Supporting Information

Reversible and Persistent Electrical Bistability in Single-Crystals of a Self-Assembled π-Conjugated Tetraaryl System: A Sub-Micron Scale Electrical Characterization

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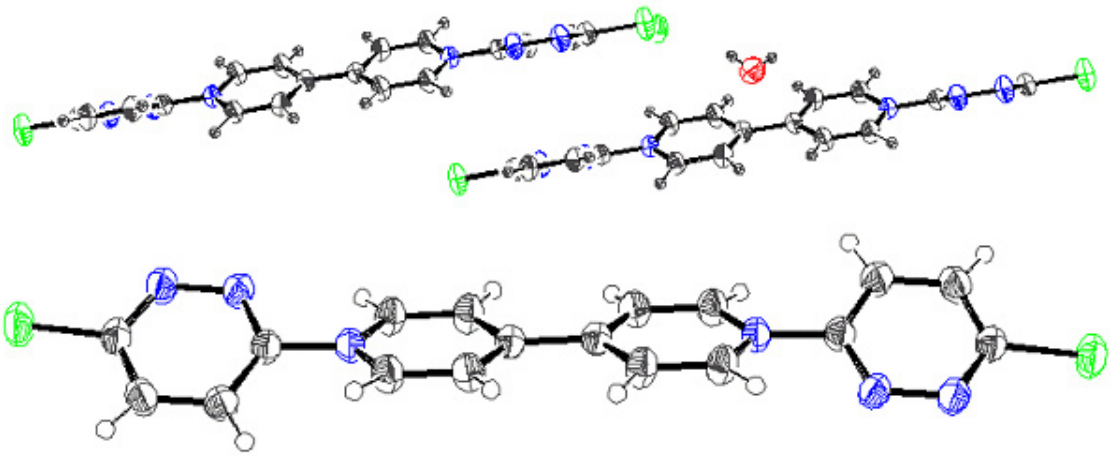
Materials $2^{2+}\cdot 2PF_6^-$ and $2^{2+}\cdot 2Cl^-$

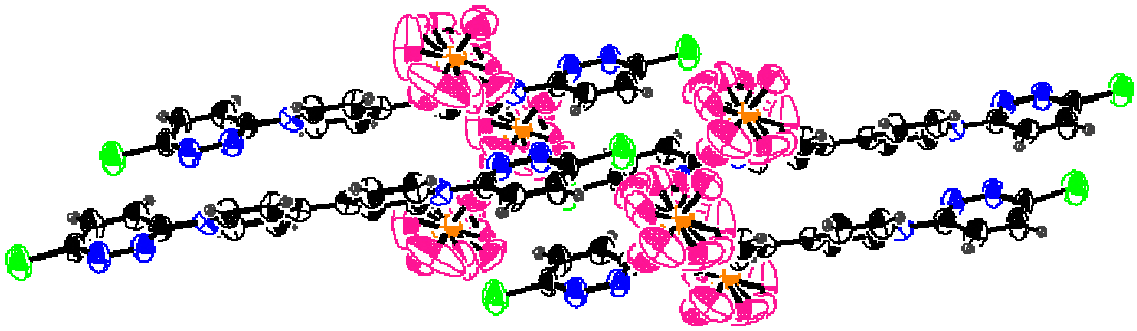
A 10:1 mixture of 3,6-dichloropyridazine and 4,4'-bipyridine was heated to 120°C under an inert atmosphere for two days. The crude was chromatographed (Silica, $5gL^{-1}$ ammonium chloride in a

2:3 water:methanol solution). The fraction of the eluent that contained the product were combined and concentrated under reduced pressure. The product was precipitated from the concentrated solution by adding a concentrated solution of ammonium hexafluorophosphate. The resulting precipitate, N,N'-(3,3'-di-(6-chloropyridazine))-4,4'-bipyridinium bis hexafluorophosphate, $\mathbf{2}^{2+}\cdot\mathbf{2PF_6}^-$, was obtained in 80% yield. The dichloride salt $\mathbf{2}^{2+}\cdot\mathbf{2Cl}^-$ was obtained by adding a saturated acetone solution of $\mathbf{2}^{2+}\cdot\mathbf{2PF_6}^-$ to an acetone solution of tetrabutyl ammonium chloride.

