Supporting Information for

BNB-Doped Phenalenyls – Aromaticity Switch upon One-Electron Reduction

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Content

1 Experimental Section

General procedures. All manipulations before the aqueous work-up were performed under an atmosphere of dry argon using standard Schlenk techniques or in an MBraun glovebox. Solvents (dichloromethane, *n*-pentane, *n*-hexane, toluene, THF, and diethylether) were dried and degassed by means of an MBraun SPS-800 solvent purification system. $CDCl_3$ and C_6D_6 for NMR spectroscopy were dried and degassed at reflux over CaH_2 or Na, respectively, and freshly distilled prior to use. *n*-Butyllithium solutions (1.6 M and 2.5 M in hexanes), trichloroborane, 1-bromonaphthalene, 2,4,6-trimethylphenyl bromide, 2,4,6-triisopropylphenyl bromide and 1,3,5-tris(trifluoromethyl)benzene were commercially purchased and used as received. Triethylamine and diisopropylamine were dried and degassed at reflux over Na and freshly distilled prior to use. Trimethylsilyl chloride and TMEDA were purified by inert-gas distillation. Dichloro(diisopropylamino)borane,[1] 1,8-dilithio-naphthalene,[2] naphtho[1,8-*cd*]-*N*-isopropyl-*B,B'*-dichloro-[1,2,6]-azadiborinine,[3] 2,4,6-trimethyl-phenyllithium,[4] 2,4,6-triisopropylphenyllithium,[5] and 2,4,6-tris(trifluoromethyl)phenyllithium[6] were prepared according to literature procedures. NMR spectra were recorded at 25 °C on a Bruker Avance III HD spectrometer operating at 300 MHz or on a Bruker Avance 500 spectrometer operating at 500 MHz. Chemical shifts were referenced to residual protic impurities in the solvent (^{1}H) or the deuterio solvent itself (^{13}C) and reported relative to external $SiMe_4$ (^{1}H, ^{13}C, ^{29}Si), $BF_3{\cdot}OEt_2$ (^{11}B), or $CFCl_3$ (^{19}F) standards. Mass spectra were obtained with the use of a Thermo Scientific Exactive Plus Orbitrap MS system employing atmospheric pressure chemical ionization (APCI). UV–vis spectra were obtained using a Jasco V-630 spectrophotometer. Emission spectra were recorded using an Edinburgh Instruments FLSP920 spectrometer equipped with a double monochromator for both excitation and emission, operating in right-angle geometry mode, and all spectra were fully corrected for the spectral response of the instrument. Fluorescence quantum yields were measured using a calibrated integrating sphere from Edinburgh Instruments combined with the FLSP920 spectrometer described above. Elemental analyses were performed on an Elementar vario MICRO cube elemental analyzer. Cyclic voltammetry experiments were performed using a Gamry Instruments Reference 600 potentiostat. The scans were referenced after the addition of a small amount of ferrocene as internal standard. The potentials are reported relative to the ferrocene/ferrocenium couple. Differential scanning calorimetry (DSC) was performed using a DSC 204 F1 Phoenix calorimeter.

Crystals suitable for single-crystal X-ray diffraction were selected, coated in perfluoropolyether oil, and mounted on MiTeGen sample holders. Diffraction data were collected on Bruker X8 Apex II 4-circle diffractometers with CCD area detectors using Mo-Kα radiation. The crystals were cooled using an Oxford Cryostreams low-temperature device. Data were collected at 100 K. The images were processed and corrected for Lorentz-polarization effects and absorption as implemented in the Bruker software packages. The structures were solved using the intrinsic phasing method (SHELXT)[7] and Fourier expansion technique. All non-hydrogen atoms were refined in anisotropic approximation, with hydrogen atoms 'riding' in idealized positions, by full-matrix least squares against F2 of all data, using SHELXL[8] software and the SHELXLE graphical user interface.[9] Other structural information was extracted using OLEX2 software.[10]

Synthesis of naphtho[1,8-*cd*]-*N*-isopropyl-*B,B'*-bis(2,4,6-trimethylphenyl)-[1,2,6]-azadiborinine (4a). To a solution of 1*H*-naphtho[1,8-*bc*]boret-1-amine **2** (2.00 mmol) in DCM (4 mL) was added a solution of BCl_3 (17.6 mmol) in DCM (5 mL) at −78 °C. The mixture was stirred for 5 days and all volatile components were removed *in vacuo*. The residue was dissolved in toluene (10 mL) and a solution of 2,4,6-trimethylphenyllithium (4.64 mmol) in toluene (25 mL) was added at −78 °C. The mixture was subsequently warmed to ambient temperature and stirred overnight. All volatile components were removed *in vacuo* and the residue was dissolved in DCM. It was washed with water and the organic phase was evaporated to dryness using a rotary evaporator. The product was received as colourless crystals after purification *via* column chromatography (silica; *n*-hexane) and crystallization from $CHCl_3$/MeOH. Yield: 0.3622 g (0.82 mmol, 41%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.07 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, C$^{4/5}$H Naph), 7.64 (d, $^3J_{HH}$ = 6.9 Hz, 2 H, C$^{2/7}$H Naph), 7.52 (pseudo t, $^3J_{HH}$ = 8.1 Hz, 2 H, C$^{3/6}$H), 6.97 (s, 4 H, CH Mes), 4.21 (sept, $^3J_{HH}$ = 7.0 Hz, 1 H, C*H*-$(CH_3)_2$), 2.43 (s, 6 H, *p*-CH_3 Mes), 2.23 (s, 12 H, *o*-CH_3 Mes), 1.23 ppm (d, $^3J_{HH}$ = 7.0 Hz, 6 H, CH-(C*H*$_3)_2$) ppm; ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ = 50.8 ppm (s); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ = 140.2 (*ipso*-C Mes), 139.9 (C$^{2/7}$ Naph), 138.8 (*p*-C Mes), 136.9 (C^{8a} Naph), 136.7 (*o*-C Mes), 135.2 (C$^{1/8}$ Naph), 132.6 (C$^{4/5}$ Naph), 131.1 (C^{4a} Naph), 127.0 (CH Mes), 126.1 (C$^{3/6}$ Naph), 53.3 (N*C*H$(CH_3)_2$), 23.7 (NCH(*C*$H_3)_2$), 23.5 (*o*-CH_3 Mes), 21.3 (*p*-CH_3 Mes) ppm; HR-MS (APCI): m/z = 444.3029 [M+H$^+$], calcd. for $C_{31}H_{35}B_2N$: 443.2956; UV/vis (DCM): $\lambda_{abs,max}$ = 234 (ε = 66539 L mol^{-1} cm^{-1}), 321 (ε = 13129 L mol^{-1} cm^{-1}), 341 nm (ε = 13891 L mol^{-1} cm^{-1}); fluorescence (DCM): λ_{ex} = 321, λ_{em1} = 352, λ_{em2} = 370, λ_{em3} = 386 nm (Φ_f = 17 %).

Synthesis of naphtho[1,8-*cd*]-*N*-isopropyl-*B,B'*-bis(2,4,6-triisopropylphenyl)-[1,2,6]azadiborinine (4b). To a solution of 1*H*-naphtho[1,8-*bc*]boret-1-amine **2** (2.04 mmol) in DCM (4 mL) was added a solution of BCl_3 (17.6 mmol) in DCM (5 mL) at −78 °C. The mixture was stirred for 5 days and all volatile components were removed *in vacuo*. The residue was dissolved in toluene (10 mL) and a solution of 2,4,6-triisopropylphenyllithium (4.03 mmol) in toluene (15 mL) was added at −78 °C. The mixture was subsequently warmed to ambient temperature and stirred overnight. All volatile components were removed *in vacuo* and the residue was dissolved in *n*-hexane. It was washed with water and the organic phase was evaporated to dryness using a rotary evaporator. The product was received as colourless crystals after purification *via* column chromatography (silica; *n*-hexane) and crystallization from $CHCl_3$/MeOH. Yield: 0.4778 g (0.78 mmol, 38%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.05 (d, $^3J_{HH}$ = 8.2 Hz, 2 H, C$^{4/5}$H Naph), 7.63 (d, $^3J_{HH}$ = 6.9 Hz, 2 H, C$^{2/7}$H Naph), 7.52 (pseudo t, $^3J_{HH}$ = 8.1 Hz, 2 H, C$^{3/6}$H Naph), 7.08 (s, 4 H, CH Tip), 4.38 (sept, $^3J_{HH}$ = 6.9 Hz, 1 H, NC*H*$(CH_3)_2$), 3.01 (sept, $^3J_{HH}$ = 6.9 Hz, 2 H, *p*-C*H*$(CH_3)_2$ Tip), 2.67 (sept, $^3J_{HH}$ = 6.7 Hz, 4 H, *o*-C*H*$(CH_3)_2$ Tip), 1.37 (d, $^3J_{HH}$ = 6.9 Hz, 12 H, *p*-CH(C*H*$_3)_2$ Tip), 1.30 (d, $^3J_{HH}$ = 6.7 Hz, 12 H, *o*-CH(C*H*$_3)_2$ Tip), 1.24 (d, $^3J_{HH}$ = 6.9 Hz, 6 H, NCH(C*H*$_3)_2$), 0.96 ppm (d, $^3J_{HH}$ = 6.6 Hz, 12 H, *o*-CH(C*H*$_3)_2$ Tip) ppm; ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ = 50.8 ppm (s); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ = 149.7 (*o*-C Tip), 148.4 (*p*-C Tip), 141.9 (C$^{2/7}$ Naph), 138.3 (*ipso*-C Tip), 136.5 (C^{8a} Naph), 136.2 (C$^{1/8}$ Naph), 132.6 (C$^{4/5}$ Naph), 130.9 (C^{4a} Naph), 125.2 (C$^{3/6}$ Naph), 120.1 (CH Tip), 52.8 (N*C*H$(CH_3)_2$), 35.0 (*o*-*C*H$(CH_3)_2$ Tip), 34.2 (*p*-*C*H$(CH_3)_2$), 25.5/23.5 (*o*-CH(*C*H$_3)_2$ Tip), 24.9 (NCH(*C*H$_3)_2$), 24.2 ppm (*p*-CH(*C*H$_3)_2$ Tip); HR-MS (APCI): m/z = 612.4897 [M+H$^+$], calcd. for $C_{43}H_{59}B_2N$: 611.4834; UV/vis (DCM): $\lambda_{abs,max}$ = 236 (ε = 68240 L mol^{-1} cm^{-1}), 326 (ε = 12397 L mol^{-1} cm^{-1}), 342 nm (ε = 13846 L mol^{-1} cm^{-1}); fluorescence (DCM): λ_{ex} = 326, λ_{em1} = 353, λ_{em2} = 369, λ_{em3} = 382 nm (Φ_f = 26 %).

Synthesis of naphtho[1,8-*cd*]-*N*-isopropyl-*B,B'*-bis(2,4,6-tris(trifluoromethyl)phenyl)-[1,2,6]aza-diborinine (4c). To a solution of 1*H*-naphtho[1,8-*bc*]boret-1-amine **2** (4.00 mmol) in DCM (8 mL) was added a solution of BCl_3 (35.2 mmol) in DCM (10 mL) at −78 °C. The mixture was stirred for 5 days and all volatile components were removed *in vacuo*. The residue was dissolved in toluene (10 mL)

and a solution of freshly prepared 2,4,6-tris(trifluoromethyl)phenyllithium (ca. 9 mmol) in toluene (15 mL) was added at −78 °C. The mixture was subsequently warmed to ambient temperature and stirred for 5 days. All volatile components were removed *in vacuo* and the residue was dissolved in *n*-hexane. It was washed with water and the organic phase was evaporated to dryness using a rotary evaporator. The product was received as yellowish crystals after purification *via* column chromatography (silica; *n*-hexane/ethyl acetate, 90:10) and crystallization from $CHCl_3$/MeOH. Yield: 0.5166 g (0.67 mmol, 17%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.21 (s, 4H, CH ^{F}Mes), 8.12 (d, $^3J_{HH}$ = 8.3 Hz, 2H, C$^{4/5}$H Naph), 7.52 (pseudo t, $^3J_{HH}$ = 7.0 Hz, 2H, C$^{3/6}$H Naph), 7.21 (d, $^3J_{HH}$ = 7.0 Hz, 2H, C$^{2/7}$H Naph), 3.73 (sept, $^3J_{HH}$ = 6.9 Hz, 1H, NC*H*$(CH_3)_2$), 1.04 (d, $^3J_{HH}$ = 6.8 Hz, 6H, NCH(C*H*$_3)_2$) ppm; ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ = 47.5 ppm (s); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ = 142.8 (*ipso*-C ^{F}Mes), 139.1 (C$^{2/7}$ Naph), 135.9 (C^{4a} Naph), 135.2 (q, $^1J_{CF}$ = 31.5 Hz, *o*-C ^{F}Mes), 133.9 (C$^{1/8}$ Naph), 133.6 (C$^{4/5}$ Naph), 132.2 (q, $^1J_{CF}$ = 34.5 Hz, *p*-C ^{F}Mes), 130.9 (C^{8a} Naph), 126.5 (*m*-C Naph), 126,0 (C$^{3/6}$ Naph), 123.7 (q, $^1J_{CF}$ = 275.8 Hz, *o*-CF_3), 122.8 (q, $^1J_{CF}$ = 272.2 Hz, *p*-CF_3), 54.4 (N*C*H(CH3)2), 23.8 (NCH(*C*H3)2) ppm; ^{19}F{^{1}H} NMR (376 MHz, $CDCl_3$): δ = −56.7 (s, 12F, *o*-CF_3), −63.2 (s, 6F, *p*-CF_3) ppm; HR-MS (APCI): m/z = 768.1322 [M+H$^+$], calcd. for $C_{31}H_{17}B_2F_{18}N$: 767.1260; UV/vis (DCM): $\lambda_{abs,max}$ = 231 (ε = 45827 L mol^{-1} cm^{-1}), 320 (ε = 14312 L mol^{-1} cm^{-1}), 339 nm (ε = 13654 L mol^{-1} cm^{-1}); fluorescence (DCM): λ_{ex} = 320, λ_{em1} = 349, λ_{em2} = 363 nm (Φ_f = 30 %).

Molecular structures in the solid state determined by single-crystal X-ray diffraction

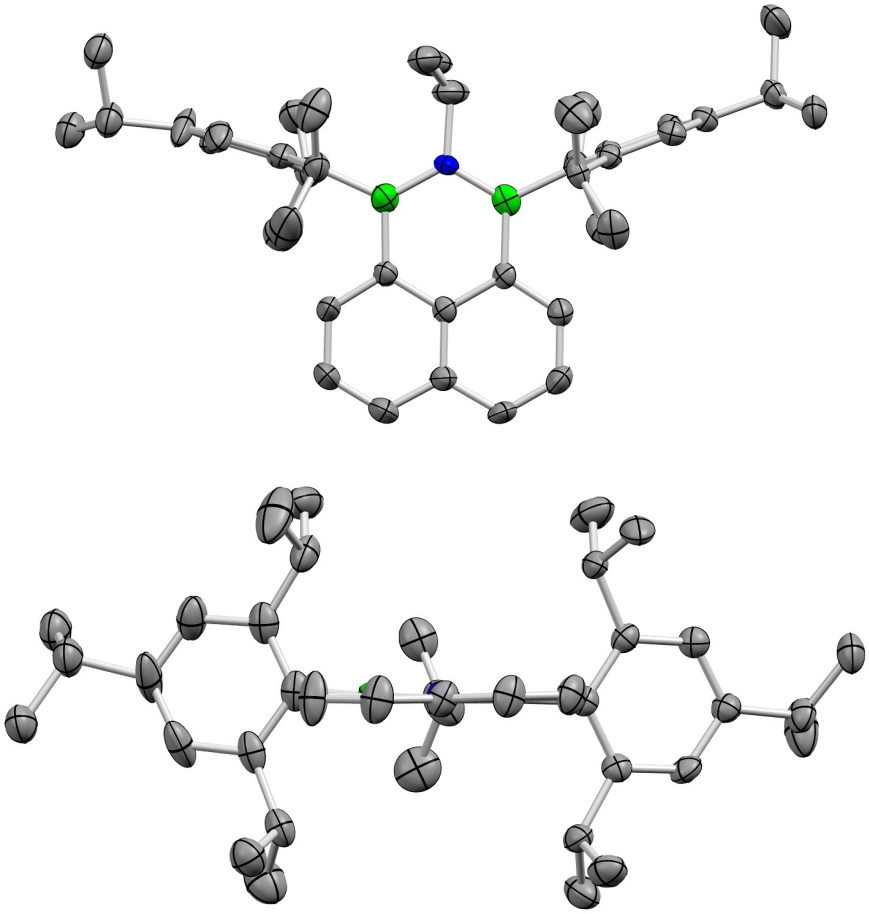

Figure S1. Molecular structure of **4b** in the solid state.

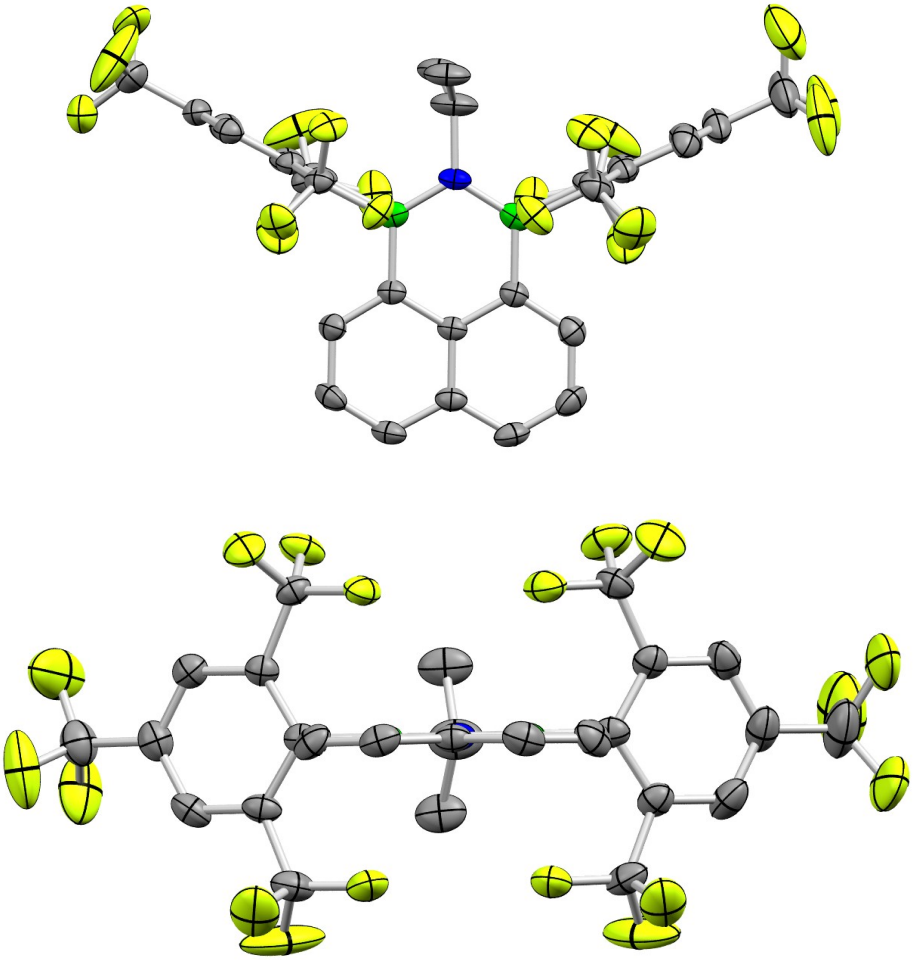

Figure S2. Molecular structure of **4c** in the solid state.

Table S1: Crystallographic data of **4b** and **4c**.

No.	**4b**	**4c**
CCDC number	2023745	2031332
Size / mm	0.22 x 0.17 x 0.07	0.41 x 0.21 x 0.15
Empiric Formula	$C_{43}H_{58.68}B_2N$	$C_{31}H_{17}B_2F_{18}N$, 0.46($C_1H_1Cl_3$)
***M* / g mol^{-1}**	611.21	821.34
Crystal system	monoclinic	monoclinic
Space group	P 21/c	P 1 21/n 1
***a* / Å**	25.774(3)	20.0781(7)
***b* / Å**	17.2923(18)	7.6006(3)
***c* / Å**	17.0060(18)	22.0644(7)
α / deg	90	90
β / deg	92.749(3)	100.5340(10)
γ / deg	90	90
***V* / Å^3**	7570.7(14)	3310.4(2)
Z	8	4
μ / mm^{-1}	0.060	0.273
***T* / K**	173	100
$\theta_{min,max}$	0.79, 25.37	2.52, 25.88
Completeness	99.8	99.8
Reflections: total / independent	13877, 7180	7036, 5352
R_{int}	0.1480	0.0374
Final *R*1 and *wR*2	0.0694, 0.1824	0.0663, 0.1801
Largest peak and hole / e Å^{-3}	0.386, -0.291	1.366, -0.731
ρ_{calc} / g cm^{-3}	1.072	1.648

NMR spectra

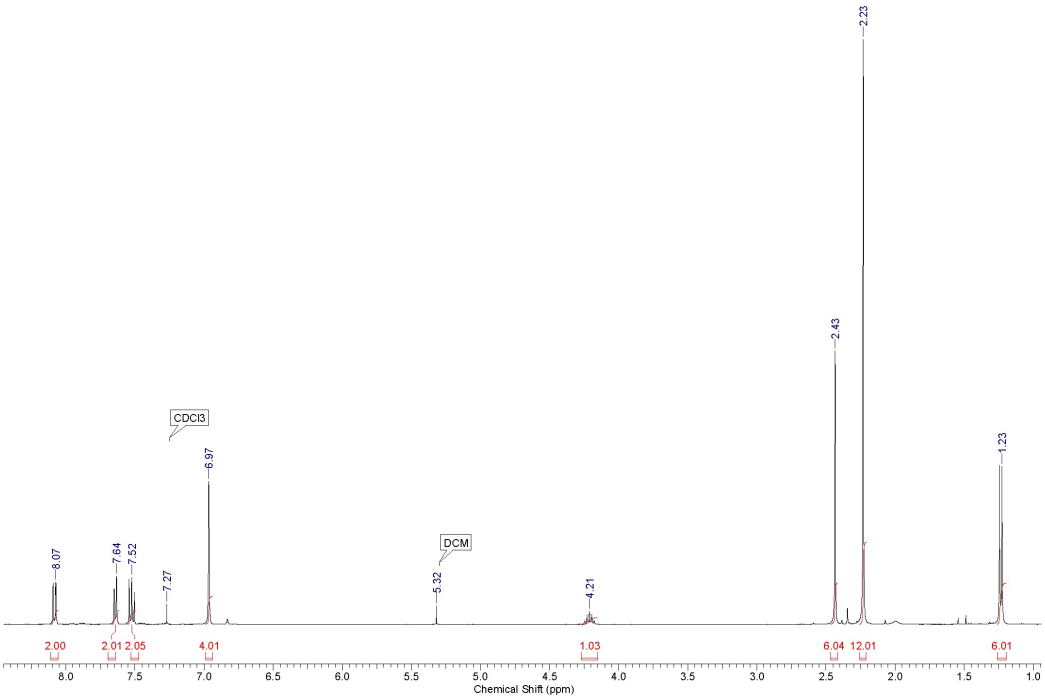

Figure S3. ^{1}H NMR spectrum of **4a**.

