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Supporting Information

Halogen bonding two-point recognition with terphenyl derivatives

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Contents:

A) Synthesis and Experimental Data

A.0) General Information

A.0.1) Chemicals

Chemicals were obtained from *ABCR*, *Alfa Aesar*, *Carbolutions*, *Fluorochem*, *Merck*, *Sigma Aldrich* or *VWR*. Commercially available reagents and starting materials were, unless mentioned otherwise, used without further purification. Solvents which were used in moisture sensitive experiments were taken from a solvent drying system by *M. Braun* (type: *MB SPS-800*), dried over molecular sieve or bought dry and stored under and argon atmosphere. Other solvents were used after single distillation.

For reactions including oxygen or moisture sensitive reagents, glassware was dried under high-vacuum conditions (10^{-2} mbar) and procedures carried out under an argon atmosphere. Reagents were injected via a septum or added under argon counterflow.

A.0.2) Appliances and materials

Thin layer chromatography (TLC) was performed on plates from *Merck* (silica gel 60, F254). Detection of the substances was obtained by fluorescence detection under UV light (wavelength $\lambda = 254$ nm). The corresponding R_f values and solvents used as eluents are listed in the experimental part. Column chromatographies were performed with silica gel (grain size 0.04-0.063 cm, *Merck, Si60*). The used eluent relations are listed with the respective experiments.

^{1}H, ^{19}F and ^{13}C-Nuclear magnetic resonance spectra (NMR spectra) were recorded on either Bruker Avance III 300, DPX 250 or DRX 400 spectrometers at 22°C. All shift values are in ppm and all coupling constants (J) are printed in Hertz (Hz) with their multiplicity: s

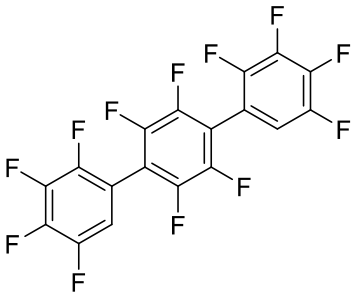
(singlet), bs (broad singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet). GC/MS spectra were measured on a Hewlett-Packard 5972 GC/MS System equipped with a Phenomenex Zebron ZB-5HT Inferno (25 m) column. Infrared spectra were measured on a Shimadzu FTIR-8400s spectrometer equipped with a Specac Quest ATR through attenuated total reflection (ATR). Elemental analyses were performed on a vario MICRO cube from Elementar Analysensysteme GmbH.

A.1) Synthesis of starting materials and guest molecules for Titration experiments

2,3,4,5-tetrafluoroboronic acid[1], 5,5-dimethyl-2-(2,3,4,5-tetrafluorophenyl)-1,3,2-dioxaborinane[2], 1,3-diiodotetrafluorobenzene[3], 3,6-diphenylpyridazin[4], pyridazine[5] were prepared according to literature. Benzohydrazide[6] was prepared according to literature but was purified using column chromatography with ethyl acetate. 2-phenyl-5-(p-tolyl)-1,3,4-oxadiazole[7] was synthesized according to literature as following: A mixture of 4-methylbenzoic acid (3.2 mmol, 436 mg) and benzohydrazide (3.2 mmol, 436 mg) was suspended in 10 ml $POCl_3$ and heated to reflux overnight. The excess solvent was removed, the residue was neutralized with $NaHCO_3$ and extracted three times with dichloromethane and the combined organic layers were washed with saturated NaCl-solution and dried over $MgSO_4$. The crude product mixture was purified via column chromatography using a petrol ether/ethyl acetate (10:1) mixture as eluent. The spectroscopic data matched the previously described data.[8] 2-5-diphenyl-1,3,4-oxadiazol was bought from *ABCR* and used without further purification.

A.2) Synthesis of halogen bond donors

A.2.1) 2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-1,1':4',1''-terphenyl



An argon purged 250 ml round bottom flask was charged with 60 ml THF and 60 ml toluene and deoxygenated via the freeze-pump-thaw technique. Afterwards 12.5 mg Bis(dibenzylideneacetone)palladium(0) (Pd_2dba_3) (12.4 µmol, 5 mol %) and 15.32 mg 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (SPhos) (37.33 µmol, 30 mol %) were added. The solution was stirred for 2 hours at 50°C to prepare the active catalyst. During that time the colour of the solution changed from dark red to orange. Subsequently 20 ml ddH_2O, 68.78 mg K_2CO_3 (497.68 µmol, 200 mol %), 100 mg 1,4-diiodotetrafluorobenzene (248.84 µmol) and 430 mg 5,5-dimethyl-2-(2,3,4,5-tetrafluorophenyl)-1,3,2-dioxaborinane (1.64 mmol, 660 mol %) were added. The flask was equipped with a reflux condenser, septum and an argon filled balloon and the biphasic mixture was refluxed at 95°C for 60 hours. After cooling to room temperature, the mixture was filtered into a separatory funnel and the organic and aqueous phase were separated. The aqueous layer was extracted 3 times with diethyl ether and the combined organic layers were washed with saturated NaCl-solution and dried over $MgSO_4$. The Solvents were removed under reduced pressure and the residue was filtered through a plug of silica with pentane as eluent. The pentane was removed *in vacuo* and the product was obtained as white solid (98.17 mg, 220.02 µmol, 88.42% yield).

^{1}H NMR (250 MHz, DMSO-d_6) δ = 7.90 (q, *J* = 8.6, 8.2 Hz, 2H).

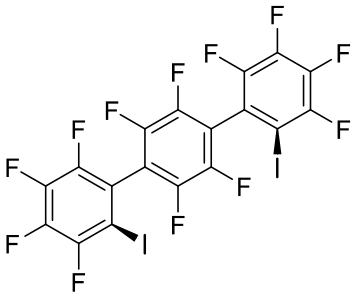
^{19}F NMR (235 MHz, DMSO-d_6) δ = -137.87 (br s, 2F), -138.42 (dtd, *J* = 22.6, 11.4, 3.0 Hz, 2F), -140.19 (s, 4F), -151.93 (tdd, *J* = 21.9, 8.3, 5.0 Hz, 2F), -154.56 (t, *J* = 21.5 Hz, 2F).

^{13}C NMR (63 MHz, Chloroform-*d*) δ = 149.33 (ddd, *J* = 10.2, 3.7, 2.5 Hz), 147.76 (ddd, *J* = 11.3, 3.7, 1.5 Hz), 146.23 (ddd, *J* = 15.7, 6.8, 4.2 Hz), 145.37 (ddd, *J* = 10.4, 3.7, 2.5 Hz), 143.73 (tdd, *J* = 16.6, 12.3, 3.7 Hz), 142.56 – 141.82 (m), 140.18 – 139.10 (m), 113.18 (d, *J* = 20.6 Hz), 111.34 – 110.58 (m).

EI-MS: m/z [+] calc. = 466.0 [M^+] found = 466.0 [M^+]

Elemental Analysis: Calc.: C: 48.45 H: 0.45
Found: C: 48.99 H: 0.78

A.2.2) <u>2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-6,6''-diiodo-1,1':4',1''-terphenyl</u>



A 250 ml round bottom flask was charged with 25.6 ml (290.9 mmol, 20000 mol %) trifluoromethanesulfonic acid and cooled to 0°C. Then 649 mg 2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-1,1':4',1''-terphenyl (1.45 mmol) was added. Over the course of 1 hour 1.31 g of *N*-iodosuccinimide (5.82 mmol, 400 mol %) was added. The solution was stirred overnight and allowed to warm to room temperature. The reaction mixture was poured onto crushed ice and the aqueous phase was extracted three times with diethyl ether. The combined organic layers were neutralized with saturated $NaHCO_3$-solution, washed with saturated NaCl-solution and dried over $MgSO_4$. The solvent was removed under reduced pressure and the residue was purified using column chromatography with pentane as eluent. Removal of the solvent yielded 280 mg of

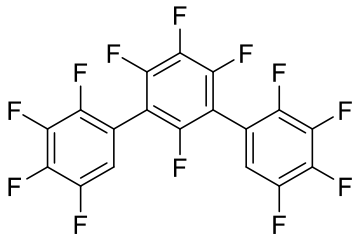
2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-6,6''-diiodo-1,1':4',1''-terphenyl as white powder (401 µmol, 21 %).

^{19}F NMR (235 MHz, Chloroform-*d*) δ = -111.62 (ddd, *J* = 22.7, 10.1, 4.6 Hz, 2 F), -131.60 (ddd, *J* = 21.4, 10.1, 4.7 Hz, 2 F), -137.18 (m, 4 F), -148.76 (ddd, *J* = 22.7, 19.4, 4.9 Hz, 2 F), -151.87 – -152.16 (ddd, *J* = 21.0, 19.7, 4.7 Hz, 2 F).

^{13}C NMR (101 MHz, Chloroform-*d*) δ = 148.55 (dd, *J* = 245.6, 11.2 Hz), 147.02 – 143.85 (m), 145.63 – 142.62 (m), 142.71 – 139.55 (m), 117.37 (dd, *J* = 16.2, 3.4 Hz), 116.69 (dt, *J* = 16.8, 9.4 Hz), 81.43 (dd, *J* = 25.5, 4.5 Hz).

Elemental Analysis: Calc.: C: 30.97
Found: C: 31.21

A.2.3) <u>2,2',2'',3,3'',4,4',4'',5,5',5'',6'-dodecafluoro-1,1':3',1''-terphenyl</u>



An argon purged 250 ml round bottom flask was charged with 60 ml THF and 60 ml toluene and deoxygenated via the freeze-pump-thaw technique. Afterwards 39.72 mg Bis(dibenzylideneacetone)palladium(0) (Pd_2dba_3) (43.37 µmol, 5 mol %) and 106.83 mg 2-dicyclohexylphosphino-2',6'-dimethoxybiphenyl (SPhos) (260.23 µmol, 30 mol %) were added. The solution was stirred for 2 hours at 50°C to prepare the active catalyst. During that time the colour of the solution changed from dark red to orange. Subsequently 20 ml ddH_2O, 239.7 mg K_2CO_3 (1.73 mmol, 200 mol %), 348.59 mg 1,3-diiodotetrafluorobenzene (867.42 µmol) and 1.5 g 5,5-dimethyl-2-(2,3,4,5-tetrafluorophenyl)-1,3,2-dioxaborinane (5.72 mmol, 660 mol %) were added. The flask was equipped with a reflux condenser, septum and an argon filled balloon and the biphasic mixture was refluxed at 95°C for 60

hours. After cooling to room temperature, the mixture was filtered into a separatory funnel and the organic and aqueous phase were separated. The aqueous layer was extracted 3 times with diethyl ether and the combined organic layers were washed with saturated NaCl-solution and dried over $MgSO_4$. The Solvents were removed under reduced pressure and the residue was purified via column chromatography using pentane as eluent. The pentane was removed *in vacuo* and the product was obtained as a white solid (325 mg, 680 µmol, 78.42% yield).

^{1}H NMR (250 MHz, Acetone-d_6) δ = 7.58 (dddd, J = 10.7, 8.3, 6.0, 2.6 Hz, 2H).

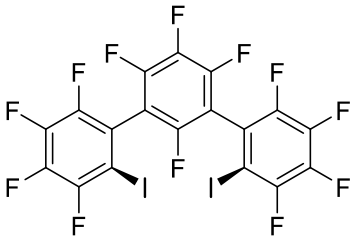
^{19}F NMR (235 MHz, Acetone-d_6) δ = -117.96 (d, J = 67.4 Hz, 1F) -132.68 (ddt, J = 21.3, 8.4, 4.1 Hz, 2F), -139.00 (s, 2F), -140.43 (dt, J = 22.0, 11.1 Hz, 2F), -154.92 (tdd, J = 20.1, 8.0, 5.1 Hz, 2F), -156.79 (t, J = 19.9 Hz, 2F), -165.12 (s, 1F).

^{13}C NMR (75 MHz, Chloroform-d) δ = 153.72, 151.43 – 150.67 (m), 150.38 (q, J = 6.8, 6.3 Hz), 149.23 – 148.74 (m), 147.59 (ddd, J = 14.8, 9.0, 3.4 Hz), 145.69 (ddd, J = 10.3, 3.7, 2.5 Hz), 144.40 – 143.93 (m), 143.69 – 142.85 (m), 140.28 – 139.28 (m), 113.36 (d, J = 20.5 Hz), 111.13 (dt, J = 13.4, 5.7 Hz), 108.02 (t, J = 21.9 Hz).

EI-MS: m/z [+] calc. = 466.0 [M^+] found = 466.0 [M^+]

Elemental Analysis: Calc.: C: 48.45 H: 0.45
Found: C: 48.74 H: 0.52

A.2.4) 2,2',2'',3,3'',4,4',4'',5,5',5'',6'-dodecafluoro-6,6''-diiodo-1,1':3',1''-terphenyl



A 250 ml round bottom flask was charged with 37.7 ml (427.17mmol, 20000 mol %) trifluoromethanesulfonic acid and cooled to 0°C. Then 831 mg 2,2',2'',3,3'',4,4',4'',5,5',5'',6'-dodecafluoro-1,1':3',1''-terphenyl (1.45 mmol) was added. Over the course of 1 hour 1.67 g of *N*-iodosuccinimide (5.82 mmol, 400 mol %) was added. The solution was stirred overnight and allowed to warm to room temperature. The reaction mixture was poured onto crushed ice and the aqueous phase was extracted three times with diethyl ether. The combined organic layers were neutralized with saturated $NaHCO_3$-solution, washed with saturated NaCl-solution and dried over $MgSO_4$. The solvent was removed under reduced pressure and the residue was purified using column chromatography with pentane as eluent. Removal of the solvent yielded 360 mg of syn-2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-6,6''-diiodo-1,1':4',1''-terphenyl as white powder (515 µmol, 30 %) and 325 mg of anti-2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-6,6''-diiodo-1,1':4',1''-terphenyl as a colorless oil (465 µmol, 25 %).

^{19}F NMR (235 MHz, Chloroform-*d*) δ = -111.93 (ddd, *J* = 22.8, 10.1, 4.5 Hz), -113.72 (dt, *J* = 10.9, 2.7 Hz), -127.71 (dt, *J* = 22.2, 1.8 Hz), -131.64 (dddd, *J* = 21.2, 9.7, 4.5, 2.3 Hz), -149.19 (ddd, *J* = 23.0, 19.6, 4.9 Hz), -152.38 (ddd, *J* = 21.3, 19.6, 4.5 Hz), -161.30 (td, *J* = 22.2, 10.8 Hz).

^{13}C NMR (63 MHz, Chloroform-*d*) δ = 154.21 – 153.62 (m), 151.81 (ddd, *J* = 11.4, 8.7, 6.1 Hz), 148.37 (dddd, *J* = 245.6, 11.2, 4.2, 2.4 Hz), 147.70 (dt, *J* = 11.1, 5.2 Hz), 143.72 (d, *J* = 11.5 Hz), 143.10 (ddd, *J* = 17.3, 12.7, 3.9 Hz), 139.43 – 138.50 (m), 138.03 (dtd, *J* = 253.3, 15.5, 5.0 Hz), 117.43 (dd, *J* = 16.2, 3.4 Hz), 110.63 (ddd, *J* = 22.6, 13.1, 10.0 Hz), 82.07 (dd, *J* = 25.2, 4.7 Hz).

Elemental Analysis: Calc.: C: 30.97
Found: C: 31.31

A.3) Complexes preparation (m-1/4a and m-1/4b)

The halogen-bonded complexes were obtained by co-crystallization of the donor and acceptor mixed in 2:1 stoichiometric ratio with THF/ETOH 1:2 mixture followed by slow evaporation to yield single crystals.

A.3.1) Complex m-1/4a for $C_{32}H_{10}F_{10}I_4N_2O$

Calcd(%). C: 33.83, N: 2.47, H: 0.89. Found(%). C: 33.75, N: 2.31, H: 0.80.

A.3.2) Complex m-1/4b for $C_{33}H_{12}F_{10}I_4N_2O$

Calcd(%). C: 34.46, N: 2.44, H: 1.05. Found (%). C: 34.21, N: 2.35, H: 0.93.

B) Structural Characterization

B.1) Crystal Structure Determination

The data collection of the X-ray diffraction experiment were carried out in an Agilent Supernova diffractometer with Cu (λ= 1.5418 Å; for **m-1/4a**) and Mo (λ= 0.71073 Å; for **m-1/4b**) radiations at 293 K. Data were indexed, integrated and scaled with the CrysAlisPRO program.[9] The observed intensities were corrected with a numerical absorption correction based on Gaussian integration over a multifaceted crystal model with CrysAlisPRO.[9] Both crystal structures were solved by the SHELXTL routine and refined with the full-matrix least-squares technique on *F*[10] by using the SHELXL-2013 program[11] within the WINGX[12] software package. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were set on geometrical positions and refined with a riding model. Residual electron density is located close to the iodine atoms of the **m-1** ligand in both compounds. A summary of the crystallographic data and structure refinement is given in Table S1. The final geometrical calculations and the graphical manipulation were carried out with DIAMOND[13] and MERCURY[14] programs, respectively.

CCDC numbers 1824277 and 1824278, for **m-1/4a** and **m-1/4b**, respectively, contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK: fax: (+44)1123-336-033; e-mail: deposit@ccdc.cam.ac.uk).

