Electronic Supplementary Material (ESI) for CrystEngComm

Preparation and crystal structures of the isomeric series 4-tolyl-1,2,3,5-dithiadiazolyl, (*o*-$MeC_6H_4CNSSN)_2$, (*m*-$MeC_6H_4CNSSN)_2$ and (*p*-$MeC_6H_4CNSSN)_2$

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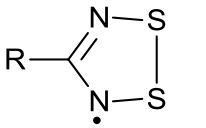
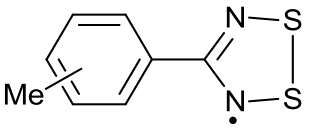
Electronic Supplementary Information



1,2,3,5-DTDA



1 *p*-Me
2 *m*-Me
3 *o*-Me

Table S1 Selected crystal data for **1**, **2** and **3**

	1	**2**	**3**
common name	4-*p*-tolyl-1,2,3,5-dithiadiazolyl	4-*m*-tolyl-1,2,3,5-dithiadiazolyl	4-*o*-tolyl-1,2,3,5-dithiadiazolyl
chemical formula	$C_8H_7N_2S_2$	$C_8H_7N_2S_2$	$C_8H_7N_2S_2$
formula weight	195.28	195.28	195.28
crystal system	monoclininc	monoclinic	monoclinic
space group	*C*2/*c*	$P2_1$	$P2_1/c$
Z	16	4	32
Z'	2	2	8
a (Å)	20.940(4)	5.912(1)	7.859(2)
b (Å)	10.563(2)	13.360(3)	14.917(3)
c (Å)	14.998(3)	10.963(3)	55.36(1)
α (°)	90.00	90.00	90.00
β (°)	91.14(3)	105.11(3)	92.445(3)
γ (°)	90.00	90.00	90.00
temperature (K)	153(2)	173(2)	105(2)
calculated density (g cm^{-3})	1.564	1.552	1.600
μ (mm^{-1})	0.579	0.574	0.592
independent reflections	36732	9329	41346
R_{int}	0.0597	0.0507	0.1111
R1 [I>2σ(I)]	0.0330	0.0362	0.0746

Table S2 Selected structural parameters for **1**, **2** and **3**

	1	**2**	**3**
twist angle between aryl and heterocyclic ring planes (º)	7.1(1) 6.4(1)	5.2(1) 10.9(1)	19.9(1) 24.4(1) 25.6(1) 24.5(2) 19.4(1) 25.7(1) 28.1(1) 27.1(1)
intradimer S…S (Å)	3.0230(9) 3.0928(9)	3.000(1) 3.156(1)	3.123(2) 3.091(2) 3.216(2) 3.131(2) 3.114(2) 3.084(2) 3.207(2) 2.969(2)
S...N	S11…N21[a] 3.223(2) N11…S21[a] 3.168(2)	S11…N12[b] 3.548(2) S21…N22[b] 3.517(2)	S11…N52 3.440(4) S12…N52 3.234(4) S21…N62 3.690(4) S21…N62 3.340(4) S31…N72 3.519(5) S31…N72 3.288(4) S41…N82 3.486(5) S41…N82 3.279(4) S52…N12[c] 3.261(4) S62…N12[c] 3.619(4) S62…N22[c] 3.454(5) S72…N22[c] 3.628(4) S72…N32[c] 3.361(5) S82…N32[c] 3.292(4) S82…N42[c] 3.481(5)

a (1-x, -y, -z) b (-1+x, y, z) c (1+x, y, z)

Figure S1: Variable Temperature EPR Spectra for 3 on heating from 300 to 350 K

All spectra recorded on a Bruker EMXplus X-band EPR spectrometer with modulation amplitude of 1 G_{pp} , modulation frequency 100 kHz, microwave power 6.633-6.649 mW* (single scan).

* All spectra were recorded using the same attenuation but the microwave frequency varied slightly 9.3516 – 9.3506 GHz on warming as the cavity was retuned at each temperature.