Supporting Information

Halogen bonding two-point recognition with terphenyl derivatives

J. Stoesser, a G. Rojas M., b D. Bulfield, a P. I. Hidalgo, b J. Pasán G., b C. Ruiz-Pérez, b C. A. Jiménez,*b and S. M. Huber* a

a Department of Chemistry and Biochemistry, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum, Germany. E-mail: stefan.m.huber@rub.de.

b Depto. de Química Orgánica, Facultad de Ciencias Químicas Universidad de Concepción, Chile. Email: cjimenez@udec.cl

c Laboratorio de Rayos X y Materiales Moleculares, Dep. de Física, Facultad de Ciencias, Universidad de La Laguna, Avda. Astrofísico Francisco Sánchez, 38200, La Laguna, Spain.

Contents:

A) Synthesis and Experimental Data
B.) Structural Characterization
C.) NMR-Spectra
D ) Titration Experiments
E) DFT Calculations
F ) References
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 \(R_t\) 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-diphenylpyridazine[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 POCl₃ and heated to reflux overnight. The excess solvent was removed, the residue was neutralized with NaHCO₃ and extracted three times with dichloromethane and the combined organic layers were washed with saturated NaCl-solution and dried over MgSO₄. 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$_2$dba$_3$) (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$_2$O, 68.78 mg K$_2$CO$_3$ (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-$d_6$) $\delta = 7.90$ (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) 2,2',2'',3,3',3'',4,4'',5,5',5'',6'-dodecafluoro-6,6''-diiodo-1,1':4',1''-terphenyl

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

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

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

**Elemental Analysis:**

Calc.: C: 30.97

Found: C: 31.21

A.2.3) 2,2',2'',3,3',4,4',4'',5,5',5'',6'-dodecafluoro-1,1':3',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 39.72 mg Bis(dibenzylideneacetone)palladium(0) (Pd_{2}dba_{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_{2}O, 239.7 mg K_{2}CO_{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 MgSO₄. 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).

¹H NMR (250 MHz, Acetone-δ₆) δ = 7.58 (dddd, J = 10.7, 8.3, 6.0, 2.6 Hz, 2H).

¹⁹F NMR (235 MHz, Acetone-δ₆) 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).

¹³C NMR (75 MHz, Chloroform-δ) 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 (427.17 mmol, 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 NaHCO₃-solution, washed with saturated NaCl-solution and dried over MgSO₄. 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) $\delta = -111.93$ (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 (ddddd, $J = 21.2, 9.7, 4.5, 2.3$ Hz), -149.19 (ddd, $J = 23.0, 19.6, 4.9$ Hz), -152.38 (ddddd, $J = 21.3, 19.6, 4.5$ Hz), -161.30 (td, $J = 22.2, 10.8$ Hz).

$^{13}$C NMR (63 MHz, Chloroform-d) $\delta = 154.21 – 153.62$ (m), 151.81 (ddd, $J = 11.4, 8.7, 6.1$ Hz), 148.37 (ddddd, $J = 245.6, 11.2, 4.2, 2.4$ Hz), 147.70 (dt, $J = 11.1, 5.2$ Hz), 143.72 (d, $J = 11.5$ Hz), 143.10 (ddddd, $J = 17.3, 12.7, 3.9$ Hz), 139.43 – 138.50 (m), 138.03 (ddt, $J = 253.3, 15.5, 5.0$ 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 \( \text{C}_{32}\text{H}_{10}\text{F}_{10}\text{I}_{4}\text{N}_{2}\text{O} \)
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 \( \text{C}_{33}\text{H}_{12}\text{F}_{10}\text{I}_{4}\text{N}_{2}\text{O} \)
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. The observed intensities were corrected with a numerical absorption correction based on Gaussian integration over a multifaceted crystal model with CrysAlisPRO. Both crystal structures were solved by the SHELXTL routine and refined with the full-matrix least-squares technique on F by using the SHELXL-2013 program within the WINGX 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 and MERCURY 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.

<table>
<thead>
<tr>
<th></th>
<th>m-1/4a</th>
<th>m-1/4b</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Formula</strong></td>
<td>C₃₂H₁₀F₁₀aN₂O</td>
<td>C₅₁H₁₂F₂₀aN₂O</td>
</tr>
<tr>
<td><strong>FW</strong></td>
<td>1136.02</td>
<td>2063.83</td>
</tr>
<tr>
<td><strong>Crystal system</strong></td>
<td>Triclinic</td>
<td>Triclinic</td>
</tr>
<tr>
<td><strong>Space group</strong></td>
<td>P -1</td>
<td>P -1</td>
</tr>
<tr>
<td><strong>a (Å)</strong></td>
<td>12.9014(2)</td>
<td>11.0666(3)</td>
</tr>
<tr>
<td><strong>b (Å)</strong></td>
<td>16.0841(4)</td>
<td>11.7332(3)</td>
</tr>
<tr>
<td><strong>c (Å)</strong></td>
<td>18.1379(4)</td>
<td>22.9011(6)</td>
</tr>
<tr>
<td><strong>α (º)</strong></td>
<td>79.028(2)</td>
<td>90.760(2)</td>
</tr>
<tr>
<td><strong>β (º)</strong></td>
<td>83.942(2)</td>
<td>99.480(2)</td>
</tr>
<tr>
<td><strong>γ (º)</strong></td>
<td>67.838(2)</td>
<td>98.949(2)</td>
</tr>
<tr>
<td><strong>V (Å³)</strong></td>
<td>3419.61(14)</td>
<td>2895.01(13)</td>
</tr>
<tr>
<td><strong>Z</strong></td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td><strong>α(mm⁻¹)</strong></td>
<td>29.397</td>
<td>4.389</td>
</tr>
<tr>
<td><strong>T(K)</strong></td>
<td>293(2)</td>
<td>293(2)</td>
</tr>
<tr>
<td><strong>ρ₂₀ (g cm⁻³)</strong></td>
<td>2.207</td>
<td>2.368</td>
</tr>
<tr>
<td><strong>ρ (Å)</strong></td>
<td>1.5418</td>
<td>0.71073</td>
</tr>
<tr>
<td><strong>Index ranges</strong></td>
<td>-16≤ h≤ 13</td>
<td>-14≤ h≤ 14</td>
</tr>
<tr>
<td></td>
<td>-20≤ k≤ 20</td>
<td>-15≤ k≤ 15</td>
</tr>
<tr>
<td></td>
<td>-22≤ l≤ 22</td>
<td>-30≤ l≤ 28</td>
</tr>
<tr>
<td><strong>Total Reflections</strong></td>
<td>42308</td>
<td>49854</td>
</tr>
<tr>
<td><strong>Indep. Reflections (R_mm)</strong></td>
<td>14185(0.035)</td>
<td>13462 (0.027)</td>
</tr>
<tr>
<td><strong>Obs. reflect.</strong></td>
<td>12240</td>
<td>8975</td>
</tr>
<tr>
<td>([I/2σ(I)]</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Parameters</strong></td>
<td>883</td>
<td>739</td>
</tr>
<tr>
<td><strong>Goodness-of-fit</strong></td>
<td>1.025</td>
<td>1.009</td>
</tr>
<tr>
<td><strong>R [I&gt; 2σ(I)]</strong></td>
<td>0.0378</td>
<td>0.0487</td>
</tr>
<tr>
<td><strong>Rw [I&gt; 2σ(I)]</strong></td>
<td>0.1014</td>
<td>0.0973</td>
</tr>
<tr>
<td><strong>R (all data)</strong></td>
<td>0.0434</td>
<td>0.0806</td>
</tr>
<tr>
<td><strong>Rw (all data)</strong></td>
<td>0.1078</td>
<td>0.1116</td>
</tr>
</tbody>
</table>
Figure S1. View of asymmetric unit of m-1/4a, a 1:1 stoichiometry complex with two crystallographically independent two-point halogen bonding dimers.
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 \textit{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.)  