Table S1. Crystallographic data for complexes **m-1/4a** and **m-1/4b**.

	m-1/4a	**m-1/4b**
Formula	$C_{32}H_{10}F_{10}I_4N_2O$	$C_{51}H_{12}F_{20}I_8N_2O$
FW	1136.02	2063.83
Crystal system	Triclinic	Triclinic
Space group	*P* -1	*P* -1
a(Å)	12.9014(2)	11.0666(3)
b(Å)	16.0841(4)	11.7332(3)
c(Å)	18.1379(4)	22.9011(6)
(º)	79.028(2)	90.760(2)
(º)	83.942(2)	99.480(2)
(º)	67.838(2)	98.949(2)
V(Å^3)	3419.61(14)	2895.01(13)
Z	4	2
(mm^{-1})	29.397	4.389
T(K)	293(2)	293(2)
$_{cal}$ (g cm^{-3})	2.207	2.368
(Å)	1.5418	0.71073
Index ranges	$-16 \le h \le 13$	$-14 \le h \le 14$
	$-20 \le k \le 20$	$-15 \le k \le 15$
	$-22 \le l \le 22$	$-30 \le l \le 28$
Total Reflections	42308	49854
Indep. Reflections (R_{int})	14185(0.035)	13462 (0.027)
Obs. reflect. [I> 2σ(I)]	12240	8975
Parameters	883	739
Goodness-of-fit	1.025	1.009
R [I> 2σ(I)]7	0.0378	0.0487
R_w [I> 2σ(I)]	0.1014	0.0973
R (all data)	0.0434	0.0806
R_w (all data)	0.1078	0.1116

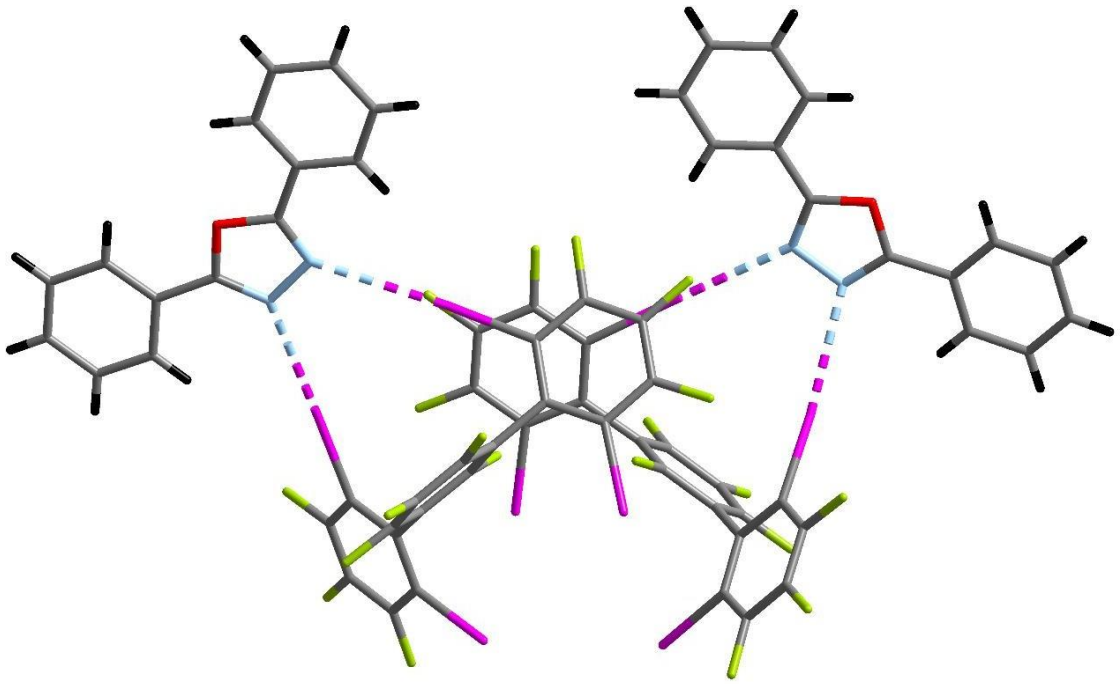
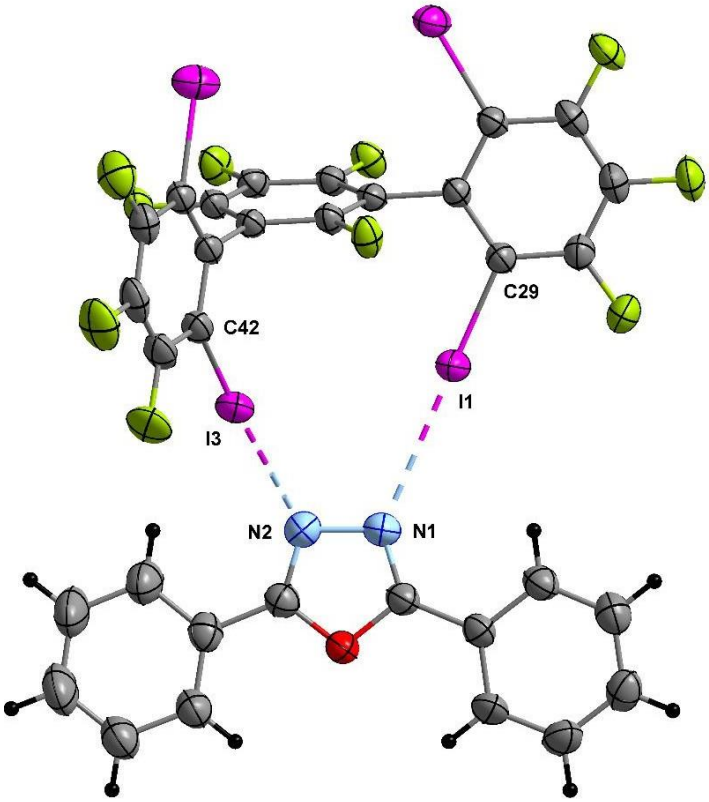
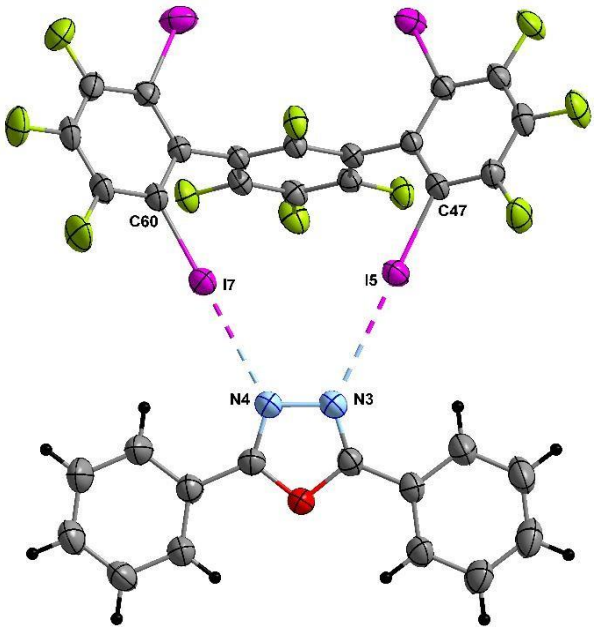


Figure S1. View of asymmetric unit of **m-1/4a**, a 1:1 stoichiometry complex with two crystallographically independent two-point halogen bonding dimers.



a)



b)

Figure S2. View of second dimer of two crystallographically independent two-points halogen bonding dimers in **m-1/4a** complex. (atoms involving in noncovalent interaction have been numbered).

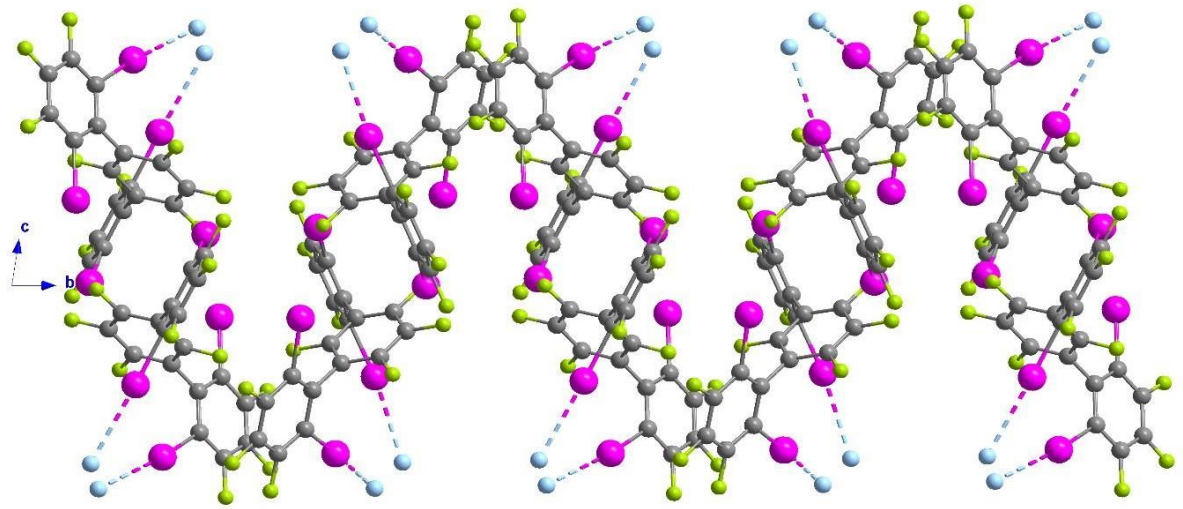


Figure S3. Pairs of **m-1** molecules forming a corrugated layer within the crystallographic *ab* plane

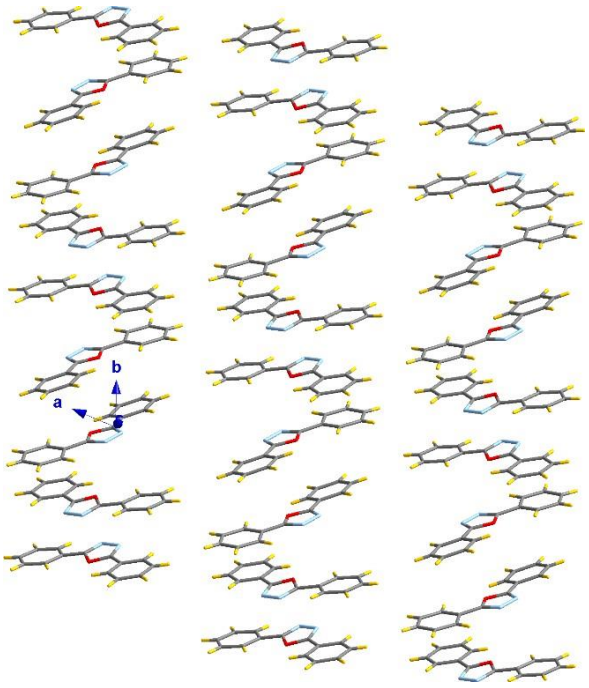


Figure S4. Oxadiazole molecules are occupying the interlayer space being stacked along the *b* axis.

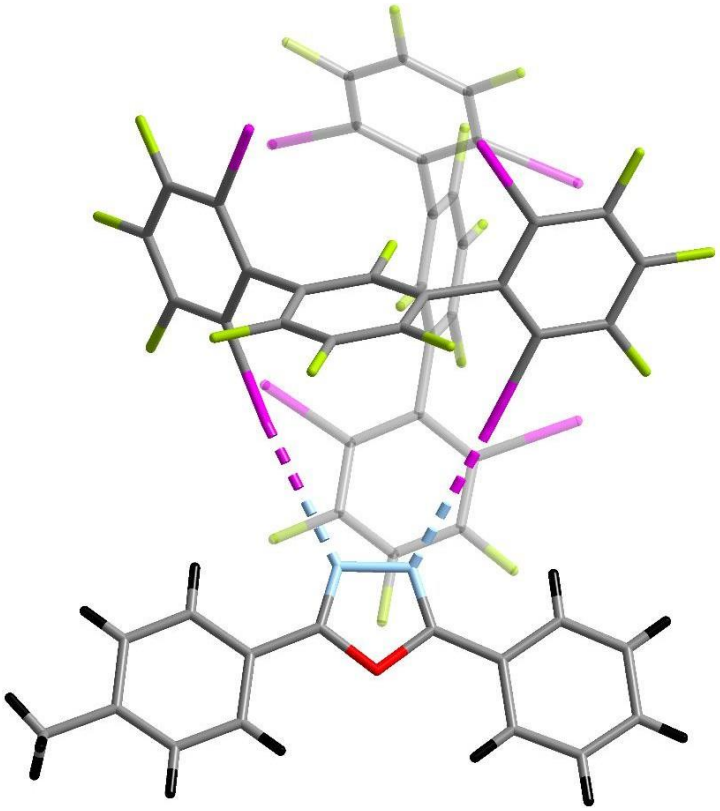


Figure S5. View of asymmetric unit of **m-1/4b**, a 2:1 stoichiometry complex with one two-point halogen bonding dimer.

C.) NMR-Spectra

C.1.) 2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-1,1':4',1''-terphenyl

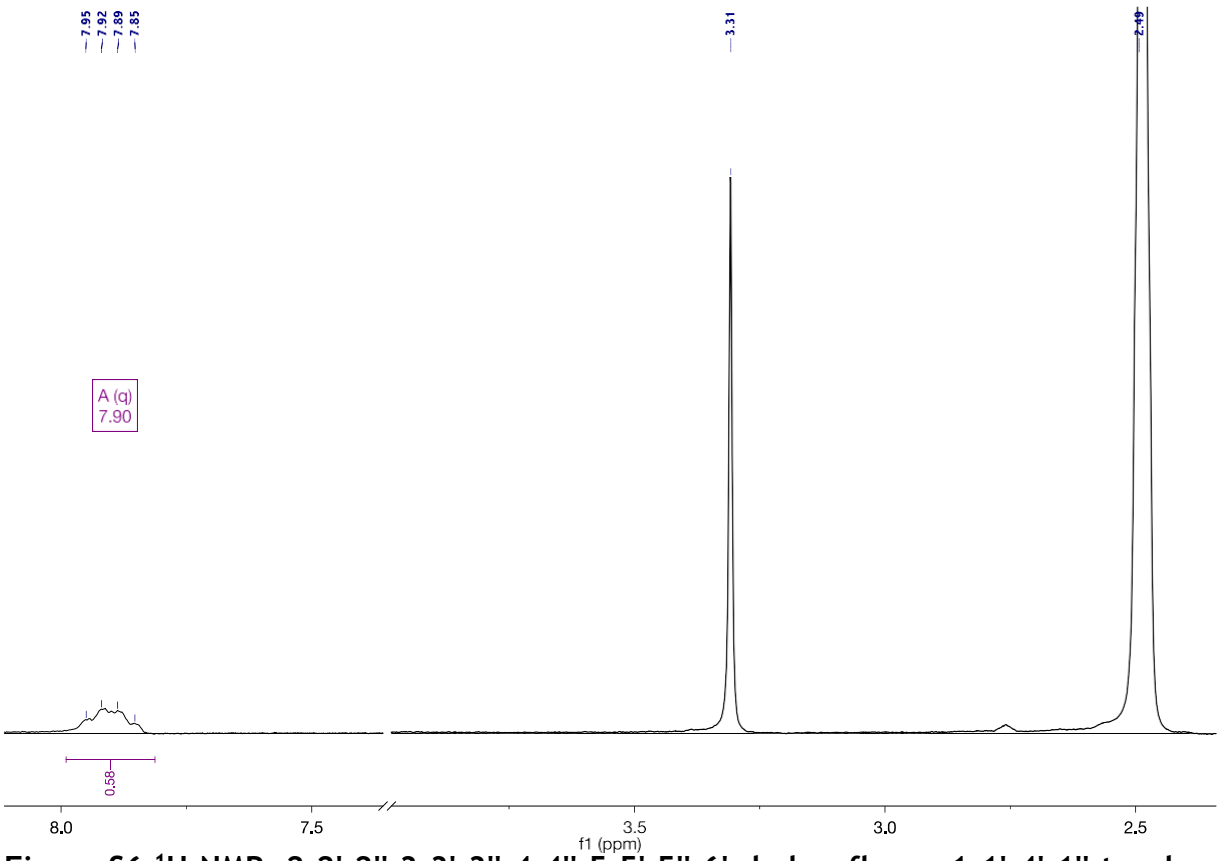


Figure S6 ^{1}H-NMR: 2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-1,1':4',1''-terphenyl

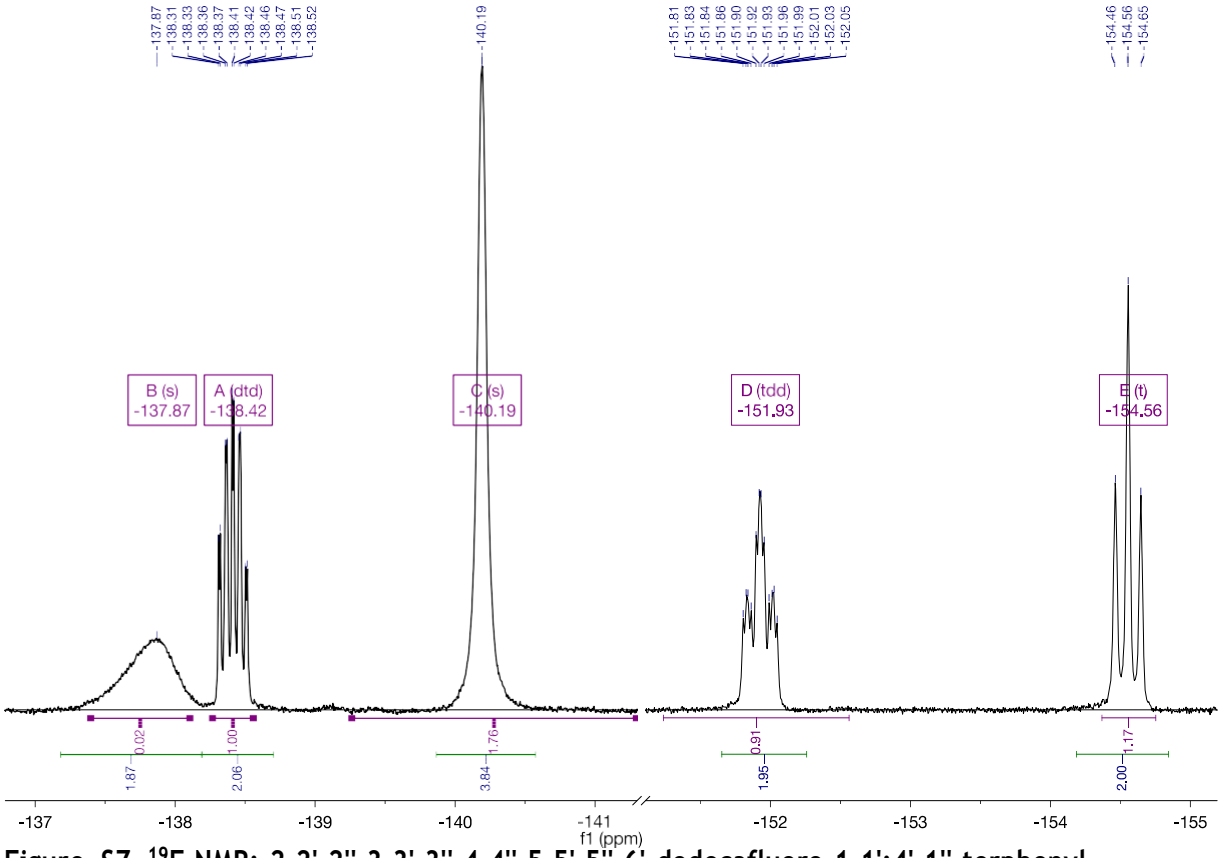


Figure S7 ^{19}F-NMR: 2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-1,1':4',1''-terphenyl