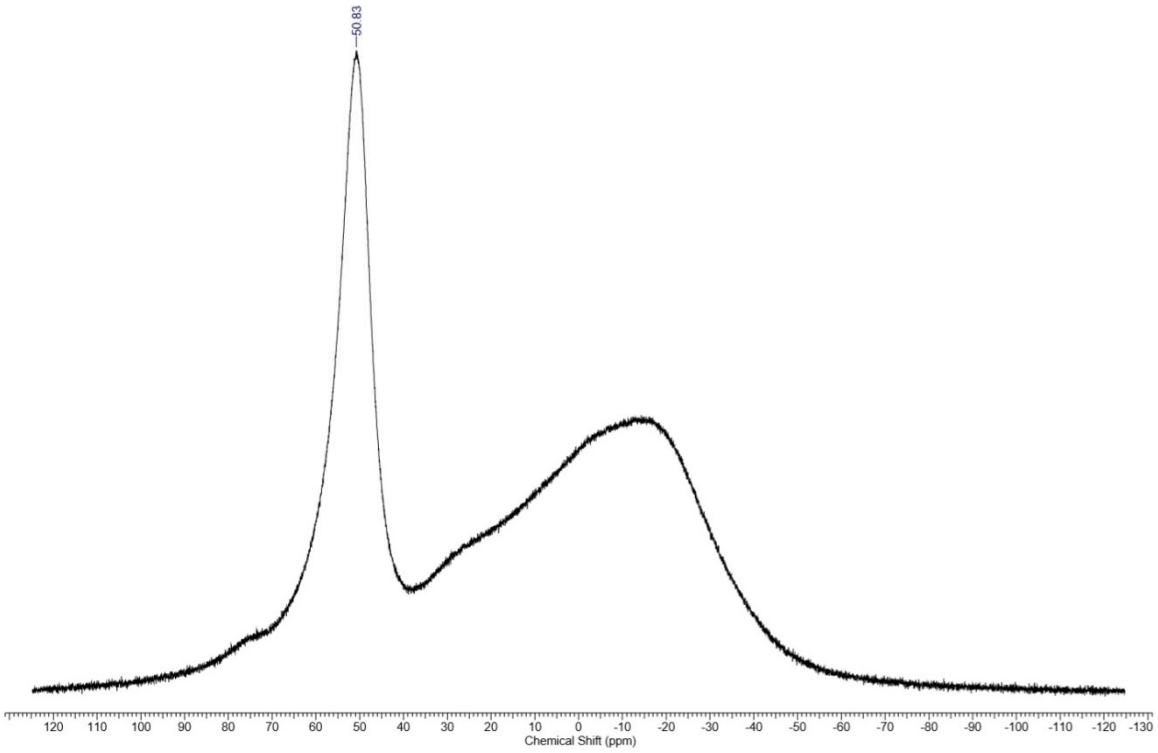

Figure S4. ^{11}B{^{1}H} NMR spectrum of **4a**.

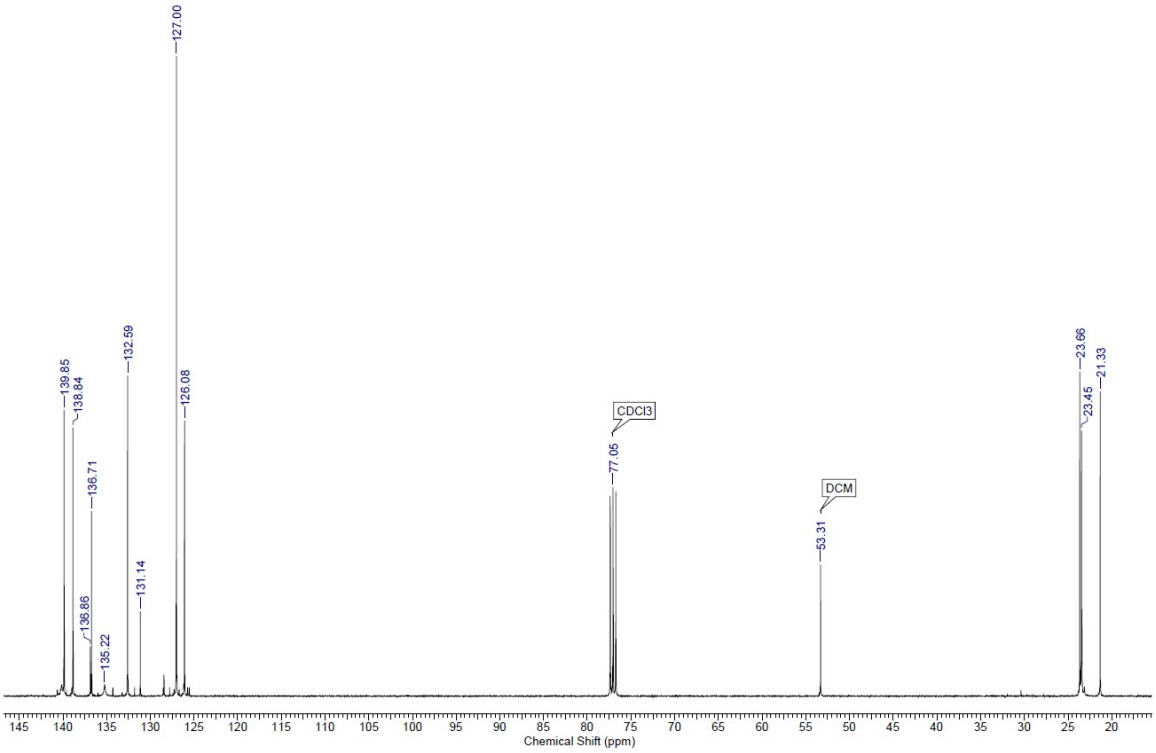

Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of **4a**.

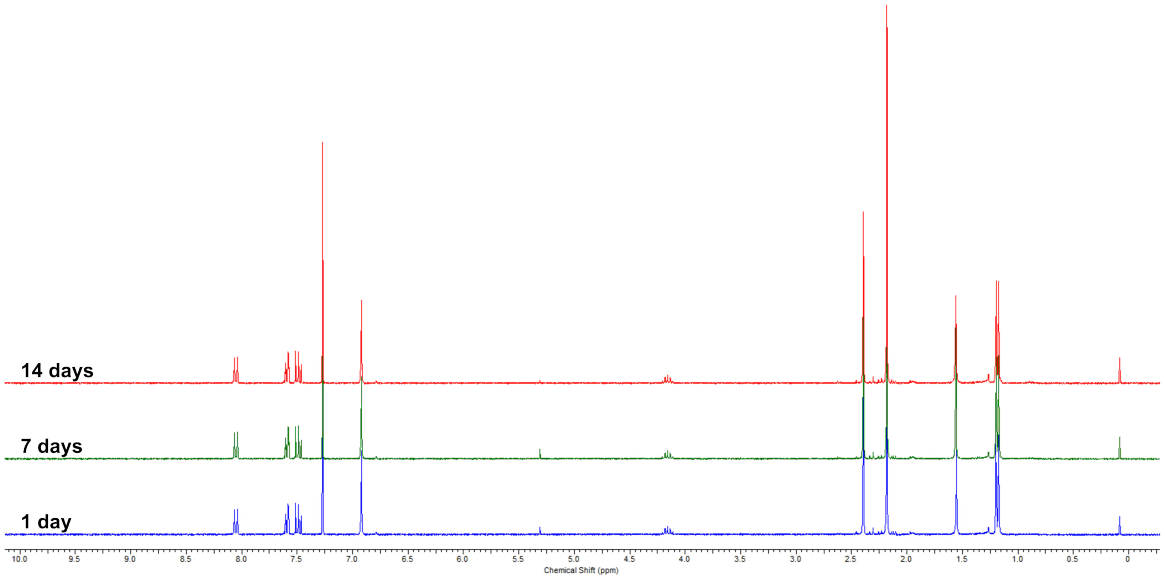

Figure S6. ^{1}H NMR spectrum of **4a** in moist solution over time.

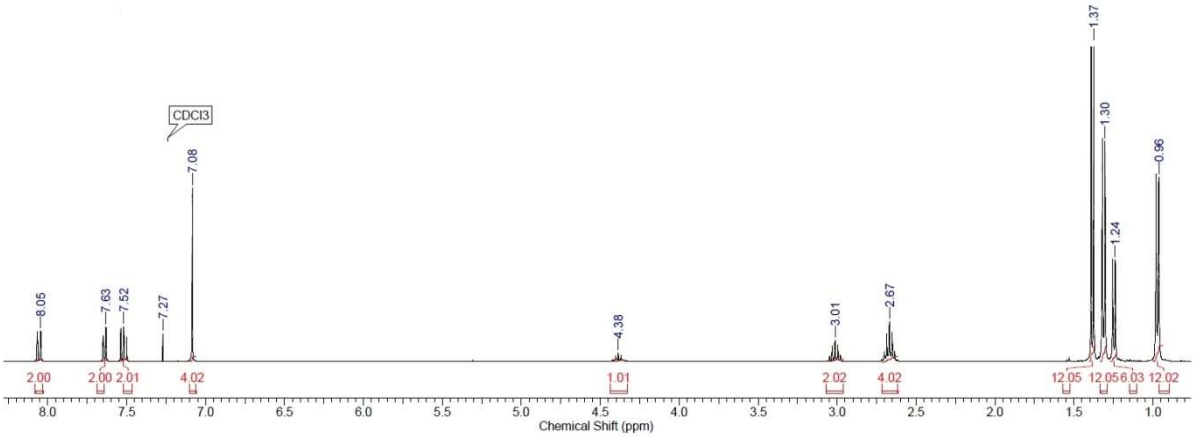

Figure S7. ^{1}H NMR spectrum of **4b**.

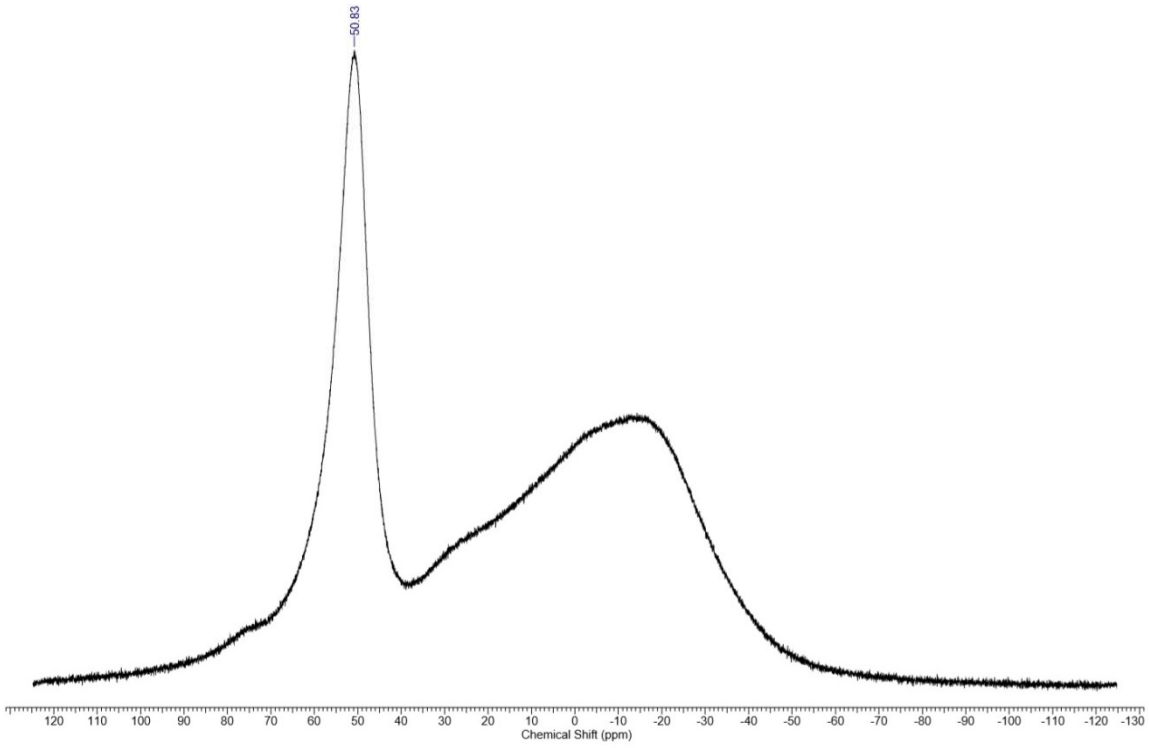

Figure S8. ^{11}B{^{1}H} NMR spectrum of **4b**.

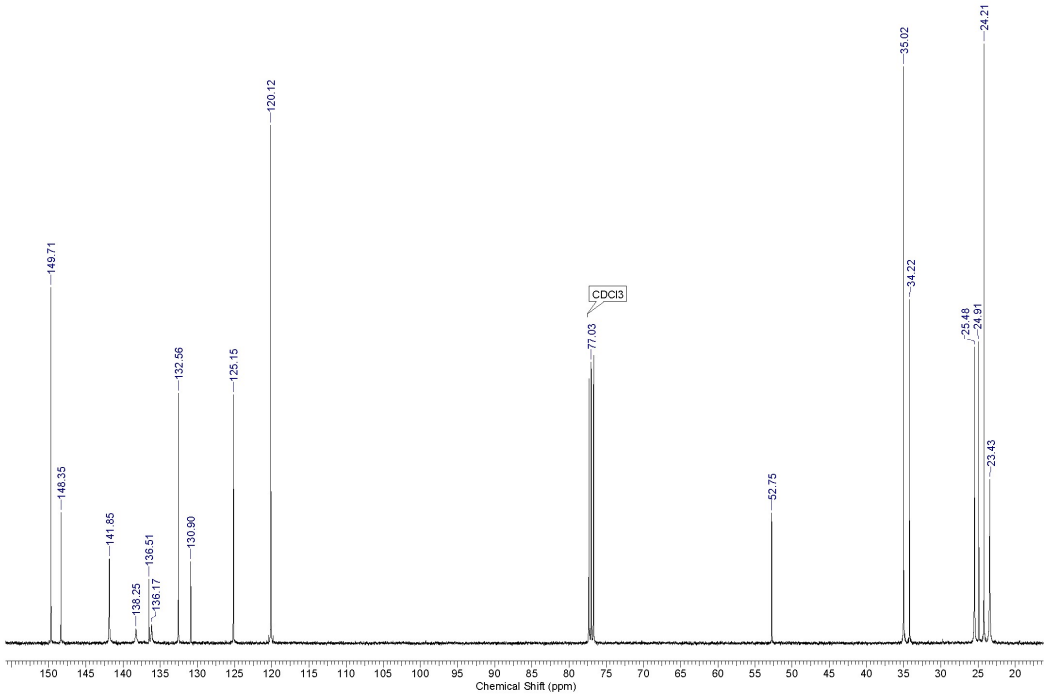

Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of **4b**.

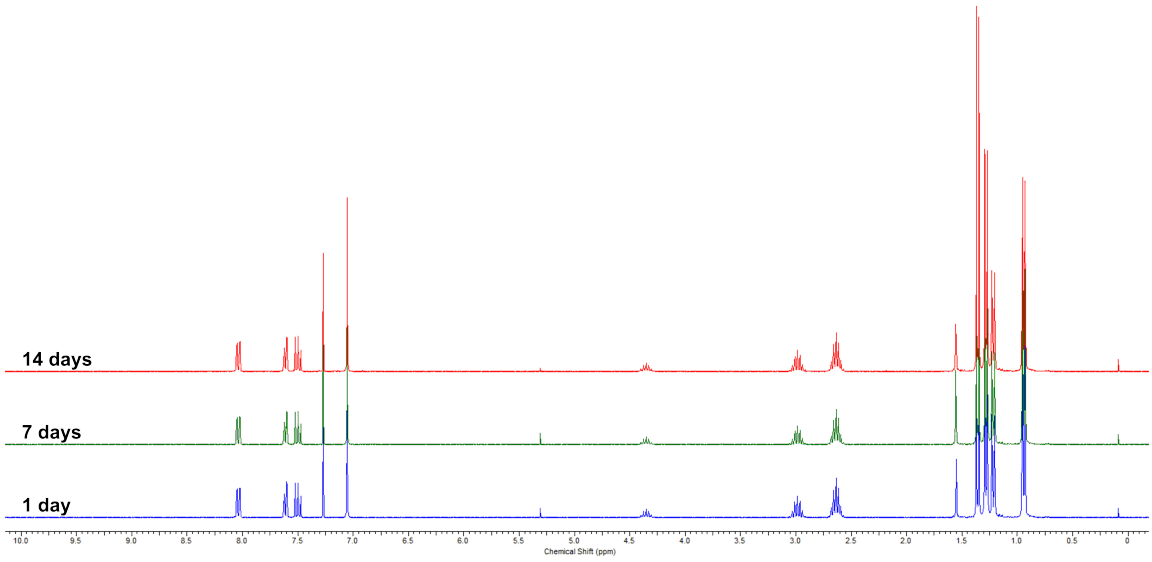

Figure S10. ^{1}H NMR spectrum of **4b** in moist solution over time.

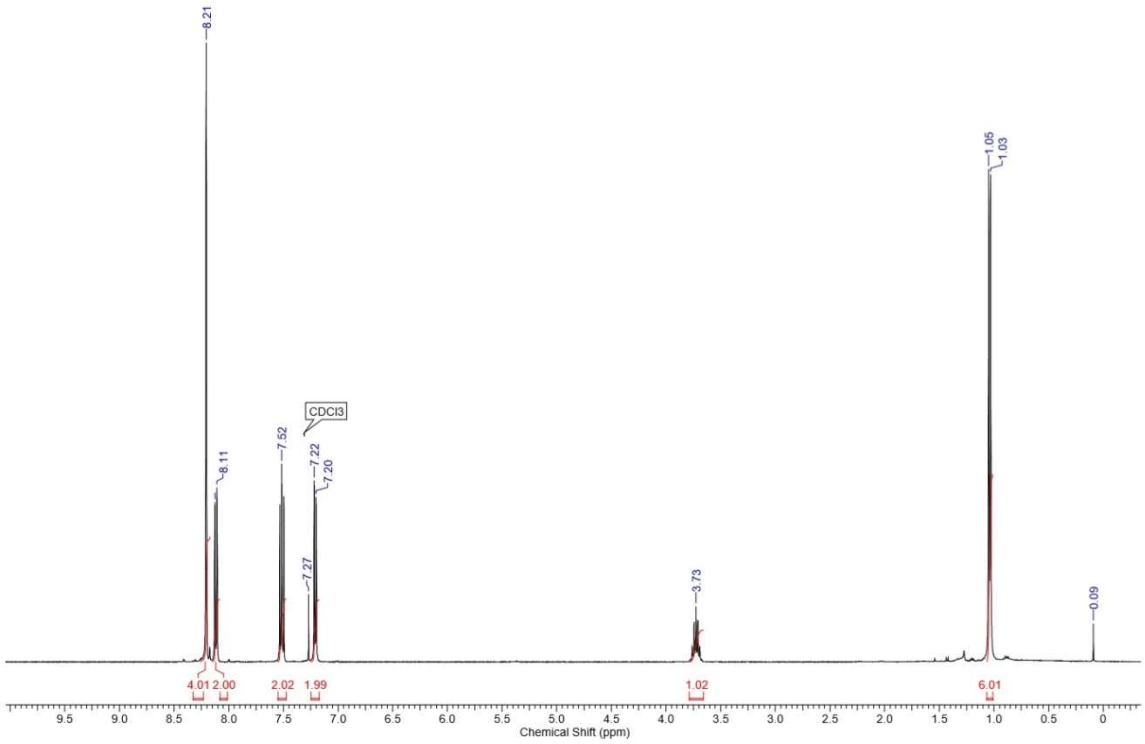

Figure S11. ^{1}H NMR spectrum of **4c**.

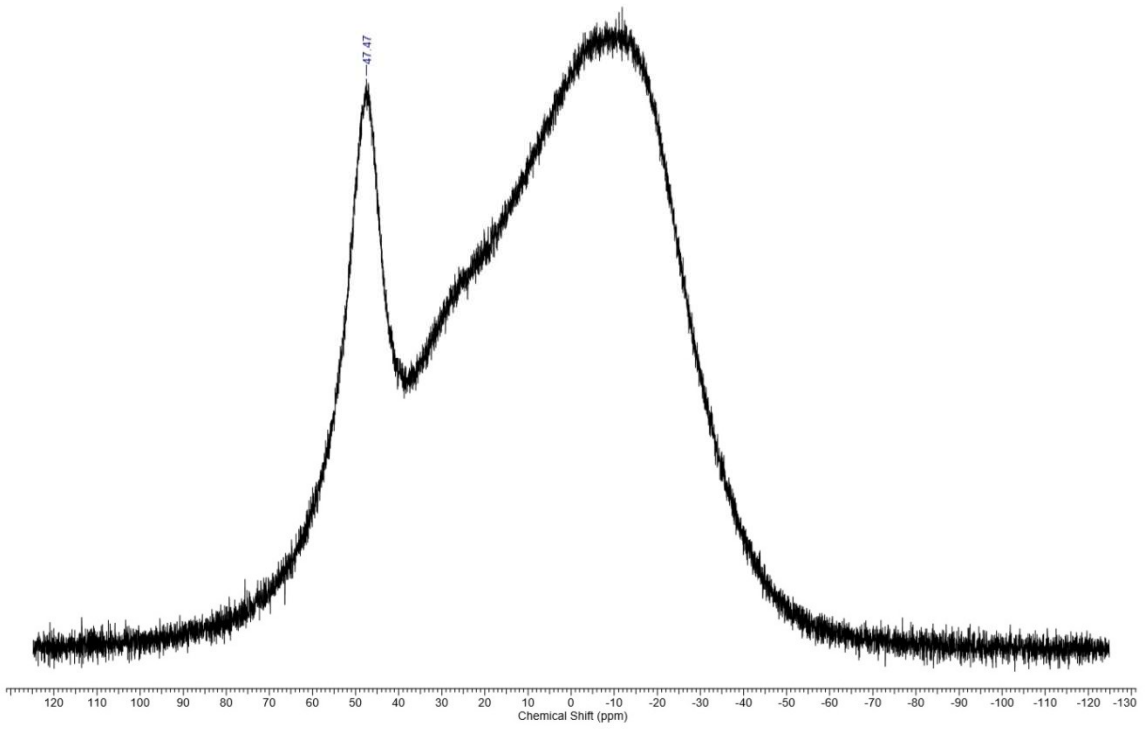

Figure S12. ^{11}B{^{1}H} NMR spectrum of **4c**.