\[ 2,2',2'',3,3'',4,4',4'',5,5',5'',6'-\text{dodecafluoro}-6,6''-\text{diiodo}-1,1':3',1''-\text{terphenyl} \]

---

**Figure S14**  
\[^{19}\text{F-NMR}:\]  
\[ 2,2',2'',3,3'',4,4',4'',5,5',5'',6'-\text{dodecafluoro}-6,6''-\text{diiodo}-1,1':3',1''-\text{terphenyl} \]

---

**Figure S15**  
\[^{13}\text{C-NMR}:\]  
\[ 2,2',2'',3,3'',4,4',4'',5,5',5'',6'-\text{dodecafluoro}-6,6''-\text{diiodo}-1,1':3',1''-\text{terphenyl} \]

23
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

<table>
<thead>
<tr>
<th>Donor</th>
<th>Guest</th>
<th>Binding constant $K$ [mol$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>p-7</td>
<td>4a</td>
<td>0.94</td>
</tr>
<tr>
<td>m-7</td>
<td>4a</td>
<td>1.99</td>
</tr>
<tr>
<td>p-7</td>
<td>8</td>
<td>0.79</td>
</tr>
<tr>
<td>m-7</td>
<td>8</td>
<td>0.91</td>
</tr>
</tbody>
</table>

Figure S16: Titration molecules. (Hosts and Guests)
Figure S17: Titration of p7 with 4a in toluene-d8, $K = 0.94 \text{ M}^{-1}$ (shift of F substituents para to iodine).

Figure S18: Titration of m7 with 4a in toluene-d8, $K = 1.99 \text{ M}^{-1}$ (shift of isolated F substituent of central core).
**Figure S19:** Titration of p7 with 8 in toluene-d8, $K = 0.79 \text{ M}^{-1}$ (shift of F substituents para to iodine).

**Figure S20:** Titration of m7 with 8 in toluene-d8, $K = 0.91 \text{ M}^{-1}$ (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 ΔGXB) are provided below (for the corresponding Lewis structures, compare Figure 1 in the manuscript):

<table>
<thead>
<tr>
<th>Halogen bond donor m-1</th>
<th>G = -2874.8284644 ht</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>1.49452600</td>
</tr>
<tr>
<td>I</td>
<td>3.02335300</td>
</tr>
<tr>
<td>I</td>
<td>-3.02341200</td>
</tr>
<tr>
<td>I</td>
<td>-1.49447100</td>
</tr>
<tr>
<td>F</td>
<td>0.000000500</td>
</tr>
<tr>
<td>F</td>
<td>2.30376400</td>
</tr>
<tr>
<td>F</td>
<td>-2.30378200</td>
</tr>
<tr>
<td>F</td>
<td>5.44959400</td>
</tr>
<tr>
<td>F</td>
<td>-5.44962800</td>
</tr>
<tr>
<td>F</td>
<td>-0.00001400</td>
</tr>
<tr>
<td>F</td>
<td>4.27902700</td>
</tr>
<tr>
<td>F</td>
<td>-5.99535800</td>
</tr>
<tr>
<td>F</td>
<td>5.99537300</td>
</tr>
<tr>
<td>F</td>
<td>-4.27896900</td>
</tr>
<tr>
<td>C</td>
<td>2.47725400</td>
</tr>
<tr>
<td>C</td>
<td>1.20760300</td>
</tr>
<tr>
<td>C</td>
<td>-1.20760600</td>
</tr>
<tr>
<td>C</td>
<td>3.38576800</td>
</tr>
<tr>
<td>C</td>
<td>0.00000100</td>
</tr>
<tr>
<td>C</td>
<td>-2.47725100</td>
</tr>
<tr>
<td>C</td>
<td>2.77677200</td>
</tr>
<tr>
<td>C</td>
<td>1.17855400</td>
</tr>
<tr>
<td>C</td>
<td>-2.77674500</td>
</tr>
<tr>
<td>C</td>
<td>4.56907300</td>
</tr>
<tr>
<td>C</td>
<td>-3.38578700</td>
</tr>
<tr>
<td>C</td>
<td>-1.17856700</td>
</tr>
<tr>
<td>C</td>
<td>-4.56908800</td>
</tr>
<tr>
<td>C</td>
<td>3.96445200</td>
</tr>
<tr>
<td>C</td>
<td>4.86309200</td>
</tr>
</tbody>
</table>
Halogen bond donor p-1
G = -2874.827507 ht

Disulphide 2
G = -876.142480 ht
Thioacetal 3
G = -953.514681 h

Oxadiazole 4
G = -724.036448 h
Pyridazin 5
G = -726.171613 ht

C  0.68453500  1.30276500  0.42369500
C  -0.68451800  1.30276500  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  -2.80658400  0.02087800  0.00044600
C  -3.61509200  1.14909200  -0.18139800
C  -4.99693200  1.03760300  -0.21527900
C  3.42890400  -1.22487400  0.13938200
C  4.80924800  -1.22489400  0.13947300
C  5.60337100  1.92041300  -0.36606600
C  5.27268300  -2.30429100  0.26899500
H  3.15893100  2.11986400  -0.32456300
H  -2.80655000  -2.09866000  0.26895000
H  -3.15897200  0.02087800  0.00044600
H  -3.42886000  -1.22487400  0.13938200
H  -4.80922800  -1.33372500  0.10947300
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  0.61181000  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
\[
\begin{array}{ccc}
C & 0.19777400 & 0.80597100 \\
& -2.28389000 & 0.97011500 \\
& 3.07326500 & -0.54465900 \\
& 1.25336000 & 0.70575200 \\
& -2.50374000 & -0.87255600 \\
& 4.85550900 & 1.57167600 \\
& -3.22185300 & -0.55233600 \\
& -1.11769600 & 2.08292800 \\
& -4.34400000 & -1.00829600 \\
& 4.32432500 & -1.14079300 \\
& 5.21545600 & -0.99237500 \\
& 3.62469100 & -1.67124200 \\
& 0.02317600 & 2.85917600 \\
& -4.55044200 & -1.73555900 \\
F & 3.27610700 & 1.04954200 \\
& -1.63130000 & 0.82346000 \\
\end{array}
\]

**Halogen bond donor p-7**

\[G = -2479.245961 \text{ ht}\]

\[
\begin{array}{cccc}
I & 2.77955300 & -2.21949200 & -0.19961200 \\
F & 1.33898000 & -0.20676700 & 2.20417600 \\
F & 1.33586400 & 1.90939800 & -1.98870800 \\
F & 5.54203100 & 3.29348200 & 0.22863800 \\
F & 6.99695000 & 1.01627900 & 0.07317400 \\
C & 2.88989400 & 0.82710900 & 0.08513700 \\
C & 1.40924700 & 0.83207700 & 0.09679600 \\
C & -0.69093300 & 0.30242400 & 1.15956300 \\
C & 3.65015300 & -0.34350400 & -0.00357500 \\
C & 0.69090500 & 0.30241700 & 1.15955800 \\
C & 3.55246300 & 2.04280500 & 0.15526600 \\
C & 0.69155600 & 1.38382300 & -0.95350300 \\
C & 5.03120300 & -0.26640900 & -0.00365500 \\
C & -1.40928000 & 0.83209600 & 0.09681100 \\
C & 4.93483900 & 2.12155800 & 0.15342400 \\
C & 5.67644600 & 0.95849500 & 0.07625200 \\
C & -0.69159600 & 1.38382900 & -0.95350000 \\
C & -2.88993000 & 0.82710900 & 0.08518100 \\
C & -3.65014900 & -0.34351900 & -0.00367800 \\
C & -3.55253900 & 2.04277100 & 0.15551200 \\
C & -5.03120000 & -0.26647700 & -0.00372400 \\
C & -4.93492000 & 2.12147200 & 0.15370200 \\
C & -5.67648700 & 0.95839400 & 0.07636700 \\
F & -1.33392300 & -0.20676200 & 2.20418200 \\
F & -5.78373000 & -1.35490900 & -0.09049200 \\
F & -6.99699200 & 1.01613100 & 0.07331900 \\
F & -5.54215300 & 3.29336200 & 0.22910200 \\
I & -2.77946300 & -2.21944400 & -0.19993900 \\
F & 2.86163800 & 3.17399400 & 0.23840000 \\
F & -2.86175900 & 3.17397500 & 0.23882600 \\
\end{array}
\]
Complex of m-1 with disulphide 2
\[ G = -3750.964241 \mathrm{ht} \]

\[ \Delta G_{\text{XB}} = 2.4 \text{ kcal/mol} \]