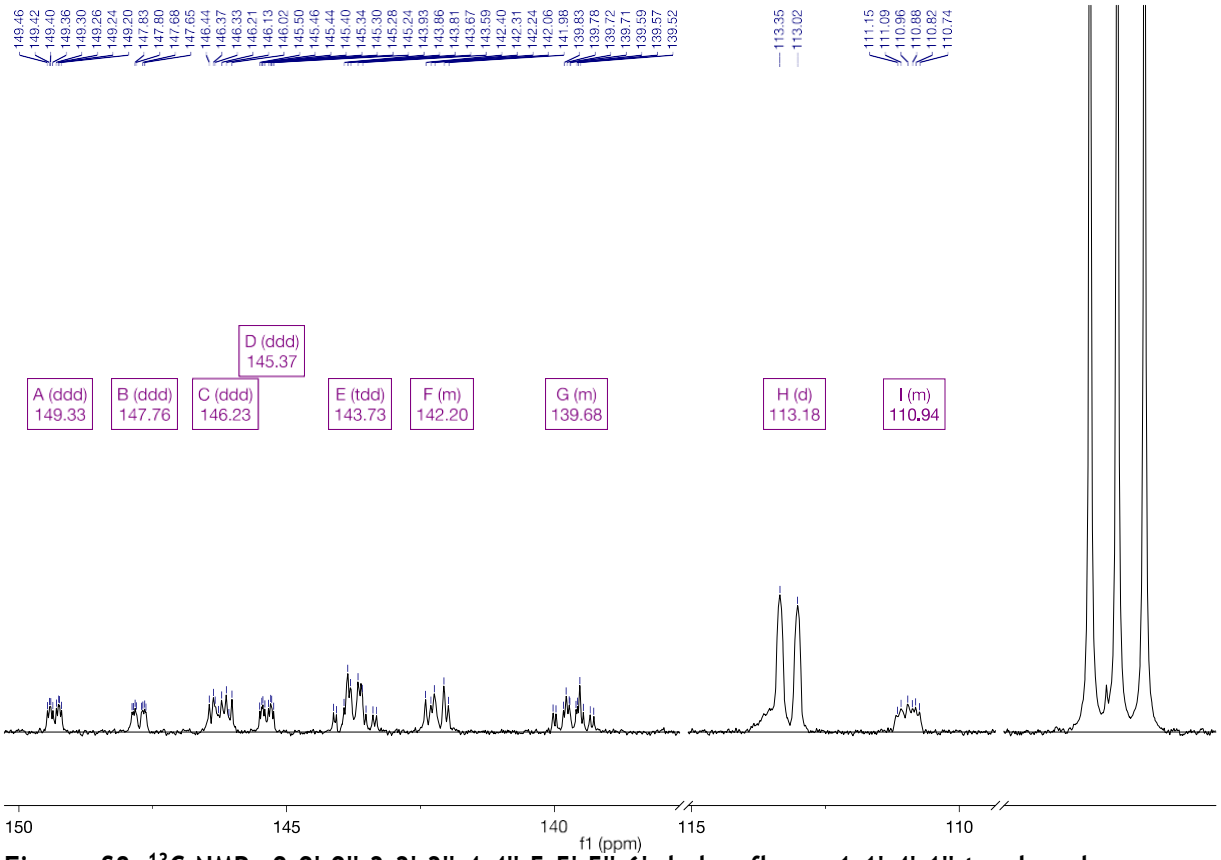


Figure S8 ^{13}C-NMR: 2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-1,1':4',1''-terphenyl

C.2.) 2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-6,6''-diiodo-1,1':4',1''-terphenyl

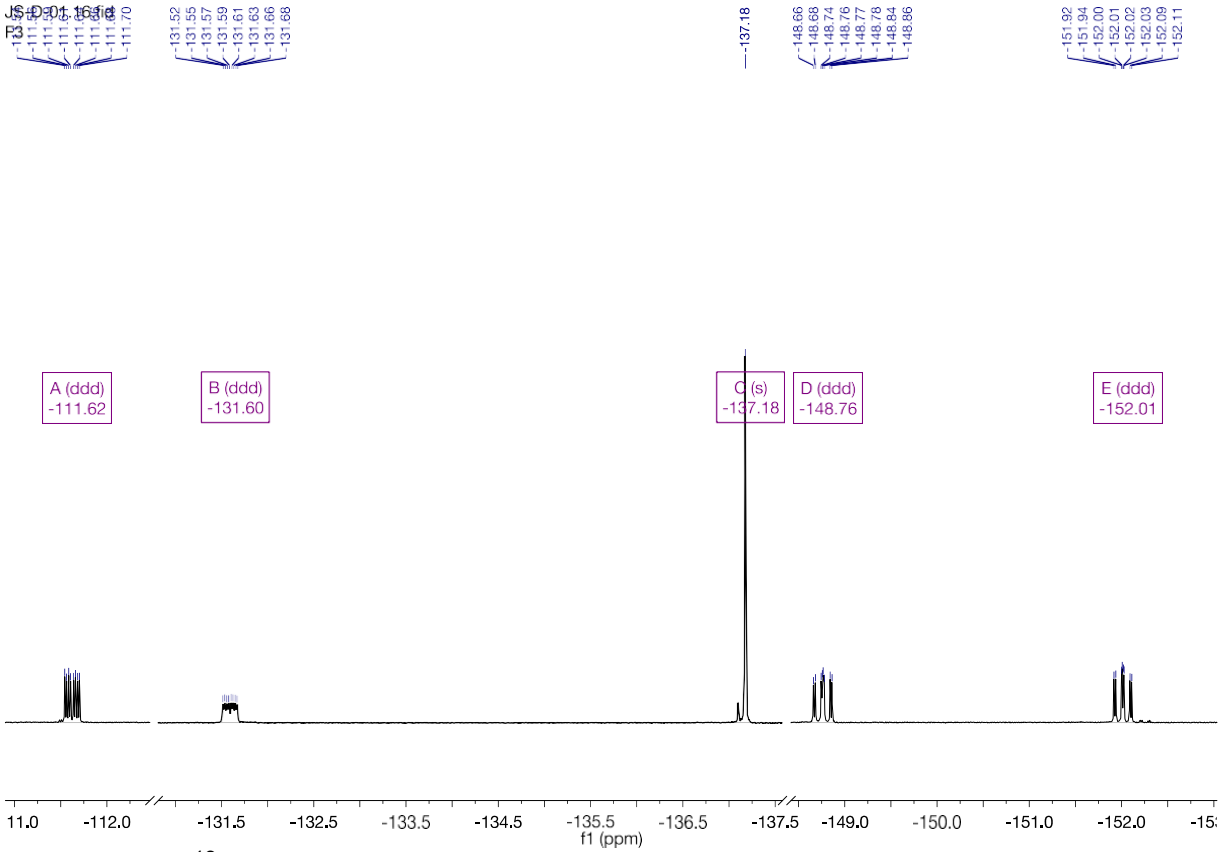


Figure S9 ^{19}F-NMR: 2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-6,6''-diiodo-1,1':4',1''-terphenyl

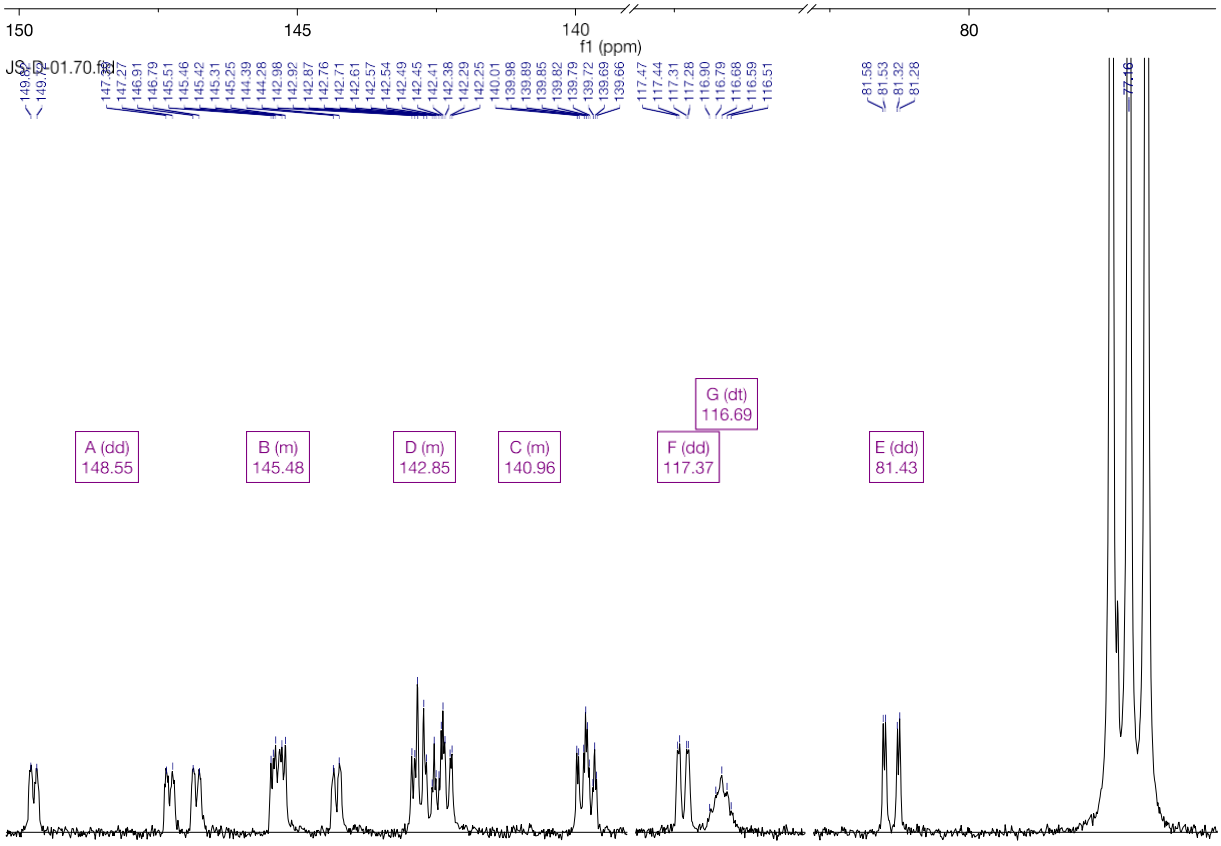


Figure S10 **^{13}C-NMR:** 2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-6,6''-diiodo-1,1':4',1''-terphenyl

C.3.) 2,2',2'',3,3'',4,4',4'',5,5',5'',6'-dodecafluoro-1,1':3',1''-terphenyl

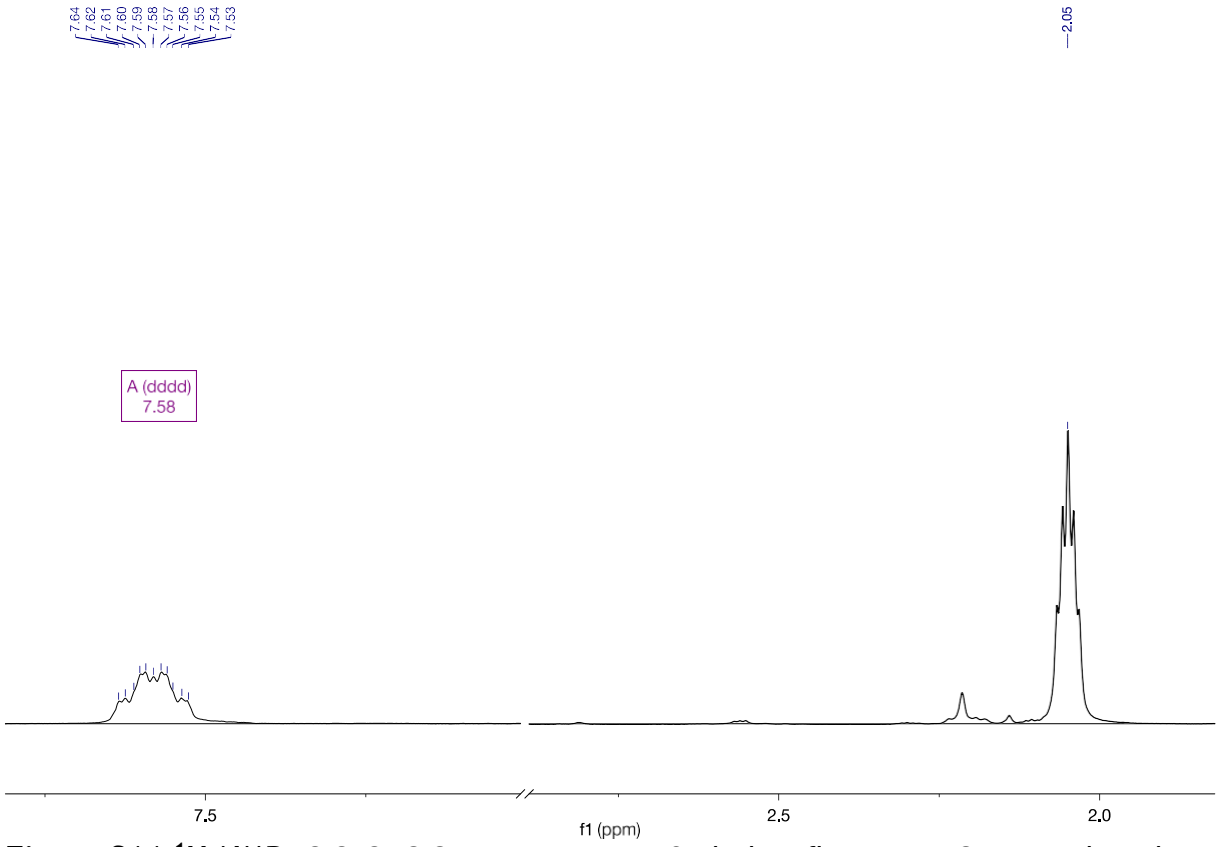


Figure S11 ^{1}H-NMR: 2,2',2'',3,3'',4,4',4'',5,5',5'',6'-dodecafluoro-1,1':3',1''-terphenyl

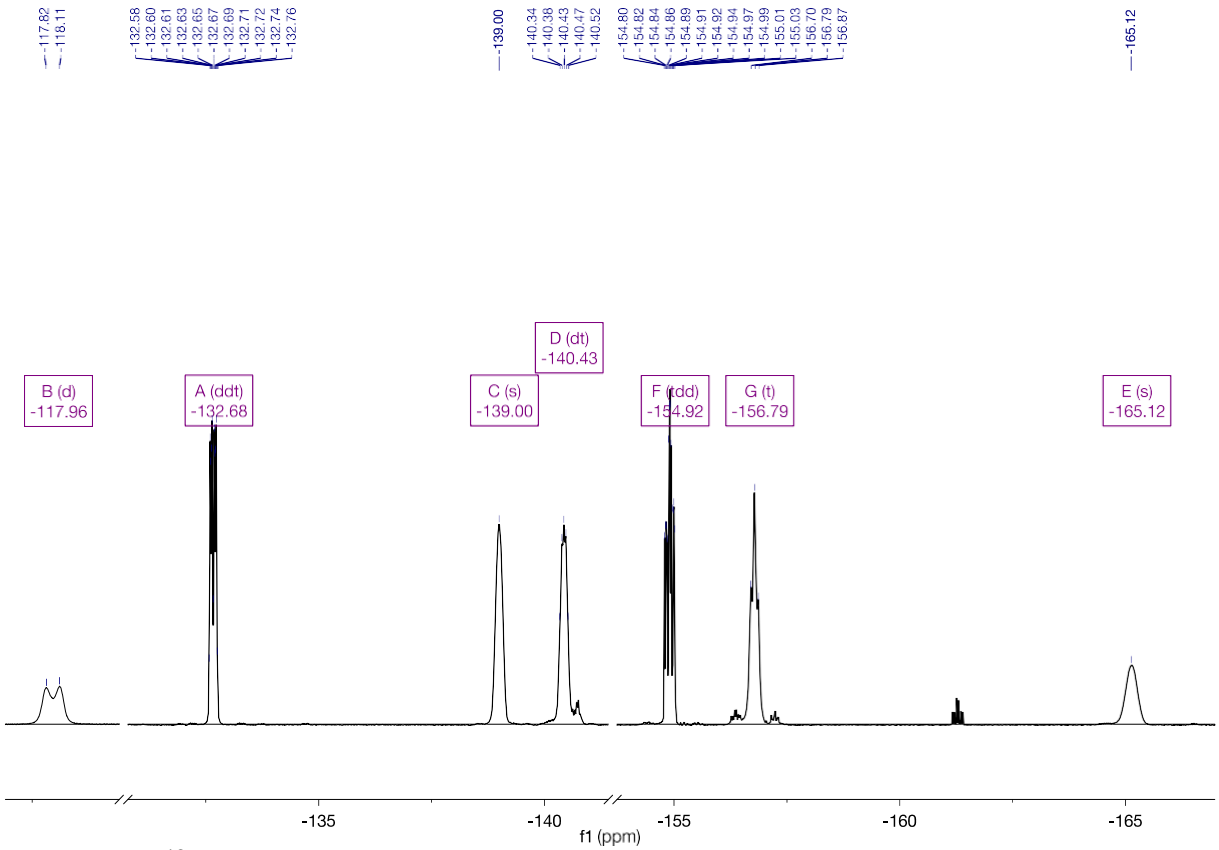


Figure S12 ^{19}F-NMR: 2,2',2'',3,3'',4,4',4'',5,5',5'',6'-dodecafluoro-1,1':3',1''-terphenyl

