# Electronic Supporting Information

**Dichotomy of π-Stacking-Directing Noncovalent Forces in Inorganic–Organic Planar Assemblies. The Case of Platinum(II) Square-Plane π-Stacked with Halo-Substituted Benzoquinones**

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# S1. CRYSTAL DATA AND STRUCTURE REFINEMENT

**Table S1.** Crystal data and structure refinement for **1·QF**, **1·QCl**, **1·QBr**, and **1·QI**.

| | **1·QF** | **1·QCl** | **1·QBr** | **1·QI** |
|---|---|---|---|---|
| Empirical formula | $C_{24}H_{12}F_4N_2O_3PtS_2$ | $C_{24}H_{12}Cl_4N_2O_3PtS_2$ | $C_{24}H_{12}Br_4N_2O_3PtS_2$ | $C_{24}H_{12}I_4N_2O_3PtS_2$ |
| Formula weight | 711.57 | 777.37 | 955.21 | 1143.17 |
| Temperature/K | 100(2) | 100(2) | 100(2) | 100(2) |
| Crystal system | triclinic | monoclinic | monoclinic | orthorhombic |
| Space group | P-1 | P2$_1$ | P2$_1$ | Pna2$_1$ |
| a/Å | 7.30130(10) | 7.94224(9) | 7.69860(10) | 18.1811(3) |
| b/Å | 8.15735(11) | 18.6997(2) | 17.1871(2) | 8.19870(10) |
| c/Å | 18.77600(17) | 8.20079(9) | 9.55470(10) | 17.8672(3) |
| α/° | 101.8971(10) | 90 | 90 | 90 |
