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Halogen Bonding Provides Heterooctameric Supramolecular Aggregation of Diaryliodonium Thiocyanate

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Supporting Information

Table 1. Cartesian atomic coordinates for model heterooctameric cluster {PhI(p-(MeO)C_6H_4}$_4$·{SCN}$_4$.

Atom	X	Y	Z
I	19.999111	7.692282	6.214580
O	14.602375	10.710973	6.772765
C	18.183534	8.724229	6.484626
C	19.991704	8.065478	4.134347
C	20.495334	9.279908	3.709484
H	20.846722	9.903890	4.334330
C	19.465650	7.128373	3.260134
H	19.124754	6.299483	3.575210
C	20.478258	9.572046	2.348374
H	20.826149	10.399702	2.035203
C	19.452895	7.443142	1.899568
H	19.098009	6.819983	1.276083
C	19.954467	8.656955	1.451035
H	19.937391	8.860834	0.523766
C	15.823183	10.113736	6.703383
C	17.024446	10.795323	6.741883
H	17.034527	11.739011	6.845684
C	18.212131	10.093574	6.628151
H	19.042461	10.554000	6.649782
C	16.990500	8.023920	6.468028
H	16.987209	7.077146	6.385858
C	15.806518	8.725875	6.573598
H	14.977217	8.262157	6.557273
C	14.588385	12.129488	6.973292
H	15.102713	12.563992	6.260699

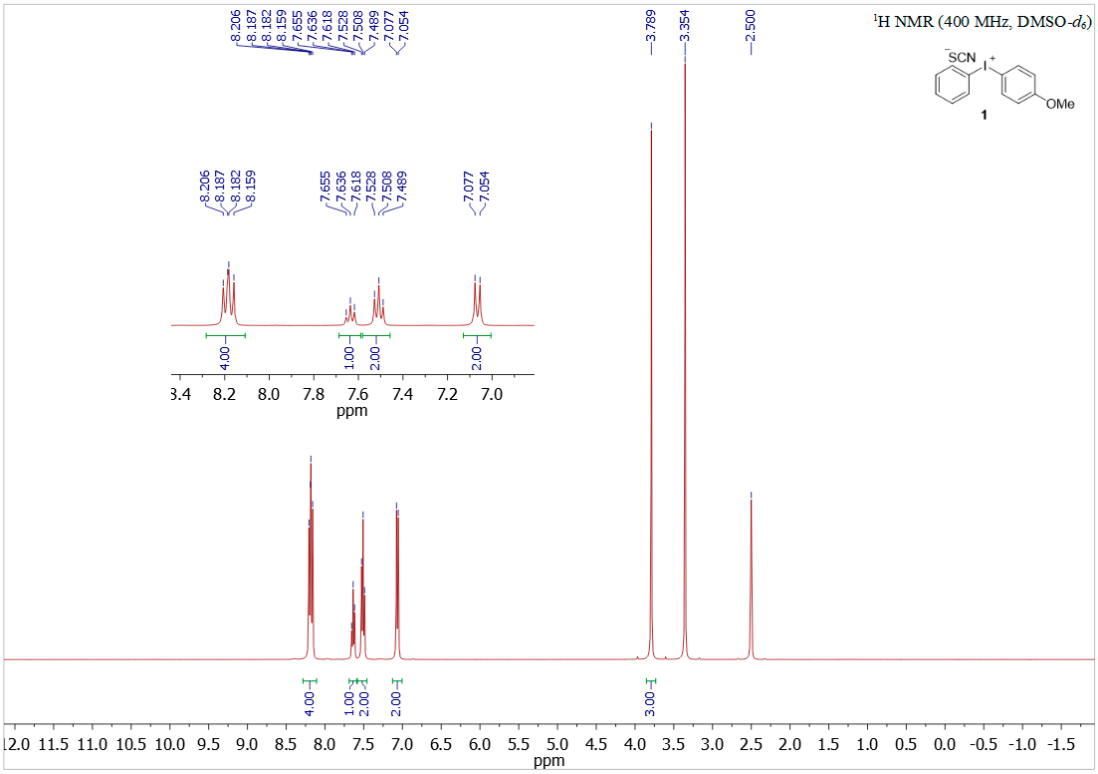
H	14.989561	12.339745	7.841519
H	13.664653	12.452897	6.954518
S	19.392410	7.287815	11.724050
N	19.980183	7.933193	9.054070
C	19.727957	7.648461	10.148536
I	18.024093	4.569286	10.790795
O	15.005402	−0.827450	10.232610
C	16.992146	2.753709	10.520749
C	17.650897	4.561879	12.871028
C	16.436467	5.065509	13.295891
H	15.812485	5.416897	12.671045
C	18.588002	4.035825	13.745241
H	19.416892	3.694929	13.430165
C	16.144329	5.048433	14.657001
H	15.316673	5.396324	14.970172
C	18.273233	4.023070	15.105807
H	18.896392	3.668184	15.729292
C	17.059420	4.524642	15.554340
H	16.855541	4.507566	16.481609
C	15.602639	0.393358	10.301992
C	14.921052	1.594621	10.263492
H	13.977364	1.604702	10.159691
C	15.622801	2.782306	10.377224
H	15.162375	3.612636	10.355593
C	17.692455	1.560675	10.537347
H	18.639229	1.557384	10.619517
C	16.990500	0.376693	10.431777
H	17.454218	−0.452608	10.448102
C	13.586887	−0.841440	10.032083
H	13.152383	−0.327112	10.744676
H	13.376630	−0.440264	9.163856
H	13.263478	−1.765172	10.050857
S	18.428560	3.962585	5.281325
N	17.783182	4.550358	7.951305
C	18.067914	4.298132	6.856839
I	21.147089	2.594268	6.214580
O	26.543825	−0.424423	6.772765
C	22.962666	1.562321	6.484626
C	21.154496	2.221072	4.134347
C	20.650866	1.006642	3.709484
H	20.299478	0.382660	4.334330
C	21.680550	3.158177	3.260134
H	22.021446	3.987067	3.575210
C	20.667942	0.714504	2.348374
H	20.320051	−0.113152	2.035203
C	21.693305	2.843408	1.899568
H	22.048191	3.466567	1.276083
C	21.191733	1.629595	1.451035
H	21.208809	1.425716	0.523766
C	25.323017	0.172814	6.703383