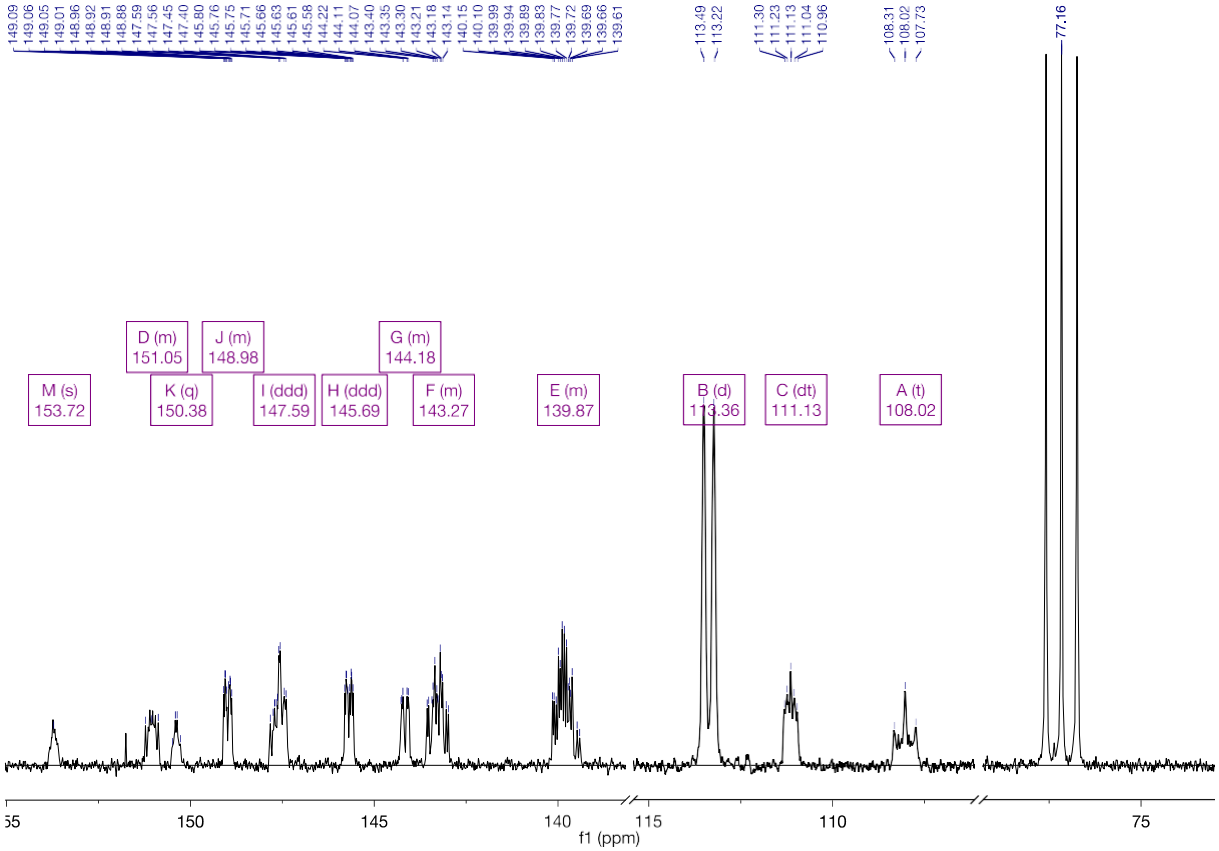


Figure S13 ^{13}C-NMR: 2,2',2'',3,3'',4,4',4'',5,5',5'',6'-dodecafluoro-1,1':3',1''-terphenyl

C.3.) 2,2',2",3,3",4,4',4",5,5',5",6'-dodecafluoro-6,6"-diiodo-1,1':3',1"-terphenyl

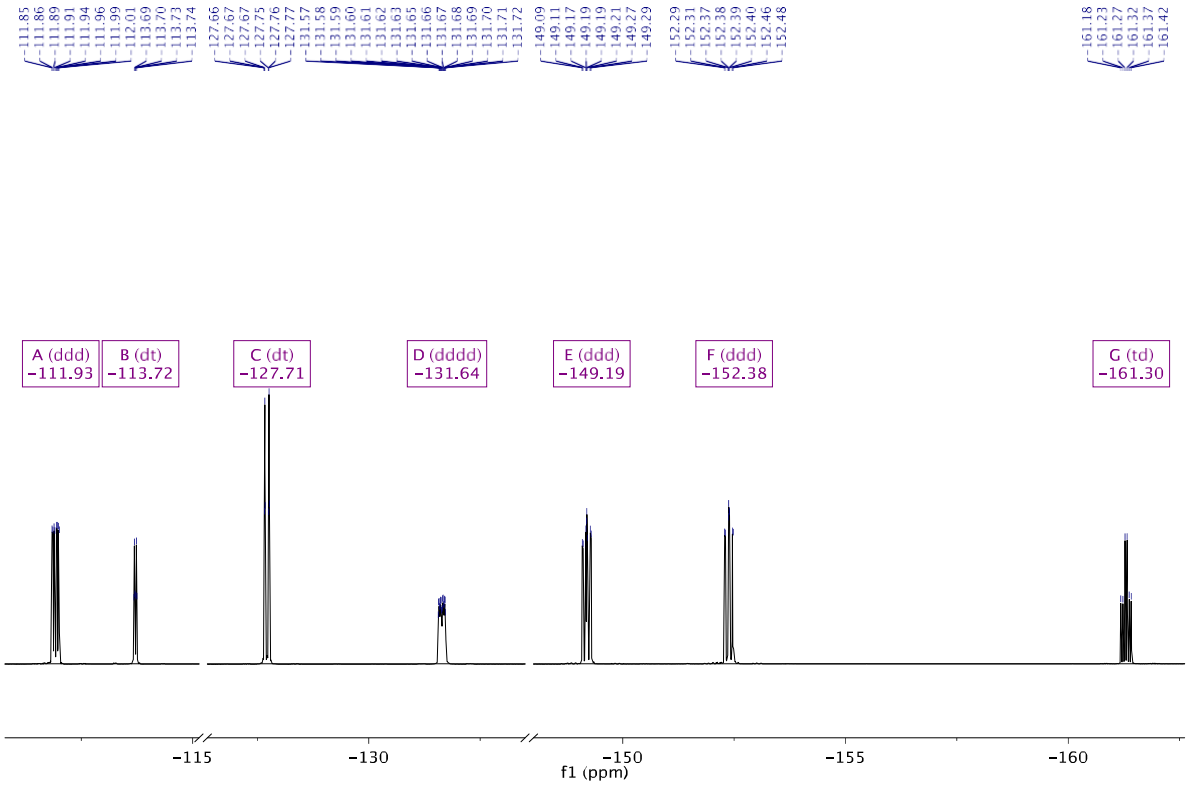


Figure S14 ^{19}F-NMR: 2,2',2",3,3",4,4',4",5,5',5",6'-dodecafluoro-6,6"-diiodo-1,1':3',1"-terphenyl

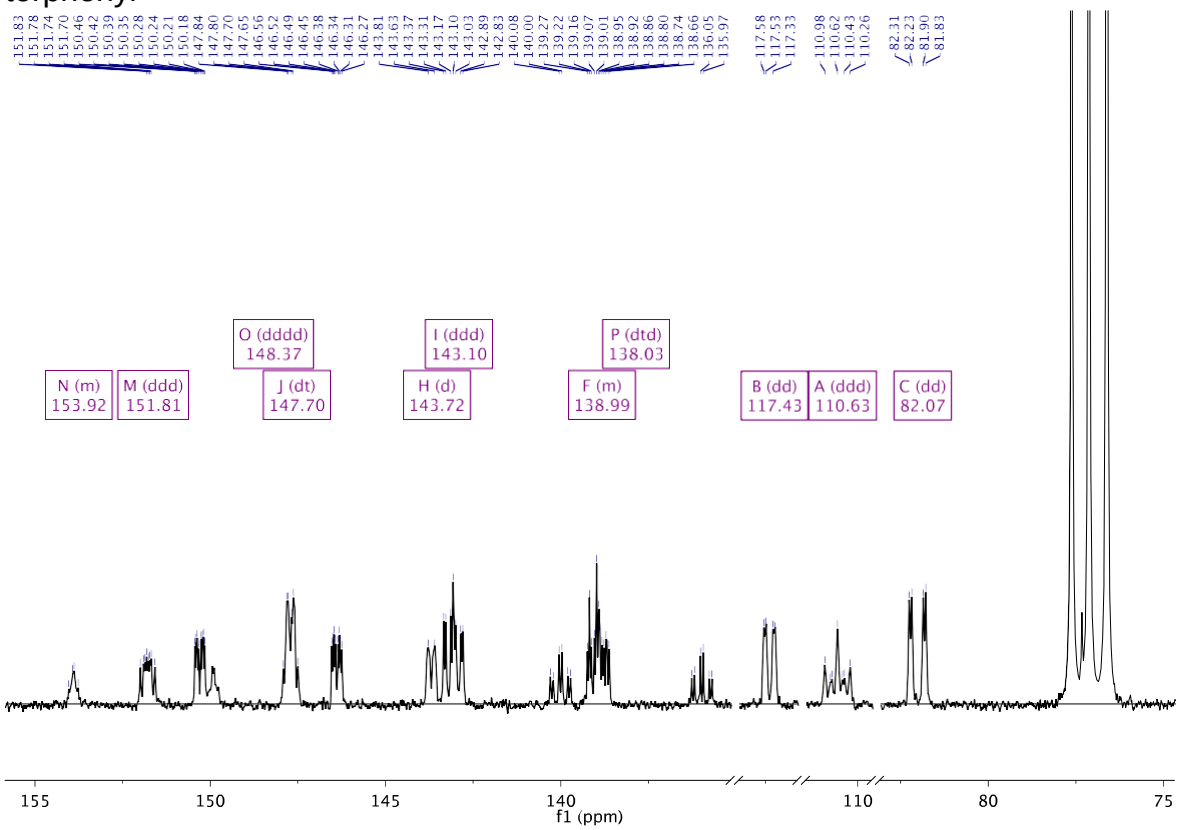


Figure S15 ^{13}C-NMR: 2,2',2",3,3",4,4',4",5,5',5",6'-dodecafluoro-6,6"-diiodo-1,1':3',1"-terphenyl

D. 1) NMR-Titrations

D. 1.1) General information

Chemicals

All deuterated solvents were purchased from *Deutero GmbH*, dried and stored over molecular sieve.

General Procedure

For pipetting *Hamilton*®-syringes were used. All experiments were conducted at ambient temperature and in *Norell*® 502 NMR-Tubes. 30 µmol of the Host (XB-Donor) were dissolved in 1 ml of deuterated solvent. Stock solutions of the Guest (XB-Acceptor) were prepared as 0.3 M solutions in the corresponding deuterated solvent. As internal standard a solution of 2 µl 1,3,5-trifluorobenzene in 1 ml deuterated solvent was used. The NMR-Tube was charged with 50 µl of the Host-solution and 550 µl of the 1,3,5-trifluorobenzene solution. For each measured point a certain amount of Guest solution was added. The NMR-spectra were measured with a *Bruker* DPX-250. Each ^{19}F-NMR-spectra was measured with 32 scans. In addition, ^{1}H-Spectra were measured and the host to guest ratio was checked by integration of the signals and corrected if necessary.

For the determination of the binding constants the shifts of all fluorine atoms were observed relative to the signal of the standard. The collected data (measured shifts (Δppm) vs. guest equivalents) was fitted via the website supramolecular.org, fitting the shift of several nuclei simultaneously: for both **p-7** and **m-7**, all fluorine substituents on the outer phenyl rings were considered, and for **m-7** additionally the isolated fluorine substituent at the central core was included.

For the calculations of the binding constants (K) a 1:1 stochiometry was assumed.

D. 1.2) Titration results

Table S2. Titration experiments and corresponding binding constants

Donor	Guest	Binding constant K [mol^{-1}]
p-7	4a	0,94
m-7	4a	1,99
p-7	8	0,79
m-7	8	0,91

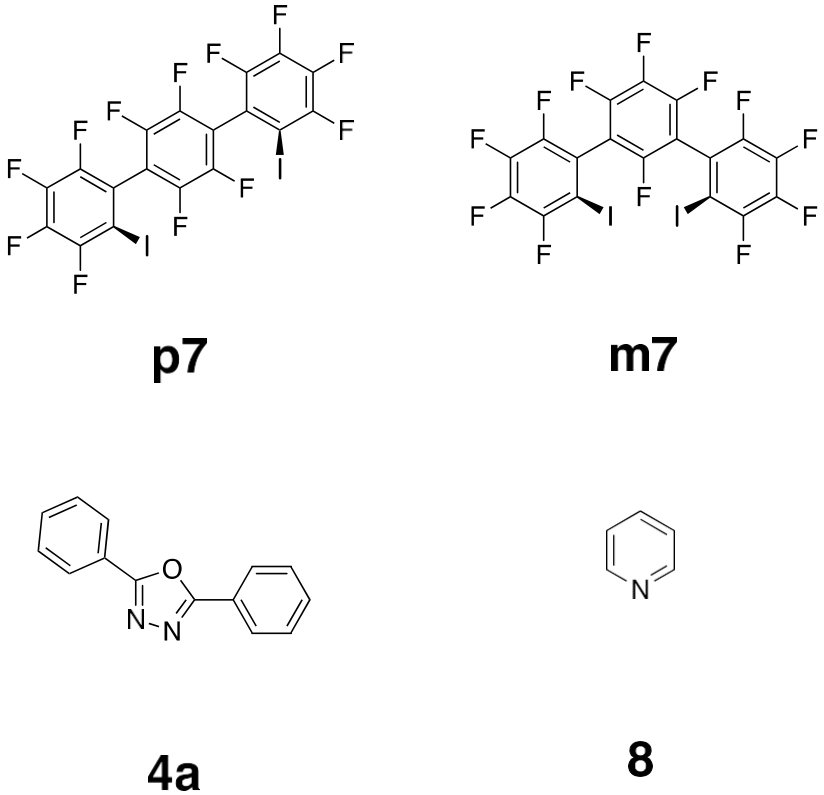


Figure S16: Titration molecules. (Hosts and Guests)

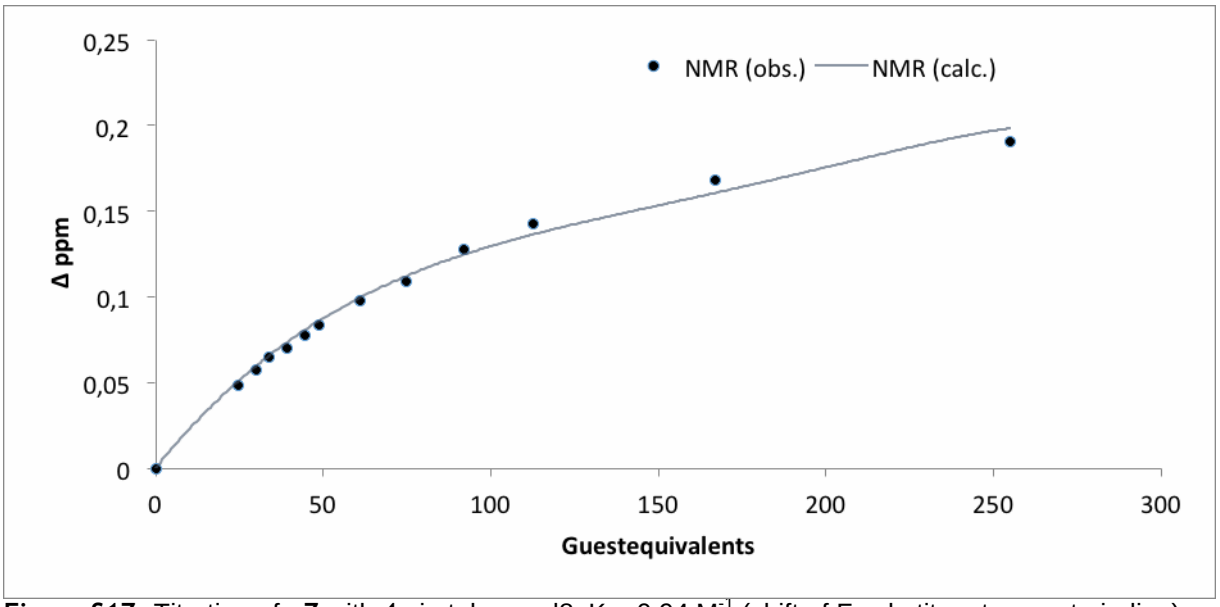


Figure S17: Titration of **p7** with **4a** in toluene-d8, K = 0,94 M^{-1} (shift of F substituents *para* to iodine)

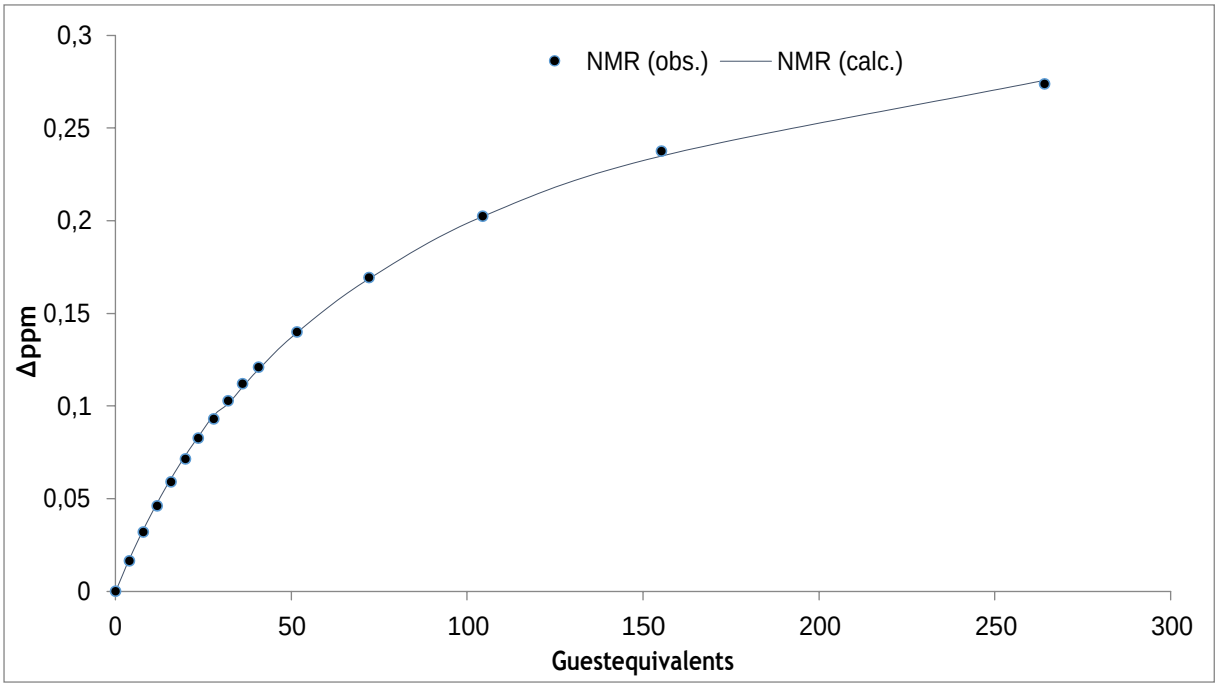


Figure S18: Titration of **m7** with **4a** in toluene-d8, K = 1,99 M^{-1} (shift of isolated F substituent of central core).