| β/° | 92.8080(9) | 101.1165(11) | 101.2610(10) | 90 |
| γ/° | 101.3060(11) | 90 | 90 | 90 |
| Volume/Å$^3$ | 1068.36(2) | 1195.11(2) | 1239.91(3) | 2663.31(7) |
| Z | 2 | 2 | 2 | 4 |
| $\rho_{calc}$g/cm$^3$ | 2.212 | 2.160 | 2.559 | 2.851 |
| μ/mm$^{-1}$ | 14.743 | 17.023 | 19.996 | 47.995 |
| F(000) | 680.0 | 744.0 | 888.0 | 2064.0 |
| Crystal size/mm$^3$ | 0.08 × 0.06 × 0.05 | 0.15 × 0.1 × 0.1 | 0.16 × 0.14 × 0.12 | 0.07 × 0.06 × 0.05 |
| Radiation | CuKα (λ = 1.54184) | CuKα (λ = 1.54184) | CuKα (λ = 1.54184) | Cu Kα (λ = 1.54184) |
| 2Θ range for data collection/° | 4.83 to 139.934 | 9.46 to 139.66 | 9.438 to 139.998 | 9.73 to 139.994 |
| Index ranges | -8 ≤ h ≤ 8, -9 ≤ k ≤ 9, -22 ≤ l ≤ 22 | -9 ≤ h ≤ 9, -22 ≤ k ≤ 22, -9 ≤ l ≤ 9 | -9 ≤ h ≤ 9, -20 ≤ k ≤ 20, -11 ≤ l ≤ 11 | -22 ≤ h ≤ 16, -9 ≤ k ≤ 5, -21 ≤ l ≤ 20 |
| Reflections collected | 25786 | 24743 | 17227 | 15387 |
| Independent reflections | 4019 [R$_{int}$ = 0.0557, R$_{sigma}$ = 0.0316] | 4402 [R$_{int}$ = 0.0502, R$_{sigma}$ = 0.0319] | 4691 [R$_{int}$ = 0.0458, R$_{sigma}$ = 0.0436] | 4529 [R$_{int}$ = 0.0447, R$_{sigma}$ = 0.0380] |
