	1.115194000
1	-12.770266000	1.136261000	0.293604000
1	-12.347336000	1.445187000	1.986499000
1	-12.388628000	-0.206978000	1.370864000
6	-7.307482000	1.476547000	2.467364000
1	-7.789863000	1.472270000	3.447220000
1	-6.791913000	2.437463000	2.360664000
1	-6.541228000	0.694140000	2.468545000

7	-1.229009000	6.284846000	-0.298635000
7	6.286567000	1.228381000	-0.290473000
7	1.236326000	-6.283572000	-0.286346000
7	-6.287079000	-1.234990000	-0.305416000
16	-4.216192000	2.834229000	-0.369557000
16	2.835590000	4.214285000	-0.396229000
16	4.219089000	-2.835147000	-0.425591000
16	-2.834849000	-4.214660000	-0.388953000

34: Coordinates for optimized structure **5b**.

Atomic no	X	Y	Z
16	-4.650902000	-0.366161000	-0.582201000
16	4.650199000	-0.363929000	0.585478000
16	1.803069000	0.265840000	-2.146038000
16	-1.804258000	0.266223000	2.149199000
7	2.488322000	-1.846192000	2.261354000
7	-4.067509000	1.922840000	1.306059000
7	-2.488517000	-1.849086000	-2.255779000
6	-0.157278000	-0.369242000	2.328468000
6	-3.450795000	2.950686000	1.886816000
7	4.065767000	1.923357000	-1.303403000
6	-5.441919000	-1.690155000	-1.437404000
6	-6.197637000	0.223625000	0.034715000
6	-2.011592000	3.045742000	2.018426000
6	-4.804373000	-2.705144000	-2.236130000
6	-1.202529000	1.927760000	1.995366000
6	6.196750000	0.225414000	-0.032488000
6	-1.549424000	5.407845000	1.257101000
6	-8.501124000	1.367983000	2.253834000
6	-1.066588000	6.694504000	1.521551000
6	1.352582000	-2.304799000	2.802396000
6	-0.055651000	-1.668888000	-2.748208000
6	0.055096000	-1.667709000	2.752693000
6	-5.422231000	2.195943000	1.387925000
6	-5.979402000	-4.930886000	-1.977697000
6	-0.806343000	0.677258000	-2.084598000
6	1.851016000	-3.344033000	-2.534670000
6	5.713901000	-3.785819000	2.763876000
6	4.804419000	-2.701670000	2.241217000
6	1.200452000	1.926967000	-1.990440000
6	0.156284000	-0.370611000	-2.323323000
6	7.240116000	-0.589916000	0.419711000
6	4.403054000	3.948432000	-2.373862000
6	0.482272000	7.031863000	-2.735353000

6	-5.639292000	3.464990000	2.079101000
6	-7.793732000	0.518596000	3.285755000
6	2.009027000	3.045209000	-2.015008000
6	-4.405609000	3.950839000	2.370908000
6	-6.824890000	-1.652078000	-1.218267000
6	-5.713469000	-3.788608000	-2.760877000
6	0.848867000	4.735086000	-3.496074000
6	-7.240641000	-0.593080000	-0.415757000
6	-10.527258000	2.537885000	1.541120000
6	-1.850295000	-3.344101000	2.536954000
6	-6.411410000	1.398069000	0.837832000
6	-2.882530000	-3.871157000	-3.364037000
6	3.463922000	-2.774469000	2.587235000
6	1.552439000	5.407181000	-1.252817000
6	-1.436237000	4.409853000	2.251098000
6	2.196545000	5.127804000	0.086509000
6	5.979778000	-4.927493000	1.976693000
6	-7.151503000	-4.665770000	-4.500101000
6	1.115597000	-2.430934000	-3.316602000
6	5.637032000	3.462403000	-2.083416000
6	-0.857703000	4.734554000	3.503671000
6	5.420507000	2.195285000	-1.388683000
6	0.804993000	0.679455000	2.092245000
6	0.239343000	1.911317000	1.959539000
6	1.434843000	4.409988000	-2.246235000
6	-0.479925000	7.029636000	2.743394000
6	-3.463815000	-2.777594000	-2.581979000
6	7.146193000	-4.673056000	4.502473000
6	1.566314000	-3.584641000	3.494573000
6	7.422400000	-5.810670000	3.742408000
6	1.070122000	6.695122000	-1.515315000
6	8.496766000	1.354422000	-2.258001000
6	-8.525476000	2.592250000	0.137631000
6	-9.831540000	1.748725000	2.460440000
6	-7.844540000	1.792746000	1.079980000
6	-0.241334000	1.909403000	-1.951825000
6	-1.352771000	-2.306806000	-2.797484000
6	6.410066000	1.397799000	-0.838685000
6	7.842971000	1.789842000	-1.086520000
6	-1.116107000	-2.430801000	3.319778000
6	-1.566083000	-3.586350000	-3.490295000
6	0.694688000	-1.271323000	-5.550318000
6	-0.390454000	6.033958000	3.720847000
6	-2.194317000	5.130214000	-0.082192000
6	-6.038807000	-2.441874000	-4.898756000
6	3.301949000	-3.827300000	-4.442569000