^{1}H NMR (DMSO-d_6): δ_{ppm} 9.92 (4H, d), 9.12 (4H, d), 8.76 (2H, d), 8.56 (2H, d). ^{13}C NMR (DMSO-d_6): δ_{ppm} 158.69, 156.15, 151.4, 144.59, 132.55, 127.1, 126.97.

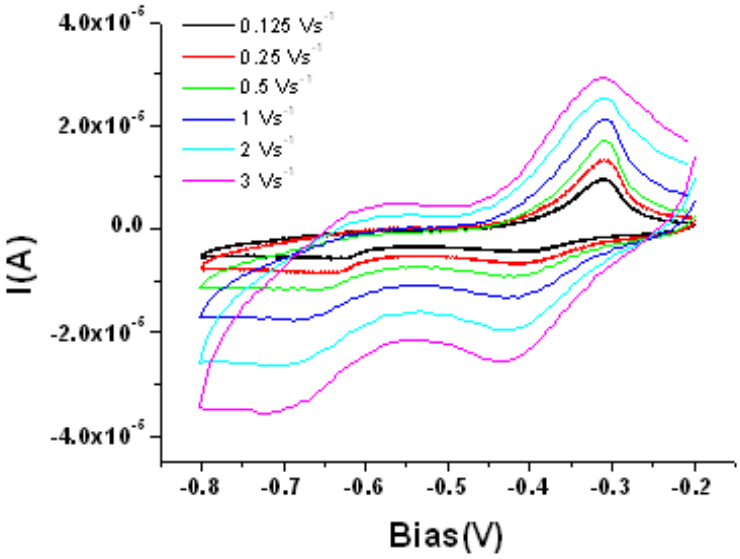


***Supplementary* Figure 1**. Crystal structure of $\mathbf{2}^{2+}\cdot\mathbf{2Cl}^-$.



***Supplementary* Figure 2**. Crystal structure of $\mathbf{2}^{2+}\cdot\mathbf{2PF_6}^-$.

Material 1^{2+}



Supplementary **Figure 3.** Cyclic voltammogram of **1** in acetonitrile in different scan rates. Upon decreasing the scan rate, the oxidation peak of the doubly reduced species disappears while the oxidation of the singly reduced species is increased, an indication of a disproportionation reaction. Electrolyte=$1*10^{-2}$M $N(Bu)_4^+PF_6^-$; scan rate=0.125 - $3Vs^{-1}$; reference electrode=$Ag/AgNO_3$; working and counter electrodes=Pt.

Cif file of $\mathbf{1^{2+}\cdot 2I_3^-\text{-}A}$:

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N21 N22 C23 129.1(5) . . ?
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'x, -y-1/2, z-1/2'