| Data/restraints/parameters | 4019/0/325 | 4402/1/325 | 4691/1/325 | 4529/1/325 |
| Goodness-of-fit on F$^2$ | 1.044 | 1.124 | 1.076 | 1.052 |
| Final R indexes [I>=2σ (I)] | R$_1$ = 0.0216, wR$_2$ = 0.0509 | R$_1$ = 0.0312, wR$_2$ = 0.0814 | R$_1$ = 0.0222, wR$_2$ = 0.0515 | R$_1$ = 0.0278, wR$_2$ = 0.0708 |
| Final R indexes [all data] | R$_1$ = 0.0234, wR$_2$ = 0.0516 | R$_1$ = 0.0322, wR$_2$ = 0.0820 | R$_1$ = 0.0229, wR$_2$ = 0.0518 | R$_1$ = 0.0285, wR$_2$ = 0.0712 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.98/-0.70 | 2.49/-1.28 | 0.80/-0.61 | 0.86/-0.78 |
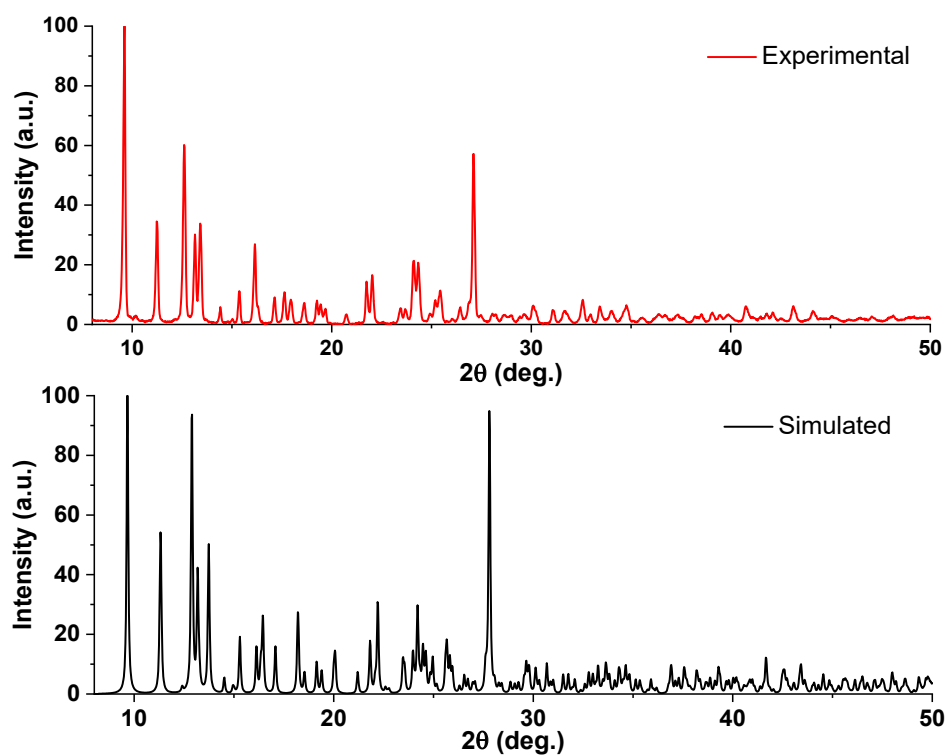
**Figure S1**. Powder XRD patterns of **1**·QF.
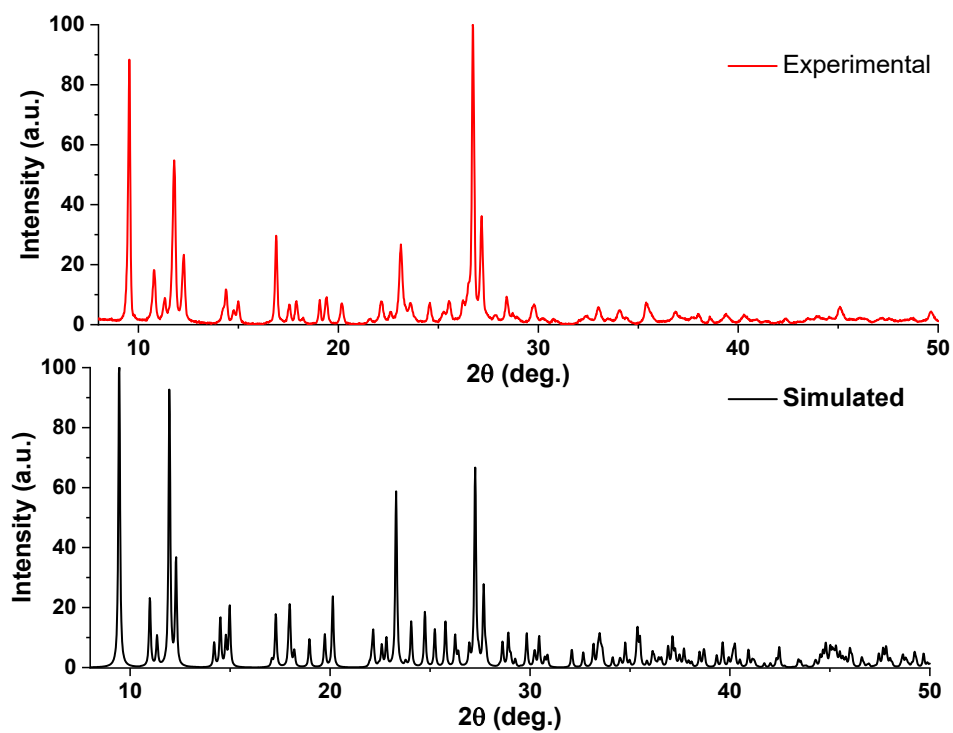


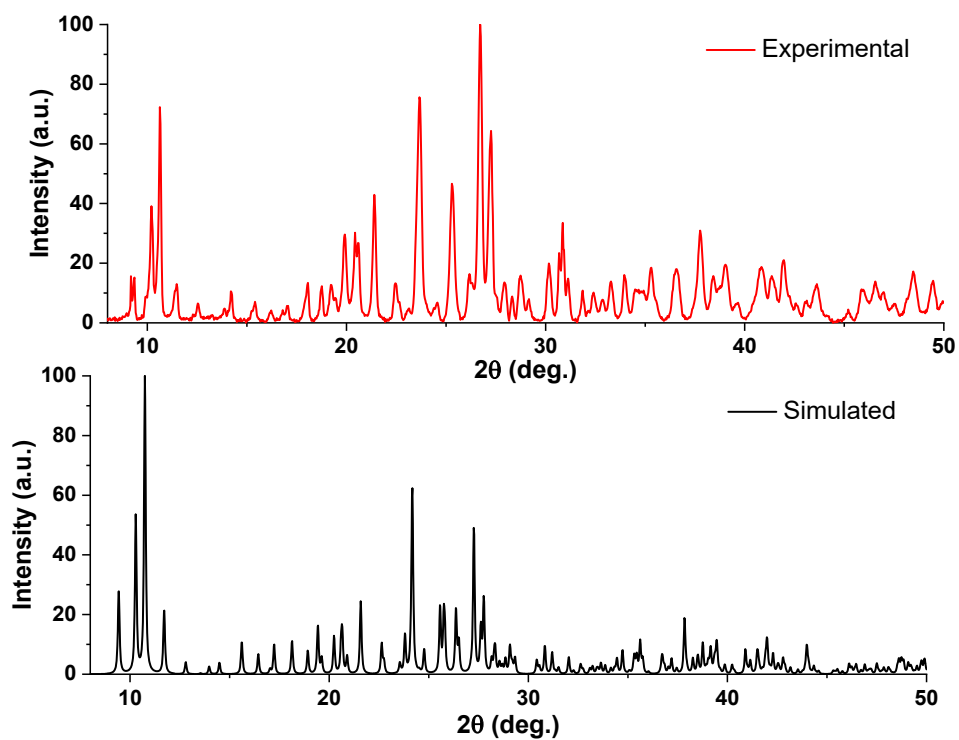**Figure S2**. Powder XRD patterns of **1**·QCl.

**Figure S3**. Powder XRD patterns of **1**·QBr.
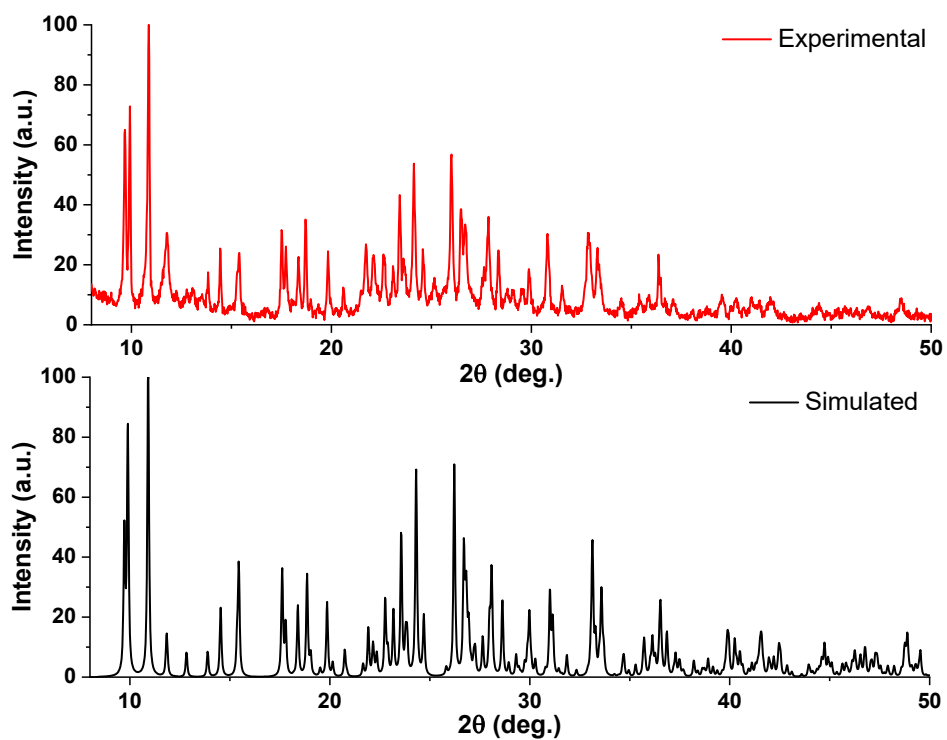


**Figure S4**. Powder XRD patterns of **1**·QI.

**Table S2**. Refined unit cell parameters at room temperature from PXRD and cell parameters at 100 K from single-crystal XRD (in square brackets).