6	3.448587000	2.950050000	-1.885607000
6	6.824753000	-1.647702000	1.223984000
6	5.441707000	-1.686428000	1.442549000
6	-3.302539000	-3.828881000	4.443472000
6	-9.853287000	2.952280000	0.389012000
6	2.882906000	-3.868798000	3.368495000
6	0.381661000	6.034241000	-3.710657000
6	6.301665000	-3.656778000	4.038377000
6	8.529517000	2.588724000	-0.147702000
6	2.931053000	-4.022255000	-3.111200000
6	6.031308000	-2.450809000	4.909454000
6	-11.972514000	2.911017000	1.772556000
6	6.825994000	-5.918184000	2.481604000
6	7.786449000	0.496993000	-3.281167000
6	5.350278000	-5.100613000	0.613272000
6	8.340276000	-6.894762000	4.256410000
6	0.748927000	3.729775000	-4.623012000
6	-6.305384000	-3.653720000	-4.034754000
6	10.528541000	2.520053000	-1.554412000
6	-0.006005000	8.434480000	-3.011994000
6	7.850882000	3.072427000	1.113423000
6	0.054587000	8.418969000	3.000280000
6	-1.471096000	-2.226648000	4.673699000
6	-1.483424000	-3.605590000	1.097507000
6	-4.491744000	-4.547692000	5.035219000
6	-2.930410000	-4.023169000	3.112364000
6	-5.351905000	-5.108375000	-0.613900000
6	-2.552837000	-2.931120000	5.208723000
6	2.551053000	-2.929770000	-5.206899000
6	1.485454000	-3.606226000	-1.095014000
6	-7.840426000	3.073893000	-1.120807000
6	1.469312000	-2.226139000	-4.670736000
6	-7.424773000	-5.808809000	-3.743987000
6	-6.829250000	-5.919655000	-2.484943000
6	11.956273000	2.935993000	-1.819452000
6	4.491135000	-4.545180000	-5.035489000
6	-8.315219000	-6.903173000	-4.283540000
6	-0.769440000	3.730750000	4.632894000
6	9.829480000	1.725822000	-2.466759000
6	-0.697837000	-1.271609000	5.554244000
6	9.859452000	2.939316000	-0.401216000
1	-1.156687000	7.453774000	0.748338000
1	-1.866958000	0.465213000	-2.081245000
1	8.273482000	-0.401020000	0.158961000
1	-6.600714000	3.913374000	2.286679000
1	-8.479104000	0.231009000	4.087229000