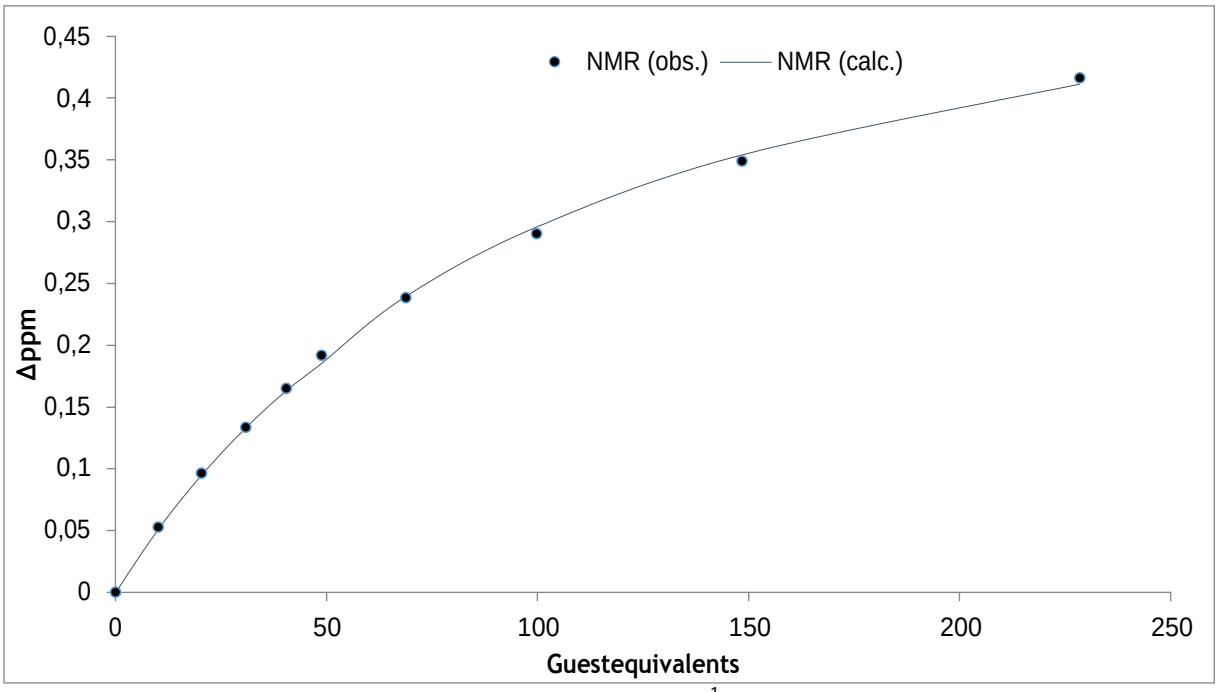


Figure S19: Titration of **p7** with **8** in toluene-d8, K = 0,79 M^{-1} (shift of F substituents *para* to iodine).

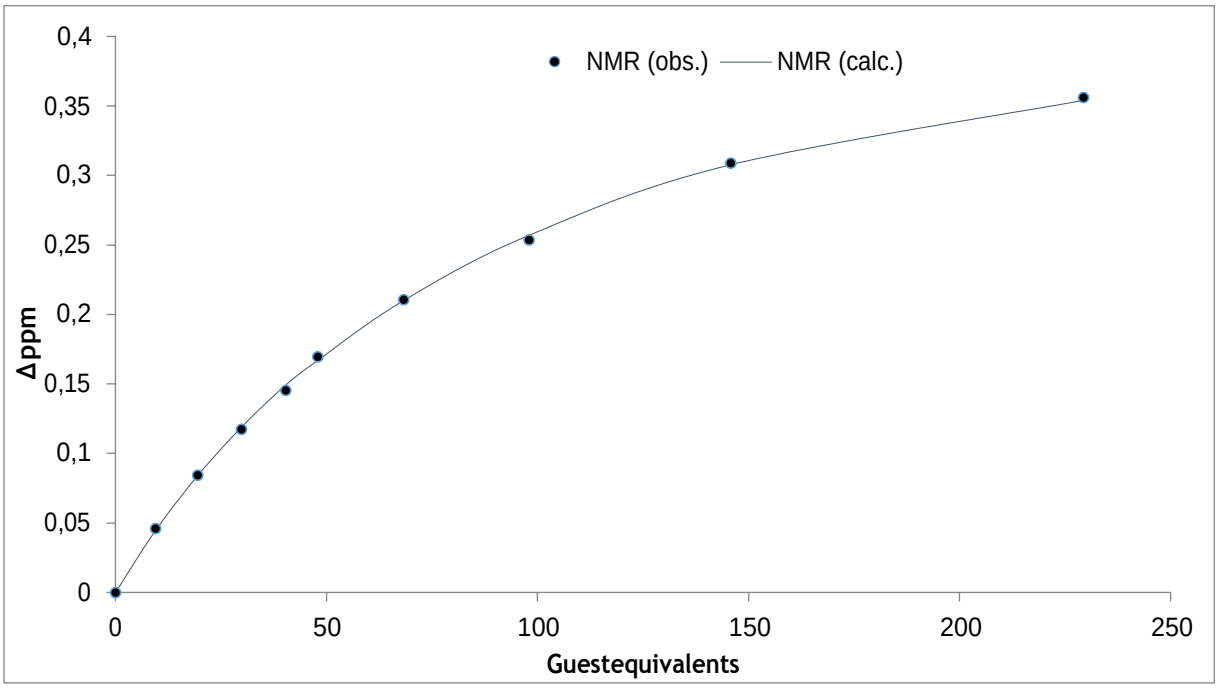


Figure S20: Titration of **m7** with **8** in toluene-d8, K = 0,91 M^{-1} (shift of isolated F substituent of central core).

E) DFT Calculations

The halogen-bonded complexes were modelled by density functional theory using the M062X functional[15] with D3 dispersion corrections by Grimme[16] and the triple-zeta TZVPP basis set (including the corresponding pseudopotential for iodine).[17] All geometries were fully optimized and the nature of the minima was confirmed by the absence of relevant imaginary frequencies (note: in very few cases, small imaginary frequencies < 10 cm^{-1} were obtained which could not be eliminated by further optimization and which were consequently disregarded as "noise"). All figures shown below were generated with CYLview.[18] Free energy values G refer to the Gibbs free energy in hartree, as provided in the Gaussian09 output.

Coordinates, Gibbs free energies of the respective minima (denoted G), halogen bonding interaction details and Gibbs free energies of binding (denoted ΔG_{XB}) are provided below (for the corresponding Lewis structures, compare Figure 1 in the manuscript):

Halogen bond donor m-1

G = -2874.828464 ht

I	1.49452600	-3.21474800	-0.52465500
I	3.02335300	2.57255300	0.68198900
I	-3.02341200	-2.57255500	0.68193900
I	-1.49447100	3.21474000	-0.52462200
F	0.00000500	0.00002700	-1.27944900
F	2.30376400	-0.33706600	2.77568700
F	-2.30378200	0.33694300	2.77568500
F	5.44959400	1.50383200	-0.97396500
F	-5.44962800	-1.50375800	-0.97399500
F	-0.00001400	-0.00009000	4.12310500
F	4.27902700	-2.88800800	-1.90798400
F	-5.99535800	0.85317400	-2.10235900
F	5.99537300	-0.85307600	-2.10235700
F	-4.27896900	2.88806800	-1.90796000
C	2.47725400	-0.35507500	-0.03594100
C	1.20760300	-0.17437500	0.70821500
C	-1.20760600	0.17434100	0.70821400
C	3.38576800	0.70027700	-0.14979300
C	0.00000100	-0.00000300	0.05237900
C	-2.47725100	0.35507600	-0.03594200
C	2.77677200	-1.58073100	-0.63635400
C	1.17855400	-0.17265400	2.09439300
C	-2.77674500	1.58074600	-0.63634000
C	4.56907300	0.52278500	-0.84677800
C	-3.38578700	-0.70025600	-0.14981000
C	-1.17856700	0.17256000	2.09439300
C	-4.56908800	-0.52273100	-0.84679400
C	3.96445200	-1.73849300	-1.33059900
C	4.86309200	-0.69257900	-1.43777100

C	-3.96442000	1.73854000	-1.33058700
C	-0.00000900	-0.00006200	2.79786200
C	-4.86308100	0.69264600	-1.43777300

Halogen bond donor p-1

G = -2874.827507 ht

I	-2.63431700	-3.05030400	-0.04660800
I	-2.63438400	3.05032200	0.04667200
F	-1.34074500	-0.33532100	2.32204900
F	-1.34072100	0.33536800	-2.32209200
F	-5.67735600	2.32003700	0.02559800
F	1.34074100	0.33536500	-2.32208000
F	-5.67728500	-2.32009900	-0.02566700
F	-6.99705300	-0.00005100	-0.00005400
C	-2.88932900	0.00001200	-0.00002800
C	-1.40538400	0.00002700	-0.00002100
C	0.69130300	-0.16888000	1.17525500
C	-3.59389300	1.20545700	0.01308100
C	-0.69131900	-0.16887900	1.17525000
C	-3.59385400	-1.20545900	-0.01313500
C	-0.69130700	0.16892500	-1.17528500
C	-4.97867900	1.19526200	0.01226100
C	1.40538000	0.00002500	-0.00000700
C	-4.97864200	-1.19530300	-0.01233300
C	-5.67444100	-0.00003200	-0.00004500
C	0.69131500	0.16892400	-1.17528000
C	2.88932600	0.00000700	-0.00000900
C	3.59389400	1.20545300	0.01284100
C	3.59385000	-1.20547000	-0.01286100
C	4.97868000	1.19525500	0.01202800
C	4.97863700	-1.19531700	-0.01206000
C	5.67443800	-0.00004300	-0.00001900
F	1.34071900	-0.33533000	2.32206100
I	2.63430900	-3.05032000	-0.04598600
F	5.67735900	2.32003000	0.02512700
F	6.99705000	-0.00006500	-0.00002400
F	5.67727800	-2.32011600	-0.02515900
I	2.63439700	3.05033700	0.04600400

Disulphide 2

G = -876.142480 ht

S	-0.89323300	-0.49843100	-0.48729900
S	0.89322300	-0.49842600	0.48730300
C	-1.80504500	0.80172300	0.37982400
H	-2.79447900	0.84113500	-0.07440900
H	-1.89699400	0.55798000	1.43455200
H	-1.31727300	1.76547500	0.25600700
C	1.80506100	0.80170900	-0.37983300
H	1.31728600	1.76546300	-0.25604500
H	2.79448300	0.84112100	0.07442700

H	1.89704000	0.55794300	-1.43455400

Thioacetal 3

G = -953.514681 ht

C	0.00000400	1.69536700	-0.27618200
C	-1.27150500	1.06262800	0.27572500
C	0.00004000	-1.34426500	0.45192600
C	1.27144400	1.06260800	0.27586200
H	-1.27805800	1.11283100	1.36742300
H	-2.15162700	1.59468200	-0.08209100
H	0.00007100	1.62989600	-1.36498900
H	-0.00001200	2.75498300	-0.00499400
H	0.00006800	-1.22765600	1.53644300
H	0.00004800	-2.40681600	0.22016400
H	1.27782500	1.11266000	1.36757000
H	2.15161100	1.59472800	-0.08174300
S	-1.52157700	-0.65700900	-0.22877200
S	1.52158800	-0.65694900	-0.22883900

Oxadiazole 4

G = -724.036448 ht

O	-0.00000500	0.18609300	-0.00005600
N	0.68932700	-1.89176800	-0.00004000
C	2.41198700	-0.11524500	-0.00003200
N	-0.68932200	-1.89177500	-0.00002800
C	1.05872400	-0.65706000	-0.00005200
C	3.49294900	-0.99589500	-0.00001500
H	3.30269600	-2.06026700	-0.00003900
C	-1.05872700	-0.65707000	-0.00004000
C	2.63074700	1.25964500	0.00000000
H	1.78837500	1.93730300	-0.00001500
C	4.78374200	-0.49739300	0.00003400
H	5.62228200	-1.18016900	0.00005100
C	3.92721300	1.75087400	0.00005300
H	4.09619200	2.81892800	0.00008500
C	-2.41199100	-0.11525500	-0.00002000
C	-2.63074000	1.25963700	-0.00008000
H	-1.78836000	1.93728600	-0.00016100
C	-3.92720000	1.75087700	-0.00004700
H	-4.09617200	2.81893200	-0.00009900
C	-5.00371800	0.87529200	0.00005000
H	-6.01416300	1.26101300	0.00007700
C	-3.49295800	-0.99589700	0.00006900
H	-3.30271400	-2.06027000	0.00011100
C	-4.78375000	-0.49738400	0.00011000
H	-5.62229600	-1.18015300	0.00019300
C	5.00372200	0.87528300	0.00007200
H	6.01417100	1.26099500	0.00011600

Pyridazin 5

G = -726.171613 ht

C	0.68453500	1.30276500	0.42369500
C	-0.68451800	1.30277600	0.42369500
C	-1.34099100	0.12793100	0.04177700
C	1.34099000	0.12790900	0.04177400
H	1.24381700	2.17107400	0.74191800
H	-1.24378100	2.17109600	0.74191900
N	0.65564200	-0.96745900	-0.28095300
N	-0.65566000	-0.96744900	-0.28095200
C	2.81719700	0.02085600	0.00044400
C	3.61509200	1.14909200	-0.18144200
C	3.42890400	-1.22488200	0.13942400
C	4.99693200	1.03761000	-0.21532200
H	3.15893100	2.11986400	-0.32464000
C	4.80924800	-1.33370900	0.10951600
H	2.80658400	-2.09867300	0.26907200
C	5.59795100	-0.20377800	-0.06596200
H	5.60337100	1.92041300	-0.36606600
H	5.27268300	-2.30429100	0.22438500
H	6.67573000	-0.29148200	-0.09078700
C	-2.81719800	0.02087800	0.00044600
C	-3.42888600	-1.22487400	0.13938200
C	-3.61511200	1.14910700	-0.18139800
C	-4.80922800	-1.33372500	0.10947300
H	-2.80655000	-2.09866000	0.26899500
C	-4.99695100	1.03760300	-0.21527900
H	-3.15897200	2.11989300	-0.32456300
C	-5.59795000	-0.20379900	-0.06596200
H	-5.27264600	-2.30431800	0.22430800
H	-5.60340400	1.92040300	-0.36598900
H	-6.67572700	-0.29152000	-0.09078800

Halogen bond donor m-7

G = -2479.24799 ht

I	1.83511400	-2.19854200	-0.77534500
I	-2.96513100	-1.86739500	0.78548600
F	0.28090000	0.82677400	-1.20978600
F	2.33914400	0.61118100	2.98553100
F	-2.29029800	0.97871400	2.69292000
F	5.70006700	2.57820000	-0.09705100
F	-5.25137500	-0.87595700	-1.11110700
F	-0.05978500	0.80350300	4.18145700
F	4.71889600	-1.63070500	-1.85503800
F	-5.62598500	1.37707400	-2.49329600
F	6.40877500	0.41319100	-1.55869400
F	-3.81318000	3.38251100	-2.36346700
C	2.69379400	0.57401600	0.19723300
C	1.37142900	0.69666700	0.85008900
C	-1.05957800	0.88484300	0.69588500
C	3.60167200	1.61155800	0.34132700

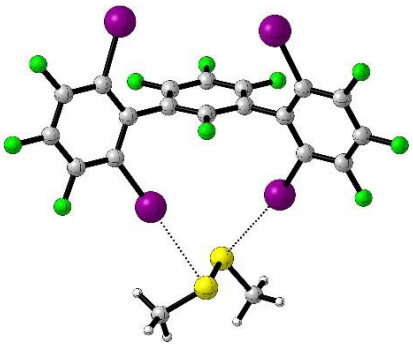
C	0.19777400	0.80597100	0.11859300
C	-2.28389000	0.97011500	-0.13169500
C	3.07326500	-0.54465900	-0.55233600
C	1.25336000	0.70575200	2.23228300
C	-2.50374000	2.12079300	-0.87255600
C	4.85550900	1.57167600	-0.24484400
C	-3.22185300	-0.06393800	-0.21371900
C	-1.11769600	0.88635500	2.08292800
C	-4.34400000	0.08575600	-1.00829600
C	4.32432500	-0.58514800	-1.14079300
C	5.21545600	0.46704800	-0.99237500
C	-3.62469100	2.27185900	-1.67124200
C	0.02317600	0.79940200	2.85917600
C	-4.55044200	1.24819400	-1.73555900
F	3.27610700	2.68726800	1.04954200
F	-1.63130000	3.12125500	-0.82346000