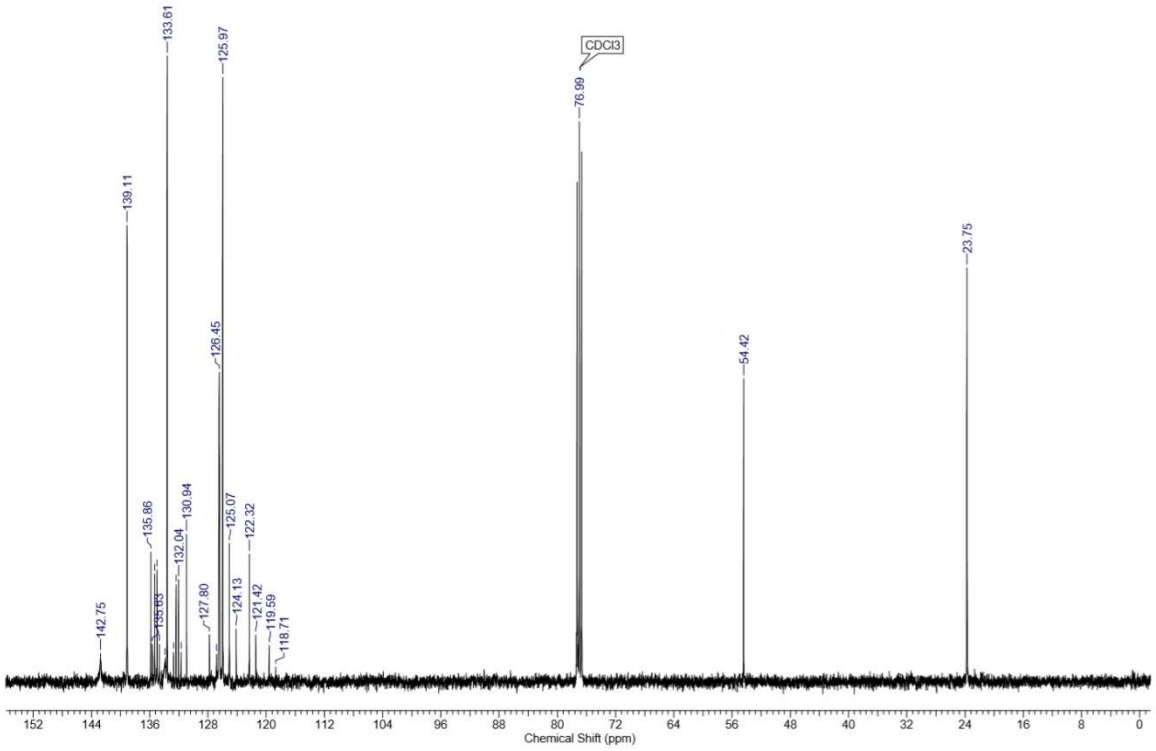

Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum of **4c**.

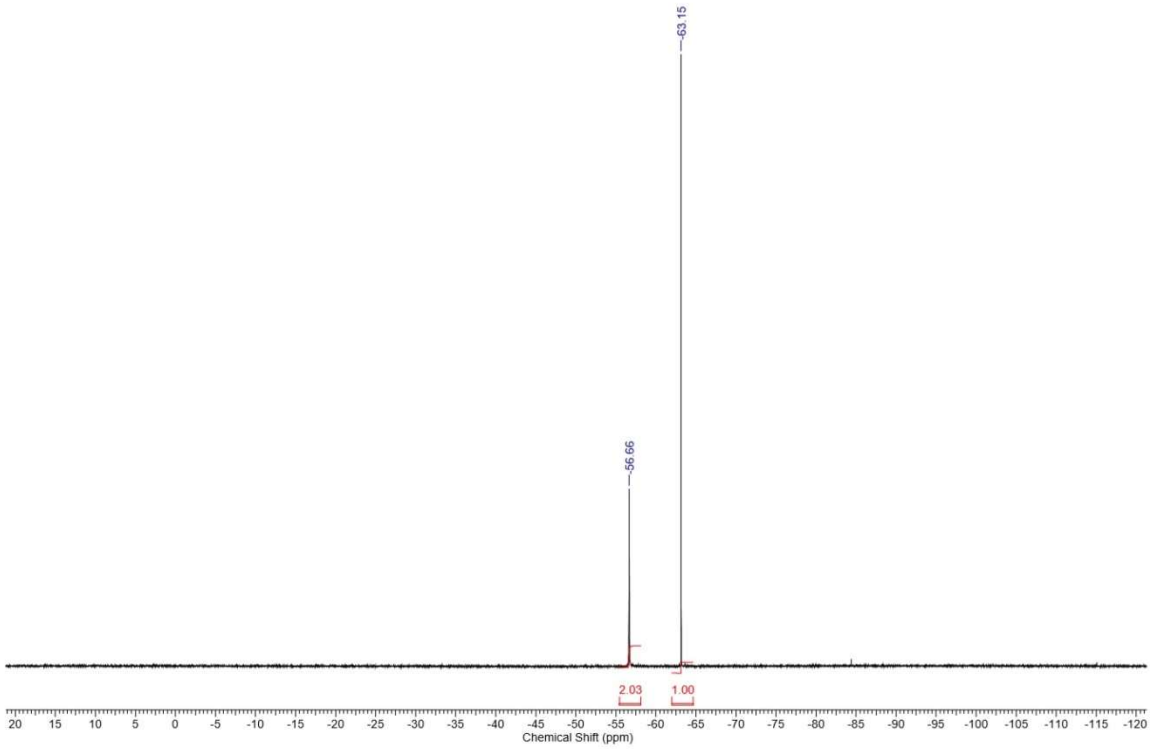

Figure S14. $^{19}F\{^{1}H\}$ NMR spectrum of **4c**.

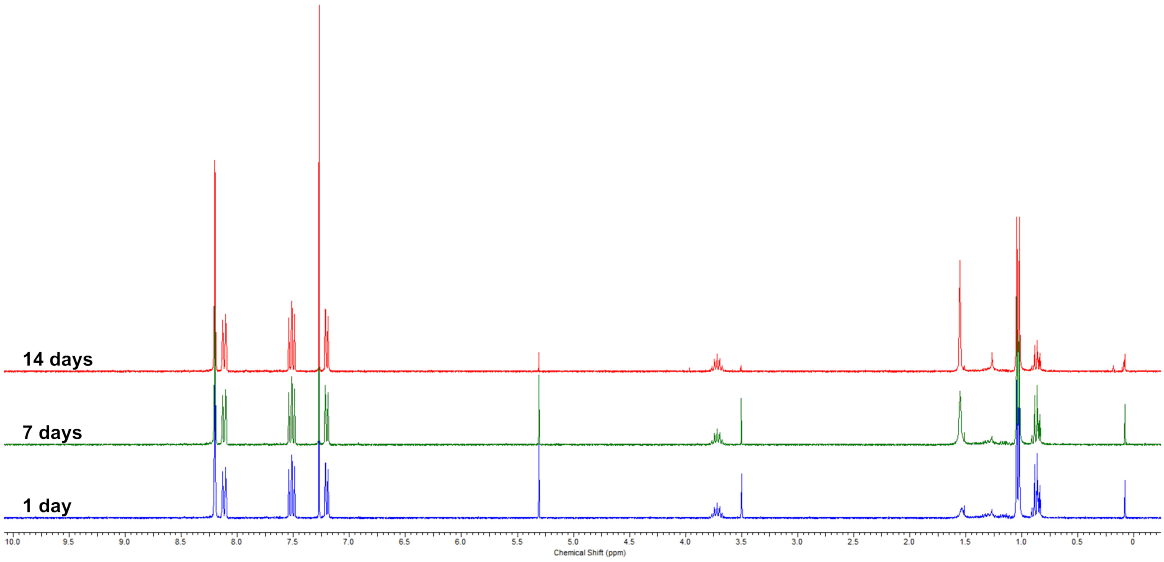

Figure S15. ^{1}H NMR spectrum of **4c** in moist solution over time.

Mass spectra

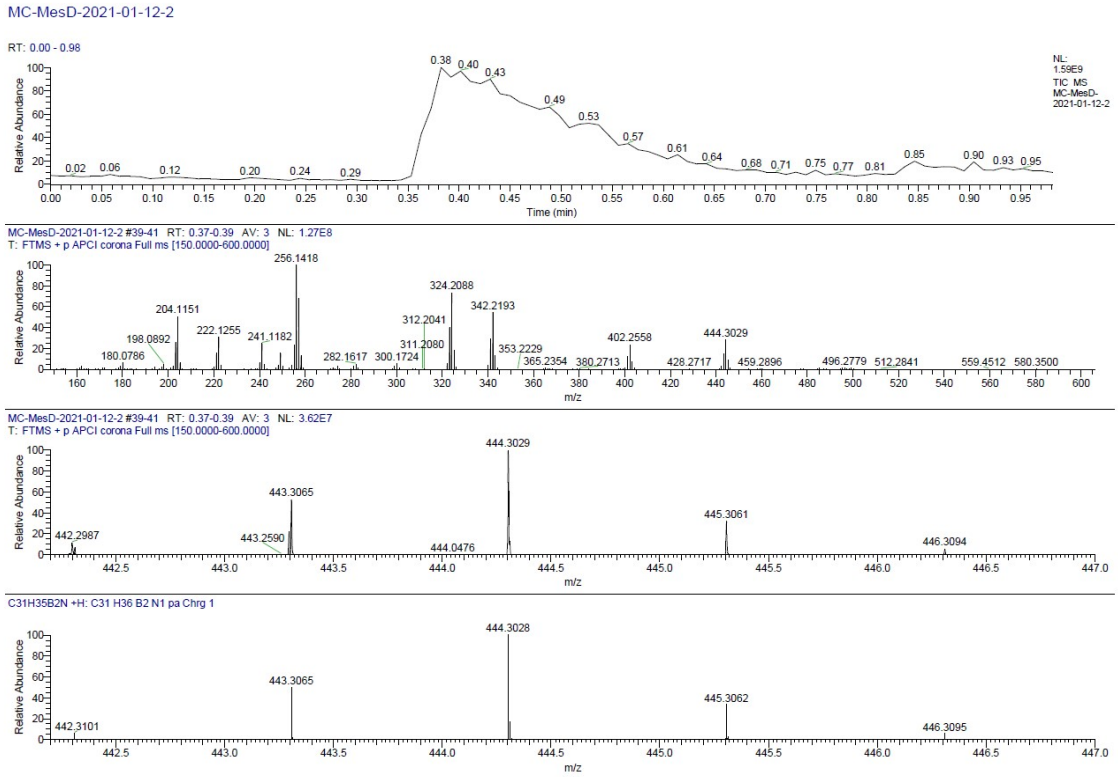

Figure S16. APCI HRMS spectrum of **4a**.

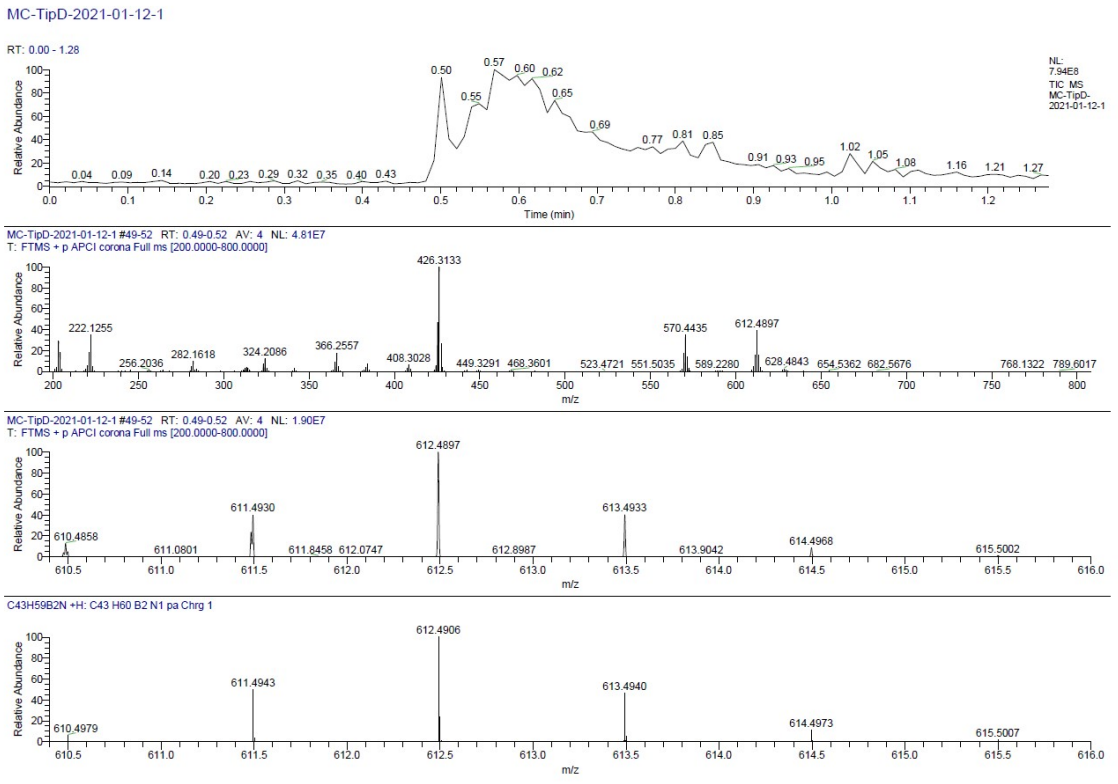

Figure S17. APCI HRMS spectrum of **4b**.

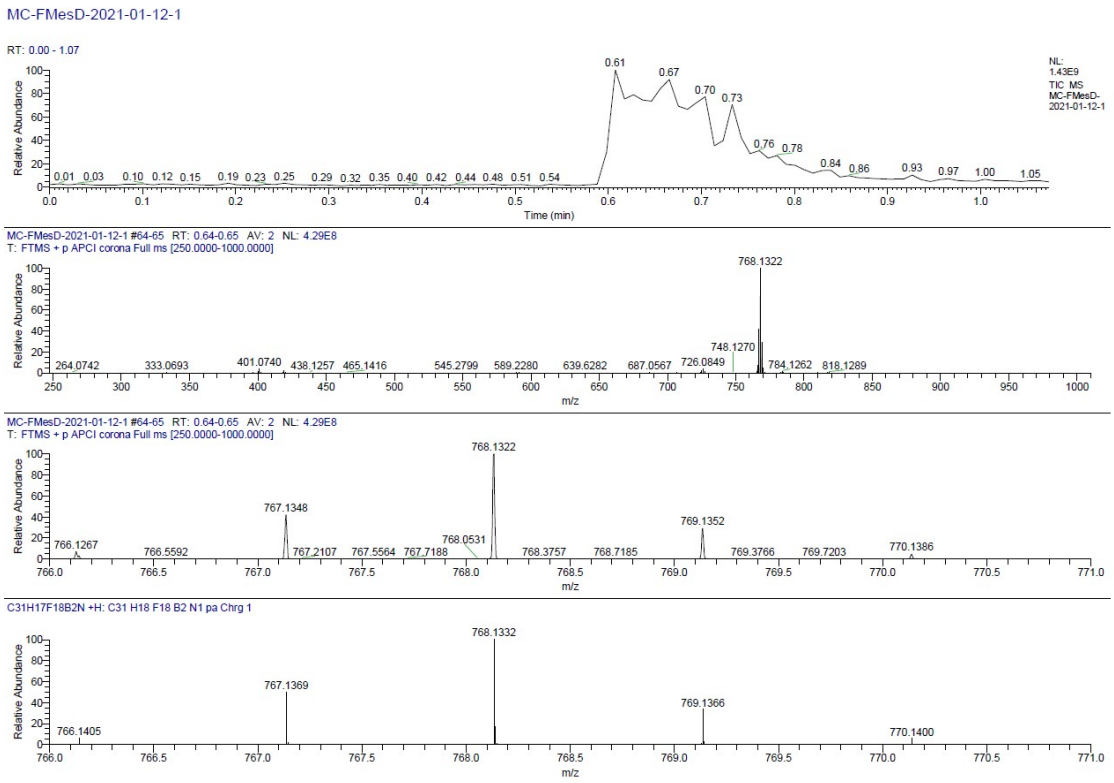

Figure S18. APCI HRMS spectrum of **4c**.

UV/vis and fluorescence spectra

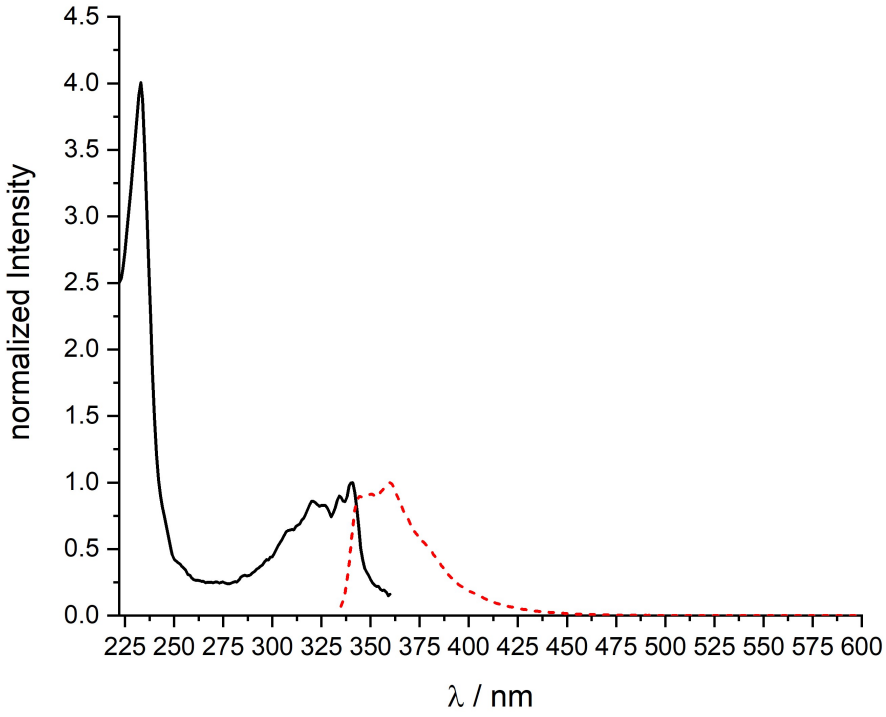

Figure S19. UV/vis and fluorescence spectrum of **4a** in hexane.

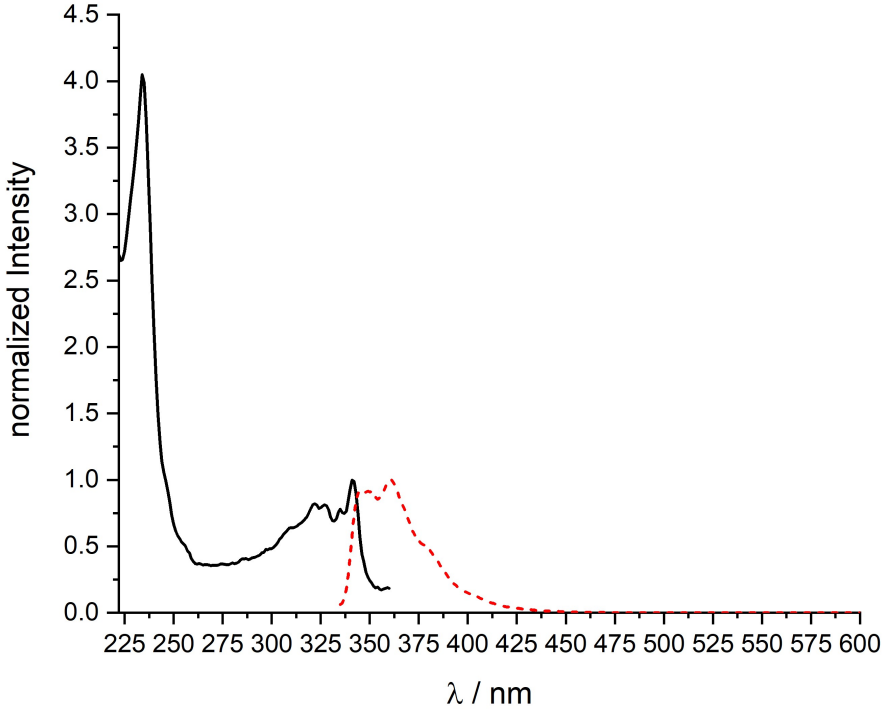

Figure S20. UV/vis and fluorescence spectrum of **4b** in hexane.

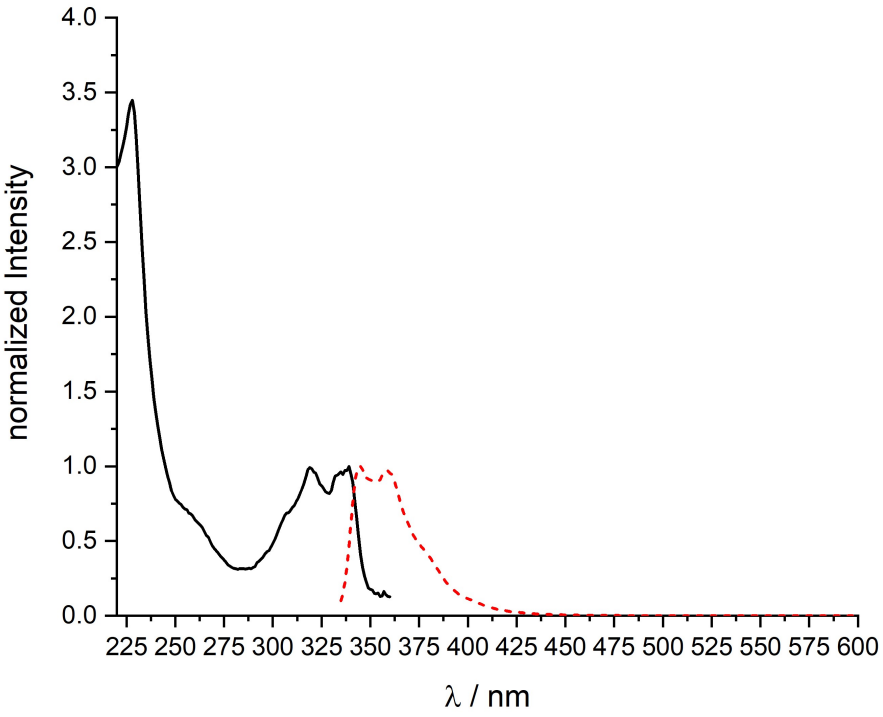

Figure S21. UV/vis and fluorescence spectrum of **4c** in hexane.

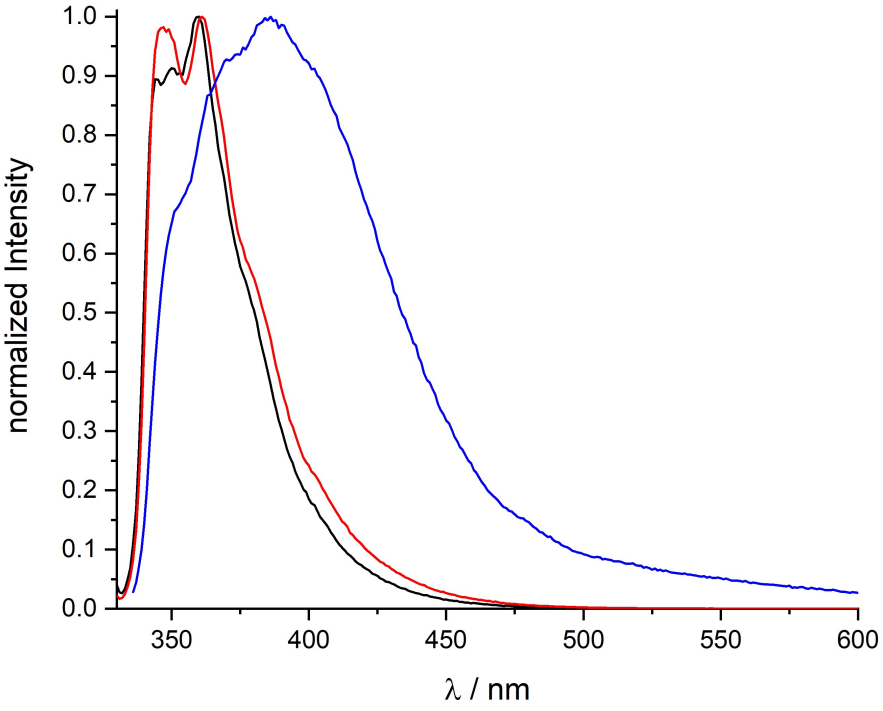

Figure S22. Fluorescence spectra of **4a** in hexane (black), Et_2O (red) and DCM (blue) showing the solvatochromic effect.

