Electronic Supplementary Information for Dalton Transactions

$NC\text{-}(CF_2)_4\text{-}CNSSN^{\bullet}$ Containing 1,2,3,5-Dithiadiazolyl Radical Dimer Exhibiting Triplet Excited States at Low Temperature and Thermal Hysteresis on Melting – Solidification: Structural, Spectroscopic, and Magnetic Characterization

by

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Table S1. Temperature dependent data obtained from solid-state EPR experiment and magnetic susceptibility measurements for [**1a**]$_2$.

EPR data		Magnetism data	
T/K	Integral/a.u.*	T/K	χ/emu/mol
188	82.16	2	0.00482
196	131.63	4	0.00296
203	221	6.01	0.00238
211	332.31	8	0.0021
216	468.88	10	0.00192
222	542.19	14	0.00173
227	674.83	18	0.00162
237	1121.47	22	0.00156
242	1290.5	26	0.00151
247	1542.06	30	0.00148
252	1801.63	40	0.00143
198	91.52	50	0.0014
206	192.38	60.1	0.00137
220	421.67	70.1	0.00136
229	732.6	80.1	0.00135
240	1276.33	90.1	0.00133
250	1699.26	100	0.00133
		120	0.00131
		140	0.0013
		160	0.0013
		180	0.00129
		200	0.00129
		220	0.0013
		240	0.00132
		260	0.00135
		280	0.00139
		300	0.00144

* a.u. stands for arbitrary units.

Table S2. Experimental and calculated [MPW1PW91/6-311+G*] vibrational frequencies of monomeric $NCC_4F_8CNSSN^{\bullet}$.

Calc IR	Exp IR	Tentative Assignment
19 (0)		
31 (0)		
41 (<1)		
43 (<1)		
64 (<1)		
104 (2)		
159 (<1)		
170 (<1)		
175 (0)		
191 (8)		
210 (1)		
227 (1)		
238 (1)		
240 (1)		
263 (0)		
309 (<1)		
319 (2)		
338 (2)		
355 (<1)		
363 (11)	364m	ν [NCC_4F_8]
388 (24)	392m	δ_s [NC-C] oop
400 (<1)		ν [S-S]
402 (1)	434vw	ν [NCC_4F_8]
479 (3)	480w	ν [NCC_4F_8]
487 (1)		ν [NCC_4F_8]
516 (10)	515m	ν [-CNSSN] ring twist
553 (19)	557m	ν [C_4F_8]
566 (9)		ν [NCC_4F_8]
598 (13)	596mw	ν [NCC_4F_8]
612 (2)		δ_s [NC-C] ip
637 (49)	628m	ν [NCC_4F_8]
689 (15)	689m	ν [NCC_4F_8]
721 (23)	790m	ν [NCC_4F_8]
767 (157)	768ms	ν [NCC_4F_8]
810 (9)	821m	δ_s [NSSN] ip
838 (57)	897m	δ_{as} [NSSN] ip
907 (16)	918w	ν [NCC_4F_8]
1031 (3)	970w	ν [C_4F_8]
1132 (160)	1098mw	ν [C_4F_8]
1151 (36)	1120m	ν [C_4F_8]
1159 (17)	1133m	ν [C_4F_8]
1168 (9)		ν [C_4F_8]
1185 (130)	1152m	ν [C_4F_8]
1201 (397)	1170ms	ν [C_4F_8]
1204 (297)	1199s	ν [C_4F_8]

1210 (99)	1184ms	ν [C_4F_8]
1272 (4)	1221m	ν [C_4F_8]
1300 (6)	1303w	ν [C_4F_8]
1332 (10)	1313w	ν [C=N]
1401 (6)		ν [C(N)-C(F)]
2362 (22)	2269mw	ν [C≡N)