I-S distances (Å): 3.42 and 3.47
C-I-S angles (°): 178 and 169

<table>
<thead>
<tr>
<th>I</th>
<th>F</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>C</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>-1.27664900</td>
<td>-4.10324200</td>
<td>-0.32930600</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>3.30758400</td>
<td>-0.15253600</td>
<td>0.39690200</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>-4.54191400</td>
<td>-0.44930400</td>
<td>0.70902200</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>0.41775700</td>
<td>2.86158000</td>
<td>-0.66522100</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-0.53395600</td>
<td>-0.47994800</td>
<td>-1.32993600</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>1.04081300</td>
<td>-2.20703000</td>
<td>2.71835600</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-2.09990800</td>
<td>1.23125900</td>
<td>2.73288500</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>4.62305600</td>
<td>-2.51741400</td>
<td>-1.22141200</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-5.69537100</td>
<td>1.94926400</td>
<td>-0.92422400</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-0.53786700</td>
<td>-0.49814600</td>
<td>4.07304700</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>1.11674900</td>
<td>-5.50670800</td>
<td>-1.78894700</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-4.57586600</td>
<td>4.06958800</td>
<td>-2.09763100</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>3.66936500</td>
<td>-4.82392800</td>
<td>-2.17196800</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-1.93838800</td>
<td>4.45839000</td>
<td>-1.98106900</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.18336000</td>
<td>-2.30089400</td>
<td>-0.09190200</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.28949800</td>
<td>-1.38231700</td>
<td>0.65537300</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.35822100</td>
<td>0.41816200</td>
<td>0.66029700</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.52089600</td>
<td>-1.95472000</td>
<td>-0.30185400</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.53615700</td>
<td>-0.48276500</td>
<td>0.00205200</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.21155600</td>
<td>1.38254700</td>
<td>-0.07611300</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.69857600</td>
<td>-3.50885500</td>
<td>-0.59660600</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.26784800</td>
<td>-1.36914700</td>
<td>2.04088400</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.63847700</td>
<td>2.49489900</td>
<td>-0.70081300</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.34935700</td>
<td>-2.81327900</td>
<td>-1.00300000</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.59378700</td>
<td>1.19114800</td>
<td>-0.15128800</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.33717000</td>
<td>0.39076000</td>
<td>2.04662600</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.38224700</td>
<td>2.10257300</td>
<td>-0.83312100</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.54387100</td>
<td>-4.35273100</td>
<td>-1.29710200</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.86833700</td>
<td>-4.01048800</td>
<td>-1.50192900</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.44619600</td>
<td>3.39149500</td>
<td>-1.37872900</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.53703700</td>
<td>-0.49377600</td>
<td>2.74717600</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.81454500</td>
<td>3.20380800</td>
<td>-1.44720500</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>S</td>
<td>3.76955600</td>
<td>3.54790500</td>
<td>-0.64017700</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Complex of m-1 with thioacetal 3

$G = -3828.336919$ kcal/mol

$\Delta G_{XB} = 3.9$ kcal/mol

I-S distances (Å): 3.43 and 3.41

C-I-S angles (°): 159 and 162
<table>
<thead>
<tr>
<th>Element</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.92808500</td>
<td>-3.02805700</td>
<td>-0.78956800</td>
</tr>
<tr>
<td>C</td>
<td>0.16374400</td>
<td>-1.80231000</td>
<td>1.82034500</td>
</tr>
<tr>
<td>C</td>
<td>0.97172900</td>
<td>4.32502000</td>
<td>-1.47028600</td>
</tr>
<tr>
<td>C</td>
<td>-0.89606600</td>
<td>4.18719000</td>
<td>-1.57802900</td>
</tr>
<tr>
<td>C</td>
<td>-2.24423000</td>
<td>4.49698300</td>
<td>-1.59241900</td>
</tr>
<tr>
<td>C</td>
<td>-1.33053200</td>
<td>-4.62984200</td>
<td>0.96524600</td>
</tr>
<tr>
<td>C</td>
<td>0.15361100</td>
<td>0.03892600</td>
<td>2.47399400</td>
</tr>
<tr>
<td>C</td>
<td>-0.15085100</td>
<td>-5.03542200</td>
<td>-1.56247300</td>
</tr>
<tr>
<td>C</td>
<td>3.59995500</td>
<td>0.87501700</td>
<td>2.05920700</td>
</tr>
<tr>
<td>C</td>
<td>4.67565800</td>
<td>-0.20308400</td>
<td>2.05193100</td>
</tr>
<tr>
<td>C</td>
<td>6.12626000</td>
<td>1.28910900</td>
<td>0.26421100</td>
</tr>
<tr>
<td>C</td>
<td>4.14263700</td>
<td>2.28351300</td>
<td>1.86713800</td>
</tr>
<tr>
<td>H</td>
<td>5.42873400</td>
<td>-0.00926100</td>
<td>2.81885800</td>
</tr>
<tr>
<td>H</td>
<td>4.23854400</td>
<td>-1.18013300</td>
<td>2.25634600</td>
</tr>
<tr>
<td>H</td>
<td>2.84831700</td>
<td>0.65747900</td>
<td>1.30618500</td>
</tr>
<tr>
<td>H</td>
<td>3.10164700</td>
<td>0.83977300</td>
<td>3.04189700</td>
</tr>
<tr>
<td>H</td>
<td>6.84044000</td>
<td>1.50721200</td>
<td>1.05882700</td>
</tr>
<tr>
<td>H</td>
<td>6.64792400</td>
<td>1.32974400</td>
<td>-0.68900700</td>
</tr>
<tr>
<td>H</td>
<td>4.89440800</td>
<td>2.52054700</td>
<td>2.62325100</td>
</tr>
<tr>
<td>H</td>
<td>3.34176000</td>
<td>3.01682000</td>
<td>1.95546800</td>
</tr>
<tr>
<td>S</td>
<td>5.51691000</td>
<td>-0.39562600</td>
<td>0.45910500</td>
</tr>
<tr>
<td>S</td>
<td>4.86417700</td>
<td>2.57475000</td>
<td>0.23161400</td>
</tr>
</tbody>
</table>

Complex of m-1 with oxadiazole 4
G = -3'598.865273 ht

\[ \Delta G_{\text{HB}} = -0.2 \text{ kcal/mol} \]