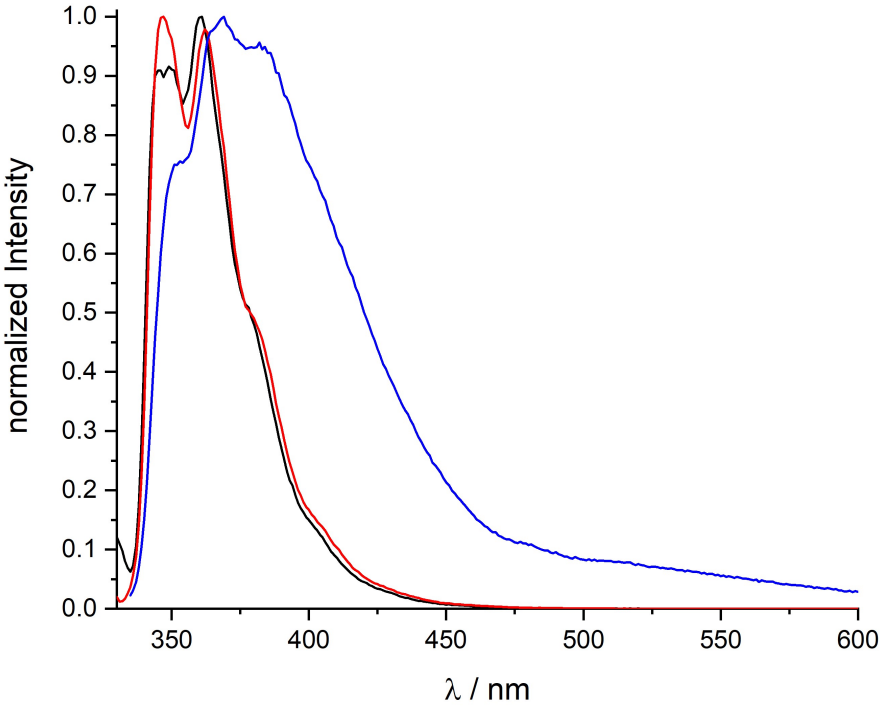

Figure S23. Fluorescence spectra of **4b** in hexane (black), Et_2O (red) and DCM (blue) showing the solvatochromic effect.

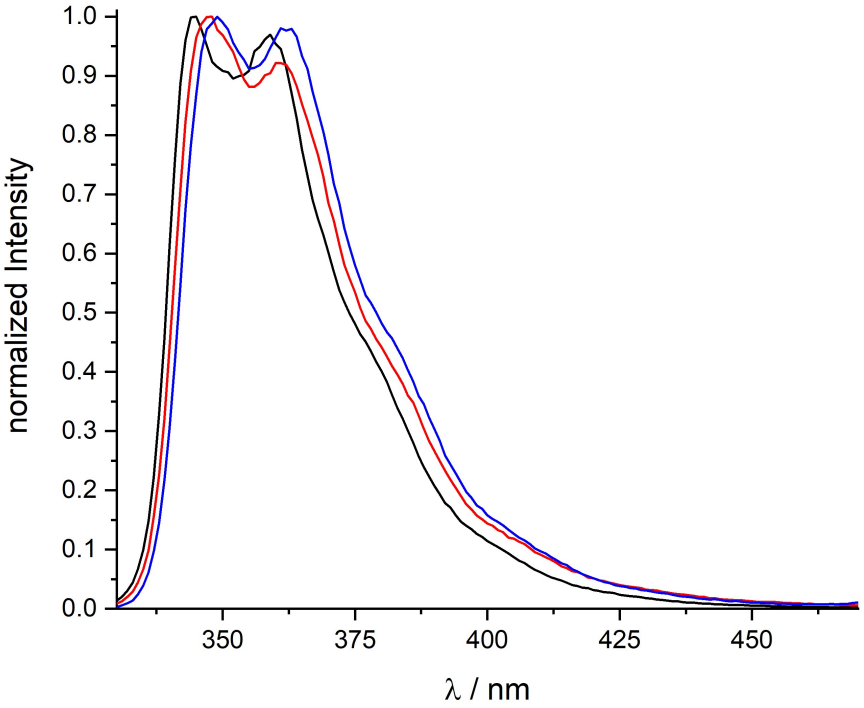

Figure S24. Fluorescence spectra of **4c** in hexane (black), Et_2O (red) and DCM (blue) showing the solvatochromic effect.

Table S2. Investigation of the solvatochromic effect on the absorption and emission maxima of **4a**, **4b** and **4c**.

Compound	λ_{abs} [nm] hexane	λ_{abs} [nm] Et_2O	λ_{abs} [nm] DCM	λ_{em} [nm] hexane	λ_{em} [nm] Et_2O	λ_{em} [nm] DCM
4a	321	321	321	344	347	351
	341	341	341	360	361	386
4b	322	323	326	345	347	353
	341	342	342	361	362	369
4c	319	320	320	345	348	349
	339	339	339	359	360	361

Table S3. Fluorescence lifetime data for compounds **4a**, **4b** and **4c** in hexane, Et_2O and DCM.

Compound	hexane	Et_2O	DCM
4a	1.11 ns (12 %)	3.33 ns (100 %)	2.81 ns (69%)
	3.74 ns (88%)		4.72 ns (31%)
4b	1.17 ns (11 %)	3.02 ns (100 %)	2.08 ns (10%)
	3.20 ns (89 %)		4.36 ns (88%)
4c	1.40 ns (5 %)	4.40 ns (100 %)	2.44 ns (100%)
	5.26 ns (95 %)		

Table S4. Fluorescence quantum yields of compounds **4a**, **4b** and **4c** in hexane, Et_2O and DCM.

Compound	hexane	Et_2O	DCM
4a	34 %	20 %	17 %
4b	36 %	26 %	26 %
4c	47 %	36 %	30 %

CV traces

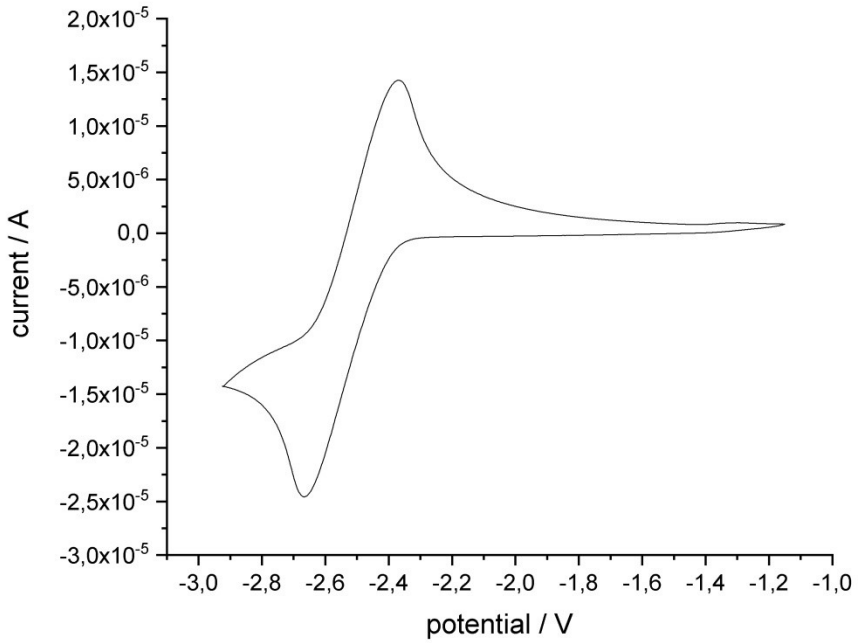

Figure S25. Cyclic voltammogram of **4a**.

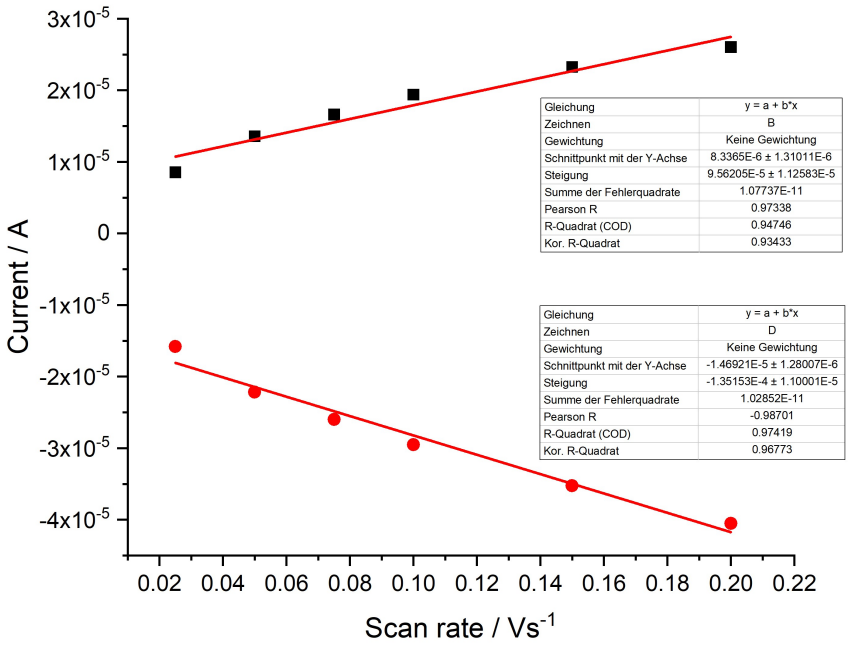

Figure S26. Plot of oxidation and reduction peak current of **4a** vs. CV scan rate showing the linear dependence.

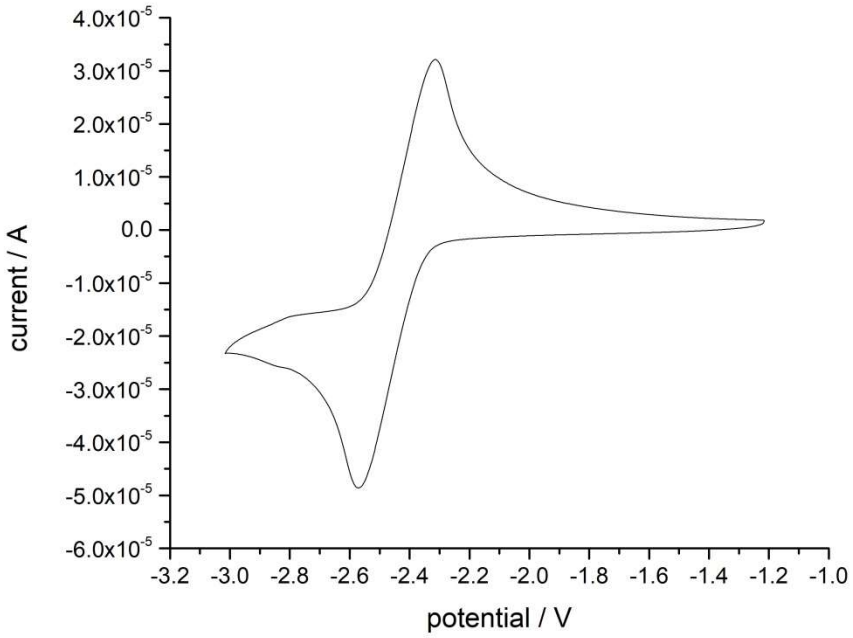

Figure S27. Cyclic voltammogram of **4b**.

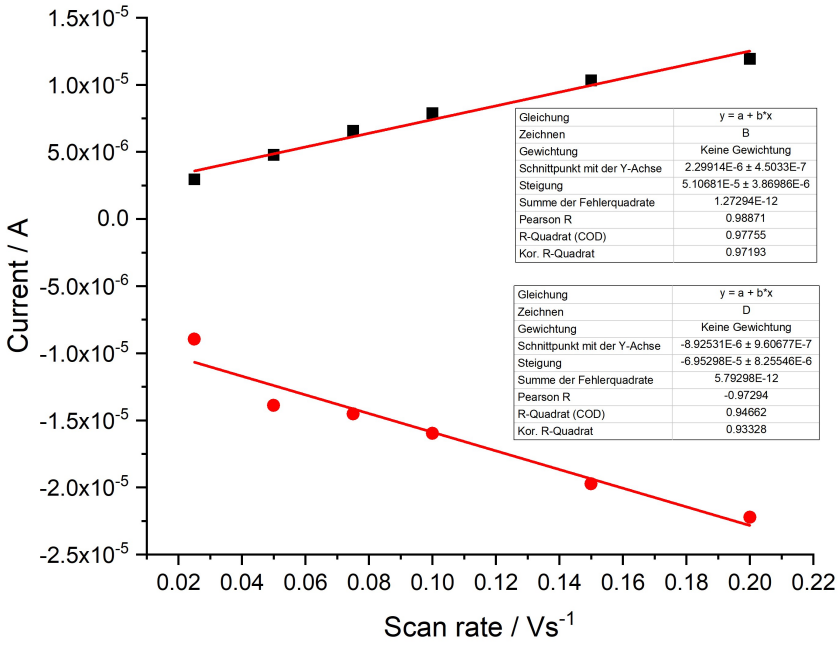

Figure S28. Plot of oxidation and reduction peak current of **4b** vs. CV scan rate showing the linear dependence.

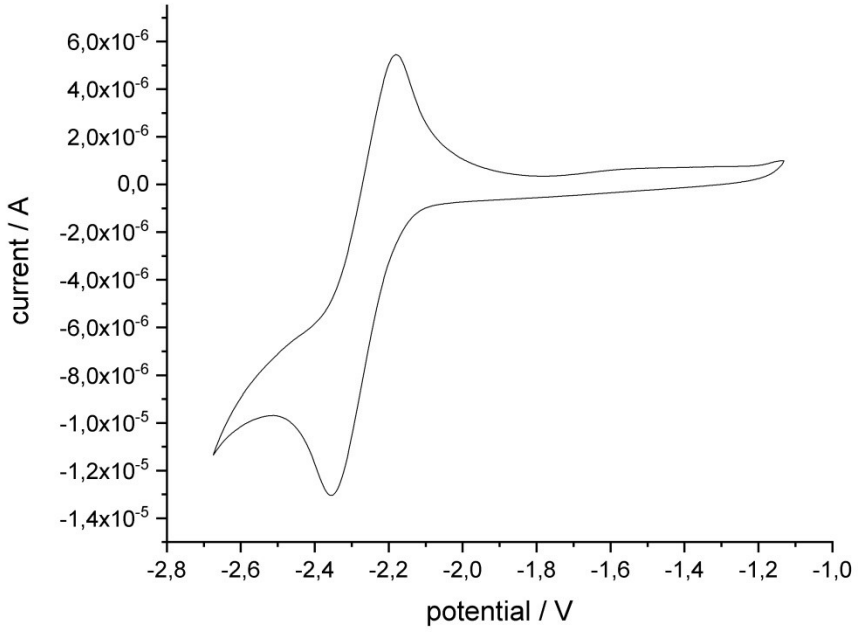

Figure S29. Cyclic voltammogram of **4c**.

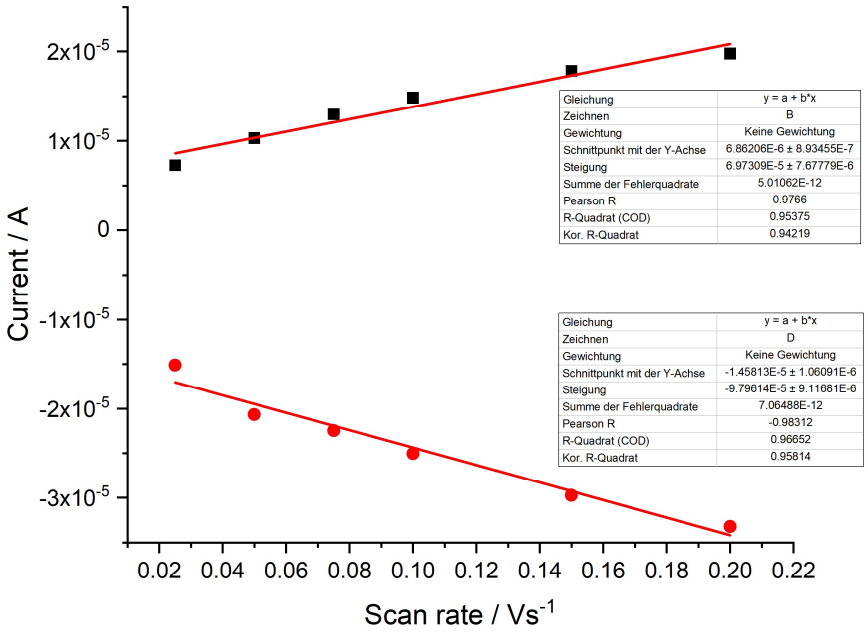

Figure S30. Plot of oxidation and reduction peak current of **4c** vs. CV scan rate showing the linear dependence.

Table S5. Differences in potential between the respective anodic and cathodic peaks for 4a, 4b and 4c in V.

Scan rate / Vs^{-1}	4a	4b	4c
0.025	0.1868	0.1248	0.2374
0.050	0.2328	0.1575	0.2979
0.075	0.2631	0.1520	0.3235
0.100	0.2884	0.1666	0.3696
0.150	0.3284	0.1926	0.4086
0.200	0.3436	0.2264	0.4398

Differential scanning calorimetry

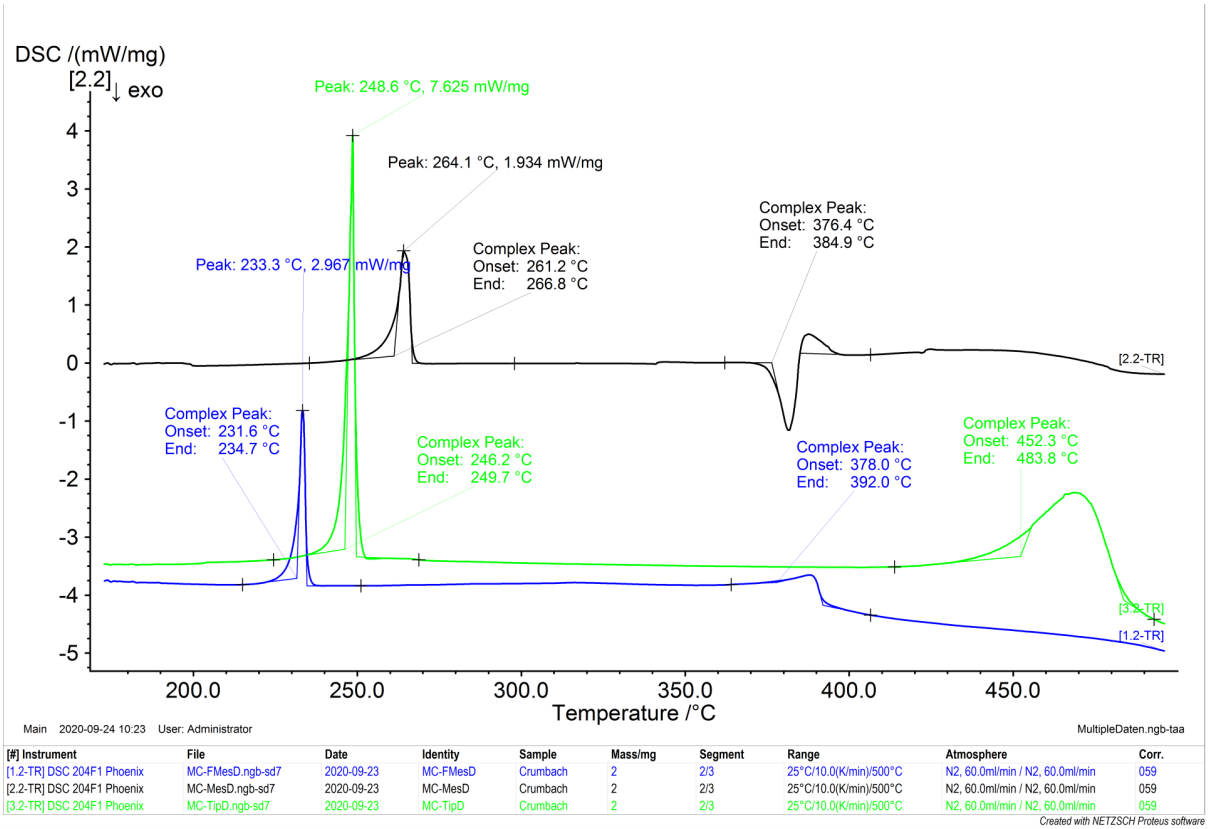

Figure S31. Differential scanning calorimetry graphs for **4a** (black), **4b** (green), and **4c** (blue).

2 Computational Information

Computational methods. Optimizations were carried out with the TURBOMOLE V7.0.1 program package.[11] NICS Scan,[12] NICS XY-Scan[13] and ACID[14] calculations were carried out using the Gaussian 09 program package, revision D.01.[15] Becke's three parameter exchange-correlation hybrid functional B3LYP[16] was used in combination with the 6-31+G* basis set in Gaussian 09 and the valence-double-ζ basis set def2-SV(P)[17] in TURBOMOLE. The empirical dispersion correction DFT-D3 by Grimme was used including the three-body term and with Becke-Johnson (BJ) damping.[18] The stationary points were characterized as minima by an analytical vibrational frequency calculation,[19] which revealed the absence of imaginary frequencies.

Computational results:

NICS and ACID plots

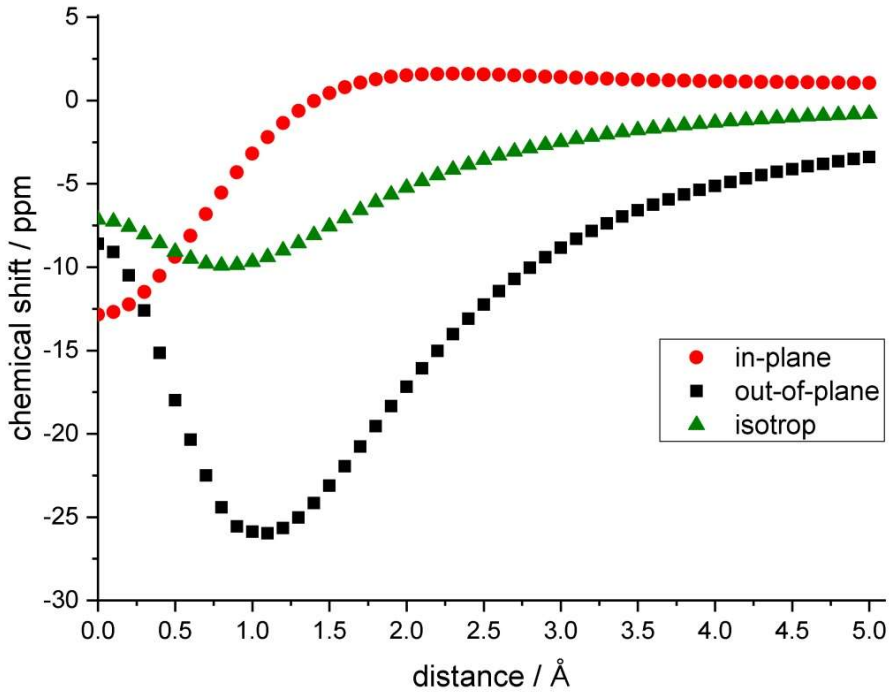

Figure S32. NICS Scan of naphthalenic rings of neutral **4a**.