Halogen bond donor p-7

G = -2479.245961 ht

I	2.77955300	-2.21949200	-0.19961200
F	1.33389800	-0.20676700	2.20417600
F	1.33586400	1.90939800	-1.98870300
F	5.78377100	-1.35482600	-0.09028700
F	-1.33590000	1.90939400	-1.98870800
F	5.54203100	3.29348200	0.22863800
F	6.99695000	1.01627900	0.07317400
C	2.88989400	0.82710900	0.08513700
C	1.40924700	0.83207700	0.09679600
C	-0.69093300	0.30242400	1.15956300
C	3.65015300	-0.34350400	-0.00357500
C	0.69090500	0.30241700	1.15955800
C	3.55246300	2.04280500	0.15526600
C	0.69155600	1.38382300	-0.95350300
C	5.03120300	-0.26640900	-0.00365500
C	-1.40928000	0.83209600	0.09681100
C	4.93483900	2.12155800	0.15342400
C	5.67644600	0.95849500	0.07625200
C	-0.69159600	1.38382900	-0.95350000
C	-2.88993000	0.82710900	0.08518100
C	-3.65014900	-0.34351900	-0.00367800
C	-3.55253900	2.04277100	0.15551200
C	-5.03120000	-0.26647700	-0.00372400
C	-4.93492000	2.12147200	0.15370200
C	-5.67648700	0.95839400	0.07636700
F	-1.33392300	-0.20676200	2.20418200
F	-5.78373000	-1.35490900	-0.09049200
F	-6.99699200	1.01613100	0.07331900
F	-5.54215300	3.29336200	0.22910300
I	-2.77946300	-2.21944400	-0.19993900
F	2.86163800	3.17399400	0.23840000
F	-2.86175900	3.17397500	0.23882600

Complex of m-1 with disulphide 2
G = -3750.964241 ht



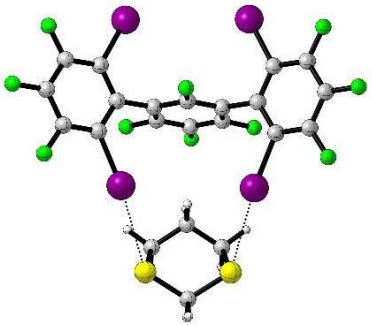
ΔG_{XB} = 2.4 kcal/mol
I···S distances (Å): 3.42 and 3.47
C-I···S angles (°): 178 and 169

I	-1.27664900	-4.10324200	-0.32930600
I	3.30758400	-0.15253600	0.39690200
I	-4.54191400	-0.44930400	0.70902200
I	0.41775700	2.86158000	-0.66522100
F	-0.53395600	-0.47994800	-1.32993600
F	1.04081300	-2.20703000	2.71835600
F	-2.09990800	1.23125900	2.73288500
F	4.62305600	-2.51741400	-1.22141200
F	-5.69537100	1.94926400	-0.92422400
F	-0.53786700	-0.49814600	4.07304700
F	1.11674900	-5.50670800	-1.78894700
F	-4.57586600	4.06958800	-2.09763100
F	3.66936500	-4.82392800	-2.17196800
F	-1.93838800	4.45839000	-1.98106900
C	1.18336000	-2.30089400	-0.09190200
C	0.28949800	-1.38231700	0.65537300
C	-1.35822100	0.41816200	0.66029700
C	2.52089600	-1.95472000	-0.30185400
C	-0.53615700	-0.48276500	0.00205200
C	-2.21155600	1.38254700	-0.07611300
C	0.69857600	-3.50885500	-0.59660600
C	0.26784800	-1.36914700	2.04088400
C	-1.63847700	2.49489900	-0.70081300
C	3.34935700	-2.81327900	-1.00300000
C	-3.59378700	1.19114800	-0.15128800
C	-1.33717000	0.39076000	2.04662600
C	-4.38224700	2.10257300	-0.83312100
C	1.54387100	-4.35273100	-1.29710200
C	2.86833700	-4.01048800	-1.50192900
C	-2.44619600	3.39149500	-1.37872900
C	-0.53703700	-0.49377600	2.74717600
C	-3.81454500	3.20380800	-1.44720500
S	3.76955600	3.54790500	-0.64017700

S	4.05860200	3.10045300	1.32915100
C	3.48586400	5.33467600	-0.59464200
H	3.26743900	5.63305000	-1.61931600
H	2.63391800	5.56239300	0.04044600
H	4.37368400	5.85642400	-0.24727300
C	5.84861200	3.29543300	1.50869000
H	6.14094100	4.32558500	1.32303700
H	6.08215900	3.03419200	2.53995100
H	6.36947700	2.62314200	0.83286400

Complex of m-1 with thioacetal 3

G = -3828.336919 ht



ΔG_{XB} = 3.9 kcal/mol

I···S distances (Å): 3.43 and 3.41

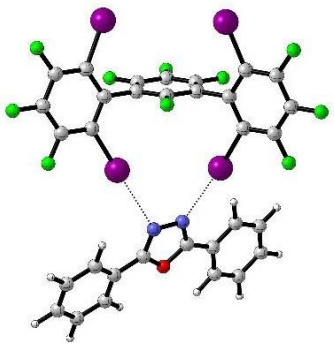
C-I···S angles (°): 159 and 162

I	1.62004600	2.69688700	-0.89442900
I	-4.10103900	1.43475800	0.80086400
I	2.67049900	-1.88107400	-0.69434600
I	-3.20859700	-2.90558600	0.59599600
F	-1.27848100	-0.28110200	-1.32614300
F	-0.31992800	2.31913900	2.44041100
F	0.66589300	-2.23204600	2.45409900
F	-4.41977000	4.02089200	-0.93744700
F	2.08383300	-4.65380100	-2.05523600
F	0.62867400	0.14480000	3.70955700
F	-0.07046000	4.98154000	-2.24388800
F	-0.09751800	-6.18471400	-2.21624700
F	-2.67819900	5.55662200	-2.25558800
F	-2.38577100	-5.42408300	-1.07045100
C	-1.33212900	2.26666000	-0.19750000
C	-0.84025200	1.06711500	0.52444100
C	-0.32043200	-1.31874500	0.52936000
C	-2.69181900	2.58204400	-0.20983500
C	-0.81698200	-0.17858900	-0.08152900
C	-0.26378300	-2.61752600	-0.18613900
C	-0.43095900	3.08125600	-0.88774500
C	-0.34150000	1.14945600	1.81432600
C	-1.39588800	-3.42929800	-0.27832300
C	-3.13655300	3.69309400	-0.90643500

C	0.92808500	-3.02805700	-0.78956800
C	0.16374400	-1.18023100	1.82034500
C	0.97172900	-4.23250200	-1.47028600
C	-0.89606600	4.18719000	-1.57802900
C	-2.24423000	4.49698300	-1.59241900
C	-1.33053200	-4.62984200	-0.96524600
C	0.15361100	0.03892600	2.47399400
C	-0.15085100	-5.03542200	-1.56247300
C	3.59995500	0.87501700	2.06920700
C	4.67565800	-0.20308400	2.05193100
C	6.12626000	1.28910900	0.26421100
C	4.14263700	2.28351300	1.86713800
H	5.42873400	-0.00926100	2.81885800
H	4.23854400	-1.18013300	2.25634600
H	2.84831700	0.65747900	1.30618500
H	3.10164700	0.83977300	3.04189700
H	6.84044000	1.50721200	1.05882700
H	6.64792400	1.32974400	-0.68900700
H	4.89440800	2.52054700	2.62325100
H	3.34176000	3.01682000	1.95546800
S	5.51691000	-0.39562600	0.45910500
S	4.86417700	2.57475000	0.23161400

Complex of m-1 with oxadiazole 4

G = -3'598.865273 ht



ΔG_{XB} = -0.2 kcal/mol

I···N distances (Å): 3.06 and 3.03

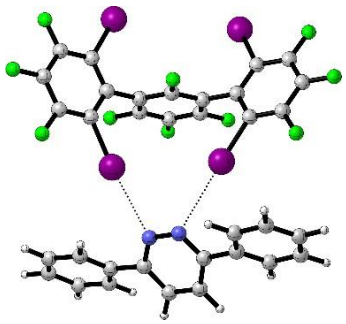
C-I···N angles (°): 178 and 175

I	1.35488900	2.02169700	-0.36651100
I	-4.58213800	2.48050000	0.99979900
I	1.35064700	-2.17299200	-0.54995900
I	-4.72892000	-2.29793000	-0.11090800
F	-1.75161300	0.19959200	-1.35899700
F	-1.43602700	1.91665400	2.98027000
F	-1.52431600	-2.69210800	2.30818000
F	-3.91537700	5.26406400	-0.26932600
F	0.52473500	-4.60729700	-2.38502400
F	-1.39097300	-0.58289700	3.97532900
F	0.59183700	4.91941800	-1.32109400
F	-1.83167400	-5.68367800	-3.02980900

F	-1.67923100	6.31900900	-1.27833600
F	-4.10441400	-4.68541200	-2.04477000
C	-1.61743800	2.49924000	0.23261000
C	-1.59641200	1.11994600	0.77943600
C	-1.64434700	-1.29434000	0.42842600
C	-2.79922000	3.24373800	0.24561000
C	-1.66429000	0.00756100	-0.04374800
C	-1.69747000	-2.45905900	-0.49017200
C	-0.45377700	3.06126400	-0.30066300
C	-1.50373400	0.88977900	2.14300800
C	-2.92266000	-3.03090800	-0.83751600
C	-2.81107700	4.53063800	-0.26466700
C	-0.51439400	-2.98828700	-1.01343900
C	-1.55163900	-1.46672300	1.80002000
C	-0.57490100	-4.07525700	-1.86821600
C	-0.49079800	4.34935500	-0.80667200
C	-1.65993200	5.08752100	-0.79130900
C	-2.95874200	-4.11779200	-1.69441600
C	-1.48083200	-0.39060100	2.66601600
C	-1.78848800	-4.64338600	-2.21131600
O	5.99883300	-0.05288100	0.33799600
N	4.00865300	0.48253500	-0.38188500
C	5.82706400	2.14034500	-0.69072600
N	3.94854700	-0.78009500	0.16742900
C	5.23088700	0.88046500	-0.26745500
C	5.07132100	3.03039200	-1.45222600
H	4.05920900	2.77009400	-1.72953400
C	5.13613100	-1.06380700	0.58390200
C	7.13646200	2.45659700	-0.33649800
H	7.71680600	1.76204800	0.25469600
C	5.62624100	4.23414100	-1.84943300
H	5.03925300	4.92514900	-2.43831100
C	7.68494400	3.66310200	-0.74069000
H	8.70081800	3.90986000	-0.46488400
C	5.60979300	-2.27237900	1.24498400
C	6.96076500	-2.43192000	1.54315700
H	7.66512200	-1.65453000	1.28203600
C	7.39385300	-3.58913800	2.17047400
H	8.44269600	-3.71381300	2.40139700
C	6.48440100	-4.58446000	2.49987100
H	6.82496900	-5.48670300	2.98934400
C	4.69511600	-3.27064100	1.57699000
H	3.64772100	-3.13376000	1.34484700
C	5.13641800	-4.42315300	2.20250800
H	4.42714200	-5.19732600	2.46021500
C	6.93166400	4.55233600	-1.49469500
H	7.36192300	5.49391700	-1.80763500

Complex of m-1 with Pyridazin 5

G = -3'600.999794 ht



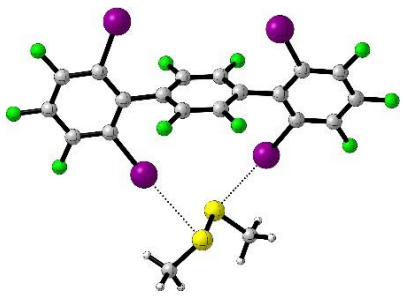
ΔG_{XB} = 0.2 kcal/mol
I···N distances (Å): 3.19 and 3.04
C-I···N angles (°): 172 and 175

I	-1.68745100	-2.10930800	-0.65492000
I	4.38352000	-2.55054600	-0.17833300
I	-1.30669600	2.05416100	-0.54550200
I	4.53229600	2.21065000	1.24691300
F	1.63659100	0.11590500	-1.36893500
F	1.07159500	-2.83858900	2.20993500
F	1.34069900	1.74296700	3.00686400
F	3.65212000	-4.85360000	-2.17626300
F	-0.34798600	4.92518600	-1.38469400
F	1.06559400	-0.76790300	3.93059200
F	-0.96358800	-4.52727100	-2.54476800
F	1.97383500	6.21890300	-1.14380300
F	1.33782500	-5.70641700	-3.20129500
F	4.07907600	5.04405900	0.00327400
C	1.34968800	-2.54822900	-0.57714000
C	1.35502700	-1.40803300	0.37271000
C	1.50011900	0.99224200	0.78906700
C	2.54695700	-3.17254600	-0.93265500
C	1.49720000	-0.10125500	-0.06222900
C	1.63041000	2.37825000	0.27700800
C	0.14436500	-2.99881400	-1.12241900
C	1.21106600	-1.60758700	1.73628100
C	2.83978300	3.06780200	0.39200800
C	2.53439500	-4.23655300	-1.81798600
C	0.53660400	3.00369100	-0.32945500
C	1.35112200	0.73554300	2.14287800
C	0.66648500	4.29752100	-0.80485400
C	0.15749200	-4.06511800	-2.00546200
C	1.34234500	-4.68665500	-2.35568900
C	2.94571600	4.36203000	-0.08824000
C	1.20726800	-0.55129000	2.62935200
C	1.86315600	4.98069300	-0.68637900
C	-6.03068500	0.09303000	1.45444900
C	-5.95918600	1.33871500	0.89565600
C	-4.98399900	1.56414300	-0.08443000
C	-5.13044100	-0.88284900	1.00651300
H	-6.77938200	-0.15576700	2.19353600
H	-6.64956900	2.12430400	1.16940600
N	-4.22457100	-0.60221600	0.07475800

N	-4.14766800	0.59877800	-0.45630100
C	-5.15524200	-2.26521800	1.52866000
C	-5.44067500	-2.51005300	2.87037800
C	-4.89648600	-3.33822000	0.67826500
C	-5.45955000	-3.80808400	3.35646000
H	-5.61973700	-1.68171700	3.54419300
C	-4.92049200	-4.63511300	1.16501500
H	-4.68641800	-3.14785200	-0.36516600
C	-5.20044500	-4.87257300	2.50410800
H	-5.66812700	-3.98779000	4.40221900
H	-4.72069300	-5.46172800	0.49701900
H	-5.21494600	-5.88527100	2.88343600
C	-4.83375000	2.87001200	-0.75935900
C	-4.44704600	2.92047300	-2.09741200
C	-5.04530200	4.05757500	-0.06284300
C	-4.27295300	4.14201300	-2.72613400
H	-4.27558500	1.99521700	-2.63058300
C	-4.86207900	5.27927100	-0.69197100
H	-5.31748200	4.02908100	0.98464800
C	-4.47625500	5.32308700	-2.02441200
H	-3.97123500	4.17351100	-3.76405000
H	-5.00966000	6.19666700	-0.13883400
H	-4.32940600	6.27614400	-2.51396200

Complex of p-1 with disulphide 2

G = -3750.966145 ht



ΔG_{XB} = 4.2 kcal/mol

I···S distances (Å): 3.43

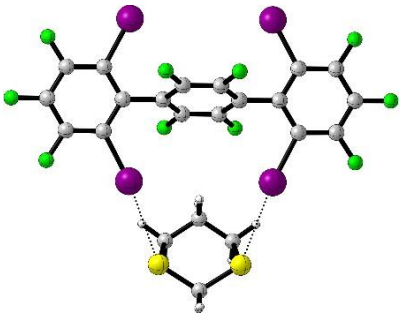
C-I···S angles (°): 177

I	2.95076500	-3.71310400	-0.50678300
I	2.27853500	2.26441800	0.53108700
F	1.34477100	-0.83221700	-2.34440800
F	1.33605200	-0.83139500	2.34868000
F	5.40375100	1.88129700	0.39164000
F	-1.34318500	-0.83311900	2.34397000
F	5.90214700	-2.66404600	-0.40719000
F	6.96445000	-0.24662000	-0.01407700
C	2.88360900	-0.69767100	0.00388500
C	1.40606700	-0.83438300	0.00230600
C	-0.68804900	-0.85438300	-1.18831500

C	3.45109500	0.56378400	0.20968800
C	0.69411400	-0.85243800	-1.18603500
C	3.71084100	-1.80080400	-0.20745700
C	0.68966800	-0.85320000	1.18788400
C	4.82780900	0.70217500	0.20159100
C	-1.40447800	-0.83606400	-0.00274800
C	5.08629000	-1.63853900	-0.21186300
C	5.64872100	-0.39153900	-0.00839000
C	-0.69250100	-0.85290100	1.18560300
C	-2.88219300	-0.70123300	-0.00438400
C	-3.45130800	0.55936300	-0.21093600
C	-3.70801300	-1.80529600	0.20765700
C	-4.82819700	0.69599900	-0.20289900
C	-5.08366700	-1.64478500	0.21200600
C	-5.64770500	-0.39863500	0.00777400
F	-1.33445700	-0.83372400	-2.34911800
I	-2.94551300	-3.71645300	0.50809200
F	-5.40565400	1.87426800	-0.39364700
F	-6.96361800	-0.25539800	0.01340700
F	-5.89820300	-2.67121400	0.40799700
I	-2.28100600	2.26137600	-0.53318700
S	0.22282300	4.96823400	0.99558200
S	-0.23189800	4.97096400	-0.99358000
C	1.52388900	6.22230900	1.09463200
H	1.84889000	6.24200700	2.13406800
H	2.35876100	5.94794900	0.45551600
H	1.13605400	7.19946300	0.81917300
C	-1.53794200	6.22021900	-1.08800100
H	-1.15400100	7.19787900	-0.80891000
H	-1.86304600	6.24248400	-2.12735300
H	-2.37169000	5.94014900	-0.44989100