1	-7.385011000	-0.396172000	2.843844000
1	-6.951327000	1.053727000	3.736240000
1	-4.151504000	4.871119000	2.878448000
1	-7.498026000	-2.382956000	-1.646291000
1	-8.274023000	-0.404179000	-0.155118000
1	-3.420328000	-4.726393000	-3.747353000
1	2.045190000	4.092994000	0.400247000
1	3.280373000	5.290249000	0.044880000
1	1.786653000	5.785846000	0.856921000
1	-7.609081000	-4.555359000	-5.480814000
1	1.865754000	0.468122000	2.090569000
1	0.801538000	2.829623000	1.842436000
1	7.597915000	-4.569121000	5.486399000
1	0.804716000	-4.156399000	4.005279000
1	1.160026000	7.453130000	-0.740913000
1	-10.334717000	1.420002000	3.367135000
1	-0.804048000	2.827159000	-1.832889000
1	-0.804365000	-4.157487000	-4.001516000
1	1.070579000	-1.299572000	-6.576587000
1	-0.372253000	-1.517223000	-5.573709000
1	0.776436000	-0.240057000	-5.190372000
1	0.041787000	6.278527000	4.688844000
1	-1.789567000	5.793052000	-0.851085000
1	-2.037953000	4.097146000	-0.399387000
1	-3.278954000	5.286359000	-0.037971000
1	-4.985352000	-2.385172000	-5.192807000
1	-6.642181000	-2.473340000	-5.809804000
1	-6.269934000	-1.511200000	-4.370386000
1	-10.372690000	3.575232000	-0.335929000
1	3.420991000	-4.724033000	3.751435000
1	-0.061065000	6.277568000	-4.674307000
1	3.493205000	-4.724038000	-2.498966000
1	6.637437000	-2.483902000	5.818619000
1	6.256372000	-1.516342000	4.385227000
1	4.978447000	-2.400787000	5.206954000
1	-12.206171000	2.964493000	2.840044000
1	-12.212704000	3.879464000	1.323494000
1	-12.649728000	2.170692000	1.328296000
1	7.023005000	-6.797866000	1.872279000
1	7.377138000	-0.413448000	-2.830976000
1	6.944035000	1.029720000	-3.734489000
1	8.469836000	0.201865000	-4.081603000
1	5.578949000	-4.258165000	-0.047458000
1	5.707020000	-6.016051000	0.134044000
1	4.258672000	-5.158543000	0.685089000
1	8.672069000	-6.686728000	5.277196000

1	7.843150000	-7.871339000	4.257775000
1	9.233809000	-6.991664000	3.628575000
1	0.539071000	4.236471000	-5.568873000
1	1.675996000	3.160684000	-4.738166000
1	-0.050368000	3.000247000	-4.453271000
1	-1.012675000	8.431277000	-3.443595000
1	-0.031774000	9.036713000	-2.099529000
1	0.647431000	8.948397000	-3.727565000
1	8.527986000	3.692301000	1.706747000
1	6.959425000	3.665865000	0.884824000
1	7.521701000	2.235823000	1.738853000
1	-0.414677000	9.156298000	2.342420000
1	-0.119081000	8.729439000	4.035449000
1	1.137077000	8.467684000	2.827415000
1	-0.444868000	-3.938562000	1.015140000
1	-2.121267000	-4.383497000	0.669097000
1	-1.588261000	-2.710017000	0.476410000
1	-4.334609000	-4.779097000	6.093433000
1	-5.398572000	-3.933265000	4.969777000
1	-4.695989000	-5.485272000	4.509588000
1	-3.491629000	-4.725078000	2.499419000
1	-4.260467000	-5.170720000	-0.685031000
1	-5.577622000	-4.266110000	0.048053000
1	-5.712479000	-6.023197000	-0.136353000
1	2.813039000	-2.771101000	-6.250882000
1	0.446977000	-3.939242000	-1.011854000
1	2.123673000	-4.384379000	-0.667612000
1	1.590816000	-2.710940000	-0.473564000
1	-8.514860000	3.691863000	-1.719137000
1	-6.950504000	3.668464000	-0.889067000
1	-7.507503000	2.235989000	-1.742460000
1	-7.029948000	-6.798955000	-1.876715000
1	12.518018000	3.057105000	-0.888280000
1	12.479139000	2.200616000	-2.438153000
1	11.997867000	3.895496000	-2.350192000
1	4.695380000	-5.483607000	-4.511362000
1	4.333984000	-4.774879000	-6.094064000
1	5.397986000	-3.930887000	-4.969049000
1	-9.090637000	-6.500272000	-4.942165000
1	-7.738984000	-7.630885000	-4.868663000
1	-8.807777000	-7.453521000	-3.476418000
1	-0.563195000	4.238015000	5.579251000
1	-1.699447000	3.165519000	4.743313000
1	0.028003000	2.997790000	4.469078000
1	10.332826000	1.383047000	-3.368124000
1	0.369286000	-1.516648000	5.578270000

1	-0.780183000	-0.240238000	5.194728000
1	-1.074418000	-1.300628000	6.580237000
1	10.385465000	3.555949000	0.324358000
1	7.498190000	-2.377380000	1.653545000
1	6.598341000	3.909545000	-2.294130000
1	4.148550000	4.867556000	-2.883275000
1	-2.815801000	-2.772949000	6.252534000

35: Coordinates for optimized structure 5d.