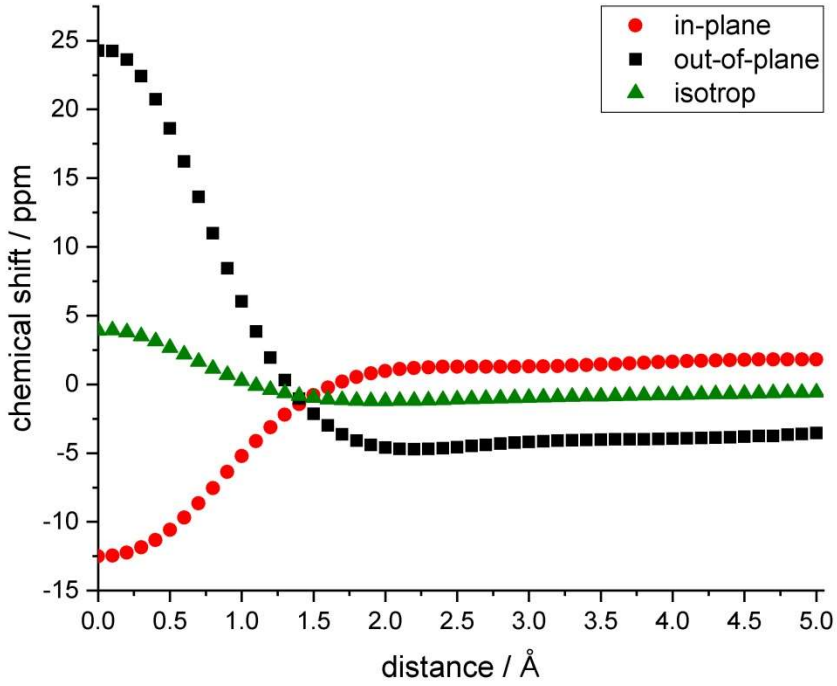

Figure S33. NICS Scan of hetero ring of neutral **4a**.

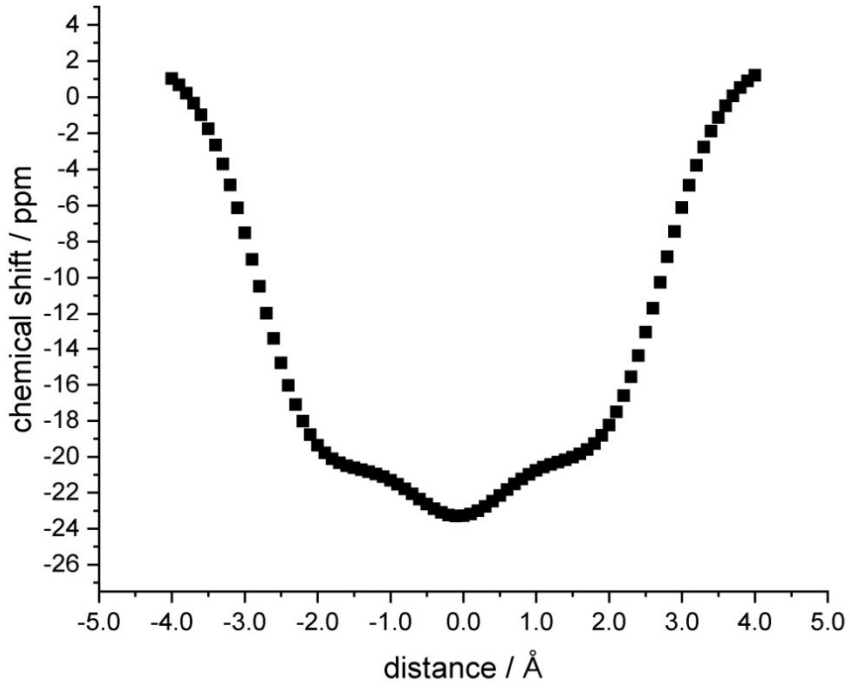

Figure S34. NICS XY-Scan of naphthalenic rings of neutral **4a**.

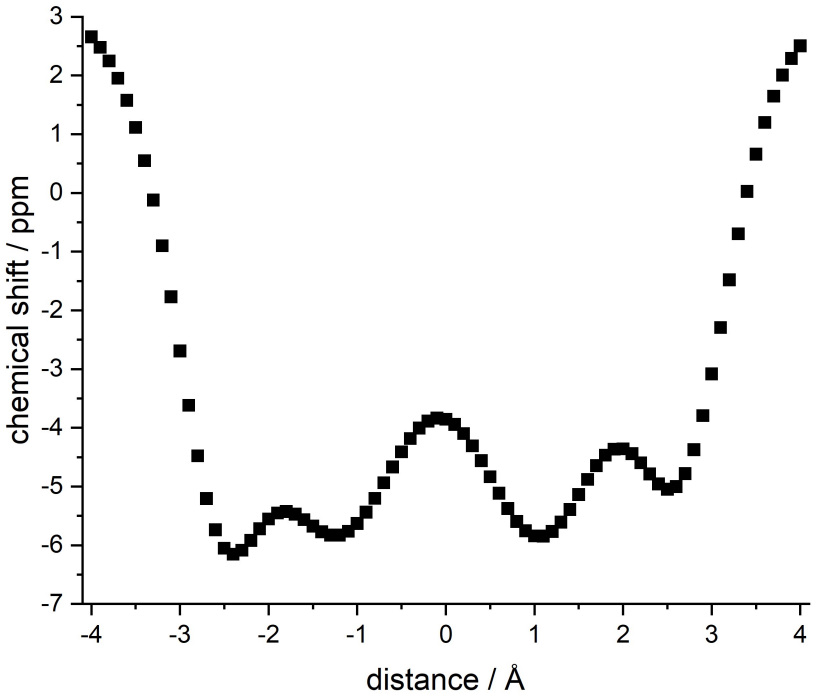

Figure S35. NICS XY-Scan of hetero ring of neutral **4a**.

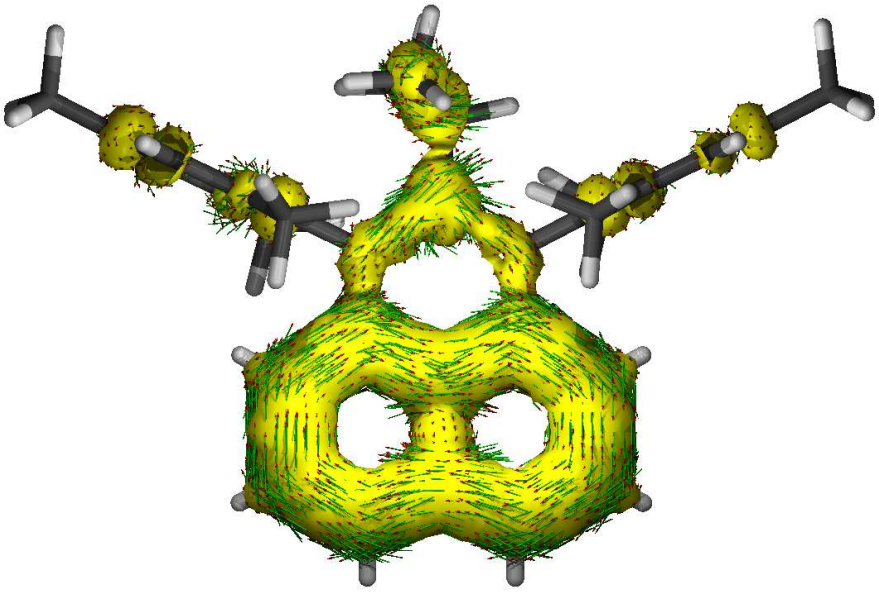

Figure S36. ACID map of neutral **4a** (isovalue 0.015).

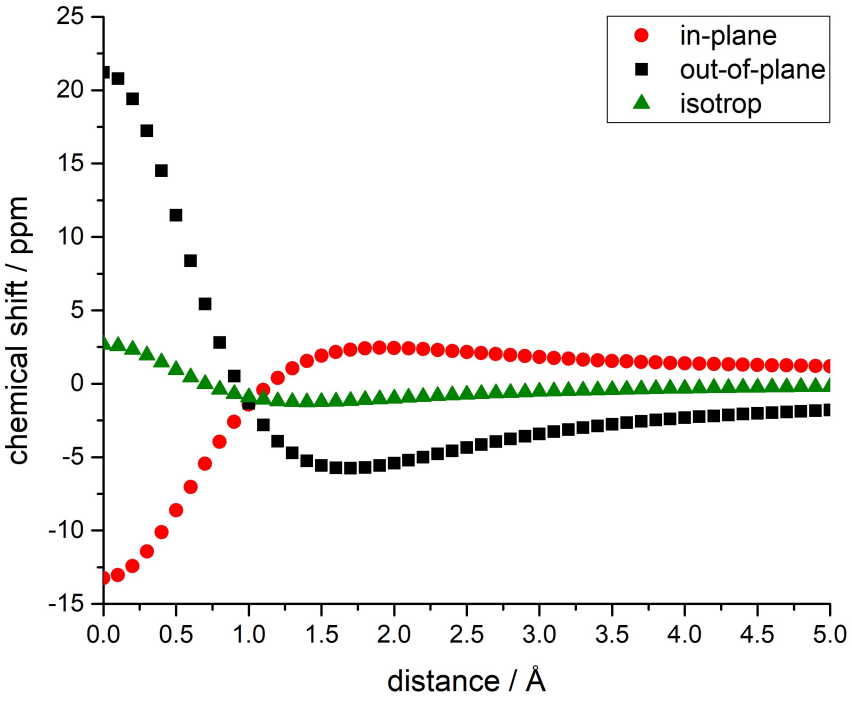

Figure S37. NICS Scan of naphthalenic rings of mono anionic **4a**.

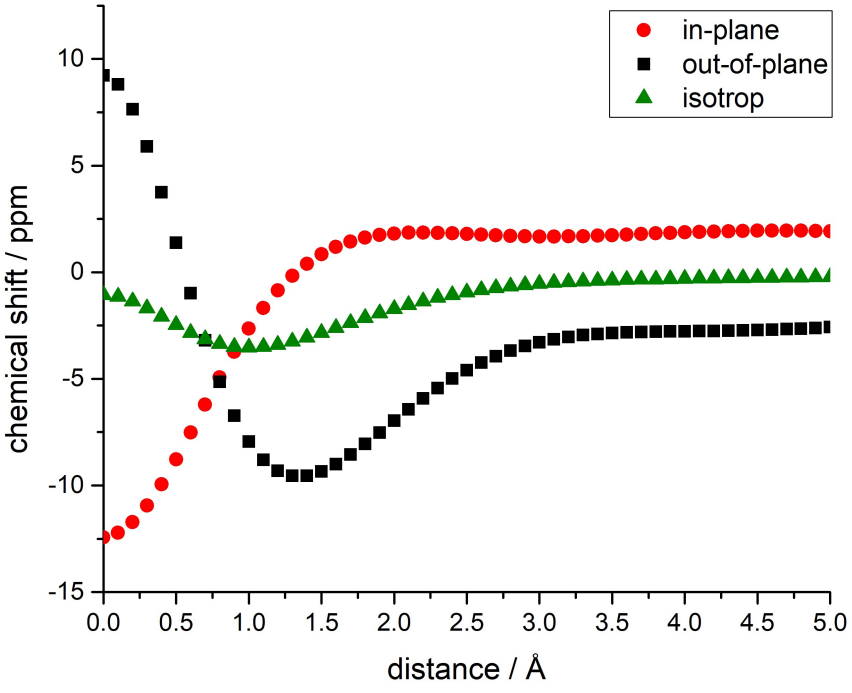

Figure S38. NICS Scan of hetero ring of mono anionic **4a**.

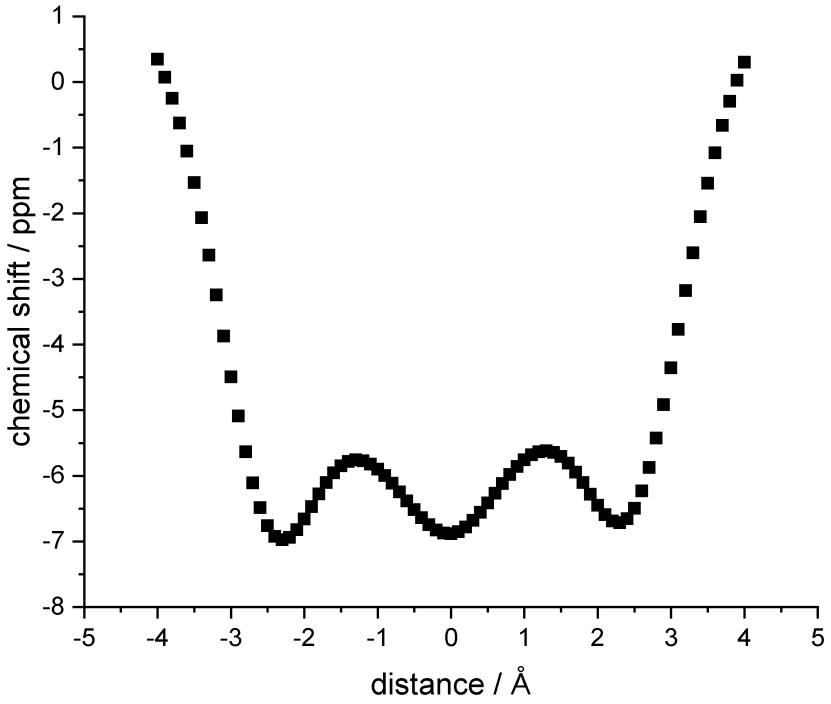

Figure S39. NICS XY-Scan of naphthalenic rings of mono anionic **4a**.

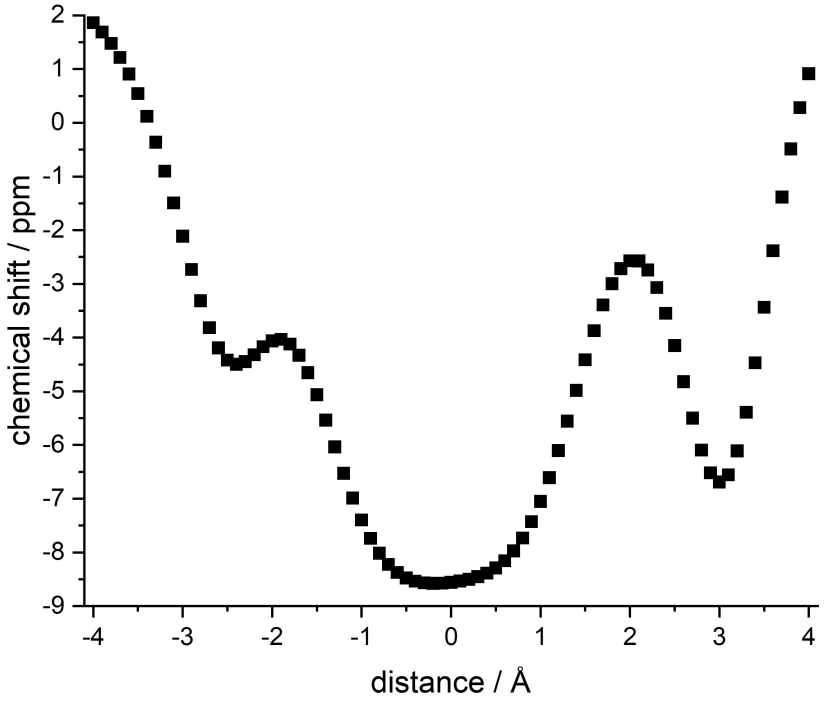

Figure S40. NICS XY-Scan of hetero ring of mono anionic **4a**.

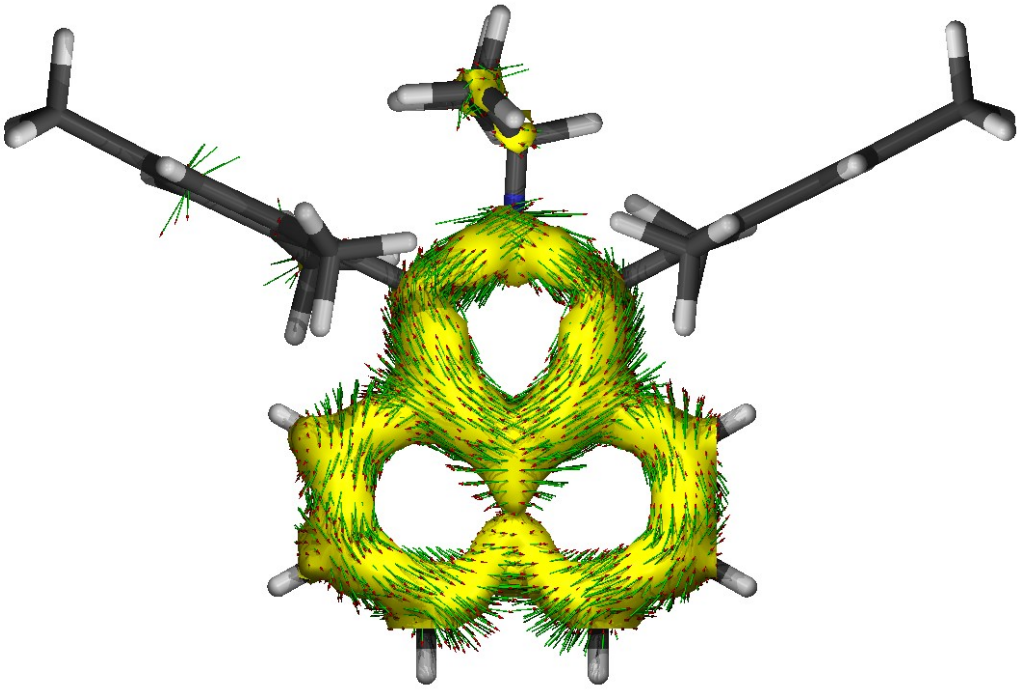

Figure S41. ACID map of mono anionic **4a** (isovalue 0.015).

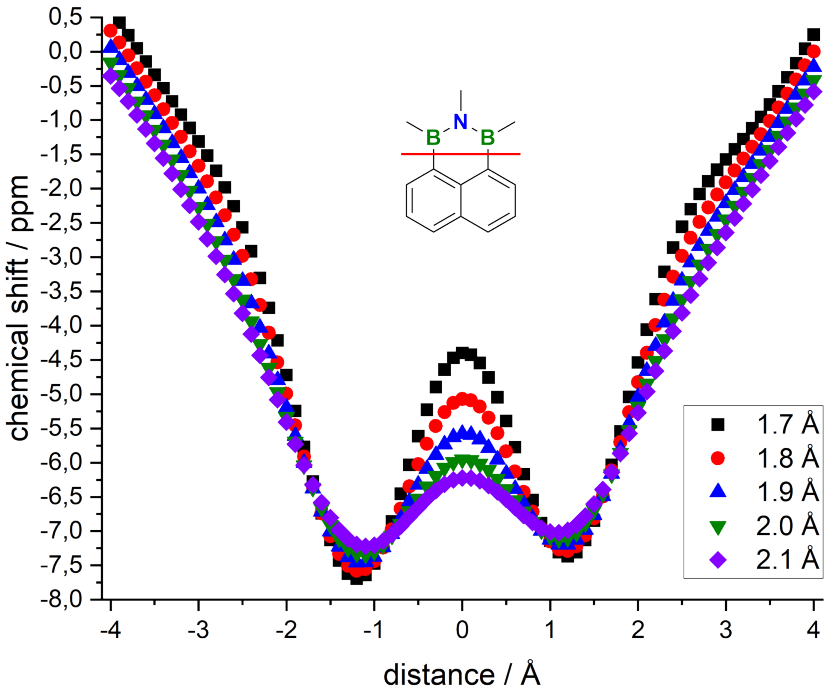

Figure S42. NICS-*X*-height-scan for the hetero ring of a model compound with only methyl groups on boron and nitrogen (see structure as inset). This indicates that a scan-height of 2.1 Å or higher is more appropriate in this case. With increasing scan-height, the maximum at 0.0 Å decreases, whereas the minima almost stay at the same level. A scan-height of 1.7 Å corresponds to the NICS-*X*-height scans reported for all-carbon systems by Stanger *et al.*[17b] As the naphthalenic rings lose a major part of the π-effects at the height of 2.1 Å (cf. Figure S43), all NICS-*X*-scans were performed at 1.7 Å above the ring plane.

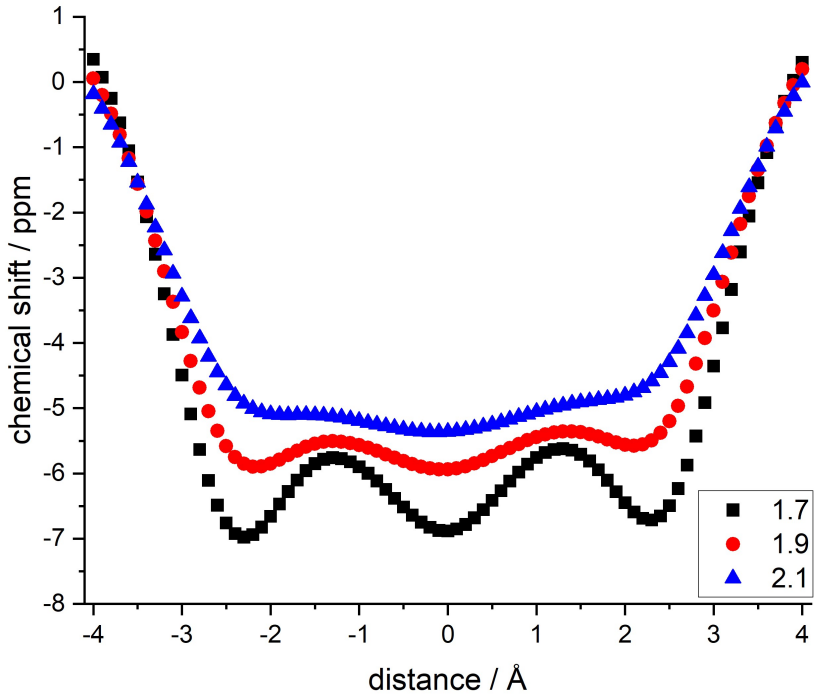

Figure S43. NICS-X-height-scan of naphthalenic rings of mono anionic **4a**, indicating a scan-height of 1.7 Å for all-carbon systems to be the most appropriate, as shown by Stanger *et al.*[17b] Upon increasing the scan-height, the minima as well as the maxima decrease, which shows that the system loses major parts of its π-effects at this height. Therefore, all NICS-X-Scans were performed at a height of 1.7 Å.