I-N distances (Å): 3.06 and 3.03
C-I-N angles (°): 178 and 175
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>-1.67923100</td>
<td>6.31900900</td>
<td>-1.2783600</td>
</tr>
<tr>
<td>F</td>
<td>-4.10414000</td>
<td>-4.68541200</td>
<td>-2.04477000</td>
</tr>
<tr>
<td>C</td>
<td>-1.61743800</td>
<td>2.49924000</td>
<td>0.23261000</td>
</tr>
<tr>
<td>C</td>
<td>-1.59641200</td>
<td>1.11994600</td>
<td>0.77943600</td>
</tr>
<tr>
<td>C</td>
<td>-1.64434700</td>
<td>-1.29434000</td>
<td>0.42842600</td>
</tr>
<tr>
<td>C</td>
<td>-2.79922000</td>
<td>3.24373800</td>
<td>0.24561000</td>
</tr>
<tr>
<td>C</td>
<td>-1.66429000</td>
<td>0.00756100</td>
<td>-0.04374800</td>
</tr>
<tr>
<td>C</td>
<td>-1.69747000</td>
<td>-2.45905900</td>
<td>-0.49017200</td>
</tr>
<tr>
<td>C</td>
<td>-0.45377700</td>
<td>3.06126400</td>
<td>-0.30066300</td>
</tr>
<tr>
<td>C</td>
<td>-1.50373400</td>
<td>0.88977900</td>
<td>2.14300800</td>
</tr>
<tr>
<td>C</td>
<td>-2.92266000</td>
<td>-3.03908000</td>
<td>-0.83751600</td>
</tr>
<tr>
<td>C</td>
<td>-2.81107700</td>
<td>4.53063800</td>
<td>-0.26466700</td>
</tr>
<tr>
<td>C</td>
<td>-0.51439400</td>
<td>-2.98827800</td>
<td>-1.01343900</td>
</tr>
<tr>
<td>C</td>
<td>-1.55163900</td>
<td>-1.46672300</td>
<td>1.80002000</td>
</tr>
<tr>
<td>C</td>
<td>-0.57490100</td>
<td>-4.07525700</td>
<td>-1.86821600</td>
</tr>
<tr>
<td>C</td>
<td>-0.49079800</td>
<td>4.34935500</td>
<td>-0.80667200</td>
</tr>
<tr>
<td>C</td>
<td>-1.65993200</td>
<td>5.08752100</td>
<td>-0.79130900</td>
</tr>
<tr>
<td>C</td>
<td>-2.95847200</td>
<td>-4.11779200</td>
<td>1.69416000</td>
</tr>
<tr>
<td>C</td>
<td>-1.48083200</td>
<td>-0.39060100</td>
<td>2.66601600</td>
</tr>
<tr>
<td>C</td>
<td>-1.78848800</td>
<td>-4.64338600</td>
<td>-2.21131600</td>
</tr>
<tr>
<td>O</td>
<td>5.99883300</td>
<td>-0.05288100</td>
<td>0.33799600</td>
</tr>
<tr>
<td>N</td>
<td>4.00865300</td>
<td>0.48253500</td>
<td>-0.38188500</td>
</tr>
<tr>
<td>C</td>
<td>5.82706400</td>
<td>2.14034500</td>
<td>-0.69072600</td>
</tr>
<tr>
<td>N</td>
<td>3.94854700</td>
<td>-0.78009500</td>
<td>0.16742900</td>
</tr>
<tr>
<td>C</td>
<td>5.23088700</td>
<td>0.88046500</td>
<td>-0.26745500</td>
</tr>
<tr>
<td>C</td>
<td>5.07132100</td>
<td>3.03039200</td>
<td>-1.45222600</td>
</tr>
<tr>
<td>H</td>
<td>4.05920900</td>
<td>2.77009400</td>
<td>-1.72953400</td>
</tr>
<tr>
<td>C</td>
<td>5.13613100</td>
<td>-1.06380700</td>
<td>0.58390200</td>
</tr>
<tr>
<td>C</td>
<td>7.13646200</td>
<td>2.45659700</td>
<td>-0.33649800</td>
</tr>
<tr>
<td>H</td>
<td>7.71680600</td>
<td>1.76204800</td>
<td>0.25469600</td>
</tr>
<tr>
<td>C</td>
<td>5.62624100</td>
<td>4.23414100</td>
<td>-1.84943300</td>
</tr>
<tr>
<td>H</td>
<td>5.03925300</td>
<td>4.92514900</td>
<td>-2.43831100</td>
</tr>
<tr>
<td>C</td>
<td>7.68494400</td>
<td>3.66310200</td>
<td>-0.74069000</td>
</tr>
<tr>
<td>H</td>
<td>8.70081800</td>
<td>3.90986000</td>
<td>-0.46488400</td>
</tr>
<tr>
<td>C</td>
<td>5.60979300</td>
<td>-2.27237900</td>
<td>1.24498400</td>
</tr>
<tr>
<td>C</td>
<td>6.96076500</td>
<td>-2.43192000</td>
<td>1.54315700</td>
</tr>
<tr>
<td>H</td>
<td>7.66512200</td>
<td>-1.65453000</td>
<td>1.28203600</td>
</tr>
<tr>
<td>C</td>
<td>7.39385300</td>
<td>-3.58913800</td>
<td>2.17047400</td>
</tr>
<tr>
<td>H</td>
<td>8.44269600</td>
<td>-3.71381300</td>
<td>2.40139700</td>
</tr>
<tr>
<td>C</td>
<td>6.48440100</td>
<td>-4.58446000</td>
<td>2.49987100</td>
</tr>
<tr>
<td>H</td>
<td>6.82496900</td>
<td>-5.48670300</td>
<td>2.98934400</td>
</tr>
<tr>
<td>C</td>
<td>4.69511600</td>
<td>-3.27064100</td>
<td>1.57699000</td>
</tr>
<tr>
<td>H</td>
<td>3.64772100</td>
<td>-3.13760000</td>
<td>1.34484700</td>
</tr>
<tr>
<td>C</td>
<td>5.13641800</td>
<td>-4.42315300</td>
<td>2.20250800</td>
</tr>
<tr>
<td>H</td>
<td>4.42714200</td>
<td>-5.19732600</td>
<td>2.46021500</td>
</tr>
<tr>
<td>C</td>
<td>6.93166400</td>
<td>4.55233600</td>
<td>-1.49469500</td>
</tr>
<tr>
<td>H</td>
<td>7.36192300</td>
<td>5.49391700</td>
<td>-1.80763500</td>
</tr>
</tbody>
</table>

Complex of m-1 with Pyridazin 5

G = -3'600.999794 ht
\[ \Delta G_{\text{XB}} = 0.2 \text{ kcal/mol} \]