Complex of p-1 with thioacetal 3

G = -3'828.336256 ht



ΔG_{XB} = 3.7 kcal/mol

I···S distances (Å): 3.45

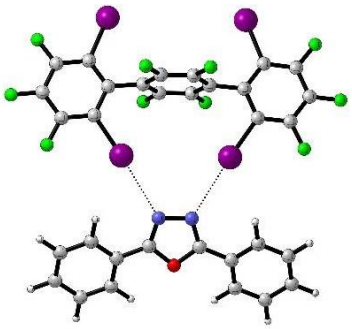
C-I···S angles (°): 154

I	-2.65089600	-3.78797400	0.45660200
I	-2.63841600	2.22388800	-0.67996700
F	-1.33624200	0.25993900	1.96490800

F	-1.33615000	-1.82373500	-2.24405600
F	-5.67868300	1.47518400	-0.65356900
F	1.33639700	-1.82358200	-2.24406000
F	-5.68165100	-3.08389600	0.20594800
F	-6.99893500	-0.81167600	-0.26666600
C	-2.89228100	-0.79126500	-0.15339100
C	-1.40855000	-0.78828000	-0.13823400
C	0.69126900	-0.26090100	0.92443100
C	-3.59500500	0.39246200	-0.39300100
C	-0.69119800	-0.26096600	0.92442400
C	-3.59757200	-1.97982400	0.05281000
C	-0.69101300	-1.31089900	-1.20246500
C	-4.97905700	0.37254500	-0.42844700
C	1.40868300	-0.78812800	-0.13823200
C	-4.98158600	-1.97602500	0.01204800
C	-5.67636700	-0.80496200	-0.22982600
C	0.69120700	-1.31081900	-1.20246700
C	2.89241300	-0.79091700	-0.15339300
C	3.59497400	0.39293600	-0.39285400
C	3.59786700	-1.97940300	0.05267200
C	4.97902800	0.37322000	-0.42827900
C	4.98188200	-1.97540200	0.01193100
C	5.67650300	-0.80421200	-0.22978500
F	1.33625200	0.26005300	1.96493000
I	2.65146300	-3.78774500	0.45621300
F	5.67850200	1.47598500	-0.65326000
F	6.99907200	-0.81073900	-0.26660400
F	5.68210200	-3.08319700	0.20570600
I	2.63812700	2.22425700	-0.67965400
C	-0.00050600	3.69237700	1.99413400
C	1.27064500	4.52669900	1.91115500
C	-0.00039100	6.29037500	0.24395100
C	-1.27168800	4.52662600	1.91089400
H	1.27971300	5.29388300	2.68866500
H	2.15022300	3.90056500	2.05337400
H	-0.00041500	2.93709000	1.20403100
H	-0.00058300	3.16181700	2.94998800
H	-0.00049400	7.02102200	1.05333500
H	-0.00030800	6.82498100	-0.70296100
H	-1.28096900	5.29379800	2.68841400
H	-2.15125800	3.90043400	2.05291400
S	1.52515500	5.33276800	0.30906000
S	-1.52591300	5.33269100	0.30874800

Complex of p-1 with oxadiazole 4

G = -3598.857999 ht



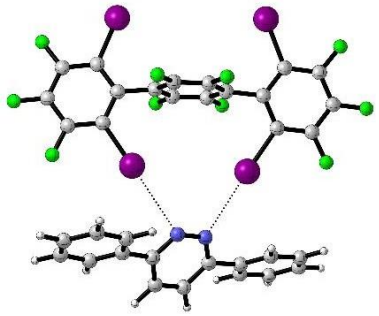
ΔG_{XB} = 3.7 kcal/mol
I···N distances (Å): 3.08
C-I···N angles (°): 176

I	1.33246600	-2.27891600	-0.41925500
I	-4.68951400	-2.94200200	0.33323100
F	-1.39926900	-1.34126800	2.28797800
F	-2.16853600	-1.34157200	-2.34082200
F	-3.65207900	-5.90029300	0.18696900
F	-2.16864500	1.34141600	-2.34080900
F	0.92820200	-5.40139400	-0.38194700
F	-1.22080000	-6.96153500	-0.12114200
C	-1.65708300	-2.88166300	-0.04693400
C	-1.78894700	-1.40399800	-0.02565400
C	-1.60996600	0.69092700	1.14817000
C	-2.77210000	-3.70802300	0.08814100
C	-1.60991700	-0.69107500	1.14816700
C	-0.38792600	-3.44523000	-0.20778100
C	-1.99861200	-0.69121700	-1.19445500
C	-2.61568700	-5.08363000	0.06176900
C	-1.78905700	1.40385200	-0.02564100
C	-0.25700700	-4.82300000	-0.23056700
C	-1.36162400	-5.64480700	-0.09697900
C	-1.99866900	0.69106500	-1.19444800
O	5.87035700	0.00026500	0.25243300
N	3.96769200	-0.68972500	-0.56690900
C	5.61573500	-2.40961900	0.13290000
N	3.96756800	0.68988100	-0.56693800
C	5.10395400	-1.06186500	-0.08078500
C	4.97786600	-3.48943400	-0.47490200
H	4.12588400	-3.31450700	-1.11634100
C	5.10376300	1.06224600	-0.08083700
C	6.72989900	-2.61925200	0.94246300
H	7.22218300	-1.77715300	1.40867200
C	5.44683600	-4.77354800	-0.25844700
H	4.94878800	-5.61076000	-0.72746000
C	7.19534700	-3.90746100	1.15067600
H	8.05802500	-4.07090800	1.78157800
C	5.61529600	2.41010600	0.13277800
C	6.72922100	2.62004100	0.94259500
H	7.22152000	1.77809200	1.40906100
C	7.19439600	3.90835900	1.15073800
H	8.05688400	4.07204500	1.78184000

C	6.55257300	4.98523000	0.55424900
H	6.91650100	5.98998800	0.72060600
C	4.97740900	3.48972200	-0.47534700
H	4.12564300	3.31453700	-1.11699600
C	5.44610300	4.77395000	-0.25895700
H	4.94803600	5.61100800	-0.72822600
C	6.55355300	-4.98452500	0.55450400
H	6.91769000	-5.98919700	0.72091600
C	-1.65728600	2.88152200	-0.04689600
C	-2.77234500	3.70782900	0.08813300
C	-0.38814900	3.44514500	-0.20767300
C	-2.61598700	5.08344600	0.06179200
C	-0.25727900	4.82291900	-0.23042400
C	-1.36193900	5.64467900	-0.09687600
F	-1.39935700	1.34112400	2.28798700
I	1.33226700	2.27887400	-0.41915200
F	-3.65242100	5.90006100	0.18694900
F	-1.22116700	6.96141200	-0.12100700
F	0.92791200	5.40136700	-0.38173700
I	-4.68974100	2.94173400	0.33312400

Complex of p-1 with pyridazin 5

G = -3'600.998255 ht



ΔG_{XB} = 0.5 kcal/mol

I···N distances (Å): 3.24 and 3.08

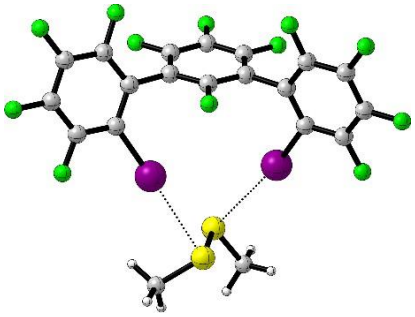
C-I···N angles (°): 173 and 177

I	1.34854400	2.41164900	-0.36422000
I	4.72989400	-2.68445400	-0.32977500
F	2.06027800	-0.38707900	2.12662000
F	1.88256200	-1.25821200	-2.48154800
F	6.85087600	-0.41056400	-0.74262900
F	-0.46997800	-2.50440300	-2.15426200
F	4.28616200	3.45824200	-0.75720200
F	6.65608800	2.24735200	-0.92266000
C	3.26546100	0.00028700	-0.38119900
C	2.02834000	-0.79449500	-0.18504500
C	0.24698000	-1.56775600	1.23930300
C	4.51129200	-0.62088800	-0.47068200
C	1.45685700	-0.92189800	1.07028100
C	3.17061600	1.39178700	-0.47957700

C	1.36629600	-1.36151300	-1.26136900
C	5.65007000	0.14454600	-0.65448700
C	-0.43044200	-2.10631700	0.15829600
C	4.32488300	2.13468900	-0.66075200
C	5.56159500	1.52145700	-0.74886300
C	0.15614400	-2.00734200	-1.09222900
C	-1.79668200	-2.66186900	0.31725600
C	-2.00317900	-4.00633500	0.62265100
C	-2.89280700	-1.80878800	0.15806900
C	-3.29340800	-4.48870200	0.76516800
C	-4.17371400	-2.31257800	0.30527100
C	-4.37945500	-3.64704300	0.60751400
F	-0.29002600	-1.63642900	2.45340200
I	-2.66083600	0.21255200	-0.30229100
F	-3.52815700	-5.76087200	1.05438300
F	-5.61013200	-4.11713000	0.74579100
F	-5.24133900	-1.53893400	0.16302400
I	-0.42309400	-5.33359700	0.87534000
C	-2.74370300	5.45356100	1.12694200
C	-3.80539500	4.83550000	0.52700800
C	-3.53575000	3.79725700	-0.37344500
C	-1.45397200	5.01772800	0.79547500
H	-2.87834400	6.28170300	1.80878600
H	-4.82347800	5.15089900	0.70815400
N	-1.26610900	4.01602900	-0.05909300
N	-2.28791300	3.41204300	-0.62752200
C	-0.24923900	5.66166400	1.36002400
C	0.87250500	5.86723100	0.56017600
C	-0.22528200	6.07457500	2.69055200
C	2.00381400	6.46959700	1.08637000
H	0.84787100	5.55623600	-0.47499000
C	0.90863100	6.67393600	3.21651400
H	-1.08512000	5.89977700	3.32506000
C	2.02463800	6.87208600	2.41503200
H	2.87072200	6.62234800	0.45811500
H	0.92412400	6.97797700	4.25418100
H	2.90982800	7.33809100	2.82610000
C	-4.60915600	3.07847900	-1.09104600
C	-5.82587200	2.81215800	-0.46769000
C	-4.39244500	2.62751300	-2.39182800
C	-6.80862700	2.09384400	-1.13095000
H	-5.99157600	3.13141500	0.55342500
C	-5.37994900	1.91931000	-3.05632200
H	-3.44197500	2.82892300	-2.86683200
C	-6.58727300	1.64712000	-2.42631000
H	-7.74220600	1.87248100	-0.63226800
H	-5.20517300	1.57280600	-4.06569700
H	-7.35307000	1.08434600	-2.94249800

Complex of m-7 with disulphide 2

G = -3'355.386703 ht



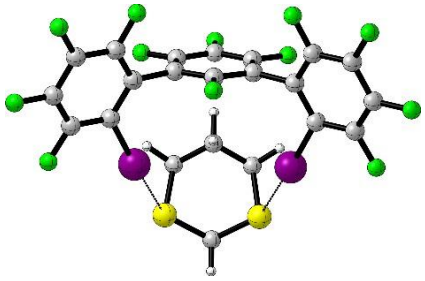
ΔG_{XB} = 2.4 kcal/mol
I···S distances (Å): 3.42 and 3.47
C-I···S angles (°): 177 and 168

I	2.43603100	1.14861000	0.39567100
I	-1.69530600	1.56877900	-0.63257400
F	-0.30948400	-1.48167000	-1.26353600
F	2.13158700	-2.11353300	2.67156800
F	-2.47951700	-1.51759000	2.88406700
F	4.93309000	0.23598700	-1.32333300
F	-5.87255900	-2.99904100	-0.38597200
F	-0.13329200	-1.95308700	4.11676200
F	4.15853900	-4.32962900	-1.91301700
F	-6.42666400	-0.67831700	-1.66532400
F	5.67251700	-2.12664700	-2.32990400
F	-4.60998300	1.27379300	-1.77234500
C	2.21545500	-1.84804900	-0.12642700
C	0.96148600	-1.79555000	0.66347200
C	-1.45683000	-1.47164700	0.77220300
C	3.00127500	-0.71328500	-0.34871200
C	-0.26929900	-1.58605900	0.06317300
C	-2.75508600	-1.21450800	0.10781200
C	2.62344400	-3.05659800	-0.66404200
C	0.98009500	-1.91931900	2.04432200
C	-3.05180400	-0.01451200	-0.54867600
C	4.16243400	-0.81961600	-1.09088000
C	-3.72592200	-2.20308300	0.15402600
C	-1.37910000	-1.61125600	2.15073400
C	-4.96570200	-2.03704100	-0.43928000
C	3.78657600	-3.16416400	-1.40884100
C	4.55900700	-2.03824500	-1.62090500
C	-4.28959100	0.14900400	-1.14279200
C	-0.17650600	-1.83347500	2.79740500
C	-5.24644400	-0.85313400	-1.09349100
S	0.42776800	4.24839500	-0.68803900
S	0.88156100	4.11374000	1.29679300
C	-0.93490900	5.43901900	-0.69230100
H	-1.26414300	5.51967200	-1.72755700
H	-1.75296400	5.07397100	-0.07697900
H	-0.59691100	6.41128800	-0.34364600
C	2.12180900	5.41619900	1.49567700
H	1.68828300	6.39109000	1.28879700
H	2.44144700	5.37690700	2.53614000

H	2.97054400	5.22975900	0.84378300
F	-3.47837200	-3.35362300	0.77183100
F	1.89677400	-4.15293000	-0.47296900

Complex of m-7 with thioacetal 3

G = -3'432.758830 ht



ΔG_{XB} = 2.4 kcal/mol

I···S distances (Å): 3.42

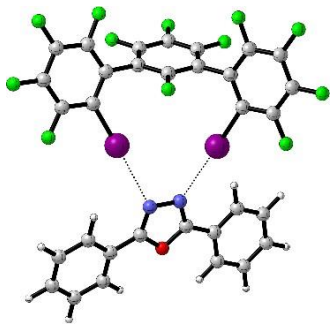
C-I···S angles (°): 163

I	-2.45099100	1.19488400	-0.80830600
I	2.45123500	1.19467100	-0.80813100
F	-0.00018300	-2.42846800	-0.69517300
F	-2.32631900	-0.13875000	2.65488300
F	2.32625200	-0.13899500	2.65484200
F	-4.67673700	-4.53392700	-0.05084700
F	5.04849600	-0.25681100	-1.88127200
F	0.00001100	0.57392200	3.79522700
F	-5.04851900	-0.25620900	-1.88134500
F	6.00732300	-2.72994000	-1.56402800
F	-6.00776700	-2.72915700	-1.56395100
F	4.67598600	-4.53457500	-0.05103300
C	-2.49678300	-1.66013200	0.28040700
C	-1.22105800	-1.31999500	0.95251300
C	1.22083500	-1.32013500	0.95250000
C	-3.01379100	-2.93691400	0.41743900
C	-0.00013600	-1.69943200	0.41811200
C	2.49651000	-1.66043400	0.28037900
C	-3.18517100	-0.73438200	-0.50989100
C	-1.19172400	-0.54721400	2.10319000
C	3.01330600	-2.93731000	0.41734100
C	-4.19732900	-3.30977700	-0.19822600
C	3.18505900	-0.73475200	-0.50985700
C	1.19160300	-0.54734500	2.10317400
C	4.36668600	-1.10627700	-1.12324700
C	-4.36685800	-1.10574400	-1.12326300
C	-4.87646300	-2.38675300	-0.97042400
C	4.19678500	-3.31033600	-0.19834100
C	-0.00003500	-0.16546400	2.69238400
C	4.87607400	-2.38738200	-0.97048400
C	0.00020000	3.22936200	1.67471600

C	1.27422100	4.01924000	1.40576200
C	0.00043300	5.36911700	-0.61212500
C	-1.27371300	4.01937000	1.40564100
H	1.29084700	4.93712500	1.99750400
H	2.15130900	3.43343400	1.67908100
H	0.00017900	2.31424000	1.07612100
H	0.00014900	2.93567500	2.72762700
H	0.00045100	6.26212000	0.01355000
H	0.00049800	5.67858300	-1.65451800
H	-1.29030900	4.93725300	1.99738700
H	-2.15088900	3.43365100	1.67886000
S	1.52773800	4.45329100	-0.33416100
S	-1.52699900	4.45345500	-0.33431000
F	-2.37611400	-3.84061400	1.15392200
F	2.37547100	-3.84094800	1.15376300

Complex of m-7 with oxadiazole 4

G = -3'203.284363 ht



ΔG_{XB} = 0.0 kcal/mol

I···N distances (Å): 3.05 and 3.03

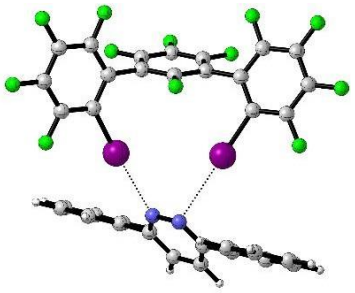
C-I···N angles (°): 178 and 179

I	0.48427500	2.02004100	-0.14744500
I	0.35375200	-2.05180900	-0.45410700
F	-2.30655100	0.26645700	-1.20673900
F	-2.99506400	2.01431200	3.08021900
F	-3.20724600	-2.58242800	2.39033500
F	-4.67193700	5.45113400	-0.03841900
F	-0.45439600	-4.47776900	-2.29973100
F	-3.35372000	-0.46686000	4.04409800
F	-0.15170200	4.94699500	-1.07988600
F	-2.79183200	-5.63341500	-2.87091800
F	-2.35633100	6.44822000	-1.02726500
F	-5.08864400	-4.68981000	-1.79277900
C	-2.48587900	2.58661000	0.38404300
C	-2.62056700	1.20680100	0.90798300
C	-2.73032500	-1.20914500	0.54844700
C	-3.61041000	3.39895900	0.40658200
C	-2.54328400	0.08737200	0.09091300
C	-2.68824600	-2.38012700	-0.35976700
C	-1.29074700	3.11062600	-0.12032900