|  | **1·QF** | **1·QCl** | **1·QBr** | **1·QI** |
|---|---|---|---|---|
| a, Å | 7.4536(10) [7.3013(1)] | 8.0004(10) [7.94224(9)] | 7.835(3) [7.6986(1)] | 18.429(2) [18.1811(3)] |
| b, Å | 8.1791(9) [8.15735(11)] | 18.694(2) [18.6997(2)] | 17.199(6) [17.1871(2)] | 8.2841(9) [8.1987(1)] |
| c, Å | 18.921(2) [18.77600(1)] | 8.3850(11) [8.20079(9)] | 9.641(3) [9.5547(1)] | 17.9630(18) [17.8672(3)] |
| α,° | 101.519(7) [101.8971(10)] | 90 [90] | 90 [90] | 90 [90] |
| β,° | 93.177(5) [92.8080(9)] | 99.822(7) [101.1165(11)] | 101.816(15) [101.261(1)] | 90 [90] |
| γ,° | 99.172(5) [101.3060(11)] | 90 [90] | 90 [90] | 90 [90] |
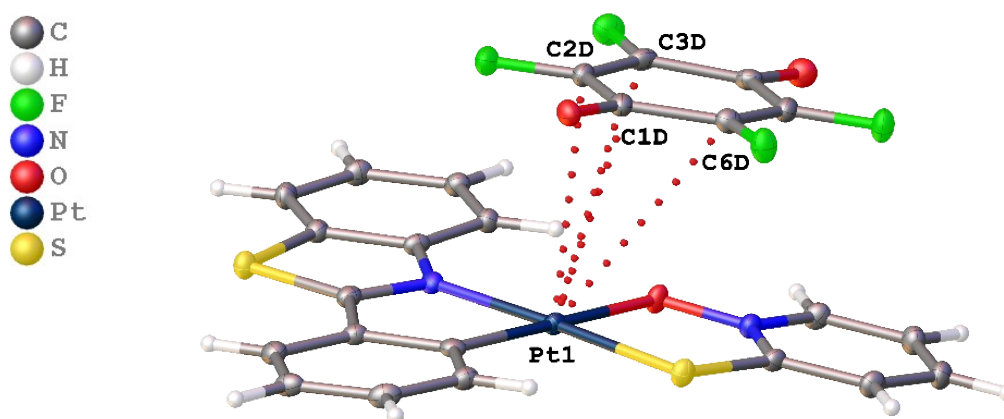


**Figure S5**. Molecular structure of **1·QF** showing C···Pt contacts (dotted lines). Here and in after non-hydrogen atoms are given as probability ellipsoids of atomic displacements ($p = 0.5$).