I-N distances (Å): 3.19 and 3.04

C-I-N angles (°): 172 and 175

<table>
<thead>
<tr>
<th>Atoms</th>
<th>X (Å)</th>
<th>Y (Å)</th>
<th>Z (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>-1.68745100</td>
<td>-2.10930800</td>
<td>-0.65492000</td>
</tr>
<tr>
<td>I</td>
<td>4.38352000</td>
<td>-2.55054600</td>
<td>-0.17833300</td>
</tr>
<tr>
<td>I</td>
<td>-1.30669600</td>
<td>2.05416100</td>
<td>-0.54550200</td>
</tr>
<tr>
<td>I</td>
<td>4.53229600</td>
<td>2.21065000</td>
<td>1.24691300</td>
</tr>
<tr>
<td>F</td>
<td>1.63659100</td>
<td>0.11590500</td>
<td>-1.36893500</td>
</tr>
<tr>
<td>F</td>
<td>1.07159500</td>
<td>-2.83858900</td>
<td>2.20993500</td>
</tr>
<tr>
<td>F</td>
<td>1.34069900</td>
<td>1.74296700</td>
<td>3.00686400</td>
</tr>
<tr>
<td>F</td>
<td>3.65212000</td>
<td>-4.85360000</td>
<td>-2.17623000</td>
</tr>
<tr>
<td>F</td>
<td>-0.34798600</td>
<td>4.92518600</td>
<td>-1.38469400</td>
</tr>
<tr>
<td>F</td>
<td>1.06559400</td>
<td>-0.76790300</td>
<td>3.93059200</td>
</tr>
<tr>
<td>F</td>
<td>-0.96358800</td>
<td>-4.52727100</td>
<td>-2.54476800</td>
</tr>
<tr>
<td>F</td>
<td>1.97383500</td>
<td>6.21890300</td>
<td>-1.14380300</td>
</tr>
<tr>
<td>F</td>
<td>1.33782500</td>
<td>-5.70641700</td>
<td>-3.20129500</td>
</tr>
<tr>
<td>F</td>
<td>4.07907600</td>
<td>5.04405900</td>
<td>0.00327400</td>
</tr>
<tr>
<td>C</td>
<td>1.34968800</td>
<td>-2.54822900</td>
<td>-0.57714000</td>
</tr>
<tr>
<td>C</td>
<td>1.35502700</td>
<td>-1.40803300</td>
<td>0.37271000</td>
</tr>
<tr>
<td>C</td>
<td>1.50011900</td>
<td>0.99224200</td>
<td>0.78906700</td>
</tr>
<tr>
<td>C</td>
<td>2.54695700</td>
<td>-3.17254600</td>
<td>-0.93265500</td>
</tr>
<tr>
<td>C</td>
<td>1.49720000</td>
<td>-0.10125500</td>
<td>-0.06222900</td>
</tr>
<tr>
<td>C</td>
<td>1.63041000</td>
<td>2.37825000</td>
<td>0.27700800</td>
</tr>
<tr>
<td>C</td>
<td>0.14436500</td>
<td>-2.99881400</td>
<td>-1.12241900</td>
</tr>
<tr>
<td>C</td>
<td>1.21106600</td>
<td>-1.60758700</td>
<td>1.73628100</td>
</tr>
<tr>
<td>C</td>
<td>2.83978300</td>
<td>3.06780200</td>
<td>0.39200800</td>
</tr>
<tr>
<td>C</td>
<td>2.53439500</td>
<td>-4.23655300</td>
<td>-1.81798600</td>
</tr>
<tr>
<td>C</td>
<td>0.53660400</td>
<td>3.00369100</td>
<td>-0.32945500</td>
</tr>
<tr>
<td>C</td>
<td>1.35112200</td>
<td>0.73554300</td>
<td>2.14287800</td>
</tr>
<tr>
<td>C</td>
<td>0.66648500</td>
<td>4.29752100</td>
<td>-0.80485400</td>
</tr>
<tr>
<td>C</td>
<td>0.15749200</td>
<td>-4.06511800</td>
<td>-2.00546200</td>
</tr>
<tr>
<td>C</td>
<td>1.34234500</td>
<td>-4.68665500</td>
<td>-2.35568900</td>
</tr>
<tr>
<td>C</td>
<td>2.94571600</td>
<td>4.36203000</td>
<td>-0.08824000</td>
</tr>
<tr>
<td>C</td>
<td>1.20726800</td>
<td>-0.55129000</td>
<td>2.62935200</td>
</tr>
<tr>
<td>C</td>
<td>1.86315600</td>
<td>4.98069300</td>
<td>-0.68637900</td>
</tr>
<tr>
<td>C</td>
<td>-6.03068500</td>
<td>0.09303000</td>
<td>1.45444900</td>
</tr>
<tr>
<td>C</td>
<td>-5.95918600</td>
<td>1.33871500</td>
<td>0.89565600</td>
</tr>
<tr>
<td>C</td>
<td>-4.98399900</td>
<td>1.56414300</td>
<td>-0.08443000</td>
</tr>
<tr>
<td>C</td>
<td>-5.13044100</td>
<td>-0.88284900</td>
<td>1.00651300</td>
</tr>
<tr>
<td>H</td>
<td>-6.77938200</td>
<td>-0.15576700</td>
<td>2.19353600</td>
</tr>
<tr>
<td>H</td>
<td>-6.64956900</td>
<td>2.12430400</td>
<td>1.16940600</td>
</tr>
<tr>
<td>N</td>
<td>-4.22457100</td>
<td>-0.60221600</td>
<td>0.07475800</td>
</tr>
</tbody>
</table>
Complex of p-1 with disulphide 2

\[ \Delta G_{298} = 4.2 \text{ kcal/mol} \]

I\(-\)S distances (Å): 3.43
C-I\(-\)S angles (°): 177
Complex of p-1 with thioacetal 3

G = -3'828.336256 ht

\[ \Delta G_{XB} = 3.7 \text{ kcal/mol} \]

I-S distances (Å): 3.45
C-I-S angles (°): 154
<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>F</td>
<td>-1.33615000</td>
<td>-1.82373500</td>
<td>-2.24405600</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-5.67868300</td>
<td>1.47518400</td>
<td>-0.65356900</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>1.33697000</td>
<td>-1.82358200</td>
<td>-2.24406000</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-5.68165100</td>
<td>-3.08396900</td>
<td>0.20594800</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-6.99893500</td>
<td>-0.81167600</td>
<td>-0.26666600</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.89228100</td>
<td>-0.79126500</td>
<td>-0.15339100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.40855000</td>
<td>-0.78828000</td>
<td>-0.13823400</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.69126900</td>
<td>-0.26090100</td>
<td>0.92443100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.59500500</td>
<td>0.39246200</td>
<td>-0.39324000</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.69119800</td>
<td>-0.26096600</td>
<td>0.92442400</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.59757200</td>
<td>-1.97982400</td>
<td>0.05281000</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.69101300</td>
<td>-1.31089900</td>
<td>-1.20246500</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.97905700</td>
<td>0.37254500</td>
<td>-0.42844700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.40868300</td>
<td>-0.78812800</td>
<td>-0.13823200</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.98158600</td>
<td>-1.97602500</td>
<td>0.01204800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-5.67636700</td>
<td>-0.80496200</td>
<td>-0.22982600</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.69120700</td>
<td>-1.31081900</td>
<td>-1.20246700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.89241300</td>
<td>-0.79091700</td>
<td>-0.15339300</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.59497400</td>
<td>0.39293600</td>
<td>-0.39285400</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.59786700</td>
<td>-1.97940300</td>
<td>0.05281000</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.98188200</td>
<td>-1.97540200</td>
<td>0.01193100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.67503000</td>
<td>-0.80421200</td>
<td>-0.22975000</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>1.33625200</td>
<td>0.26005300</td>
<td>1.96493000</td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>2.65146300</td>
<td>-3.78774500</td>
<td>0.45621300</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>5.67850200</td>
<td>1.47598500</td>
<td>-0.65326000</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>6.99907200</td>
<td>-0.81073900</td>
<td>-0.26660400</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>5.68210200</td>
<td>-3.08319700</td>
<td>0.20576000</td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>2.63812700</td>
<td>2.22425700</td>
<td>-0.67965400</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.00050600</td>
<td>3.69237700</td>
<td>1.99413400</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.27064500</td>
<td>4.52669900</td>
<td>1.91115500</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.00039100</td>
<td>6.29037500</td>
<td>0.24395100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.27168800</td>
<td>4.52662600</td>
<td>1.91089400</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.27971300</td>
<td>5.29388300</td>
<td>2.68866500</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.15022300</td>
<td>3.90056500</td>
<td>2.05337400</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.00041500</td>
<td>2.93709000</td>
<td>1.20403100</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.00058300</td>
<td>3.16181700</td>
<td>2.94988800</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.00049400</td>
<td>7.02102200</td>
<td>1.05333500</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.00030800</td>
<td>6.82498100</td>
<td>-0.70296100</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.28096900</td>
<td>5.29379800</td>
<td>2.68841400</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-2.15125800</td>
<td>3.90043400</td>
<td>2.05291400</td>
<td></td>
</tr>
<tr>
<td>S</td>
<td>1.52515500</td>
<td>5.33276800</td>
<td>0.30906000</td>
<td></td>
</tr>
<tr>
<td>S</td>
<td>-1.52591300</td>
<td>5.33269100</td>
<td>0.30874800</td>
<td></td>
</tr>
</tbody>
</table>