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HKL Denzo and Scalepack (Otwinowski & Minor 1997)
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S.Mackay, C.J.Gilmore, C.Edwards, M. Tremayne, N. Stuart, K.Shankland
"maXus": a computer program for the solution and refinement of crystal
structures from diffraction data University of Glasgow, Scotland, UK,
Nonius BV, Delft, The Netherlands and MacScience Co. Ltd.,
Yokohama, Japan (1998)
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Molecular Structure Corporation (1999).
ORTEP. TEXRAY Structure Analysis Package.
MSC, 3200 Research Forest Drive, The
Woodlands,TX 77381, USA.
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
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I3 I 0.66506(5) -0.05816(3) -0.02251(10) 0.0762(3) Uani 1 1 d . . .
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H1 H 0.4948 0.7199 0.0284 0.072 Uiso 1 1 calc R . .
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N3 N 0.4943(5) 0.59845(19) 0.1382(9) 0.0454(17) Uani 1 1 d . . .
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C2 C 0.4874(8) 0.6890(3) 0.4138(13) 0.061(3) Uani 1 1 d . . .
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C4 C 0.4917(6) 0.6403(2) 0.1952(12) 0.046(2) Uani 1 1 d . . .
C5 C 0.4382(6) 0.5714(2) 0.2189(12) 0.051(2) Uani 1 1 d . . .
H5 H 0.3986 0.5791 0.3113 0.061 Uiso 1 1 calc R . .
C6 C 0.4393(6) 0.5336(2) 0.1673(12) 0.049(2) Uani 1 1 d . . .
H6 H 0.3999 0.5152 0.2232 0.058 Uiso 1 1 calc R . .
C7 C 0.4995(6) 0.5215(2) 0.0288(10) 0.0371(18) Uani 1 1 d . . .
C8 C 0.5552(7) 0.5495(2) -0.0499(12) 0.054(2) Uani 1 1 d . . .
H8 H 0.5945 0.5424 -0.1439 0.065 Uiso 1 1 calc R . .
C9 C 0.5544(8) 0.5872(3) 0.0060(12) 0.062(3) Uani 1 1 d . . .
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O2W O 0.2572(14) 0.1773(7) -0.280(6) 0.045(6) Uiso 0.50 1 d P . .
O3W O 0.256(2) 0.1614(12) -0.133(7) 0.034(8) Uiso 0.50 1 d P . .
O4W O 0.2500 0.2500 -0.135(2) 0.065(3) Uiso 1 2 d S . .
O5W O 0.7550(10) -0.1678(6) -0.165(5) 0.025(3) Uiso 0.50 1 d P . .
O6W O 0.7470(17) -0.1766(7) 0.120(7) 0.062(8) Uiso 0.50 1 d P . .
O7W O 0.7452(12) -0.1704(8) 0.196(7) 0.015(4) Uiso 0.50 1 d P . .
O8W O 0.725(3) -0.1618(18) 0.167(9) 0.048(11) Uiso 0.50 1 d P . .
O9W O 0.741(2) -0.2695(11) -0.145(4) 0.085(10) Uiso 0.25 1 d P . .
O10W O 0.7439(11) -0.1665(9) 0.066(6) 0.034(5) Uiso 0.50 1 d P . .
O11W O 0.7528(14) -0.1595(7) -0.246(5) 0.031(6) Uiso 0.50 1 d P . .
O12W O 0.778(3) -0.1527(8) -0.320(6) 0.051(10) Uiso 0.50 1 d P . .
O13W O 0.7500 -0.2500 -0.225(3) 0.097(5) Uiso 1 2 d S . .
O14W O 0.7364(17) -0.2338(8) 0.053(4) 0.054(7) Uiso 0.25 1 d P . .
O15W O 0.7500 0.2500 0.302(16) 0.068(16) Uiso 0.25 2 d SP . .
O16W O 0.747(3) 0.2166(11) 0.056(8) 0.094(12) Uiso 0.25 1 d P . .
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O18W O 0.758(5) 0.214(2) -0.135(12) 0.054(16) Uiso 0.13 1 d P . .
O19W O 0.739(4) 0.283(2) 0.190(10) 0.056(13) Uiso 0.13 1 d P . .
O20W O 0.255(3) -0.2850(13) 0.042(9) 0.026(9) Uiso 0.13 1 d P . .
O21W O 0.2500 -0.2500 -0.009(16) 0.102(16) Uiso 0.25 2 d SP . .
O22W O 0.277(5) -0.284(2) -0.318(11) 0.07(2) Uiso 0.13 1 d P . .
O23W O 0.753(2) -0.1826(11) 0.009(9) 0.047(9) Uiso 0.25 1 d P . .
O24W O 0.7583(17) -0.1849(9) -0.118(8) 0.041(7) Uiso 0.25 1 d P . .
O25W O 0.749(5) 0.258(2) 0.225(14) 0.048(16) Uiso 0.13 1 d P . .
O26W O 0.7568(11) -0.2387(5) -0.297(3) 0.013(4) Uiso 0.25 1 d P . .
O27W O 0.757(5) 0.260(3) 0.382(16) 0.07(2) Uiso 0.13 1 d P . .
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I3 0.0752(6) 0.0928(7) 0.0607(5) -0.0006(4) -0.0033(3) 0.0007(4)
O1 0.117(6) 0.042(4) 0.072(4) -0.008(3) -0.008(4) 0.008(4)
N1 0.090(6) 0.028(4) 0.061(5) -0.004(3) 0.012(4) -0.005(4)
N2 0.083(6) 0.022(4) 0.055(4) 0.001(3) 0.002(4) 0.001(3)
N3 0.056(4) 0.032(4) 0.049(4) -0.007(3) 0.007(3) 0.000(3)
C1 0.063(6) 0.035(5) 0.088(8) -0.009(5) 0.006(5) 0.005(4)
C2 0.096(8) 0.038(5) 0.050(5) -0.008(4) -0.005(5) 0.006(5)
C3 0.083(7) 0.055(6) 0.051(6) 0.005(5) 0.008(5) 0.014(5)
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C5 0.054(5) 0.037(5) 0.061(6) 0.003(4) 0.017(4) -0.005(4)
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C8 0.067(6) 0.037(5) 0.058(6) -0.010(4) 0.022(5) -0.013(4)
C9 0.083(7) 0.044(6) 0.059(6) 0.003(4) 0.019(5) -0.004(5)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix. The cell esds are taken
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 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry. An approximate (isotropic)