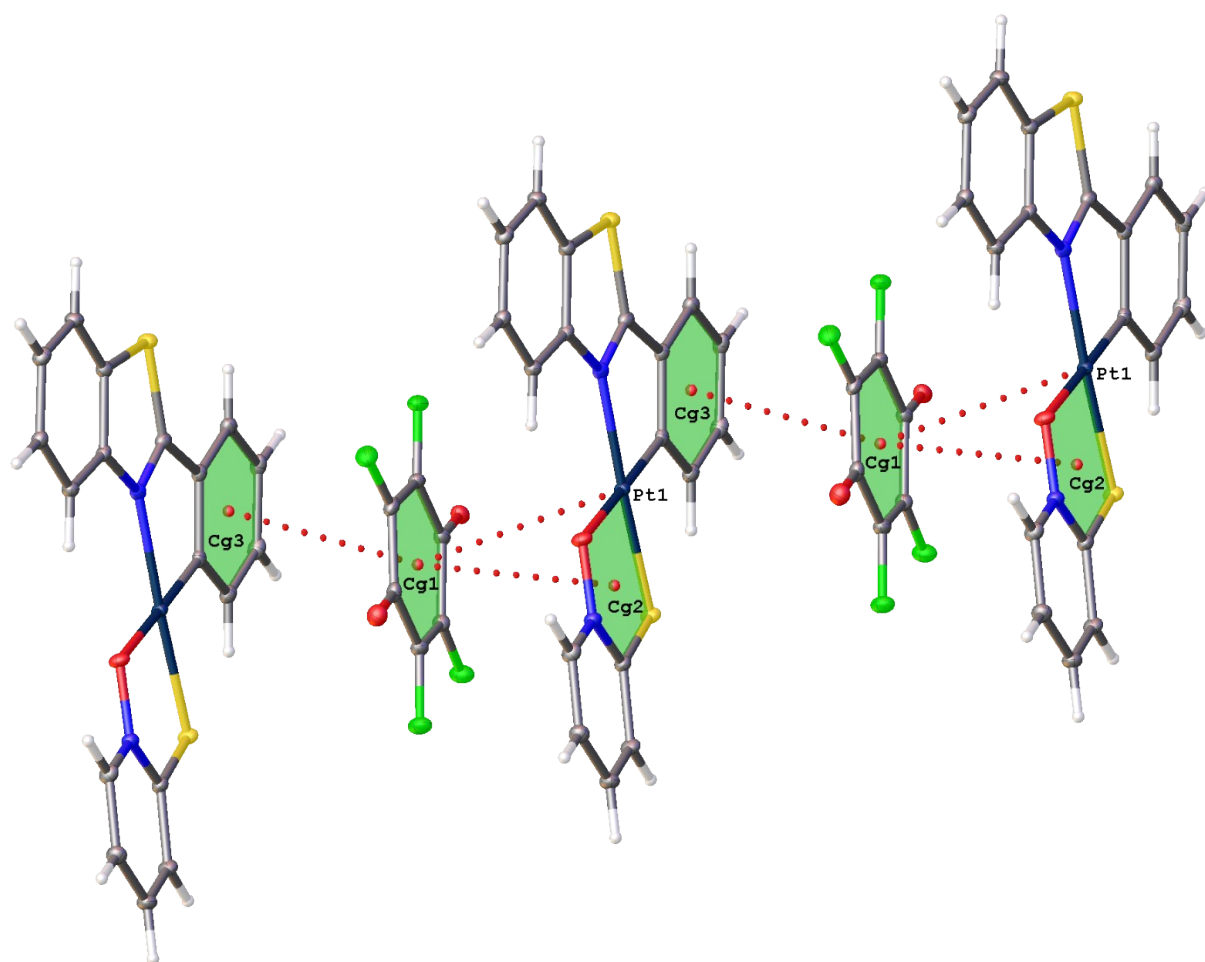
**Figure S6**. A fragment of crystal packing of **1**·QF (Cg···Pt and π-π interactions are given by dotted lines).
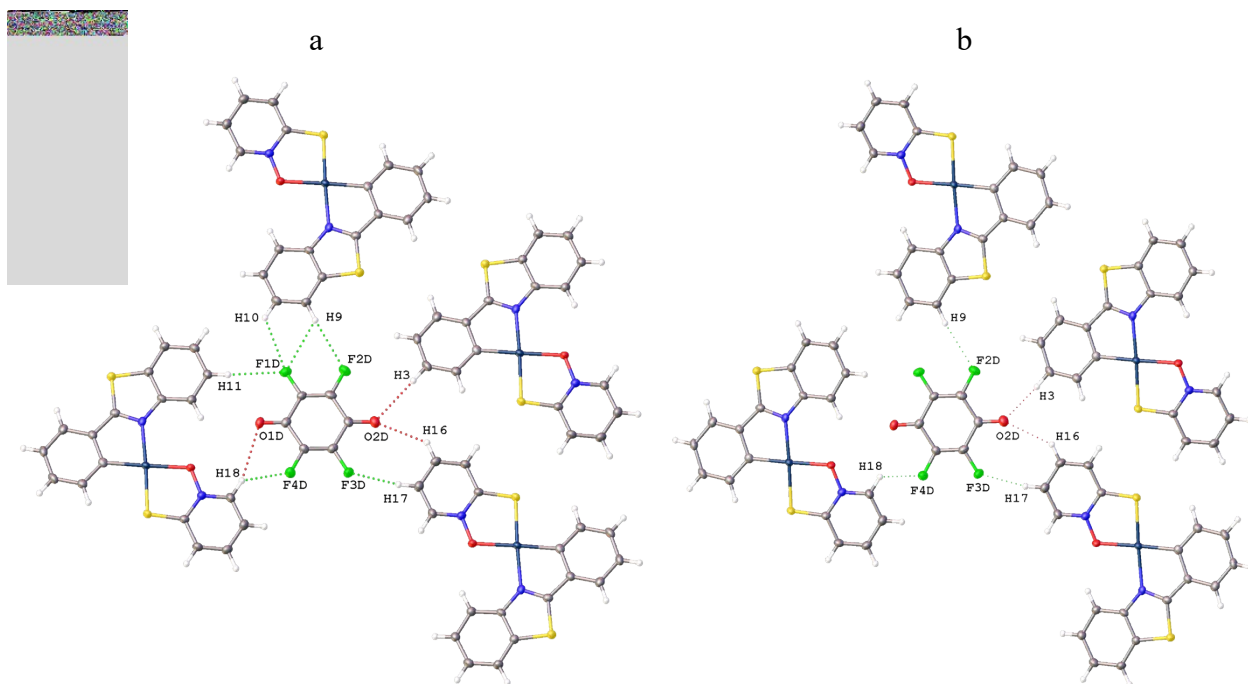