Cartesian coordinates (Å) and total energies (a.u.) of optimized stationary points

neutral 4a:

Total energy (B3LYP-D3(BJ)/def2-SV(P)): -1305.281722585

C	-0.171518	0.016715	-0.070161
C	-0.156848	0.013049	1.357787
C	1.088602	0.008046	2.064898
C	2.301405	0.008209	1.323582
C	2.281511	0.012063	-0.057595
C	1.046801	0.015586	-0.746707
C	-1.392950	0.012523	2.073926
C	-1.347465	0.005357	3.466912
C	-0.123493	0.000026	4.175060
C	1.073465	0.001814	3.486160
B	-2.763551	0.022864	1.317168
N	-2.777589	0.040308	-0.128477
B	-1.524996	0.023677	-0.847508
C	-1.466223	0.005250	-2.428935
C	-1.405563	-1.223233	-3.126128
C	-1.316632	-1.228081	-4.522716
C	-1.275329	-0.037541	-5.261907
C	-1.313337	1.172131	-4.560194
C	-1.403092	1.209327	-3.161154
C	-1.415900	-2.528228	-2.361515
C	-1.419910	2.537648	-2.438235
C	-4.063353	0.006739	2.219891
C	-4.620747	1.209532	2.699453
C	-5.762488	1.175946	3.513803
C	-6.355150	-0.031558	3.897202
C	-5.751931	-1.223318	3.470867
C	-4.613251	-1.219742	2.657456
C	-3.957493	2.536482	2.403487
C	-3.936300	-2.527608	2.311854
H	-2.285210	0.004176	4.030700
H	-0.128759	-0.005525	5.269370
H	1.048012	0.017979	-1.841126
H	3.219407	0.011966	-0.621454
H	-1.273155	-2.187696	-5.050847
C	-1.187720	-0.071431	-6.769087
H	-1.267869	2.114973	-5.116659
C	-4.035462	0.065987	-0.935098
H	-6.179732	-2.182338	3.785822
C	-7.601800	-0.062162	4.748455
H	-6.198109	2.119856	3.860783
H	-3.197578	2.767728	3.174289
H	-3.433063	2.533616	1.433995
H	-4.686021	3.366062	2.395422

H	-4.642842	-3.375150	2.344239
H	-3.474343	-2.506159	1.311142
H	-3.122852	-2.742272	3.030964
H	-1.366973	-3.396900	-3.039760
H	-0.557221	-2.589975	-1.667467
H	-2.327667	-2.632274	-1.745994
H	-0.591511	2.606408	-1.709069
H	-1.325279	3.383503	-3.140106
H	-2.356417	2.677698	-1.868325
H	2.026575	-0.002159	4.025672
H	3.252704	0.004567	1.866256
H	-7.876182	0.946854	5.100705
H	-8.463660	-0.465399	4.183323
H	-7.468845	-0.707814	5.636131
H	-1.110217	0.944447	-7.192656
H	-0.307338	-0.648056	-7.109266
H	-2.079038	-0.553675	-7.213130
H	-3.701898	0.083062	-1.981142
C	-4.892666	-1.193230	-0.774195
C	-4.870071	1.333267	-0.724425
H	-5.656135	1.383907	-1.499259
H	-5.364286	1.344938	0.259476
H	-4.248234	2.239877	-0.816790
H	-5.688616	-1.191613	-1.540541
H	-4.290592	-2.106247	-0.918560
H	-5.375477	-1.242001	0.214338

mono anionic 4a:

Total energy (B3LYP-D3(BJ)/def2-SV(P)): -1305.308885

C	-3.372033	-0.912921	1.233217
C	-2.708668	-0.596325	0.026698
C	-3.36053	-0.898362	-1.190873
C	-4.608874	-1.53597	-1.187628
C	-5.253714	-1.881374	0.006642
C	-4.621371	-1.549608	1.210593
B	-1.299073	0.157773	0.030551
C	-1.289109	1.684803	-0.001348
C	-0.040666	2.392337	-0.014812
C	-0.033748	3.839444	-0.043238
C	-1.274748	4.531981	-0.057102
C	-2.486952	3.832908	-0.04483
C	-2.496555	2.439585	-0.017645
C	1.21311	4.520749	-0.058335
C	2.417505	3.808056	-0.049054
C	2.412968	2.414882	-0.023818

C	1.199579	1.668108	-0.00445
B	1.205771	0.137178	0.024091
N	-0.053806	-0.590459	0.05343
C	-0.144217	-2.069023	0.098385
C	0.390739	-2.762954	-1.161152
C	-2.722907	-0.495199	-2.50131
C	-6.579022	-2.607444	-0.006538
C	-2.737354	-0.542252	2.554392
C	2.633567	-0.581099	0.00134
C	3.277994	-0.862383	-1.226182
C	4.541399	-1.468983	-1.242419
C	5.219168	-1.785272	-0.058042
C	4.613207	-1.434187	1.153175
C	3.349277	-0.825997	1.194183
C	2.642147	-0.431323	-2.528635
C	2.795001	-0.35731	2.520691
C	6.554972	-2.490688	-0.091317
C	0.467202	-2.692165	1.360403
H	3.36642	1.875783	-0.01842
H	3.370684	4.351675	-0.062241
H	-3.453405	1.90626	-0.006783
H	-3.433928	4.387268	-0.056706
H	-5.095743	-1.763664	-2.14427
H	-5.118188	-1.787363	2.159544
H	5.014833	-1.692998	-2.206694
H	5.14266	-1.631549	2.093771
H	3.029771	0.713739	2.670389
H	1.697397	-0.437613	2.55773
H	3.22235	-0.924107	3.368367
H	3.079834	-0.962151	-3.393937
H	1.552759	-0.593869	-2.528345
H	2.789635	0.654888	-2.678548
H	-3.312777	-0.846704	-3.367169
H	-2.629121	0.604434	-2.563186
H	-1.698076	-0.895795	-2.593752
H	-2.504165	0.537316	2.584121
H	-3.39829	-0.784402	3.406272
H	-1.778632	-1.070956	2.704131
H	1.214872	5.617284	-0.079096
H	-1.265415	5.628496	-0.078886
H	7.128999	-2.314513	0.83626
H	6.434131	-3.587662	-0.197328
H	7.172631	-2.151313	-0.943271
H	-7.14796	-2.428533	0.923738
H	-7.208939	-2.288126	-0.857077
H	-6.442681	-3.703905	-0.099305

H	-1.218255	-2.29973	0.136742
H	0.176889	-3.758047	1.426701
H	1.567414	-2.639334	1.356385
H	0.097021	-2.182742	2.266488
H	0.120007	-3.835814	-1.139227
H	-0.053193	-2.32078	-2.069391
H	1.487418	-2.690772	-1.236564

Cartesian coordinates (Å) for NICS calculations

NICS Scan of naphthalenic rings of neutral 4a:

C	3.35493100	-0.74714100	1.18911200
C	2.62253400	-0.52335000	0.00461500
C	3.23152000	-0.81374000	-1.23680400
C	4.49774600	-1.41040500	-1.27026700
C	5.20311400	-1.70447800	-0.09562200
C	4.62128800	-1.34525200	1.12551800
B	1.19817000	0.16422200	0.04725600
N	-0.05149300	-0.56061000	0.10029800
C	-0.13425400	-2.05108800	0.17331700
C	0.50160000	-2.63631800	1.43819400
C	2.55585900	-0.41512800	-2.53013600
C	6.54350900	-2.39699300	-0.14981600
C	2.81727600	-0.27918500	2.52328900
C	1.17982700	1.72938900	0.01191900
C	-0.05303600	2.45099800	0.01118700
C	-0.05305300	3.88298800	-0.01066900
C	1.19040300	4.57113400	-0.03255400
C	2.38032800	3.87008600	-0.03496600
C	2.36874500	2.45618000	-0.01369000
C	-1.29667300	4.57141400	-0.01316800
C	-2.48787900	3.87218600	0.00261200
C	-2.47738100	2.45832600	0.02076200
C	-1.28734000	1.73340600	0.02663500
B	-1.29456400	0.17330700	0.05446300
C	-2.69634800	-0.55900100	0.01585300
C	-3.38194800	-0.87628700	1.20823000
C	-4.63905800	-1.49194700	1.14784500
C	-5.24663400	-1.80312900	-0.07472100
C	-4.56777800	-1.46223000	-1.25173900
C	-3.31190600	-0.84285300	-1.22343500
C	-2.76232600	-0.54388500	2.54701900
C	-2.63247300	-0.44847100	-2.51623200

C	-6.58307900	-2.50394700	-0.12559200
C	0.38179600	-2.75702700	-1.08393600
H	3.32195500	1.91879600	-0.01677700
H	3.33460600	4.40542600	-0.05349700
H	-3.42948800	1.91872500	0.03106200
H	-3.44136500	4.40923500	-0.00016600
H	-5.03328200	-1.67921500	-2.21998900
H	-5.16045700	-1.73242300	2.08130000
H	4.94995700	-1.64787000	-2.24008600
H	5.17031700	-1.53181200	2.05557700
H	3.08658400	0.78013500	2.69713400
H	1.71760300	-0.33631100	2.57282000
H	3.22861900	-0.86937800	3.36065200
H	2.94750500	-0.98678000	-3.38922900
H	1.46360300	-0.56110500	-2.49226900
H	2.72352400	0.65896000	-2.73717300
H	-3.19222400	-0.80915500	-3.39581200
H	-2.54360200	0.65090700	-2.59827700
H	-1.60614700	-0.85232100	-2.57932800
H	-2.51088100	0.53053000	2.61648300
H	-3.44122200	-0.78868900	3.38142200
H	-1.82107500	-1.10128800	2.70660100
H	1.18916700	5.66622200	-0.04954700
H	-1.29467500	5.66652400	-0.02943600
H	7.13352900	-2.21005200	0.76419000
H	6.42271300	-3.49378500	-0.24475300
H	7.13865200	-2.06058000	-1.01739800
H	-7.16955500	-2.32488100	0.79239200
H	-7.18472800	-2.16715200	-0.98835600
H	-6.45642900	-3.59972100	-0.22547500
H	-1.20776000	-2.27350100	0.23333600
H	0.21049300	-3.69795700	1.53270500
H	1.60129700	-2.58896300	1.41050200
H	0.14894300	-2.10930800	2.34118800
H	0.11865300	-3.82892300	-1.03310200
H	-0.08435300	-2.34139500	-1.99317900
H	1.47611300	-2.68177100	-1.18075800
Bq	-1.29206900	3.17155900	0.00646500
Bq	-1.29206900	3.17155900	0.10646500
Bq	-1.29206900	3.17155900	0.20646500
Bq	-1.29206900	3.17155900	0.30646500
Bq	-1.29206900	3.17155900	0.40646500
Bq	-1.29206900	3.17155900	0.50646500
Bq	-1.29206900	3.17155900	0.60646500
Bq	-1.29206900	3.17155900	0.70646500
Bq	-1.29206900	3.17155900	0.80646500

Bq	-1.29206900	3.17155900	0.90646500
Bq	-1.29206900	3.17155900	1.00646500
Bq	-1.29206900	3.17155900	1.10646500
Bq	-1.29206900	3.17155900	1.20646500
Bq	-1.29206900	3.17155900	1.30646500
Bq	-1.29206900	3.17155900	1.40646500
Bq	-1.29206900	3.17155900	1.50646500
Bq	-1.29206900	3.17155900	1.60646500
Bq	-1.29206900	3.17155900	1.70646500
Bq	-1.29206900	3.17155900	1.80646500
Bq	-1.29206900	3.17155900	1.90646500
Bq	-1.29206900	3.17155900	2.00646500
Bq	-1.29206900	3.17155900	2.10646500
Bq	-1.29206900	3.17155900	2.20646500
Bq	-1.29206900	3.17155900	2.30646500
Bq	-1.29206900	3.17155900	2.40646500
Bq	-1.29206900	3.17155900	2.50646500
Bq	-1.29206900	3.17155900	2.60646500
Bq	-1.29206900	3.17155900	2.70646500
Bq	-1.29206900	3.17155900	2.80646500
Bq	-1.29206900	3.17155900	2.90646500
Bq	-1.29206900	3.17155900	3.00646500
Bq	-1.29206900	3.17155900	3.10646500
Bq	-1.29206900	3.17155900	3.20646500
Bq	-1.29206900	3.17155900	3.30646500
Bq	-1.29206900	3.17155900	3.40646500
Bq	-1.29206900	3.17155900	3.50646500
Bq	-1.29206900	3.17155900	3.60646500
Bq	-1.29206900	3.17155900	3.70646500
Bq	-1.29206900	3.17155900	3.80646500
Bq	-1.29206900	3.17155900	3.90646500
Bq	-1.29206900	3.17155900	4.00646500
Bq	-1.29206900	3.17155900	4.10646500
Bq	-1.29206900	3.17155900	4.20646500
Bq	-1.29206900	3.17155900	4.30646500
Bq	-1.29206900	3.17155900	4.40646500
Bq	-1.29206900	3.17155900	4.50646500
Bq	-1.29206900	3.17155900	4.60646500
Bq	-1.29206900	3.17155900	4.70646500
Bq	-1.29206900	3.17155900	4.80646500
Bq	-1.29206900	3.17155900	4.90646500
Bq	-1.29206900	3.17155900	5.00646500

NICS Scan of hetero ring of neutral 4a:

C	-3.38194756	-0.87628659	1.20823008
C	-2.69634820	-0.55900092	0.01585346

C	-3.31190670	-0.84285310	-1.22343475
C	-4.56777904	-1.46222985	-1.25173879
C	-5.24663536	-1.80312857	-0.07472060
C	-4.63905798	-1.49194730	1.14784520
B	-1.29456365	0.17330652	0.05446250
C	-1.28733956	1.73340601	0.02663466
C	-0.05303622	2.45099807	0.01118746
C	-0.05305265	3.88298784	-0.01066916
C	-1.29667305	4.57141393	-0.01316801
C	-2.48787911	3.87218596	0.00261198
C	-2.47738093	2.45832596	0.02076223
C	1.19040294	4.57113396	-0.03255423
C	2.38032802	3.87008564	-0.03496566
C	2.36874503	2.45618034	-0.01368995
C	1.17982719	1.72938870	0.01191875
B	1.19817049	0.16422154	0.04725613
N	-0.05149324	-0.56061029	0.10029763
C	-0.13425382	-2.05108822	0.17331713
C	0.38179623	-2.75702725	-1.08393588
C	-2.63247443	-0.44847118	-2.51623170
C	-6.58308011	-2.50394739	-0.12559214
C	-2.76232641	-0.54388465	2.54701933
C	2.62253359	-0.52334991	0.00461488
C	3.23152017	-0.81374048	-1.23680432
C	4.49774645	-1.41040512	-1.27026744
C	5.20311354	-1.70447754	-0.09562221
C	4.62128783	-1.34525182	1.12551764
C	3.35493147	-0.74714089	1.18911163
C	2.55585939	-0.41512847	-2.53013581
C	2.81727573	-0.27918472	2.52328923
C	6.54350907	-2.39699289	-0.14981588
C	0.50160047	-2.63631823	1.43819381
H	3.32195512	1.91879465	-0.01677730
H	3.33460649	4.40542503	-0.05349722
H	-3.42948827	1.91872531	0.03106200
H	-3.44136529	4.40923530	-0.00016527
H	-5.03328288	-1.67921447	-2.21998918
H	-5.16045670	-1.73242302	2.08129984
H	4.94995683	-1.64786973	-2.24008587
H	5.17031724	-1.53181171	2.05557704
H	3.08658378	0.78013466	2.69713414
H	1.71760267	-0.33631128	2.57282016
H	3.22861872	-0.86937786	3.36065177
H	2.94750465	-0.98677974	-3.38922922
H	1.46360324	-0.56110452	-2.49226863
H	2.72352377	0.65896036	-2.73717299

H	-3.19222533	-0.80915510	-3.39581182
H	-2.54360268	0.65090662	-2.59827670
H	-1.60614793	-0.85232146	-2.57932826
H	-2.51088087	0.53053018	2.61648317
H	-3.44122167	-0.78868867	3.38142173
H	-1.82107501	-1.10128767	2.70660082
H	1.18916684	5.66622198	-0.04954740
H	-1.29467484	5.66652376	-0.02943573
H	7.13352886	-2.21005221	0.76419018
H	6.42271335	-3.49378532	-0.24475383
H	7.13865168	-2.06057975	-1.01739860
H	-7.16955616	-2.32488121	0.79239316
H	-7.18472852	-2.16715110	-0.98835634
H	-6.45643010	-3.59972136	-0.22547514
H	-1.20775972	-2.27350050	0.23333568
H	0.21049273	-3.69795688	1.53270545
H	1.60129699	-2.58896349	1.41050227
H	0.14894282	-2.10930760	2.34118814
H	0.11865267	-3.82892286	-1.03310177
H	-0.08435275	-2.34139536	-1.99317872
H	1.47611270	-2.68177102	-1.18075764
Bq	-0.04531870	0.94580719	0.00000000
Bq	-0.04531870	0.94580719	0.10000000
Bq	-0.04531870	0.94580719	0.20000000
Bq	-0.04531870	0.94580719	0.30000000
Bq	-0.04531870	0.94580719	0.40000000
Bq	-0.04531870	0.94580719	0.50000000
Bq	-0.04531870	0.94580719	0.60000000
Bq	-0.04531870	0.94580719	0.70000000
Bq	-0.04531870	0.94580719	0.80000000
Bq	-0.04531870	0.94580719	0.90000000
Bq	-0.04531870	0.94580719	1.00000000
Bq	-0.04531870	0.94580719	1.10000000
Bq	-0.04531870	0.94580719	1.20000000
Bq	-0.04531870	0.94580719	1.30000000
Bq	-0.04531870	0.94580719	1.40000000
Bq	-0.04531870	0.94580719	1.50000000
Bq	-0.04531870	0.94580719	1.60000000
Bq	-0.04531870	0.94580719	1.70000000
Bq	-0.04531870	0.94580719	1.80000000
Bq	-0.04531870	0.94580719	1.90000000
Bq	-0.04531870	0.94580719	2.00000000
Bq	-0.04531870	0.94580719	2.10000000
Bq	-0.04531870	0.94580719	2.20000000
Bq	-0.04531870	0.94580719	2.30000000
Bq	-0.04531870	0.94580719	2.40000000

Bq	-0.04531870	0.94580719	2.50000000
Bq	-0.04531870	0.94580719	2.60000000
Bq	-0.04531870	0.94580719	2.70000000
Bq	-0.04531870	0.94580719	2.80000000
Bq	-0.04531870	0.94580719	2.90000000
Bq	-0.04531870	0.94580719	3.00000000
Bq	-0.04531870	0.94580719	3.10000000
Bq	-0.04531870	0.94580719	3.20000000
Bq	-0.04531870	0.94580719	3.30000000
Bq	-0.04531870	0.94580719	3.40000000
Bq	-0.04531870	0.94580719	3.50000000
Bq	-0.04531870	0.94580719	3.60000000
Bq	-0.04531870	0.94580719	3.70000000
Bq	-0.04531870	0.94580719	3.80000000
Bq	-0.04531870	0.94580719	3.90000000
Bq	-0.04531870	0.94580719	4.00000000
Bq	-0.04531870	0.94580719	4.10000000
Bq	-0.04531870	0.94580719	4.20000000
Bq	-0.04531870	0.94580719	4.30000000
Bq	-0.04531870	0.94580719	4.40000000
Bq	-0.04531870	0.94580719	4.50000000
Bq	-0.04531870	0.94580719	4.60000000
Bq	-0.04531870	0.94580719	4.70000000
Bq	-0.04531870	0.94580719	4.80000000
Bq	-0.04531870	0.94580719	4.90000000
Bq	-0.04531870	0.94580719	5.00000000

NICS XY-Scan of naphthalenic rings of neutral 4a:

C	-3.38194756	-0.87628659	1.20823008
C	-2.69634820	-0.55900092	0.01585346
C	-3.31190670	-0.84285310	-1.22343475
C	-4.56777904	-1.46222985	-1.25173879
C	-5.24663536	-1.80312857	-0.07472060
C	-4.63905798	-1.49194730	1.14784520
B	-1.29456365	0.17330652	0.05446250
C	-1.28733956	1.73340601	0.02663466
C	-0.05303622	2.45099807	0.01118746
C	-0.05305265	3.88298784	-0.01066916
C	-1.29667305	4.57141393	-0.01316801
C	-2.48787911	3.87218596	0.00261198
C	-2.47738093	2.45832596	0.02076223
C	1.19040294	4.57113396	-0.03255423
C	2.38032802	3.87008564	-0.03496566
C	2.36874503	2.45618034	-0.01368995
C	1.17982719	1.72938870	0.01191875
B	1.19817049	0.16422154	0.04725613

N	-0.05149324	-0.56061029	0.10029763
C	-0.13425382	-2.05108822	0.17331713
C	0.38179623	-2.75702725	-1.08393588
C	-2.63247443	-0.44847118	-2.51623170
C	-6.58308011	-2.50394739	-0.12559214
C	-2.76232641	-0.54388465	2.54701933
C	2.62253359	-0.52334991	0.00461488
C	3.23152017	-0.81374048	-1.23680432
C	4.49774645	-1.41040512	-1.27026744
C	5.20311354	-1.70447754	-0.09562221
C	4.62128783	-1.34525182	1.12551764
C	3.35493147	-0.74714089	1.18911163
C	2.55585939	-0.41512847	-2.53013581
C	2.81727573	-0.27918472	2.52328923
C	6.54350907	-2.39699289	-0.14981588
C	0.50160047	-2.63631823	1.43819381
H	3.32195512	1.91879465	-0.01677730
H	3.33460649	4.40542503	-0.05349722
H	-3.42948827	1.91872531	0.03106200
H	-3.44136529	4.40923530	-0.00016527
H	-5.03328288	-1.67921447	-2.21998918
H	-5.16045670	-1.73242302	2.08129984
H	4.94995683	-1.64786973	-2.24008587
H	5.17031724	-1.53181171	2.05557704
H	3.08658378	0.78013466	2.69713414
H	1.71760267	-0.33631128	2.57282016
H	3.22861872	-0.86937786	3.36065177
H	2.94750465	-0.98677974	-3.38922922
H	1.46360324	-0.56110452	-2.49226863
H	2.72352377	0.65896036	-2.73717299
H	-3.19222533	-0.80915510	-3.39581182
H	-2.54360268	0.65090662	-2.59827670
H	-1.60614793	-0.85232146	-2.57932826
H	-2.51088087	0.53053018	2.61648317
H	-3.44122167	-0.78868867	3.38142173
H	-1.82107501	-1.10128767	2.70660082
H	1.18916684	5.66622198	-0.04954740
H	-1.29467484	5.66652376	-0.02943573
H	7.13352886	-2.21005221	0.76419018
H	6.42271335	-3.49378532	-0.24475383
H	7.13865168	-2.06057975	-1.01739860
H	-7.16955616	-2.32488121	0.79239316
H	-7.18472852	-2.16715110	-0.98835634
H	-6.45643010	-3.59972136	-0.22547514
H	-1.20775972	-2.27350050	0.23333568
H	0.21049273	-3.69795688	1.53270545