Atomic no	X	Y	Z
16	-5.486628000	1.844760000	0.080268000
16	-3.629477000	-4.592561000	-0.249157000
7	-6.832903000	-0.996508000	0.230701000
1	-6.027118000	-0.611897000	-0.239891000
7	-1.505431000	4.313479000	-0.155809000
1	-1.513068000	5.322724000	-0.190692000
6	-2.147860000	-3.643840000	0.049744000
6	-5.161662000	3.564583000	-0.293603000
6	-8.019329000	-0.299933000	0.422644000
6	-3.926726000	4.166304000	-0.372159000
6	-0.913907000	-4.231112000	-0.105598000
6	-2.522869000	-2.322636000	0.486997000
1	-1.784352000	-1.594851000	0.798551000
6	-7.264729000	2.076474000	0.022394000
6	-12.367335000	2.369494000	0.353437000
6	-0.893452000	-6.658409000	0.614539000
6	-9.663563000	1.556960000	0.271171000
6	-3.898424000	5.653994000	-0.623750000
6	-10.467470000	1.454726000	-0.883937000
6	-7.035674000	-2.356172000	0.408154000
6	-0.851308000	-5.702385000	-0.424101000
6	-6.426089000	4.238606000	-0.439402000
1	-6.464219000	5.296090000	-0.668012000
6	-2.640721000	3.530661000	-0.221155000
6	-11.803100000	1.864768000	-0.821415000
1	-12.418332000	1.784847000	-1.715081000
6	-6.056891000	-3.397050000	0.215793000
6	-0.362645000	3.558277000	-0.012602000
6	-7.527305000	3.461899000	-0.263947000
1	-8.543309000	3.827928000	-0.338889000
6	-3.866740000	-2.101515000	0.561175000
1	-4.290388000	-1.181621000	0.947512000
6	-6.624997000	-4.775390000	0.011024000
6	-10.212832000	2.061936000	1.468484000

6	-6.715304000	-5.670789000	1.098134000
6	-0.659975000	-7.493280000	-2.043987000
1	-0.577926000	-7.814575000	-3.080086000
6	-4.689568000	-3.229700000	0.199062000
6	-0.793057000	2.219405000	0.017648000
1	-0.158451000	1.358728000	0.167256000
6	-3.750675000	6.142222000	-1.940822000
6	-11.555489000	2.455546000	1.487274000
1	-11.976777000	2.837160000	2.414894000
6	-8.224003000	1.110734000	0.234448000
6	-2.191658000	2.201162000	-0.111807000
1	-2.813118000	1.318702000	-0.135355000
6	-4.000268000	6.559266000	0.454849000
6	-0.730972000	-6.125385000	-1.766760000
6	-0.693520000	-8.455857000	-1.030668000
6	-7.267563000	-6.938733000	0.888580000
1	-7.343216000	-7.622950000	1.731009000
6	-0.812702000	-8.017310000	0.289983000
1	-0.848092000	-8.750286000	1.092919000
6	-7.091766000	-5.164752000	-1.263015000
6	-9.378161000	2.180653000	2.723617000
1	-8.878031000	1.236993000	2.962966000
1	-9.998801000	2.464783000	3.577617000
1	-8.592327000	2.935833000	2.612162000
6	-7.629077000	-6.444470000	-1.428106000
1	-7.984700000	-6.740890000	-2.412625000
6	-8.984132000	-1.254013000	0.784220000
1	-10.009801000	-1.024764000	1.031036000
6	-9.908878000	0.911257000	-2.179045000
1	-10.646474000	0.982974000	-2.982689000
1	-9.621353000	-0.140907000	-2.076748000
1	-9.012140000	1.457256000	-2.489336000
6	-8.382631000	-2.515756000	0.767179000
1	-8.845680000	-3.462632000	1.001414000
6	-7.724472000	-7.348317000	-0.366417000
6	-13.804873000	2.832330000	0.388577000
1	-14.235807000	2.724820000	1.388488000
1	-14.425637000	2.264782000	-0.311306000
1	-13.888495000	3.890790000	0.111193000
6	-6.232577000	-5.281477000	2.476725000
1	-6.657946000	-4.325727000	2.798408000
1	-5.142630000	-5.170706000	2.498483000
1	-6.506972000	-6.041791000	3.212918000
6	-3.805694000	8.437145000	-1.099571000
6	-0.698342000	-5.122210000	-2.896490000
1	-0.595518000	-5.625343000	-3.861504000

