Supplementary material (ESI) for Journal of Materials Chemistry

Supplementary material

For RBzPy[Ni(α-tpdt)$_2$], (R=H (1), Br(2), F(3))

Table1 Bond lengths of [Ni(α-tpdt)$_2$]$^-$ in the crystal structure of **1**, **2** and **3**

	1	**2**	**3**
Ni-S1	2.1634(8)	2.1673(7)	2.1731(15)
Ni-S2	2.1629(8)	2.1732(7)	2.1615(14)
Ni-S4	2.1645(8)	2.1639(7)	2.1583(14)
Ni-S5	2.1667(7)	2.1641(7)	2.1617(14)
S1-C2	1.735(3)	1.723(3)	1.726(5)
S2-C1	1.717(3)	1.723(3)	1.740(5)
S5-C5	1.726(3)	1.718(3)	1.723(5)
S4-C6	1.726(3)	1.725(3)	1.726(3)
S3-C1	1.733(3)	1.707(5)	-
S3-C2	-	-	1.730(5)
S3-C4	1.704(4)	1.558(7)	1.706(6)
S6-C5	1.732(3)	1.740(3)	1.759(5)
S6-C8	1.695(3)	1.678(4)	1.667(6)
S7-C6	1.673(19)	-	1.681(19)
S7-C8	1.52(2)	-	1.57(2)
C1-C2	1.376(4)	1.377(4)	1.367(7)
C1-C3	-	-	1.461(7)
C2-C3	1.491(4)	1.466(18)	-
C5-C6	1.373(4)	1.375(4)	1.363(7)
C3-C4	1.375(4)	1.371(15)	1.362(8)
C6-C7	1.451(12)	1.565(6)	1.49(2)
C7-C8	1.390(13)	1.221(7)	1.39(2)
S30-C2	-	1.705(7)	-
S30-C4	-	1.475(8)	-
S70-C6	-	1.528(8)	-
S70-C8	-	1.370(19)	-
C1-C30	-	1.507(17)	-
C4-C30	-	1.409(17)	-
C5-C70	-	1.579(19)	1.50(4)
C8-C70	-	1.468(8)	1.399(19)
C5-C60	1.494(17)	-	-
C8-C60	1.355(17)	-	-

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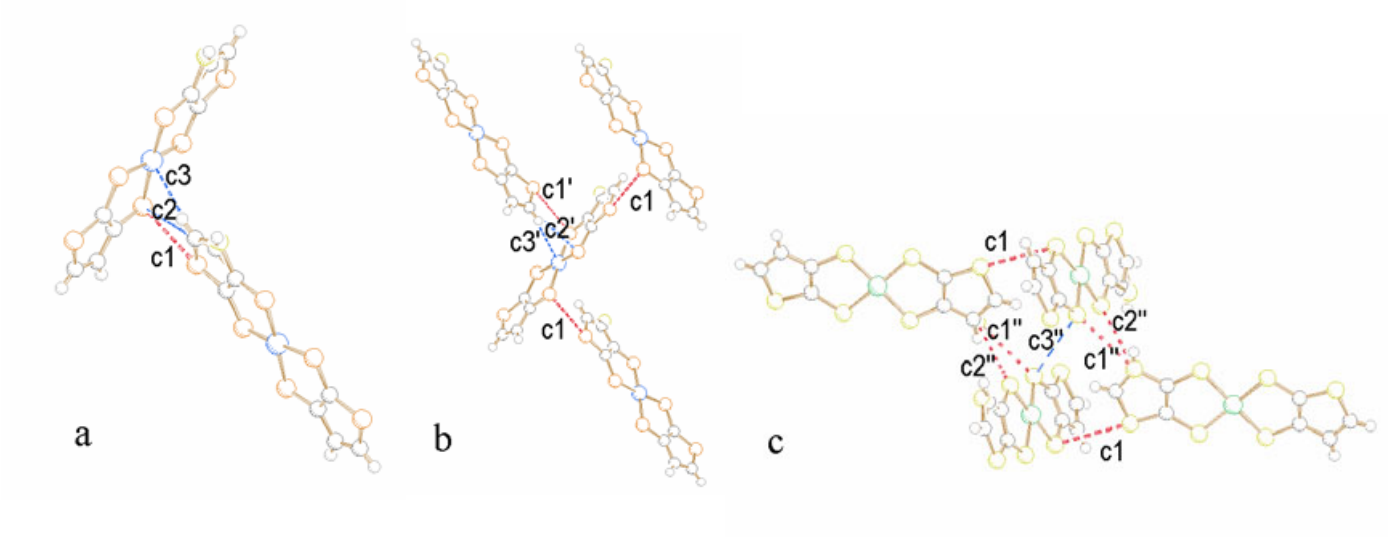

a) View of the interanionic intrachain contacts in compound **1**: c1 - sdP ≅ -0.004 and Q_W = 0.95 (83%; FM); c2 - sdP ≅ 0.0095 and Q_W = 1.09 (100%; AFM); c3 - sdP ≅ 0.008 and Q_W = 1.05 (100%; AFM); b) interchain contacts: c1' - sdP ≅ -0.004 and Q_W = 1.01 (100%; FM); c2' - sdP ≅ 0.0085 and Q_W = 1.10 (100%; AFM); c3' - sdP ≅ 0.008 and Q_W = 1.08 (100%; AFM); c) interlayer contacts: c1'' - sdP ≅ -0.0035 and Q_W = 0.96 (17%; FM); c2'' - sdP ≅ -0.0035 and Q_W = 1.02 (17%; FM); c3'' - sdP ≅ 0.008 and Q_W = 1.08 (100%; AFM).