C	24.121754	−0.508773	6.741883
H	24.111673	−1.452461	6.845684
C	22.934069	0.192976	6.628151
H	22.103739	−0.267450	6.649782
C	24.155700	2.262630	6.468028
H	24.158991	3.209404	6.385858
C	25.339682	1.560675	6.573598
H	26.168983	2.024393	6.557273
C	26.557815	−1.842938	6.973292
H	26.043487	−2.277442	6.260699
H	26.156639	−2.053195	7.841519
H	27.481547	−2.166347	6.954518
S	21.753790	2.998735	11.724050
N	21.166017	2.353357	9.054070
C	21.418243	2.638089	10.148536
I	23.122107	5.717264	10.790795
O	26.140798	11.114000	10.232610
C	24.154054	7.532841	10.520749
C	23.495303	5.724671	12.871028
C	24.709733	5.221041	13.295891
H	25.333715	4.869653	12.671045
C	22.558198	6.250725	13.745241
H	21.729308	6.591621	13.430165
C	25.001871	5.238117	14.657001
H	25.829527	4.890226	14.970172
C	22.872967	6.263480	15.105807
H	22.249808	6.618366	15.729292
C	24.086780	5.761908	15.554340
H	24.290659	5.778984	16.481609
C	25.543561	9.893192	10.301992
C	26.225148	8.691929	10.263492
H	27.168836	8.681848	10.159691
C	25.523399	7.504244	10.377224
H	25.983825	6.673914	10.355593
C	23.453745	8.725875	10.537347
H	22.506971	8.729166	10.619517
C	24.155700	9.909857	10.431777
H	23.691982	10.739158	10.448102
C	27.559313	11.127990	10.032083
H	27.993817	10.613662	10.744676
H	27.769570	10.726814	9.163856
H	27.882722	12.051722	10.050857
S	22.717640	6.323965	5.281325
N	23.363018	5.736192	7.951305
C	23.078286	5.988418	6.856839

Table S2. Crystal data and structure refinement for **1**.