**Complex of p-1 with oxadiazole 4**

G = -3598.857999 ht
\[ \Delta G_{\text{XB}} = 3.7 \text{kcal/mol} \]

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  -2.34089000
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  0.68981000  -0.56693800
C   5.10394000  -1.06186500  -0.08078500
C   4.97786600  -3.48943400  -0.47490200
H   4.12584400  -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  1.15073800
H   8.05802500  -4.07090800  1.78157800
C   5.61529600  2.41010600  0.13277800
C   6.72921000  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
Complex of p-1 with pyridazin 5

\[ G = -3'600.998255 \text{  \text{ht}} \]

\[ \Delta G_{XB} = 0.5 \text{ kcal/mol} \]

I−N distances (Å): 3.24 and 3.08

C-I−N angles (°): 173 and 177
Complex of m-7 with disulphide 2

G = -3355.386703 ht
$\Delta G_{\text{XB}} = 2.4 \text{ kcal/mol}$

I–S distances (Å): 3.42 and 3.47

C–I–S angles (°): 177 and 168

<table>
<thead>
<tr>
<th>Atom</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>2.43603100</td>
<td>1.14861000</td>
<td>0.39567100</td>
</tr>
<tr>
<td>I</td>
<td>-1.69530600</td>
<td>1.56877900</td>
<td>-0.63257400</td>
</tr>
<tr>
<td>F</td>
<td>-0.30948400</td>
<td>-1.48167000</td>
<td>-1.26353600</td>
</tr>
<tr>
<td>F</td>
<td>2.13158700</td>
<td>-2.11353300</td>
<td>2.67156800</td>
</tr>
<tr>
<td>F</td>
<td>-2.47951700</td>
<td>-1.51759000</td>
<td>2.88406700</td>
</tr>
<tr>
<td>F</td>
<td>4.93309000</td>
<td>0.23598700</td>
<td>-1.32333300</td>
</tr>
<tr>
<td>F</td>
<td>-5.87255900</td>
<td>-2.99904100</td>
<td>-0.38597200</td>
</tr>
<tr>
<td>F</td>
<td>-0.13329200</td>
<td>-1.95308700</td>
<td>4.11676200</td>
</tr>
<tr>
<td>F</td>
<td>4.15853900</td>
<td>-4.32962900</td>
<td>-1.91301700</td>
</tr>
<tr>
<td>F</td>
<td>-6.42664400</td>
<td>-0.67831700</td>
<td>-1.66532400</td>
</tr>
<tr>
<td>F</td>
<td>5.67251700</td>
<td>-2.12664700</td>
<td>-2.32990400</td>
</tr>
<tr>
<td>F</td>
<td>-4.60998300</td>
<td>1.27379300</td>
<td>-1.77234500</td>
</tr>
<tr>
<td>C</td>
<td>2.21545500</td>
<td>-1.84804900</td>
<td>0.12642700</td>
</tr>
<tr>
<td>C</td>
<td>0.96148600</td>
<td>-1.79555000</td>
<td>0.66347200</td>
</tr>
<tr>
<td>C</td>
<td>-1.45683000</td>
<td>-1.47164700</td>
<td>0.77220300</td>
</tr>
<tr>
<td>C</td>
<td>3.00127500</td>
<td>-0.71328500</td>
<td>-0.34871200</td>
</tr>
<tr>
<td>C</td>
<td>-0.26929900</td>
<td>-1.58605900</td>
<td>0.06317300</td>
</tr>
<tr>
<td>C</td>
<td>-2.75508600</td>
<td>-1.21450800</td>
<td>0.10781200</td>
</tr>
<tr>
<td>C</td>
<td>2.62344400</td>
<td>-3.05659800</td>
<td>-0.66404200</td>
</tr>
<tr>
<td>C</td>
<td>0.98009500</td>
<td>-1.91931900</td>
<td>2.04432200</td>
</tr>
<tr>
<td>C</td>
<td>-3.05180400</td>
<td>-0.01451200</td>
<td>-0.54867600</td>
</tr>
<tr>
<td>C</td>
<td>4.16243400</td>
<td>-0.81961600</td>
<td>-1.09088000</td>
</tr>
<tr>
<td>C</td>
<td>-3.72592200</td>
<td>-2.20308300</td>
<td>0.15402600</td>
</tr>
<tr>
<td>C</td>
<td>-1.37910000</td>
<td>-1.61125600</td>
<td>2.15073400</td>
</tr>
<tr>
<td>C</td>
<td>-4.96570200</td>
<td>-2.03704100</td>
<td>-0.43928000</td>
</tr>
<tr>
<td>C</td>
<td>3.78657600</td>
<td>-3.16416400</td>
<td>-1.40884100</td>
</tr>
<tr>
<td>C</td>
<td>4.55900700</td>
<td>-2.03824500</td>
<td>-1.62090500</td>
</tr>
<tr>
<td>C</td>
<td>-4.28959100</td>
<td>0.14900400</td>
<td>-1.14279200</td>
</tr>
<tr>
<td>C</td>
<td>-0.17650600</td>
<td>-1.83347500</td>
<td>2.79740500</td>
</tr>
<tr>
<td>C</td>
<td>-5.24644400</td>
<td>-0.85313400</td>
<td>-1.09349100</td>
</tr>
<tr>
<td>S</td>
<td>0.42776800</td>
<td>4.24839500</td>
<td>-0.68803900</td>
</tr>
<tr>
<td>S</td>
<td>0.88156100</td>
<td>4.11374000</td>
<td>1.29679300</td>
</tr>
<tr>
<td>C</td>
<td>-0.93490900</td>
<td>5.43901900</td>
<td>-0.69230100</td>
</tr>
<tr>
<td>H</td>
<td>-1.26414300</td>
<td>5.51967200</td>
<td>-1.72755700</td>
</tr>
<tr>
<td>H</td>
<td>-1.75296400</td>
<td>5.07397100</td>
<td>-0.07697900</td>
</tr>
<tr>
<td>H</td>
<td>-0.59691100</td>
<td>6.41128800</td>
<td>-0.34364600</td>
</tr>
<tr>
<td>C</td>
<td>2.12180900</td>
<td>5.41619900</td>
<td>1.49567700</td>
</tr>
<tr>
<td>H</td>
<td>1.68828300</td>
<td>6.39109000</td>
<td>1.28879700</td>
</tr>
<tr>
<td>H</td>
<td>2.44144700</td>
<td>5.37690700</td>
<td>2.53614000</td>
</tr>
</tbody>
</table>
Complex of m-7 with thioacetal 3

\[ G = -3'432.758830 \text{ kcal/mol} \]

\[ \Delta G_{XB} = 2.4 \text{ kcal/mol} \]

I-S distances (Å): 3.42
C-I-S angles (°): 163
Complex of m-7 with oxadiazole 4
\( G = -3'203.284363 \) \( \text{ht} \)

\[ \Delta G_{\text{XH}} = 0.0 \text{ kcal/mol} \]

I-N distances (Å): 3.05 and 3.03
C-I-N angles (°): 178 and 179
Complex of m-7 with pyridazin 5

\[ G = -3'205.419963 \text{ ht} \]
\[ \Delta G_{XB} = -0.2 \text{ kcal/mol} \]

I–N distances (Å): 3.15 and 3.03

C-I-N angles (°): 173 and 177
Complex of p-7 with disulphide 2
\[ G = -3355.382512 \text{ kcal/mol} \]

\[ \Delta G_{\text{XO}} = 3.7 \text{ kcal/mol} \]