1	0.135044000	-4.419651000	-2.788934000
1	-1.615953000	-4.524834000	-2.921200000
6	-3.710806000	7.523789000	-2.153562000
1	-3.604014000	7.894857000	-3.170573000
6	-3.953213000	7.933810000	0.195234000
1	-4.033661000	8.627387000	1.029392000
6	-7.020705000	-4.220310000	-2.440575000
1	-7.345443000	-4.716943000	-3.358711000
1	-6.001797000	-3.851191000	-2.596313000
1	-7.660291000	-3.344077000	-2.286098000
6	-3.653027000	5.195269000	-3.114871000
1	-3.526392000	5.745846000	-4.050628000
1	-4.551870000	4.575941000	-3.203247000
1	-2.807431000	4.507613000	-3.007947000
6	-1.045014000	-6.238396000	2.058904000
1	-0.928165000	-7.095543000	2.727194000
1	-2.033954000	-5.802378000	2.238126000
1	-0.306883000	-5.482096000	2.343836000
6	-8.282689000	-8.735999000	-0.576578000
1	-8.721051000	-9.135029000	0.343035000
1	-7.498111000	-9.434896000	-0.892990000
1	-9.054685000	-8.744338000	-1.352178000
6	-4.174682000	6.068217000	1.874235000
1	-5.147284000	5.582999000	2.010751000
1	-4.108229000	6.897533000	2.583169000
1	-3.413458000	5.328930000	2.142287000
6	-0.574921000	-9.926313000	-1.354559000
1	-1.026300000	-10.160529000	-2.323421000
1	-1.062414000	-10.544592000	-0.595020000
1	0.476473000	-10.237033000	-1.403155000
6	-3.720099000	9.924069000	-1.350559000
1	-2.679280000	10.270054000	-1.319450000
1	-4.273333000	10.490509000	-0.595537000
1	-4.120072000	10.188415000	-2.334062000
16	5.486583000	-1.844872000	-0.079312000
16	3.629558000	4.592676000	0.247686000
7	6.832892000	0.996320000	-0.230637000
1	6.027068000	0.611919000	0.240059000
7	1.505388000	-4.313436000	0.156066000
1	1.513027000	-5.322689000	0.190706000
6	2.147877000	3.643811000	-0.050450000
6	5.161542000	-3.564562000	0.295113000
6	8.019339000	0.299658000	-0.422144000
6	3.926587000	-4.166259000	0.373499000
6	0.913964000	4.231173000	0.104915000
6	2.522801000	2.322401000	-0.487142000