CCDC number	**1987193**
Empirical formula	$C_{14}H_{12}INOS$
Formula weight	369.21

Temperature/K	100(2)
Crystal system	tetragonal
Space group	$I4_1/a$
a/Å	20.5731(3)
b/Å	20.5731(3)
c/Å	13.6043(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	5758.1(2)
Z	16
ρ_{calc} g/cm^3	1.704
μ/mm^{-1}	2.357
F(000)	2880.0
Crystal size/mm^3	0.15 × 0.13 × 0.10
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.346 to 60.298
Index ranges	–25 ≤ h ≤ 18, –29 ≤ k ≤ 28, –18 ≤ l ≤ 18
Reflections collected	12465
Independent reflections	3819 [R_{int} = 0.0329, R_{sigma} = 0.0359]
Data/restraints/parameters	3819/0/164
Goodness-of-fit on F^2	1.040
Final R indexes [I ≥ 2σ (I)]	R_1 = 0.0250, wR_2 = 0.0484
Final R indexes [all data]	R_1 = 0.0328, wR_2 = 0.0514
Largest diff. peak/hole / e·Å^{-3}	0.47/–0.37



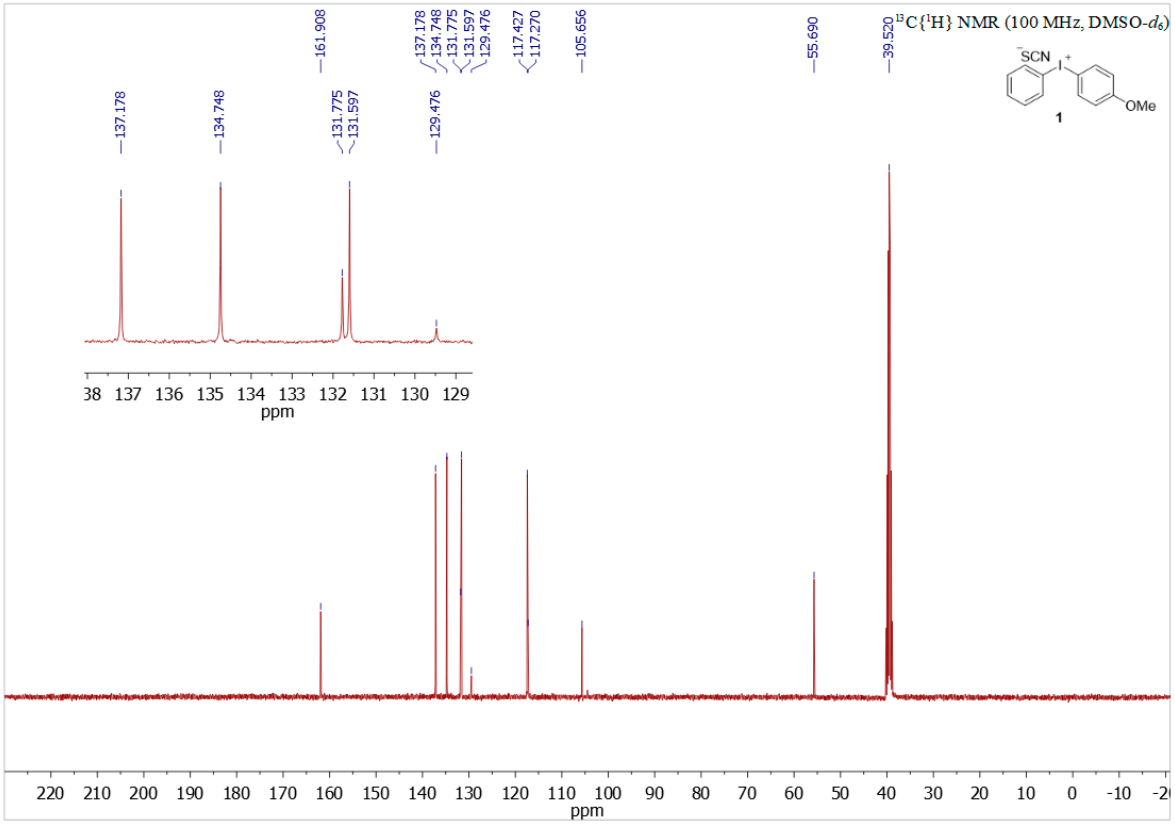


Figure S1. NMR spectra of product 1.