**Figure S7**. Fragments (a and b) of the crystal structure of **1**·QF with intermolecular HBs given by dotted lines.
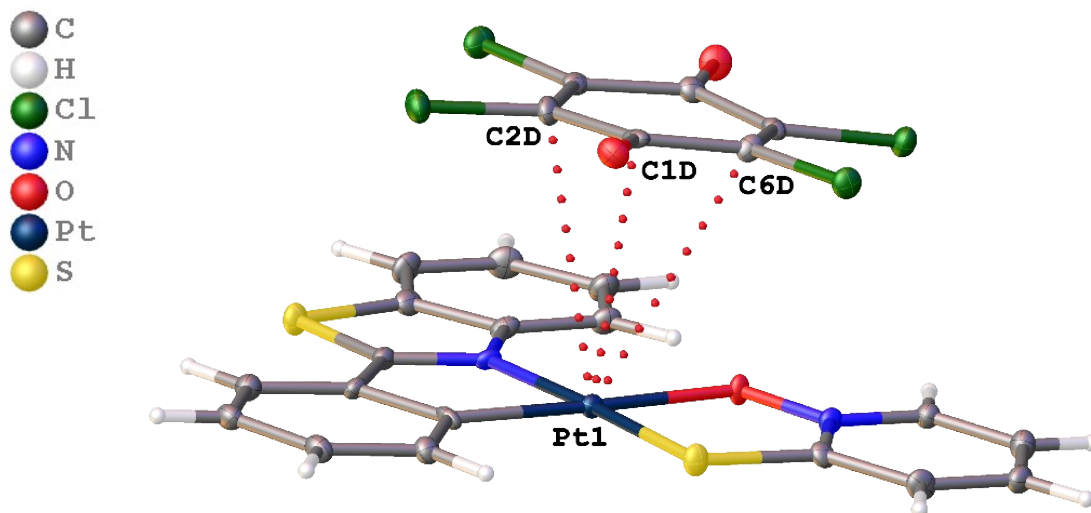