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 treatment of cell esds is used for estimating esds involving l.s. planes.
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N1 H1 0.8600 . ?
N2 C4 1.309(11) . ?
N3 C5 1.349(10) . ?
N3 C9 1.360(11) . ?
N3 C4 1.477(10) . ?
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C5 C6 1.332(11) . ?
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C8 C9 1.342(12) . ?
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N2 C4 N3 112.8(7) . . ?
C3 C4 N3 122.5(8) . . ?
C6 C5 N3 120.6(8) . . ?
C6 C5 H5 119.7 . . ?
N3 C5 H5 119.7 . . ?
C5 C6 C7 120.4(8) . . ?
C5 C6 H6 119.8 . . ?
C7 C6 H6 119.8 . . ?
C8 C7 C6 117.7(7) . . ?
C8 C7 C7 122.2(9) . 5_665 ?
C6 C7 C7 120.1(9) . 5_665 ?
C9 C8 C7 121.0(8) . . ?
C9 C8 H8 119.5 . . ?
C7 C8 H8 119.5 . . ?
C8 C9 N3 120.3(9) . . ?
C8 C9 H9 119.8 . . ?
N3 C9 H9 119.8 . . ?

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 _geom_torsion_site_symmetry_4
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C1 N1 N2 C4 -1.1(13) . . . . ?
N2 N1 C1 O1 -177.1(9) . . . . ?
N2 N1 C1 C2 4.8(14) . . . . ?
O1 C1 C2 C3 176.3(9) . . . . ?
N1 C1 C2 C3 -5.7(15) . . . . ?
C1 C2 C3 C4 3.3(15) . . . . ?
N1 N2 C4 C3 -1.8(13) . . . . ?
N1 N2 C4 N3 179.5(7) . . . . ?
C2 C3 C4 N2 0.6(15) . . . . ?
C2 C3 C4 N3 179.2(8) . . . . ?
C5 N3 C4 N2 -139.7(8) . . . . ?
C9 N3 C4 N2 41.3(11) . . . . ?
C5 N3 C4 C3 41.6(12) . . . . ?
C9 N3 C4 C3 -137.4(9) . . . . ?
C9 N3 C5 C6 -1.7(13) . . . . ?
C4 N3 C5 C6 179.3(8) . . . . ?
N3 C5 C6 C7 0.6(14) . . . . ?
C5 C6 C7 C8 -0.5(12) . . . . ?
C5 C6 C7 C7 179.8(9) . . . 5_665 ?
C6 C7 C8 C9 1.7(13) . . . . ?
C7 C7 C8 C9 -178.7(10) 5_665 . . . ?
C7 C8 C9 N3 -2.9(15) . . . . ?
C5 N3 C9 C8 2.9(14) . . . . ?
C4 N3 C9 C8 -178.1(9) . . . . ?

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_refine_diff_density_max    1.070
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