$I$-S distances (Å): 3.43

C-I-S angles (°): 174 and 176
Complex of p-7 with thioacetal 3

\[ G = -3.432.756953 \]

\[ \Delta G_{\text{XB}} = 2.3 \text{ kcal/mol} \]

I-S distances (Å): 3.44
C-I-S angles (°): 157

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.67525600</td>
<td>-1.68566300</td>
<td>-1.24389400</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.72266700</td>
<td>-2.63838000</td>
<td>-0.41595500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.75439300</td>
<td>-1.87569700</td>
<td>1.12223200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.84525100</td>
<td>-0.17620300</td>
<td>0.07816200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.38064800</td>
<td>-1.76005100</td>
<td>0.01152900</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.10022600</td>
<td>-2.49703100</td>
<td>-0.46409900</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.66150200</td>
<td>-1.25939800</td>
<td>-0.21363200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.62758900</td>
<td>-1.88347600</td>
<td>1.16831100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.85215600</td>
<td>-1.60171000</td>
<td>0.07427000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.46178000</td>
<td>-0.36132200</td>
<td>-0.14608100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.64577700</td>
<td>-2.69329900</td>
<td>0.37918000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.83747500</td>
<td>-0.25677700</td>
<td>-0.07005200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-5.02489100</td>
<td>-2.58717600</td>
<td>0.45616300</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-5.62140700</td>
<td>-1.36211800</td>
<td>0.22678600</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-1.39109100</td>
<td>-1.56831100</td>
<td>-2.32921500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-5.45431000</td>
<td>0.90191400</td>
<td>-0.26884500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-6.93745000</td>
<td>-1.24643600</td>
<td>0.29687000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-5.76966600</td>
<td>-3.64412700</td>
<td>0.74335700</td>
<td></td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>-2.33261800</td>
<td>1.35115400</td>
<td>-0.53564000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>S</td>
<td>0.17381900</td>
<td>4.00737900</td>
<td>1.03831500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>S</td>
<td>-0.27825500</td>
<td>4.06827000</td>
<td>-0.95103600</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.46459900</td>
<td>5.26838500</td>
<td>1.17694400</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.79103300</td>
<td>5.25661300</td>
<td>2.21606100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.30076500</td>
<td>5.02233500</td>
<td>0.52803900</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.06830300</td>
<td>6.25086700</td>
<td>0.93444500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.58596000</td>
<td>5.31824500</td>
<td>-1.00812500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.20365400</td>
<td>6.28707800</td>
<td>-0.69779200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.90944000</td>
<td>5.37309900</td>
<td>-2.04677300</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-2.42026600</td>
<td>5.01732900</td>
<td>-0.38026700</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-3.09217000</td>
<td>-3.88008600</td>
<td>0.60379400</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>3.20263500</td>
<td>-3.83591700</td>
<td>-0.68227900</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-5.72880000</td>
<td>0.49904800</td>
<td>-0.51595400</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-------</td>
<td>-------------</td>
<td>------------</td>
<td>-------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>1.33478900</td>
<td>-3.11262600</td>
<td>-1.70272000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-5.59544700</td>
<td>-4.02741700</td>
<td>0.60933100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-6.99604400</td>
<td>-1.78917700</td>
<td>0.01521400</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.88987300</td>
<td>-1.66564800</td>
<td>0.12380100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.40995800</td>
<td>-1.68963700</td>
<td>0.16339900</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.69072000</td>
<td>-0.98535900</td>
<td>1.11909300</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.61949900</td>
<td>-0.51427900</td>
<td>-0.19066100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.69072100</td>
<td>-0.98535500</td>
<td>1.11913500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.57778100</td>
<td>-2.84072200</td>
<td>0.38240100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.69162300</td>
<td>-2.41835100</td>
<td>-0.77167200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-5.00091500</td>
<td>-0.57064600</td>
<td>-0.22092200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.40989700</td>
<td>-1.68965400</td>
<td>0.16331900</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.96078100</td>
<td>-2.89608700</td>
<td>0.35106400</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-5.67460500</td>
<td>-1.75222800</td>
<td>0.04919000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.69149800</td>
<td>-2.41836900</td>
<td>-0.77170300</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.88980900</td>
<td>-1.66572500</td>
<td>0.12367200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.61949700</td>
<td>-0.51430500</td>
<td>-0.19045100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.57764400</td>
<td>-2.84093300</td>
<td>0.38184800</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.00090900</td>
<td>-0.57075600</td>
<td>-0.22075900</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.96063900</td>
<td>-2.89638200</td>
<td>0.35046200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.67452900</td>
<td>-1.75246800</td>
<td>0.04895600</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>1.33203800</td>
<td>-0.29603300</td>
<td>2.05881700</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>5.72886000</td>
<td>0.49898200</td>
<td>-0.51547600</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>6.99596600</td>
<td>-1.78949100</td>
<td>0.01493700</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>5.59523500</td>
<td>-4.02784000</td>
<td>0.60833500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>2.69248300</td>
<td>1.29615600</td>
<td>-0.64668100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.00011900</td>
<td>3.10061700</td>
<td>1.79499300</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.27067000</td>
<td>3.91591500</td>
<td>1.59772500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.00013800</td>
<td>5.41914500</td>
<td>-0.30974200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.27090000</td>
<td>3.91582500</td>
<td>1.59730200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.27716600</td>
<td>4.78620500</td>
<td>2.25782100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.15057300</td>
<td>3.31754900</td>
<td>1.82956300</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.00002500</td>
<td>2.24412200</td>
<td>1.11607100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.00027300</td>
<td>2.70624000</td>
<td>2.81456700</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-0.00001600</td>
<td>6.26164800</td>
<td>0.38240100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.00029200</td>
<td>5.80785500</td>
<td>-1.32528500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.27766600</td>
<td>4.78612600</td>
<td>2.25738100</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-2.15083800</td>
<td>3.31740400</td>
<td>1.82886500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>S</td>
<td>1.52754800</td>
<td>4.48437100</td>
<td>-0.10271600</td>
<td></td>
<td></td>
</tr>
<tr>
<td>S</td>
<td>-1.52725800</td>
<td>4.48423400</td>
<td>-0.10323200</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-2.91272800</td>
<td>-3.95203000</td>
<td>0.67908500</td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>2.91251600</td>
<td>-3.95229400</td>
<td>0.67816700</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Complex of p-7 with oxadiazole 4**

\[ G = -3'203.280815 \, \text{ht} \]
\[ \Delta G_{\text{XB}} = 1.0 \text{ kcal/mol} \]