**Figure S8**. Molecular structure of **1**·QCl showing C···Pt contacts in dotted lines.
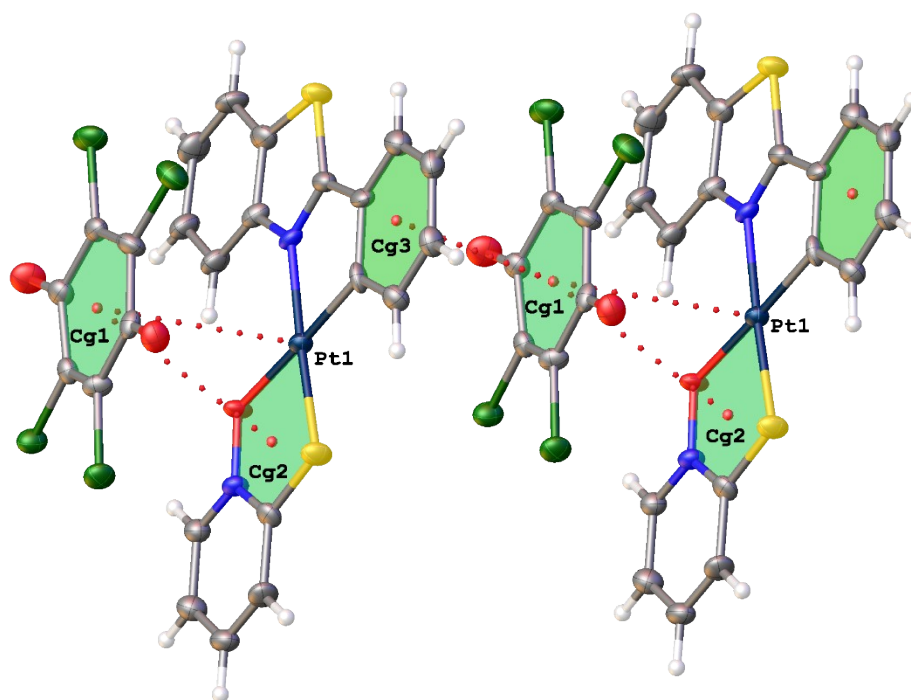
**Figure S9**. Fragment of crystal packing of **1**·QCl (Cg···Pt and π-π interactions are in dotted lines).
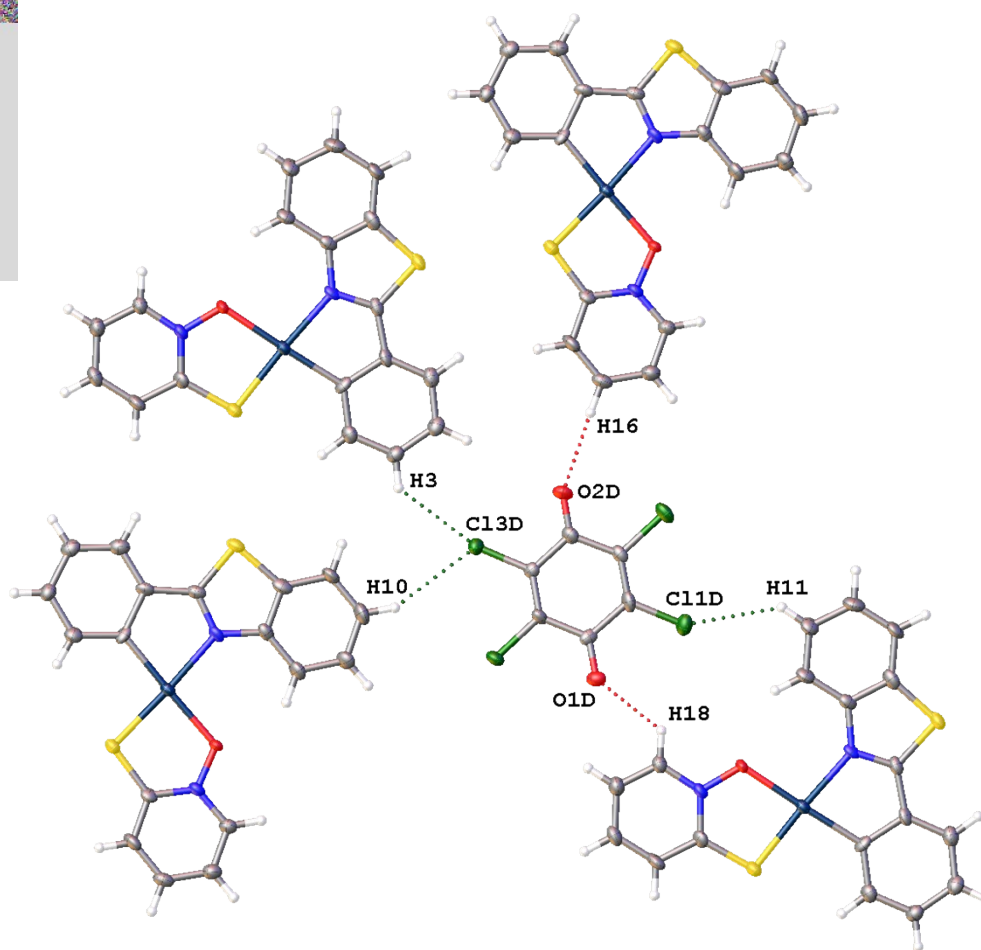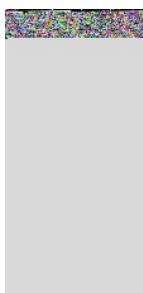
**Figure S10**. Fragment of the crystal structure of **1**·QCl showing intermolecular HBs (dotted lines).
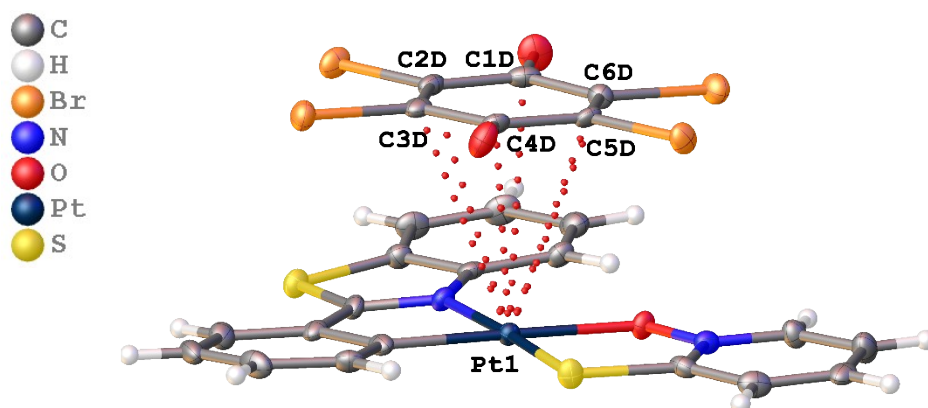