H	1.60129699	-2.58896349	1.41050227
H	0.14894282	-2.10930760	2.34118814
H	0.11865267	-3.82892286	-1.03310177
H	-0.08435275	-2.34139536	-1.99317872
H	1.47611270	-2.68177102	-1.18075764
Bq	0.00000000	3.16699296	1.70000000
Bq	-0.10000000	3.16699296	1.70000000
Bq	-0.20000000	3.16699296	1.70000000
Bq	-0.30000000	3.16699296	1.70000000
Bq	-0.40000000	3.16699296	1.70000000
Bq	-0.50000000	3.16699296	1.70000000
Bq	-0.60000000	3.16699296	1.70000000
Bq	-0.70000000	3.16699296	1.70000000
Bq	-0.80000000	3.16699296	1.70000000
Bq	-0.90000000	3.16699296	1.70000000
Bq	-1.00000000	3.16699296	1.70000000
Bq	-1.10000000	3.16699296	1.70000000
Bq	-1.20000000	3.16699296	1.70000000
Bq	-1.30000000	3.16699296	1.70000000
Bq	-1.40000000	3.16699296	1.70000000
Bq	-1.50000000	3.16699296	1.70000000
Bq	-1.60000000	3.16699296	1.70000000
Bq	-1.70000000	3.16699296	1.70000000
Bq	-1.80000000	3.16699296	1.70000000
Bq	-1.90000000	3.16699296	1.70000000
Bq	-2.00000000	3.16699296	1.70000000
Bq	-2.10000000	3.16699296	1.70000000
Bq	-2.20000000	3.16699296	1.70000000
Bq	-2.30000000	3.16699296	1.70000000
Bq	-2.40000000	3.16699296	1.70000000
Bq	-2.50000000	3.16699296	1.70000000
Bq	-2.60000000	3.16699296	1.70000000
Bq	-2.70000000	3.16699296	1.70000000
Bq	-2.80000000	3.16699296	1.70000000
Bq	-2.90000000	3.16699296	1.70000000
Bq	-3.00000000	3.16699296	1.70000000
Bq	-3.10000000	3.16699296	1.70000000
Bq	-3.20000000	3.16699296	1.70000000
Bq	-3.30000000	3.16699296	1.70000000
Bq	-3.40000000	3.16699296	1.70000000
Bq	-3.50000000	3.16699296	1.70000000
Bq	-3.60000000	3.16699296	1.70000000
Bq	-3.70000000	3.16699296	1.70000000
Bq	-3.80000000	3.16699296	1.70000000
Bq	-3.90000000	3.16699296	1.70000000
Bq	-4.00000000	3.16699296	1.70000000

Bq	0.10000000	3.16699296	1.70000000
Bq	0.20000000	3.16699296	1.70000000
Bq	0.30000000	3.16699296	1.70000000
Bq	0.40000000	3.16699296	1.70000000
Bq	0.50000000	3.16699296	1.70000000
Bq	0.60000000	3.16699296	1.70000000
Bq	0.70000000	3.16699296	1.70000000
Bq	0.80000000	3.16699296	1.70000000
Bq	0.90000000	3.16699296	1.70000000
Bq	1.00000000	3.16699296	1.70000000
Bq	1.10000000	3.16699296	1.70000000
Bq	1.20000000	3.16699296	1.70000000
Bq	1.30000000	3.16699296	1.70000000
Bq	1.40000000	3.16699296	1.70000000
Bq	1.50000000	3.16699296	1.70000000
Bq	1.60000000	3.16699296	1.70000000
Bq	1.70000000	3.16699296	1.70000000
Bq	1.80000000	3.16699296	1.70000000
Bq	1.90000000	3.16699296	1.70000000
Bq	2.00000000	3.16699296	1.70000000
Bq	2.10000000	3.16699296	1.70000000
Bq	2.20000000	3.16699296	1.70000000
Bq	2.30000000	3.16699296	1.70000000
Bq	2.40000000	3.16699296	1.70000000
Bq	2.50000000	3.16699296	1.70000000
Bq	2.60000000	3.16699296	1.70000000
Bq	2.70000000	3.16699296	1.70000000
Bq	2.80000000	3.16699296	1.70000000
Bq	2.90000000	3.16699296	1.70000000
Bq	3.00000000	3.16699296	1.70000000
Bq	3.10000000	3.16699296	1.70000000
Bq	3.20000000	3.16699296	1.70000000
Bq	3.30000000	3.16699296	1.70000000
Bq	3.40000000	3.16699296	1.70000000
Bq	3.50000000	3.16699296	1.70000000
Bq	3.60000000	3.16699296	1.70000000
Bq	3.70000000	3.16699296	1.70000000
Bq	3.80000000	3.16699296	1.70000000
Bq	3.90000000	3.16699296	1.70000000
Bq	4.00000000	3.16699296	1.70000000

NICS XY-Scan of hetero ring of neutral 4a:

C	-3.38194756	-0.87628659	1.20823008
C	-2.69634820	-0.55900092	0.01585346
C	-3.31190670	-0.84285310	-1.22343475
C	-4.56777904	-1.46222985	-1.25173879

C	-5.24663536	-1.80312857	-0.07472060
C	-4.63905798	-1.49194730	1.14784520
B	-1.29456365	0.17330652	0.05446250
C	-1.28733956	1.73340601	0.02663466
C	-0.05303622	2.45099807	0.01118746
C	-0.05305265	3.88298784	-0.01066916
C	-1.29667305	4.57141393	-0.01316801
C	-2.48787911	3.87218596	0.00261198
C	-2.47738093	2.45832596	0.02076223
C	1.19040294	4.57113396	-0.03255423
C	2.38032802	3.87008564	-0.03496566
C	2.36874503	2.45618034	-0.01368995
C	1.17982719	1.72938870	0.01191875
B	1.19817049	0.16422154	0.04725613
N	-0.05149324	-0.56061029	0.10029763
C	-0.13425382	-2.05108822	0.17331713
C	0.38179623	-2.75702725	-1.08393588
C	-2.63247443	-0.44847118	-2.51623170
C	-6.58308011	-2.50394739	-0.12559214
C	-2.76232641	-0.54388465	2.54701933
C	2.62253359	-0.52334991	0.00461488
C	3.23152017	-0.81374048	-1.23680432
C	4.49774645	-1.41040512	-1.27026744
C	5.20311354	-1.70447754	-0.09562221
C	4.62128783	-1.34525182	1.12551764
C	3.35493147	-0.74714089	1.18911163
C	2.55585939	-0.41512847	-2.53013581
C	2.81727573	-0.27918472	2.52328923
C	6.54350907	-2.39699289	-0.14981588
C	0.50160047	-2.63631823	1.43819381
H	3.32195512	1.91879465	-0.01677730
H	3.33460649	4.40542503	-0.05349722
H	-3.42948827	1.91872531	0.03106200
H	-3.44136529	4.40923530	-0.00016527
H	-5.03328288	-1.67921447	-2.21998918
H	-5.16045670	-1.73242302	2.08129984
H	4.94995683	-1.64786973	-2.24008587
H	5.17031724	-1.53181171	2.05557704
H	3.08658378	0.78013466	2.69713414
H	1.71760267	-0.33631128	2.57282016
H	3.22861872	-0.86937786	3.36065177
H	2.94750465	-0.98677974	-3.38922922
H	1.46360324	-0.56110452	-2.49226863
H	2.72352377	0.65896036	-2.73717299
H	-3.19222533	-0.80915510	-3.39581182
H	-2.54360268	0.65090662	-2.59827670

H	-1.60614793	-0.85232146	-2.57932826
H	-2.51088087	0.53053018	2.61648317
H	-3.44122167	-0.78868867	3.38142173
H	-1.82107501	-1.10128767	2.70660082
H	1.18916684	5.66622198	-0.04954740
H	-1.29467484	5.66652376	-0.02943573
H	7.13352886	-2.21005221	0.76419018
H	6.42271335	-3.49378532	-0.24475383
H	7.13865168	-2.06057975	-1.01739860
H	-7.16955616	-2.32488121	0.79239316
H	-7.18472852	-2.16715110	-0.98835634
H	-6.45643010	-3.59972136	-0.22547514
H	-1.20775972	-2.27350050	0.23333568
H	0.21049273	-3.69795688	1.53270545
H	1.60129699	-2.58896349	1.41050227
H	0.14894282	-2.10930760	2.34118814
H	0.11865267	-3.82892286	-1.03310177
H	-0.08435275	-2.34139536	-1.99317872
H	1.47611270	-2.68177102	-1.18075764
Bq	-4.09091530	0.96076164	-1.74000000
Bq	-3.99091662	0.96049724	-1.74000000
Bq	-3.89091794	0.96023284	-1.74000000
Bq	-3.79091926	0.95996844	-1.74000000
Bq	-3.69092058	0.95970404	-1.74000000
Bq	-3.59092190	0.95943964	-1.74000000
Bq	-3.49092322	0.95917524	-1.74000000
Bq	-3.39092454	0.95891084	-1.74000000
Bq	-3.29092586	0.95864644	-1.74000000
Bq	-3.19092718	0.95838204	-1.74000000
Bq	-3.09092850	0.95811764	-1.74000000
Bq	-2.99092982	0.95785324	-1.74000000
Bq	-2.89093114	0.95758884	-1.74000000
Bq	-2.79093246	0.95732444	-1.74000000
Bq	-2.69093378	0.95706004	-1.74000000
Bq	-2.59093510	0.95679564	-1.74000000
Bq	-2.49093642	0.95653124	-1.74000000
Bq	-2.39093774	0.95626684	-1.74000000
Bq	-2.29093906	0.95600244	-1.74000000
Bq	-2.19094038	0.95573804	-1.74000000
Bq	-2.09094170	0.95547364	-1.74000000
Bq	-1.99094302	0.95520924	-1.74000000
Bq	-1.89094434	0.95494484	-1.74000000
Bq	-1.79094566	0.95468044	-1.74000000
Bq	-1.69094698	0.95441604	-1.74000000
Bq	-1.59094830	0.95415164	-1.74000000
Bq	-1.49094962	0.95388724	-1.74000000

Bq	-1.39095094	0.95362284	-1.74000000
Bq	-1.29095226	0.95335844	-1.74000000
Bq	-1.19095358	0.95309404	-1.74000000
Bq	-1.09095491	0.95282987	-1.74000000
Bq	-0.99095622	0.95256524	-1.74000000
Bq	-0.89095754	0.95230084	-1.74000000
Bq	-0.79095886	0.95203644	-1.74000000
Bq	-0.69096018	0.95177204	-1.74000000
Bq	-0.59096150	0.95150764	-1.74000000
Bq	-0.49096282	0.95124324	-1.74000000
Bq	-0.39096414	0.95097884	-1.74000000
Bq	-0.29096546	0.95071444	-1.74000000
Bq	-0.19096678	0.95045004	-1.74000000
Bq	-0.09096810	0.95018564	-1.74000000
Bq	0.00903058	0.94992124	-1.74000000
Bq	0.10902926	0.94965684	-1.74000000
Bq	0.20902794	0.94939244	-1.74000000
Bq	0.30902662	0.94912804	-1.74000000
Bq	0.40902530	0.94886364	-1.74000000
Bq	0.50902398	0.94859924	-1.74000000
Bq	0.60902266	0.94833484	-1.74000000
Bq	0.70902134	0.94807044	-1.74000000
Bq	0.80902002	0.94780604	-1.74000000
Bq	0.90901870	0.94754164	-1.74000000
Bq	1.00901738	0.94727724	-1.74000000
Bq	1.10901606	0.94701284	-1.74000000
Bq	1.20901474	0.94674844	-1.74000000
Bq	1.30901342	0.94648404	-1.74000000
Bq	1.40901210	0.94621964	-1.74000000
Bq	1.50901078	0.94595524	-1.74000000
Bq	1.60900946	0.94569084	-1.74000000
Bq	1.70900814	0.94542644	-1.74000000
Bq	1.80900682	0.94516204	-1.74000000
Bq	1.90900550	0.94489764	-1.74000000
Bq	2.00900418	0.94463324	-1.74000000
Bq	2.10900286	0.94436884	-1.74000000
Bq	2.20900154	0.94410444	-1.74000000
Bq	2.30900022	0.94384004	-1.74000000
Bq	2.40899890	0.94357564	-1.74000000
Bq	2.50899758	0.94331124	-1.74000000
Bq	2.60899626	0.94304684	-1.74000000
Bq	2.70899494	0.94278244	-1.74000000
Bq	2.80899362	0.94251804	-1.74000000
Bq	2.90899230	0.94225364	-1.74000000
Bq	3.00899098	0.94198924	-1.74000000
Bq	3.10898966	0.94172484	-1.74000000

Bq	3.20898834	0.94146044	-1.74000000
Bq	3.30898702	0.94119604	-1.74000000
Bq	3.40898570	0.94093164	-1.74000000
Bq	3.50898438	0.94066724	-1.74000000
Bq	3.60898306	0.94040284	-1.74000000
Bq	3.70898174	0.94013844	-1.74000000
Bq	3.80898042	0.93987404	-1.74000000
Bq	3.90897910	0.93960964	-1.74000000
Bq	4.00897778	0.93934524	-1.74000000

NICS Scan of naphthalenic rings of mono anionicic 4a:

C	-3.38194849	-0.87628669	1.20823032
C	-2.69634918	-0.55900104	0.01585366
C	-3.31190770	-0.84285330	-1.22343552
C	-4.56778101	-1.46223112	-1.25173849
C	-5.24663628	-1.80312883	-0.07472027
C	-4.63905888	-1.49194747	1.14784550
B	-1.29456367	0.17330648	0.05446262
C	-1.28733966	1.73340596	0.02663471
C	-0.05303635	2.45099809	0.01118745
C	-0.05305286	3.88298886	-0.01066923
C	-1.29667430	4.57141489	-0.01316808
C	-2.48788033	3.87218685	0.00261198
C	-2.47738207	2.45832686	0.02076229
C	1.19040269	4.57113605	-0.03255437
C	2.38032881	3.87008679	-0.03496581
C	2.36874590	2.45618149	-0.01369004
C	1.17982709	1.72938979	0.01191873
B	1.19817048	0.16422163	0.04725618
N	-0.05149321	-0.56061127	0.10029775
C	-0.13425371	-2.05108819	0.17331732
C	0.38179633	-2.75702725	-1.08393668
C	-2.63247549	-0.44847140	-2.51623251
C	-6.58308199	-2.50394872	-0.12559174
C	-2.76232631	-0.54388466	2.54701953
C	2.62253461	-0.52335075	0.00461491
C	3.23152116	-0.81374034	-1.23680529
C	4.49774748	-1.41040592	-1.27026743
C	5.20311562	-1.70447824	-0.09562220
C	4.62128893	-1.34525151	1.12551765
C	3.35493254	-0.74714164	1.18911265
C	2.55586033	-0.41512842	-2.53013678
C	2.81727681	-0.27918444	2.52329025
C	6.54351118	-2.39699352	-0.14981589
C	0.50160065	-2.63631912	1.43819400
H	3.32195601	1.91879584	-0.01677739

H	3.33460725	4.40542623	-0.05349742
H	-3.42948938	1.91872616	0.03106212
H	-3.44136653	4.40923614	-0.00016526
H	-5.03328487	-1.67921481	-2.21998986
H	-5.16045756	-1.73242418	2.08130116
H	4.94995884	-1.64787054	-2.24008586
H	5.17031838	-1.53181132	2.05557704
H	3.08658481	0.78013596	2.69713511
H	1.71760376	-0.33631106	2.57282122
H	3.22861986	-0.86937753	3.36065280
H	2.94750559	-0.98677971	-3.38923017
H	1.46360319	-0.56110453	-2.49226956
H	2.72352464	0.65896041	-2.73717400
H	-3.19222640	-0.80915538	-3.39581259
H	-2.54360280	0.65090640	-2.59827756
H	-1.60614797	-0.85232263	-2.57932908
H	-2.51088183	0.53053018	2.61648331
H	-3.44122254	-0.78868868	3.38142296
H	-1.82107488	-1.10128762	2.70660101
H	1.18916753	5.66622307	-0.04954759
H	-1.29467615	5.66652571	-0.02943584
H	7.13353099	-2.21005278	0.76419015
H	6.42271552	-3.49378597	-0.24475379
H	7.13865375	-2.06057939	-1.01739864
H	-7.16955802	-2.32488253	0.79239357
H	-7.18473045	-2.16715249	-0.98835693
H	-6.45643192	-3.59972268	-0.22547470
H	-1.20776060	-2.27350053	0.23333591
H	0.21049296	-3.69795778	1.53270670
H	1.60129816	-2.58896432	1.41050243
H	0.14894300	-2.10930846	2.34118932
H	0.11865284	-3.82892387	-1.03310252
H	-0.08435269	-2.34139642	-1.99317952
H	1.47611280	-2.68177097	-1.18075848
Bq	-1.28733966	3.14519341	0.00000000
Bq	-1.28733966	3.14519341	0.10000000
Bq	-1.28733966	3.14519341	0.20000000
Bq	-1.28733966	3.14519341	0.30000000
Bq	-1.28733966	3.14519341	0.40000000
Bq	-1.28733966	3.14519341	0.50000000
Bq	-1.28733966	3.14519341	0.60000000
Bq	-1.28733966	3.14519341	0.70000000
Bq	-1.28733966	3.14519341	0.80000000
Bq	-1.28733966	3.14519341	0.90000000
Bq	-1.28733966	3.14519341	1.00000000
Bq	-1.28733966	3.14519341	1.10000000

Bq	-1.28733966	3.14519341	1.20000000
Bq	-1.28733966	3.14519341	1.30000000
Bq	-1.28733966	3.14519341	1.40000000
Bq	-1.28733966	3.14519341	1.50000000
Bq	-1.28733966	3.14519341	1.60000000
Bq	-1.28733966	3.14519341	1.70000000
Bq	-1.28733966	3.14519341	1.80000000
Bq	-1.28733966	3.14519341	1.90000000
Bq	-1.28733966	3.14519341	2.00000000
Bq	-1.28733966	3.14519341	2.10000000
Bq	-1.28733966	3.14519341	2.20000000
Bq	-1.28733966	3.14519341	2.30000000
Bq	-1.28733966	3.14519341	2.40000000
Bq	-1.28733966	3.14519341	2.50000000
Bq	-1.28733966	3.14519341	2.60000000
Bq	-1.28733966	3.14519341	2.70000000
Bq	-1.28733966	3.14519341	2.80000000
Bq	-1.28733966	3.14519341	2.90000000
Bq	-1.28733966	3.14519341	3.00000000
Bq	-1.28733966	3.14519341	3.10000000
Bq	-1.28733966	3.14519341	3.20000000
Bq	-1.28733966	3.14519341	3.30000000
Bq	-1.28733966	3.14519341	3.40000000
Bq	-1.28733966	3.14519341	3.50000000
Bq	-1.28733966	3.14519341	3.60000000
Bq	-1.28733966	3.14519341	3.70000000
Bq	-1.28733966	3.14519341	3.80000000
Bq	-1.28733966	3.14519341	3.90000000
Bq	-1.28733966	3.14519341	4.00000000
Bq	-1.28733966	3.14519341	4.10000000
Bq	-1.28733966	3.14519341	4.20000000
Bq	-1.28733966	3.14519341	4.30000000
Bq	-1.28733966	3.14519341	4.40000000
Bq	-1.28733966	3.14519341	4.50000000
Bq	-1.28733966	3.14519341	4.60000000
Bq	-1.28733966	3.14519341	4.70000000
Bq	-1.28733966	3.14519341	4.80000000
Bq	-1.28733966	3.14519341	4.90000000
Bq	-1.28733966	3.14519341	5.00000000

NICS Scan of hetero ring of mono anionicic 4a:

C	-3.38194849	-0.87628669	1.20823032
C	-2.69634918	-0.55900104	0.01585366
C	-3.31190770	-0.84285330	-1.22343552
C	-4.56778101	-1.46223112	-1.25173849
C	-5.24663628	-1.80312883	-0.07472027

C	-4.63905888	-1.49194747	1.14784550
B	-1.29456367	0.17330648	0.05446262
C	-1.28733966	1.73340596	0.02663471
C	-0.05303635	2.45099809	0.01118745
C	-0.05305286	3.88298886	-0.01066923
C	-1.29667430	4.57141489	-0.01316808
C	-2.48788033	3.87218685	0.00261198
C	-2.47738207	2.45832686	0.02076229
C	1.19040269	4.57113605	-0.03255437
C	2.38032881	3.87008679	-0.03496581
C	2.36874590	2.45618149	-0.01369004
C	1.17982709	1.72938979	0.01191873
B	1.19817048	0.16422163	0.04725618
N	-0.05149321	-0.56061127	0.10029775
C	-0.13425371	-2.05108819	0.17331732
C	0.38179633	-2.75702725	-1.08393668
C	-2.63247549	-0.44847140	-2.51623251
C	-6.58308199	-2.50394872	-0.12559174
C	-2.76232631	-0.54388466	2.54701953
C	2.62253461	-0.52335075	0.00461491
C	3.23152116	-0.81374034	-1.23680529
C	4.49774748	-1.41040592	-1.27026743
C	5.20311562	-1.70447824	-0.09562220
C	4.62128893	-1.34525151	1.12551765
C	3.35493254	-0.74714164	1.18911265
C	2.55586033	-0.41512842	-2.53013678
C	2.81727681	-0.27918444	2.52329025
C	6.54351118	-2.39699352	-0.14981589
C	0.50160065	-2.63631912	1.43819400
H	3.32195601	1.91879584	-0.01677739
H	3.33460725	4.40542623	-0.05349742
H	-3.42948938	1.91872616	0.03106212
H	-3.44136653	4.40923614	-0.00016526
H	-5.03328487	-1.67921481	-2.21998986
H	-5.16045756	-1.73242418	2.08130116
H	4.94995884	-1.64787054	-2.24008586
H	5.17031838	-1.53181132	2.05557704
H	3.08658481	0.78013596	2.69713511
H	1.71760376	-0.33631106	2.57282122
H	3.22861986	-0.86937753	3.36065280
H	2.94750559	-0.98677971	-3.38923017
H	1.46360319	-0.56110453	-2.49226956
H	2.72352464	0.65896041	-2.73717400
H	-3.19222640	-0.80915538	-3.39581259
H	-2.54360280	0.65090640	-2.59827756
H	-1.60614797	-0.85232263	-2.57932908