1	1.784233000	1.594464000	-0.798219000
6	7.264670000	-2.076567000	-0.020979000
6	12.367325000	-2.369772000	-0.351030000
6	0.893419000	6.658153000	-0.616277000
6	9.663548000	-1.557176000	-0.269570000
6	3.898190000	-5.653902000	0.625330000
6	10.467257000	-1.454473000	0.885638000
6	7.035665000	2.355900000	-0.408732000
6	0.851504000	5.702590000	0.422794000
6	6.425938000	-4.238521000	0.441494000
1	6.464016000	-5.295911000	0.670548000
6	2.640634000	-3.530610000	0.222048000
6	11.802890000	-1.864556000	0.823519000
1	12.417966000	-1.784280000	1.717261000
6	6.056892000	3.396882000	-0.216905000
6	0.362649000	-3.558219000	0.012582000
6	7.527189000	-3.461877000	0.265986000
1	8.543178000	-3.827867000	0.341314000
6	3.866662000	2.101228000	-0.561431000
1	4.290225000	1.181140000	-0.947396000
6	6.625033000	4.775323000	-0.012898000
6	10.213017000	-2.062652000	-1.466576000
6	6.715254000	5.670159000	-1.100484000
6	0.660639000	7.494201000	2.041944000
1	0.578865000	7.815955000	3.077922000
6	4.689562000	3.229567000	-0.199974000
6	0.793041000	-2.219334000	-0.017187000
1	0.158467000	-1.358640000	-0.166840000
6	3.749777000	-6.141916000	1.942408000
6	11.555678000	-2.456284000	-1.484969000
1	11.977123000	-2.838290000	-2.412356000
6	8.223986000	-1.110923000	-0.233281000
6	2.191594000	-2.201096000	0.112845000
1	2.813033000	-1.318634000	0.136915000
6	4.000583000	-6.559352000	-0.453070000
6	0.731528000	6.126182000	1.765299000
6	0.693952000	8.456330000	1.028191000
6	7.267583000	6.938186000	-0.891647000
1	7.343175000	7.621966000	-1.734437000
6	0.812802000	8.017202000	-0.292295000
1	0.848026000	8.749826000	-1.095558000
6	7.091951000	5.165328000	1.260886000
6	9.378568000	-2.181872000	-2.721809000
1	8.878612000	-1.238260000	-2.961715000
1	9.999334000	-2.466498000	-3.575551000
1	8.592610000	-2.936889000	-2.610137000

6	7.629334000	6.445111000	1.425256000
1	7.985078000	6.742027000	2.409581000
6	8.984166000	1.253567000	-0.784102000
1	10.009856000	1.024208000	-1.030728000
6	9.908441000	-0.910462000	2.180422000
1	10.645874000	-0.981900000	2.984240000
1	9.620993000	0.141677000	2.077652000
1	9.011612000	-1.456289000	2.490751000
6	8.382668000	2.515317000	-0.767676000
1	8.845740000	3.462086000	-1.002298000
6	7.724649000	7.348401000	0.363091000
6	13.804863000	-2.832643000	-0.385701000
1	14.235722000	-2.726388000	-1.385777000
1	14.425678000	-2.264210000	0.313423000
1	13.888514000	-3.890747000	-0.106977000
6	6.232383000	5.280139000	-2.478824000
1	6.657750000	4.324239000	-2.800064000
1	5.142437000	5.169320000	-2.500407000
1	6.506674000	6.040087000	-3.215432000
6	3.805298000	-8.436978000	1.101565000
6	0.699148000	5.123502000	2.895474000
1	0.596579000	5.627059000	3.860295000
1	-0.134290000	4.420927000	2.788428000
1	1.616744000	4.526106000	2.920216000
6	3.709850000	-7.523448000	2.155356000
1	3.602570000	-7.894354000	3.172375000
6	3.953432000	-7.933855000	-0.193250000
1	4.034290000	-8.627568000	-1.027255000
6	7.021020000	4.221490000	2.438939000
1	7.345695000	4.718643000	3.356815000
1	6.002167000	3.852306000	2.594871000
1	7.660730000	3.345267000	2.284910000
6	3.651470000	-5.194771000	3.116248000
1	3.524953000	-5.745218000	4.052098000
1	4.549973000	-4.574958000	3.204639000
1	2.805534000	-4.507572000	3.009048000
6	1.044564000	6.237492000	-2.060495000
1	0.927932000	7.094413000	-2.729111000
1	2.033290000	5.800999000	-2.239720000
1	0.306069000	5.481375000	-2.344982000
6	8.282940000	8.736174000	0.572457000
1	8.721792000	9.134446000	-0.347253000
1	7.498297000	9.435417000	0.887946000
1	9.054565000	8.745010000	1.348418000
6	4.175644000	-6.068546000	-1.872461000
1	5.148422000	-5.583599000	-2.008695000

1	4.109240000	-6.897947000	-2.581303000
1	3.414712000	-5.329101000	-2.140895000
6	0.575466000	9.926928000	1.351471000
1	1.027326000	10.161605000	2.319999000
1	1.062549000	10.544880000	0.591405000
1	-0.475918000	10.237626000	1.400465000
6	3.719652000	-9.923864000	1.352765000
1	2.678873000	-10.269923000	1.321140000
1	4.273338000	-10.490403000	0.598148000
1	4.119100000	-10.188011000	2.336534000