C	-2.90190900	0.98518200	2.24914200
C	-3.88360500	-3.01186200	-0.66561000
C	-3.58243500	4.69960300	-0.06534300
C	-1.50369200	-2.87831000	-0.91184000
C	-3.01067500	-1.36700700	1.89738400
C	-1.55646800	-3.97126200	-1.75772600
C	-1.26708700	4.41010900	-0.59431300
C	-2.40111100	5.20615200	-0.57173000
C	-3.93384500	-4.10703800	-1.51081800
C	-3.09149900	-0.28682700	2.75691700
C	-2.76101800	-4.58634300	-2.06170400
O	5.13598300	-0.21608200	0.26466600
N	3.12605700	0.50273500	-0.18910900
C	5.01536200	2.07670200	-0.52444300
N	3.03469000	-0.80327500	0.24109200
C	4.37752400	0.81700900	-0.16541300
C	4.24713500	3.09724000	-1.08264300
H	3.19089000	2.94044500	-1.25223000
C	4.23583400	-1.19571100	0.50182600
C	6.37884900	2.26323800	-0.30911900
H	6.96916700	1.46823600	0.12462300
C	4.84478600	4.29959000	-1.41729900
H	4.24792900	5.09117700	-1.84861400
C	6.96931700	3.46984300	-0.64883200
H	8.02735200	3.61548200	-0.48059600
C	4.69122900	-2.49064700	0.98936500
C	6.05202900	-2.76095900	1.11101100
H	6.77706300	-2.00532700	0.84269900
C	6.46780600	-3.99992500	1.57175000
H	7.52410300	-4.21078600	1.66505800
C	5.53137200	-4.96678800	1.91038100
H	5.85871400	-5.93312100	2.26905700
C	3.74971400	-3.46008000	1.33152500
H	2.69570800	-3.23703800	1.23742100
C	4.17384100	-4.69481900	1.78984100
H	3.44390300	-5.44702600	2.05480900
C	6.20451200	4.48804900	-1.20106300
H	6.66785700	5.42914600	-1.46428200
F	-4.76223600	2.93364300	0.88147000
F	-5.02592300	-2.56742000	-0.14945300

Complex of m-7 with pyridazin 5

G = -3'205.419963 ht



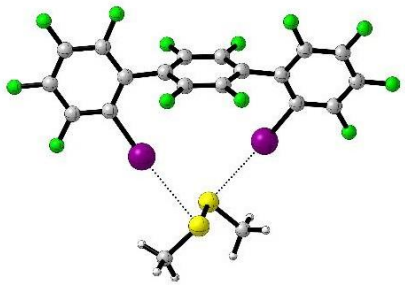
ΔG_{XB} = -0.2 kcal/mol
I···N distances (Å): 3.15 and 3.03
C-I···N angles (°): 173 and 177

I	-2.03000900	0.80292500	-0.68417300
I	2.00686600	0.37802900	-0.29971500
F	0.09803800	-2.31372200	-1.11975200
F	-3.16613300	-2.30548300	2.22608300
F	1.33296800	-2.56205800	3.38931100
F	-4.96218200	-4.45968500	-2.14342100
F	4.93445800	-0.64235900	-0.80021300
F	-1.25238600	-2.47737600	4.10993600
F	-4.30549600	0.11909600	-2.76619200
F	6.18964300	-2.93339000	-0.25465600
F	-5.58420300	-2.13886400	-3.39049200
F	4.87028200	-4.96693300	0.95093500
C	-2.63304500	-2.19628900	-0.53219000
C	-1.57454200	-2.28534600	0.50254100
C	0.78916000	-2.42327800	1.10941600
C	-3.32296600	-3.34894100	-0.87047200
C	-0.22939400	-2.33471300	0.17044900
C	2.21829200	-2.50206600	0.72744900
C	-2.96296100	-0.99777400	-1.17294100
C	-1.89514100	-2.34194300	1.84998300
C	2.90458500	-3.67487300	1.00558200
C	-4.31844200	-3.34496600	-1.83255900
C	2.90902600	-1.45221400	0.11141100
C	0.40752200	-2.47487900	2.44295200
C	4.24328900	-1.61493800	-0.21613400
C	-3.95684900	-0.99712900	-2.13458000
C	-4.63368300	-2.15985400	-2.46899600
C	4.24042300	-3.83424600	0.68038000
C	-0.92023800	-2.43193200	2.82681300
C	4.91168400	-2.79658500	0.06297700
C	0.24767900	5.29109800	1.15083300
C	1.45001700	5.15950500	0.51361300
C	1.61715300	4.07467600	-0.35694400
C	-0.74785500	4.34082600	0.88628900
H	0.04500500	6.12068600	1.81367300
H	2.24366600	5.88139100	0.64600900
N	-0.52688000	3.33686100	0.04348000
N	0.63401500	3.20201500	-0.55993800
C	-2.08427400	4.41646800	1.51269300

C	-2.22403300	4.85863900	2.82678300
C	-3.21823300	4.04733400	0.79209400
C	-3.47788700	4.92409900	3.41422700
H	-1.34704800	5.12469900	3.40322500
C	-4.47098000	4.11802900	1.37958100
H	-3.11122100	3.71675900	-0.23164200
C	-4.60350700	4.55473300	2.69103300
H	-3.57494600	5.25549800	4.43901400
H	-5.34573700	3.83284000	0.81133700
H	-5.58188500	4.60558600	3.14911400
C	2.87526400	3.84041100	-1.09560700
C	2.84014000	3.26014200	-2.36260900
C	4.10434900	4.16615100	-0.52657400
C	4.01788800	3.01056400	-3.04682000
H	1.88391600	3.00124000	-2.79648000
C	5.28233000	3.90875900	-1.21062000
H	4.14486300	4.58869800	0.46927900
C	5.24072200	3.33144300	-2.47191000
H	3.98263600	2.55963000	-4.02902700
H	6.23277200	4.14850800	-0.75401700
H	6.15981600	3.12714600	-3.00393800
F	2.28007300	-4.69268400	1.59085000
F	-3.03597000	-4.50108100	-0.27061700

Complex of p-7 with disulphide 2

G = -3'355.382512 ht



ΔG_{XB} = 3.7 kcal/mol

I···S distances (Å): 3.43

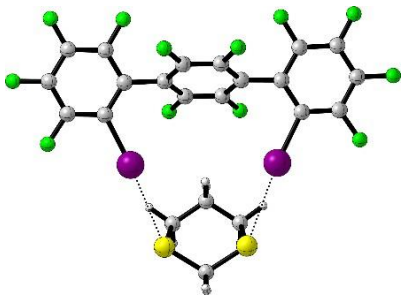
C-I···S angles (°): 174 and 176

I	2.28410200	1.35128200	0.53653000
F	1.28470500	-1.56414700	-2.41788800
F	1.44021300	-1.93290000	2.25834800
F	5.42893600	0.99474400	0.30365600
F	-1.23605700	-1.95722400	2.34667100
F	5.87412600	-3.53240700	-0.74583800
F	6.97547400	-1.11108300	-0.25676800
C	2.89792200	-1.56863200	-0.11928500
C	1.42773600	-1.75364800	-0.08251300
C	-0.70593200	-1.68659500	-1.19752400
C	3.47159600	-0.31662100	0.12625500

C	0.67525600	-1.68566300	-1.24389400
C	3.72266700	-2.63838000	-0.41595500
C	0.75439300	-1.87569700	1.12223200
C	4.84525100	-0.17620300	0.07816200
C	-1.38064800	-1.76005100	0.01152900
C	5.10022600	-2.49703100	-0.46409900
C	5.66150200	-1.25939800	-0.21363200
C	-0.62758900	-1.88347600	1.16831100
C	-2.85215600	-1.60171000	0.07427000
C	-3.46178000	-0.36132200	-0.14608100
C	-3.64577700	-2.69329900	0.37981800
C	-4.83747500	-0.25677700	-0.07005200
C	-5.02489100	-2.58717600	0.45616300
C	-5.62140700	-1.36211800	0.22678600
F	-1.39109100	-1.56831100	-2.32921500
F	-5.45453100	0.90191400	-0.26884500
F	-6.93745000	-1.24643600	0.29687000
F	-5.76696600	-3.64412700	0.74335700
I	-2.33261800	1.35115400	-0.53564000
S	0.17381900	4.00737900	1.03831500
S	-0.27825500	4.06827000	-0.95103600
C	1.46459900	5.26838500	1.17694400
H	1.79103300	5.25661300	2.21606100
H	2.30076500	5.02233500	0.52803900
H	1.06830300	6.25086700	0.93444500
C	-1.58596000	5.31824500	-1.00812500
H	-1.20365400	6.28707800	-0.69779200
H	-1.90944000	5.37309900	-2.04677300
H	-2.42026600	5.01732900	-0.38026700
F	-3.09217000	-3.88008600	0.60379400
F	3.20263500	-3.83591700	-0.66227900

Complex of p-7 with thioacetal 3

G = -3'432.756953



ΔG_{XB} = 2.3 kcal/mol

I···S distances (Å): 3.44

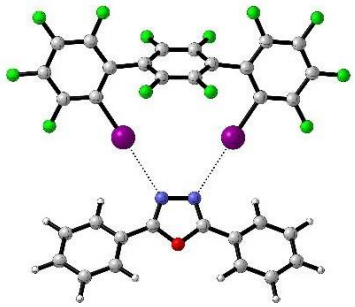
C-I···S angles (°):157

I	-2.69236700	1.29600800	-0.64732600
F	-1.33197700	-0.29601200	2.05888600
F	-1.33497300	-3.11256600	-1.70267900

F	-5.72880000	0.49904800	-0.51595400
F	1.33478900	-3.11262600	-1.70272000
F	-5.59544700	-4.02741700	0.60933100
F	-6.99604400	-1.78917700	0.01521400
C	-2.88987300	-1.66564800	0.12380100
C	-1.40995800	-1.68963700	0.16339900
C	0.69072000	-0.98535900	1.11909300
C	-3.61949900	-0.51427900	-0.19066100
C	-0.69072100	-0.98535500	1.11913500
C	-3.57778100	-2.84072200	0.38240100
C	-0.69162300	-2.41835100	-0.77167200
C	-5.00091500	-0.57064600	-0.22092200
C	1.40989700	-1.68965400	0.16331900
C	-4.96078100	-2.89608700	0.35106400
C	-5.67460500	-1.75222800	0.04919000
C	0.69149800	-2.41836900	-0.77170300
C	2.88980900	-1.66572500	0.12367200
C	3.61949700	-0.51430500	-0.19045100
C	3.57764400	-2.84093300	0.38184800
C	5.00090900	-0.57075600	-0.22075900
C	4.96063900	-2.89638200	0.35046200
C	5.67452900	-1.75246800	0.04895600
F	1.33203800	-0.29603300	2.05881700
F	5.72886000	0.49898200	-0.51547600
F	6.99596600	-1.78949100	0.01493700
F	5.59523500	-4.02784000	0.60833500
I	2.69248300	1.29615600	-0.64668100
C	-0.00011900	3.10061700	1.79499300
C	1.27067000	3.91591500	1.59772500
C	0.00013800	5.41914500	-0.30974200
C	-1.27090000	3.91582500	1.59730200
H	1.27716600	4.78620500	2.25782100
H	2.15057300	3.31754900	1.82956300
H	0.00002500	2.24412200	1.11607100
H	-0.00027300	2.70624000	2.81456700
H	-0.00001600	6.26164800	0.38240100
H	0.00029200	5.80785500	-1.32528500
H	-1.27766600	4.78612600	2.25738100
H	-2.15083800	3.31740400	1.82886500
S	1.52754800	4.48437100	-0.10271600
S	-1.52725800	4.48423400	-0.10323200
F	-2.91272800	-3.95203000	0.67908500
F	2.91251600	-3.95229400	0.67816700

Complex of p-7 with oxadiazole 4

G = -3'203.280815 ht



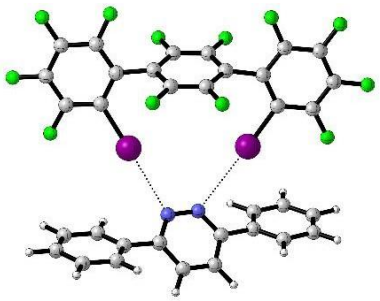
ΔG_{XB} = 1.0 kcal/mol
I···N distances (Å): 3.09
C-I···N angles (°): 176

I	2.32884800	0.37942100	-0.40370500
F	1.33611200	-1.57359100	2.31871000
F	1.33921000	-3.91064600	-1.75427500
F	5.82756900	-4.66706900	0.44552800
F	-1.33708700	-3.91138100	-1.75416500
F	5.45016000	-0.08952000	-0.38497400
F	6.96454500	-2.25944700	-0.03713200
C	2.87743100	-2.58030800	0.19341500
C	1.40684000	-2.73040800	0.27454300
C	-0.68935900	-2.16426400	1.31871000
C	3.68837600	-3.69010900	0.35478400
C	0.69077700	-2.16390200	1.31866300
C	3.46780400	-1.33735900	-0.06538100
C	0.69285300	-3.35104400	-0.73748200
C	5.06813300	-3.59554900	0.28126700
C	-1.40519500	-2.73116500	0.27465000
C	4.84525200	-1.24698300	-0.13739000
C	5.64709700	-2.36513800	0.03633800
C	-0.69095400	-3.35141700	-0.73742800
O	-0.00144000	4.88252600	0.09411000
N	0.68897100	2.97663900	-0.71843200
C	2.40866900	4.62693400	-0.02599300
N	-0.69102700	2.97643700	-0.71864900
C	1.06054400	4.11490500	-0.23667400
C	3.48478600	4.00105400	-0.65244800
H	3.30595200	3.15996300	-1.30710000
C	-1.06309300	4.11458700	-0.23699400
C	2.62247100	5.72869700	0.79924900
H	1.78303900	6.21182300	1.27967500
C	4.76982200	4.46858300	-0.43826200
H	5.60432300	3.97972400	-0.92151100
C	3.91145600	6.19300100	1.00504400
H	4.07837100	7.04577400	1.64836800
C	-2.41143500	4.62620700	-0.02672400
C	-2.62572600	5.72849400	0.79769100
H	-1.78651400	6.21233000	1.27778500
C	-3.91490900	6.19243100	1.00307800
H	-4.08219600	7.04562000	1.64575400
C	-4.98819100	5.56099200	0.38921200

H	-5.99366100	5.92381600	0.55361700
C	-3.48727500	3.99941400	-0.65274800
H	-3.30807300	3.15787700	-1.30672500
C	-4.77250700	4.46658400	-0.43897200
H	-5.60678700	3.97701600	-0.92188300
C	4.98502300	5.56245100	0.39075600
H	5.99033800	5.92555900	0.55548100
C	-2.87588100	-2.58191700	0.19366500
C	-3.68615800	-3.69218700	0.35516300
C	-3.46700900	-1.33932300	-0.06509300
C	-5.06597900	-3.59843600	0.28180600
C	-4.84451800	-1.24975100	-0.13694000
C	-5.64568900	-2.36837000	0.03691200
F	-1.33493800	-1.57429200	2.31879800
I	-2.32909800	0.37811000	-0.40359300
F	-5.82477000	-4.67039400	0.44618600
F	-6.96320700	-2.26344800	-0.03640200
F	-5.45012900	-0.09264700	-0.38447800
F	3.15103100	-4.88182900	0.59378600
F	-3.14808900	-4.88358500	0.59414200

Complex of p-7 with pyridazin 5

G = -3'205.417181 ht



ΔG_{XB} = 0.2 kcal/mol

I···N distances (Å): 3.31 and 3.08

C-I···N angles (°): 173 and 175

I	2.37470100	0.52609700	-0.45401900
F	1.56285000	-1.55278800	2.16739500
F	0.99448100	-3.68896500	-1.97728700
F	5.63878700	-4.74947300	-0.45022000
F	-1.66052200	-3.62391300	-1.64450900
F	5.43042800	-0.10569000	-0.86115800
F	6.84655600	-2.36517500	-0.87646600
C	2.80380900	-2.50979500	-0.17280600
C	1.34803000	-2.60540200	0.07633900
C	-0.58650100	-2.03126500	1.39258400
C	3.56378100	-3.66685000	-0.20027200
C	0.78287400	-2.06967900	1.22459400
C	3.42802100	-1.27781300	-0.40389400
C	0.49591300	-3.15952600	-0.86551500

C	4.92772000	-3.63270300	-0.43527500
C	-1.44097900	-2.53642300	0.42460700
C	4.79107300	-1.24940000	-0.63593800
C	5.54272800	-2.41449800	-0.65120900
C	-0.87661700	-3.12714800	-0.69349600
C	-2.90422400	-2.33926100	0.53410500
C	-3.72495600	-3.41309700	0.82966900
C	-3.47909800	-1.07937800	0.33193900
C	-5.09744300	-3.26452200	0.94357300
C	-4.84897000	-0.93251600	0.44776700
C	-5.65866500	-2.01622500	0.75431300
F	-1.08893700	-1.46160800	2.48303000
I	-2.33045900	0.57333300	-0.20818200
F	-5.86666200	-4.30216300	1.23272300
F	-6.96902700	-1.86006700	0.86023900
F	-5.43804900	0.24294300	0.26158200
C	0.43124800	5.20269200	0.95008900
C	-0.85623600	5.16971600	0.49155100
C	-1.21861600	4.12463700	-0.36731900
C	1.30763400	4.19561600	0.52497400
H	0.78756000	5.99819700	1.58965600
H	-1.57174000	5.93854000	0.74819800
N	0.89472000	3.21920800	-0.27854000
N	-0.34779000	3.17944700	-0.71136600
C	2.72919200	4.18425600	0.92986200
C	3.71232200	3.80945000	0.01689300
C	3.10048200	4.55250500	2.22134200
C	5.04558200	3.79655400	0.39306900
H	3.42270700	3.53155800	-0.98719700
C	4.43461900	4.53577100	2.59733300
H	2.34138000	4.82424900	2.94406700
C	5.40893400	4.15802600	1.68347600
H	5.80121000	3.50049700	-0.32168800
H	4.71250900	4.80885700	3.60611100
H	6.44967400	4.14315600	1.97724200
C	-2.57495100	4.01488100	-0.94341500
C	-3.69660000	4.35567400	-0.19128500
C	-2.73989100	3.52984200	-2.23940100
C	-4.96749600	4.19899600	-0.72201300
H	-3.57867300	4.70489500	0.82674000
C	-4.01042400	3.38542000	-2.77176200
H	-1.86516900	3.25869100	-2.81469900
C	-5.12603400	3.71397400	-2.01294200
H	-5.83436300	4.44368700	-0.12375100
H	-4.13138500	3.00895900	-3.77829900
H	-6.11796800	3.58847500	-2.42509900
F	2.99145600	-4.84817700	0.01036200
F	-3.20432200	-4.62106000	1.01825000

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