H	-2.51088183	0.53053018	2.61648331
H	-3.44122254	-0.78868868	3.38142296
H	-1.82107488	-1.10128762	2.70660101
H	1.18916753	5.66622307	-0.04954759
H	-1.29467615	5.66652571	-0.02943584
H	7.13353099	-2.21005278	0.76419015
H	6.42271552	-3.49378597	-0.24475379
H	7.13865375	-2.06057939	-1.01739864
H	-7.16955802	-2.32488253	0.79239357
H	-7.18473045	-2.16715249	-0.98835693
H	-6.45643192	-3.59972268	-0.22547470
H	-1.20776060	-2.27350053	0.23333591
H	0.21049296	-3.69795778	1.53270670
H	1.60129816	-2.58896432	1.41050243
H	0.14894300	-2.10930846	2.34118932
H	0.11865284	-3.82892387	-1.03310252
H	-0.08435269	-2.34139642	-1.99317952
H	1.47611280	-2.68177097	-1.18075848
Bq	-0.05000000	0.94519341	0.05000000
Bq	-0.05000000	0.94519341	0.15000000
Bq	-0.05000000	0.94519341	0.25000000
Bq	-0.05000000	0.94519341	0.35000000
Bq	-0.05000000	0.94519341	0.45000000
Bq	-0.05000000	0.94519341	0.55000000
Bq	-0.05000000	0.94519341	0.65000000
Bq	-0.05000000	0.94519341	0.75000000
Bq	-0.05000000	0.94519341	0.85000000
Bq	-0.05000000	0.94519341	0.95000000
Bq	-0.05000000	0.94519341	1.05000000
Bq	-0.05000000	0.94519341	1.15000000
Bq	-0.05000000	0.94519341	1.25000000
Bq	-0.05000000	0.94519341	1.35000000
Bq	-0.05000000	0.94519341	1.45000000
Bq	-0.05000000	0.94519341	1.55000000
Bq	-0.05000000	0.94519341	1.65000000
Bq	-0.05000000	0.94519341	1.75000000
Bq	-0.05000000	0.94519341	1.85000000
Bq	-0.05000000	0.94519341	1.95000000
Bq	-0.05000000	0.94519341	2.05000000
Bq	-0.05000000	0.94519341	2.15000000
Bq	-0.05000000	0.94519341	2.25000000
Bq	-0.05000000	0.94519341	2.35000000
Bq	-0.05000000	0.94519341	2.45000000
Bq	-0.05000000	0.94519341	2.55000000
Bq	-0.05000000	0.94519341	2.65000000
Bq	-0.05000000	0.94519341	2.75000000

Bq	-0.05000000	0.94519341	2.85000000
Bq	-0.05000000	0.94519341	2.95000000
Bq	-0.05000000	0.94519341	3.05000000
Bq	-0.05000000	0.94519341	3.15000000
Bq	-0.05000000	0.94519341	3.25000000
Bq	-0.05000000	0.94519341	3.35000000
Bq	-0.05000000	0.94519341	3.45000000
Bq	-0.05000000	0.94519341	3.55000000
Bq	-0.05000000	0.94519341	3.65000000
Bq	-0.05000000	0.94519341	3.75000000
Bq	-0.05000000	0.94519341	3.85000000
Bq	-0.05000000	0.94519341	3.95000000
Bq	-0.05000000	0.94519341	4.05000000
Bq	-0.05000000	0.94519341	4.15000000
Bq	-0.05000000	0.94519341	4.25000000
Bq	-0.05000000	0.94519341	4.35000000
Bq	-0.05000000	0.94519341	4.45000000
Bq	-0.05000000	0.94519341	4.55000000
Bq	-0.05000000	0.94519341	4.65000000
Bq	-0.05000000	0.94519341	4.75000000
Bq	-0.05000000	0.94519341	4.85000000
Bq	-0.05000000	0.94519341	4.95000000
Bq	-0.05000000	0.94519341	5.05000000

NICS XY-Scan of naphthalenic rings of mono anionicic 4a:

C	-3.38194849	-0.87628669	1.20823032
C	-2.69634918	-0.55900104	0.01585366
C	-3.31190770	-0.84285330	-1.22343552
C	-4.56778101	-1.46223112	-1.25173849
C	-5.24663628	-1.80312883	-0.07472027
C	-4.63905888	-1.49194747	1.14784550
B	-1.29456367	0.17330648	0.05446262
C	-1.28733966	1.73340596	0.02663471
C	-0.05303635	2.45099809	0.01118745
C	-0.05305286	3.88298886	-0.01066923
C	-1.29667430	4.57141489	-0.01316808
C	-2.48788033	3.87218685	0.00261198
C	-2.47738207	2.45832686	0.02076229
C	1.19040269	4.57113605	-0.03255437
C	2.38032881	3.87008679	-0.03496581
C	2.36874590	2.45618149	-0.01369004
C	1.17982709	1.72938979	0.01191873
B	1.19817048	0.16422163	0.04725618
N	-0.05149321	-0.56061127	0.10029775
C	-0.13425371	-2.05108819	0.17331732
C	0.38179633	-2.75702725	-1.08393668

C	-2.63247549	-0.44847140	-2.51623251
C	-6.58308199	-2.50394872	-0.12559174
C	-2.76232631	-0.54388466	2.54701953
C	2.62253461	-0.52335075	0.00461491
C	3.23152116	-0.81374034	-1.23680529
C	4.49774748	-1.41040592	-1.27026743
C	5.20311562	-1.70447824	-0.09562220
C	4.62128893	-1.34525151	1.12551765
C	3.35493254	-0.74714164	1.18911265
C	2.55586033	-0.41512842	-2.53013678
C	2.81727681	-0.27918444	2.52329025
C	6.54351118	-2.39699352	-0.14981589
C	0.50160065	-2.63631912	1.43819400
H	3.32195601	1.91879584	-0.01677739
H	3.33460725	4.40542623	-0.05349742
H	-3.42948938	1.91872616	0.03106212
H	-3.44136653	4.40923614	-0.00016526
H	-5.03328487	-1.67921481	-2.21998986
H	-5.16045756	-1.73242418	2.08130116
H	4.94995884	-1.64787054	-2.24008586
H	5.17031838	-1.53181132	2.05557704
H	3.08658481	0.78013596	2.69713511
H	1.71760376	-0.33631106	2.57282122
H	3.22861986	-0.86937753	3.36065280
H	2.94750559	-0.98677971	-3.38923017
H	1.46360319	-0.56110453	-2.49226956
H	2.72352464	0.65896041	-2.73717400
H	-3.19222640	-0.80915538	-3.39581259
H	-2.54360280	0.65090640	-2.59827756
H	-1.60614797	-0.85232263	-2.57932908
H	-2.51088183	0.53053018	2.61648331
H	-3.44122254	-0.78868868	3.38142296
H	-1.82107488	-1.10128762	2.70660101
H	1.18916753	5.66622307	-0.04954759
H	-1.29467615	5.66652571	-0.02943584
H	7.13353099	-2.21005278	0.76419015
H	6.42271552	-3.49378597	-0.24475379
H	7.13865375	-2.06057939	-1.01739864
H	-7.16955802	-2.32488253	0.79239357
H	-7.18473045	-2.16715249	-0.98835693
H	-6.45643192	-3.59972268	-0.22547470
H	-1.20776060	-2.27350053	0.23333591
H	0.21049296	-3.69795778	1.53270670
H	1.60129816	-2.58896432	1.41050243
H	0.14894300	-2.10930846	2.34118932
H	0.11865284	-3.82892387	-1.03310252

H	-0.08435269	-2.34139642	-1.99317952
H	1.47611280	-2.68177097	-1.18075848
Bq	-4.05000000	3.14519341	1.71000000
Bq	-3.95000000	3.14519341	1.71000000
Bq	-3.85000000	3.14519341	1.71000000
Bq	-3.75000000	3.14519341	1.71000000
Bq	-3.65000000	3.14519341	1.71000000
Bq	-3.55000000	3.14519341	1.71000000
Bq	-3.45000000	3.14519341	1.71000000
Bq	-3.35000000	3.14519341	1.71000000
Bq	-3.25000000	3.14519341	1.71000000
Bq	-3.15000000	3.14519341	1.71000000
Bq	-3.05000000	3.14519341	1.71000000
Bq	-2.95000000	3.14519341	1.71000000
Bq	-2.85000000	3.14519341	1.71000000
Bq	-2.75000000	3.14519341	1.71000000
Bq	-2.65000000	3.14519341	1.71000000
Bq	-2.55000000	3.14519341	1.71000000
Bq	-2.45000000	3.14519341	1.71000000
Bq	-2.35000000	3.14519341	1.71000000
Bq	-2.25000000	3.14519341	1.71000000
Bq	-2.15000000	3.14519341	1.71000000
Bq	-2.05000000	3.14519341	1.71000000
Bq	-1.95000000	3.14519341	1.71000000
Bq	-1.85000000	3.14519341	1.71000000
Bq	-1.75000000	3.14519341	1.71000000
Bq	-1.65000000	3.14519341	1.71000000
Bq	-1.55000000	3.14519341	1.71000000
Bq	-1.45000000	3.14519341	1.71000000
Bq	-1.35000000	3.14519341	1.71000000
Bq	-1.25000000	3.14519341	1.71000000
Bq	-1.15000000	3.14519341	1.71000000
Bq	-1.05000000	3.14519341	1.71000000
Bq	-0.95000000	3.14519341	1.71000000
Bq	-0.85000000	3.14519341	1.71000000
Bq	-0.75000000	3.14519341	1.71000000
Bq	-0.65000000	3.14519341	1.71000000
Bq	-0.55000000	3.14519341	1.71000000
Bq	-0.45000000	3.14519341	1.71000000
Bq	-0.35000000	3.14519341	1.71000000
Bq	-0.25000000	3.14519341	1.71000000
Bq	-0.15000000	3.14519341	1.71000000
Bq	-0.05000000	3.14519341	1.71000000
Bq	0.05000000	3.14519341	1.71000000
Bq	0.15000000	3.14519341	1.71000000
Bq	0.25000000	3.14519341	1.71000000

Bq	0.35000000	3.14519341	1.71000000
Bq	0.45000000	3.14519341	1.71000000
Bq	0.55000000	3.14519341	1.71000000
Bq	0.65000000	3.14519341	1.71000000
Bq	0.75000000	3.14519341	1.71000000
Bq	0.85000000	3.14519341	1.71000000
Bq	0.95000000	3.14519341	1.71000000
Bq	1.05000000	3.14519341	1.71000000
Bq	1.15000000	3.14519341	1.71000000
Bq	1.25000000	3.14519341	1.71000000
Bq	1.35000000	3.14519341	1.71000000
Bq	1.45000000	3.14519341	1.71000000
Bq	1.55000000	3.14519341	1.71000000
Bq	1.65000000	3.14519341	1.71000000
Bq	1.75000000	3.14519341	1.71000000
Bq	1.85000000	3.14519341	1.71000000
Bq	1.95000000	3.14519341	1.71000000
Bq	2.05000000	3.14519341	1.71000000
Bq	2.15000000	3.14519341	1.71000000
Bq	2.25000000	3.14519341	1.71000000
Bq	2.35000000	3.14519341	1.71000000
Bq	2.45000000	3.14519341	1.71000000
Bq	2.55000000	3.14519341	1.71000000
Bq	2.65000000	3.14519341	1.71000000
Bq	2.75000000	3.14519341	1.71000000
Bq	2.85000000	3.14519341	1.71000000
Bq	2.95000000	3.14519341	1.71000000
Bq	3.05000000	3.14519341	1.71000000
Bq	3.15000000	3.14519341	1.71000000
Bq	3.25000000	3.14519341	1.71000000
Bq	3.35000000	3.14519341	1.71000000
Bq	3.45000000	3.14519341	1.71000000
Bq	3.55000000	3.14519341	1.71000000
Bq	3.65000000	3.14519341	1.71000000
Bq	3.75000000	3.14519341	1.71000000
Bq	3.85000000	3.14519341	1.71000000
Bq	3.95000000	3.14519341	1.71000000

NICS XY-Scan of hetero ring of mono anionicic 4a:

C	-3.38194849	-0.87628669	1.20823032
C	-2.69634918	-0.55900104	0.01585366
C	-3.31190770	-0.84285330	-1.22343552
C	-4.56778101	-1.46223112	-1.25173849
C	-5.24663628	-1.80312883	-0.07472027
C	-4.63905888	-1.49194747	1.14784550
B	-1.29456367	0.17330648	0.05446262

C	-1.28733966	1.73340596	0.02663471
C	-0.05303635	2.45099809	0.01118745
C	-0.05305286	3.88298886	-0.01066923
C	-1.29667430	4.57141489	-0.01316808
C	-2.48788033	3.87218685	0.00261198
C	-2.47738207	2.45832686	0.02076229
C	1.19040269	4.57113605	-0.03255437
C	2.38032881	3.87008679	-0.03496581
C	2.36874590	2.45618149	-0.01369004
C	1.17982709	1.72938979	0.01191873
B	1.19817048	0.16422163	0.04725618
N	-0.05149321	-0.56061127	0.10029775
C	-0.13425371	-2.05108819	0.17331732
C	0.38179633	-2.75702725	-1.08393668
C	-2.63247549	-0.44847140	-2.51623251
C	-6.58308199	-2.50394872	-0.12559174
C	-2.76232631	-0.54388466	2.54701953
C	2.62253461	-0.52335075	0.00461491
C	3.23152116	-0.81374034	-1.23680529
C	4.49774748	-1.41040592	-1.27026743
C	5.20311562	-1.70447824	-0.09562220
C	4.62128893	-1.34525151	1.12551765
C	3.35493254	-0.74714164	1.18911265
C	2.55586033	-0.41512842	-2.53013678
C	2.81727681	-0.27918444	2.52329025
C	6.54351118	-2.39699352	-0.14981589
C	0.50160065	-2.63631912	1.43819400
H	3.32195601	1.91879584	-0.01677739
H	3.33460725	4.40542623	-0.05349742
H	-3.42948938	1.91872616	0.03106212
H	-3.44136653	4.40923614	-0.00016526
H	-5.03328487	-1.67921481	-2.21998986
H	-5.16045756	-1.73242418	2.08130116
H	4.94995884	-1.64787054	-2.24008586
H	5.17031838	-1.53181132	2.05557704
H	3.08658481	0.78013596	2.69713511
H	1.71760376	-0.33631106	2.57282122
H	3.22861986	-0.86937753	3.36065280
H	2.94750559	-0.98677971	-3.38923017
H	1.46360319	-0.56110453	-2.49226956
H	2.72352464	0.65896041	-2.73717400
H	-3.19222640	-0.80915538	-3.39581259
H	-2.54360280	0.65090640	-2.59827756
H	-1.60614797	-0.85232263	-2.57932908
H	-2.51088183	0.53053018	2.61648331
H	-3.44122254	-0.78868868	3.38142296

H	-1.82107488	-1.10128762	2.70660101
H	1.18916753	5.66622307	-0.04954759
H	-1.29467615	5.66652571	-0.02943584
H	7.13353099	-2.21005278	0.76419015
H	6.42271552	-3.49378597	-0.24475379
H	7.13865375	-2.06057939	-1.01739864
H	-7.16955802	-2.32488253	0.79239357
H	-7.18473045	-2.16715249	-0.98835693
H	-6.45643192	-3.59972268	-0.22547470
H	-1.20776060	-2.27350053	0.23333591
H	0.21049296	-3.69795778	1.53270670
H	1.60129816	-2.58896432	1.41050243
H	0.14894300	-2.10930846	2.34118932
H	0.11865284	-3.82892387	-1.03310252
H	-0.08435269	-2.34139642	-1.99317952
H	1.47611280	-2.68177097	-1.18075848
Bq	-4.05000000	0.94519341	1.75000000
Bq	-3.95000000	0.94519341	1.75000000
Bq	-3.85000000	0.94519341	1.75000000
Bq	-3.75000000	0.94519341	1.75000000
Bq	-3.65000000	0.94519341	1.75000000
Bq	-3.55000000	0.94519341	1.75000000
Bq	-3.45000000	0.94519341	1.75000000
Bq	-3.35000000	0.94519341	1.75000000
Bq	-3.25000000	0.94519341	1.75000000
Bq	-3.15000000	0.94519341	1.75000000
Bq	-3.05000000	0.94519341	1.75000000
Bq	-2.95000000	0.94519341	1.75000000
Bq	-2.85000000	0.94519341	1.75000000
Bq	-2.75000000	0.94519341	1.75000000
Bq	-2.65000000	0.94519341	1.75000000
Bq	-2.55000000	0.94519341	1.75000000
Bq	-2.45000000	0.94519341	1.75000000
Bq	-2.35000000	0.94519341	1.75000000
Bq	-2.25000000	0.94519341	1.75000000
Bq	-2.15000000	0.94519341	1.75000000
Bq	-2.05000000	0.94519341	1.75000000
Bq	-1.95000000	0.94519341	1.75000000
Bq	-1.85000000	0.94519341	1.75000000
Bq	-1.75000000	0.94519341	1.75000000
Bq	-1.65000000	0.94519341	1.75000000
Bq	-1.55000000	0.94519341	1.75000000
Bq	-1.45000000	0.94519341	1.75000000
Bq	-1.35000000	0.94519341	1.75000000
Bq	-1.25000000	0.94519341	1.75000000
Bq	-1.15000000	0.94519341	1.75000000

Bq	-1.05000000	0.94519341	1.75000000
Bq	-0.95000000	0.94519341	1.75000000
Bq	-0.85000000	0.94519341	1.75000000
Bq	-0.75000000	0.94519341	1.75000000
Bq	-0.65000000	0.94519341	1.75000000
Bq	-0.55000000	0.94519341	1.75000000
Bq	-0.45000000	0.94519341	1.75000000
Bq	-0.35000000	0.94519341	1.75000000
Bq	-0.25000000	0.94519341	1.75000000
Bq	-0.15000000	0.94519341	1.75000000
Bq	-0.05000000	0.94519341	1.75000000
Bq	0.05000000	0.94519341	1.75000000
Bq	0.15000000	0.94519341	1.75000000
Bq	0.25000000	0.94519341	1.75000000
Bq	0.35000000	0.94519341	1.75000000
Bq	0.45000000	0.94519341	1.75000000
Bq	0.55000000	0.94519341	1.75000000
Bq	0.65000000	0.94519341	1.75000000
Bq	0.75000000	0.94519341	1.75000000
Bq	0.85000000	0.94519341	1.75000000
Bq	0.95000000	0.94519341	1.75000000
Bq	1.05000000	0.94519341	1.75000000
Bq	1.15000000	0.94519341	1.75000000
Bq	1.25000000	0.94519341	1.75000000
Bq	1.35000000	0.94519341	1.75000000
Bq	1.45000000	0.94519341	1.75000000
Bq	1.55000000	0.94519341	1.75000000
Bq	1.65000000	0.94519341	1.75000000
Bq	1.75000000	0.94519341	1.75000000
Bq	1.85000000	0.94519341	1.75000000
Bq	1.95000000	0.94519341	1.75000000
Bq	2.05000000	0.94519341	1.75000000
Bq	2.15000000	0.94519341	1.75000000
Bq	2.25000000	0.94519341	1.75000000
Bq	2.35000000	0.94519341	1.75000000
Bq	2.45000000	0.94519341	1.75000000
Bq	2.55000000	0.94519341	1.75000000
Bq	2.65000000	0.94519341	1.75000000
Bq	2.75000000	0.94519341	1.75000000
Bq	2.85000000	0.94519341	1.75000000
Bq	2.95000000	0.94519341	1.75000000
Bq	3.05000000	0.94519341	1.75000000
Bq	3.15000000	0.94519341	1.75000000
Bq	3.25000000	0.94519341	1.75000000
Bq	3.35000000	0.94519341	1.75000000
Bq	3.45000000	0.94519341	1.75000000

Bq	3.55000000	0.94519341	1.75000000
Bq	3.65000000	0.94519341	1.75000000
Bq	3.75000000	0.94519341	1.75000000
Bq	3.85000000	0.94519341	1.75000000
Bq	3.95000000	0.94519341	1.75000000
Bq	4.05000000	0.94519341	1.75000000
Bq	4.15000000	0.94519341	1.75000000
Bq	4.25000000	0.94519341	1.75000000
Bq	4.35000000	0.94519341	1.75000000
Bq	4.45000000	0.94519341	1.75000000
Bq	4.55000000	0.94519341	1.75000000
Bq	4.65000000	0.94519341	1.75000000
Bq	4.75000000	0.94519341	1.75000000
Bq	4.85000000	0.94519341	1.75000000
Bq	4.95000000	0.94519341	1.75000000
Bq	5.05000000	0.94519341	1.75000000

References

[1] W. Gerrard, H. R. Hudson, E. F. Mooney, *J. Chem. Soc.* **1960**, 5168–5172.

[2] J. van Soolingen, R.-J. de Lang, R. den Besten, P. A. A. Klusener, N. Veldman, A. L. Spek, L. Brandsma, *Synth. Commun.* **1995**, *25*, 1741–1744.

[3] A. Hergel, H. Pritzkow, W. Siebert, *Angew. Chem. Int. Ed.* **1994**, *33*, 1247–1248; *Angew. Chem.* **1994**, *106*, 1342–1343.

[4] B. M. Lindkey, B. P. Jacobs, S. N. MacMillan, P. T. Wolczanski, *Chem. Commun.* **2016**, *52*, 3891–3894.

[5] K. Ruhlandt-Senge, J. J. Ellison, R. J. Wehmschulte, F. Pauer, P. P. Power, *J. Am. Chem. Soc.* **1993**, *115*, 11353–11357.

[6] G. E. Carr, R. D. Chambers, T. F. Holmes, D. G. Parker, *J. Organomet. Chem.* **1987**, *325*, 13–23.

[7] G. M. Sheldrick, *Acta Crystallogr. A* **2015**, *71*, 3-8.

[8] G. M. Sheldrick, *Acta Crystallogr. A* **2008**, *64*, 112-122.

[9] C. B. Hubschle, G. M. Sheldrick, B. Dittrich, *J. Appl. Crystallogr.* **2011**, *44*, 1281-1284.

[10] O. V. Dolomanov, L. J. Bourhis, R. J. Gildea, J. A. K. Howard, H. Puschmann, *J. Appl. Crystallogr.* **2009**, *42*, 339-341.

[11] R. Ahlrichs, M. Bär, M. Häser, H. Horn, C. Kölmel, *Chem. Phys. Lett.* **1989**, *162*, 165–169.

[12] A. Stanger, *J. Org. Chem.* **2006**, *71*, 883-893.

[13] R. Gershoni-Poranne, A. Stanger, *Chem. Eur. J.* **2014**, *20*, 5673-5688.

[14] D. Geuenich, K. Hess, F. Köhler, R. Herges, *Chem. Rev.* **2005**, *105*, 3758-3772.

[15] Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, *Gaussian Inc.*, *Wallingford CT*, **2016**.

[16] a) P. A. M. Dirac, *Proc. R. Soc. London, Ser. A* **1929**, *123*, 714–733; b) J. C. Slater, *Phys. Rev.* **1951**, *81*, 385–390; c) A. D. Becke, *Phys. Rev. A.* **1988**, *38*, 3098–3100; d) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785–89; e) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648–5652.

[17] A. Schäfer, H. Horn, R. Ahlrichs, *J. Chem. Phys.* **1992**, *97*, 2571–2577.

[18] a) S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104; b) S. Grimme, S. Ehrlich, L. J. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456–1465.

[19] P. Deglmann, F. Furche, R. Ahlrichs, *Chem. Phys. Lett.* **2002**, *362*, 511–518; b) P. Deglmann, F. Furche, *J. Chem. Phys.* **2002**, *117*, 9535–9538.

[20] a) R. Bauernschmitt, R. Ahlrichs, *Chem. Phys. Lett.* **1996**, *256*, 454–464; b) R. Bauernschmitt, R. Ahlrichs, *J. Chem. Phys.* **1996**, *104*, 9047–9052; c) F. Furche, D. Rappoport, *Density functional methods for excited states: equilibrium structure and electronic spectra.* In M. Olivucci, Ed., *Computational Photochemistry*, Vol. 16 of *Computational and Theoretical Chemistry*, ch. III., Elsevier, Amsterdam, **2005**.