I–N distances (Å): 3.09

C–I–N angles (°): 176

<table>
<thead>
<tr>
<th>Atom</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
<th>I–X</th>
<th>I–Y</th>
<th>I–Z</th>
<th>C–I–N</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>2.32884800</td>
<td>0.37942100</td>
<td>-0.40370500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>1.33611200</td>
<td>-1.57359100</td>
<td>2.31871000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>1.33921000</td>
<td>-3.91064600</td>
<td>-1.75427500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>5.82756900</td>
<td>-4.66706900</td>
<td>0.44552800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-1.33708700</td>
<td>-3.91138100</td>
<td>-1.75416500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>5.45016000</td>
<td>-0.08952000</td>
<td>-0.38497400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>6.96454500</td>
<td>-2.25944700</td>
<td>-0.03713200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.87743100</td>
<td>-2.58030800</td>
<td>0.19341500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.40684000</td>
<td>-2.73040800</td>
<td>0.27454300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.68935900</td>
<td>-2.16426400</td>
<td>1.31871000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.68837600</td>
<td>-3.69010900</td>
<td>0.35478400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.69077700</td>
<td>-2.16390200</td>
<td>1.31866300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.46780400</td>
<td>-1.33735900</td>
<td>-0.06538100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.06813300</td>
<td>-3.59549000</td>
<td>0.28126700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.06054400</td>
<td>-2.73116500</td>
<td>0.27465000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.64709700</td>
<td>-2.36513800</td>
<td>0.03633800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.69095400</td>
<td>-3.59549000</td>
<td>0.28126700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.69285300</td>
<td>-3.59549000</td>
<td>-0.73748200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.06813300</td>
<td>-3.59549000</td>
<td>0.28126700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.06054400</td>
<td>-2.73116500</td>
<td>0.27465000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.84525200</td>
<td>-1.24698300</td>
<td>-0.13739000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.64709700</td>
<td>-2.36513800</td>
<td>0.03633800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.69095400</td>
<td>-3.59549000</td>
<td>0.28126700</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>O</td>
<td>0.00144000</td>
<td>4.88252600</td>
<td>0.09411000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>0.68897100</td>
<td>2.97663900</td>
<td>-0.71843200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.40866900</td>
<td>4.62693400</td>
<td>-0.02599300</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>-0.69102700</td>
<td>2.97643700</td>
<td>-0.71864900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.06054400</td>
<td>4.11490500</td>
<td>-0.23667400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.48478600</td>
<td>4.00105400</td>
<td>-0.65244800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>3.30595200</td>
<td>3.15996300</td>
<td>-1.30710000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.06309300</td>
<td>4.11458700</td>
<td>-0.23699400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.62247100</td>
<td>5.72869700</td>
<td>0.79924900</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>1.78303900</td>
<td>6.21182300</td>
<td>1.27967500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.76982200</td>
<td>4.46858300</td>
<td>-0.43826200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>5.60432300</td>
<td>3.97972400</td>
<td>-0.92151100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.91145600</td>
<td>6.19300100</td>
<td>1.00504400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>4.07837100</td>
<td>7.04577400</td>
<td>1.64836800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.41143500</td>
<td>4.62620700</td>
<td>-0.02672400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.62572600</td>
<td>5.72849400</td>
<td>0.79769100</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.78651400</td>
<td>6.21233000</td>
<td>1.27778500</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.91490900</td>
<td>6.19243100</td>
<td>1.00307800</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.08219600</td>
<td>7.04562000</td>
<td>1.64575400</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.98819100</td>
<td>5.56099200</td>
<td>0.38921200</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Complex of p-7 with pyridazin 5

\[ G = -3'205.417181 \text{ kcal/mol} \]

\[ \Delta G_{XB} = 0.2 \text{ kcal/mol} \]

I-N distances (Å): 3.31 and 3.08

C-I-N angles (°): 173 and 175
<table>
<thead>
<tr>
<th>Column 1</th>
<th>Column 2</th>
<th>Column 3</th>
<th>Column 4</th>
<th>Column 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>4.92772000</td>
<td>-3.63270300</td>
<td>-0.43527500</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.44097900</td>
<td>-2.53642300</td>
<td>0.42460700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.79107300</td>
<td>-1.24940000</td>
<td>-0.63593800</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.54272800</td>
<td>-2.41449800</td>
<td>-0.65120900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.87661700</td>
<td>-3.12714800</td>
<td>-0.69349600</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.90422400</td>
<td>-2.33926100</td>
<td>0.53410500</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.72495600</td>
<td>-3.42130970</td>
<td>0.82966900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.47909800</td>
<td>-1.07937800</td>
<td>0.33193900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-5.09744300</td>
<td>-3.26452200</td>
<td>0.94357300</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.84973400</td>
<td>-0.93251600</td>
<td>0.44776700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-5.65866500</td>
<td>-2.01162250</td>
<td>0.75431300</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-1.08937300</td>
<td>-1.46160800</td>
<td>2.48303000</td>
<td></td>
</tr>
<tr>
<td>I</td>
<td>-2.33045900</td>
<td>0.57333300</td>
<td>-0.20818200</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-5.86666200</td>
<td>-4.30216300</td>
<td>1.23272300</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-6.96902700</td>
<td>-1.86006700</td>
<td>0.86023900</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-5.43804900</td>
<td>0.24294300</td>
<td>0.26158200</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.43124800</td>
<td>5.20269200</td>
<td>0.95008900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-0.85623600</td>
<td>5.16971600</td>
<td>0.49155100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-1.21861600</td>
<td>4.12463700</td>
<td>-0.36731900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>1.30763400</td>
<td>4.19561600</td>
<td>0.52497400</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>0.78756000</td>
<td>5.99819700</td>
<td>1.58965600</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.57174000</td>
<td>5.93540000</td>
<td>0.74819800</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>0.89472000</td>
<td>3.21920800</td>
<td>-0.27540000</td>
<td></td>
</tr>
<tr>
<td>N</td>
<td>-0.34779000</td>
<td>3.17944700</td>
<td>-0.71136600</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>2.72919200</td>
<td>4.18425600</td>
<td>0.92986200</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.71232200</td>
<td>3.80945000</td>
<td>0.01689900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>3.10048200</td>
<td>4.55250500</td>
<td>2.22134200</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.04582000</td>
<td>3.79655400</td>
<td>0.39306900</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>3.42270700</td>
<td>3.53155800</td>
<td>-0.98719700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>4.43461900</td>
<td>4.53577100</td>
<td>2.59733300</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>2.34138000</td>
<td>4.82424900</td>
<td>2.94406700</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>5.40893400</td>
<td>4.15802600</td>
<td>1.68347600</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>5.80121000</td>
<td>3.50049700</td>
<td>-0.32168800</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>4.71250900</td>
<td>4.80885700</td>
<td>3.60611100</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>6.44967400</td>
<td>4.14315600</td>
<td>1.97724200</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.57495100</td>
<td>4.01488100</td>
<td>-0.94341500</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-3.69660000</td>
<td>4.35567400</td>
<td>-0.19128500</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-2.73989100</td>
<td>3.52984200</td>
<td>-2.23940100</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.96749600</td>
<td>4.19896900</td>
<td>-0.72201300</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-3.57867300</td>
<td>4.70489500</td>
<td>0.82674000</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-4.01042400</td>
<td>3.38542000</td>
<td>-2.77176200</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-1.86516900</td>
<td>3.25869100</td>
<td>-2.81469900</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>-5.12603400</td>
<td>3.71397400</td>
<td>-2.01294200</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-5.83436300</td>
<td>4.44368700</td>
<td>-0.12375100</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-4.13138500</td>
<td>3.00895900</td>
<td>-3.77829900</td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>-6.11796800</td>
<td>3.58847500</td>
<td>-2.42509900</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>2.99145600</td>
<td>-4.84817700</td>
<td>0.01036200</td>
<td></td>
</tr>
<tr>
<td>F</td>
<td>-3.20432200</td>
<td>-4.62106000</td>
<td>1.01825000</td>
<td></td>
</tr>
</tbody>
</table>


F ) References


4 W. Wang, W. Meng and H. Du, Dalton T, 2016, 45, 5945

5 R.H. Mizzoni and P.E. Spoerri, JACS, 1951, 73, 1873


8 L. Wang, J. Cao, Q. Chen and M. He, J. Org. Chem., 2015, 80, 4743

9 Agilent 2011 CrysAlis PRO; Oxford Diffraction/Agilent Technologies UK Ltd; Yarnton, England


11 G. Sheldrick, Acta Crystallographica Section A, 2008, 64, 112


13 DIAMOND 2.1d; Crystal Impact - H. Putz & K. Brandenburg GbR; Kreuzherrenstr. 102, 53227 Bonn, Germany, 2000


15 Y. Zhao and D.G. Truhlar, Theor. Chem. Acc., 2008, 120, 215


18 C.Y. Legault; CYLview.1.0b; Université de Sherbrooke; 2009; Available from: http://www.cylview.org.