**Figure S11**. Molecular structure of **1**·QBr showing C···Pt contacts (dotted lines).
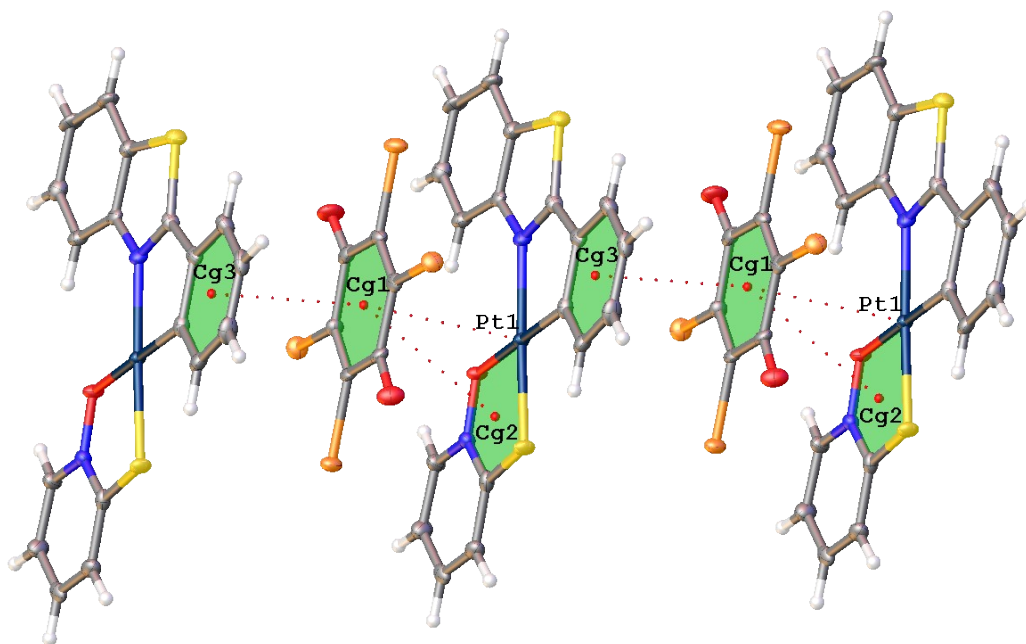


**Figure S12**. Fragment of crystal packing of **1**·QBr (Cg···Pt and π-π separations are in dotted lines).
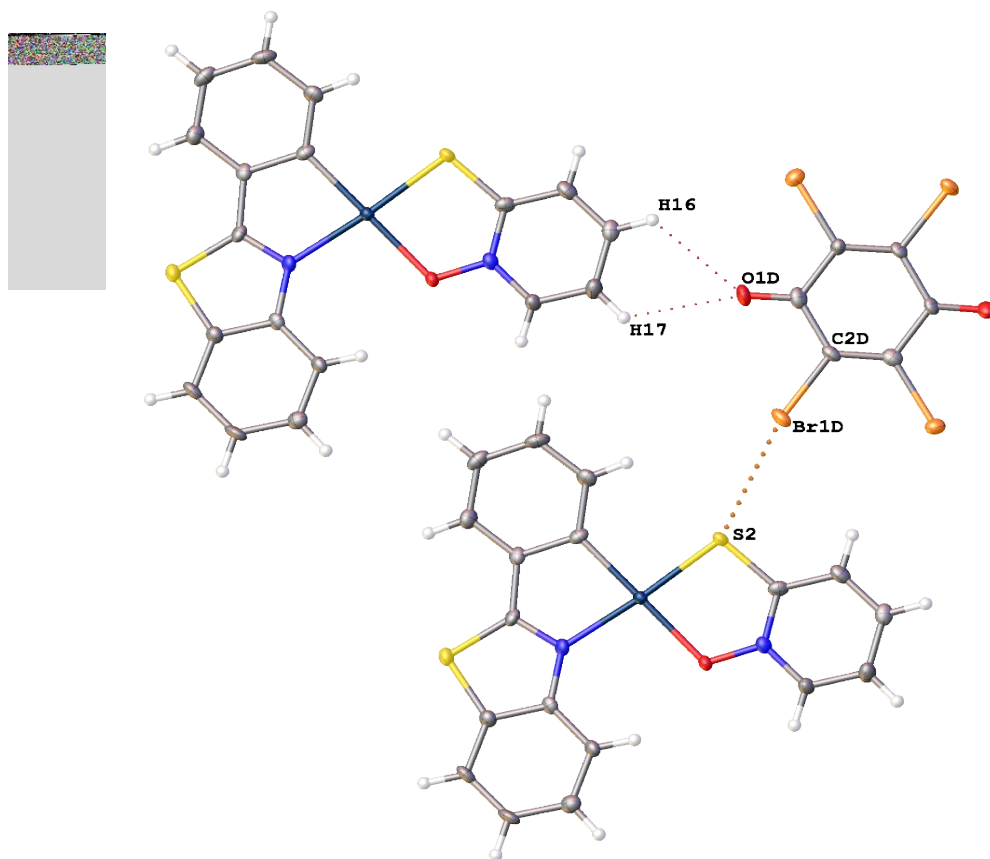
**Figure S13**. Fragment of the crystal structure of **1**·QBr showing intermolecular HBs (red dotted lines) and HaB (orange dotted line).
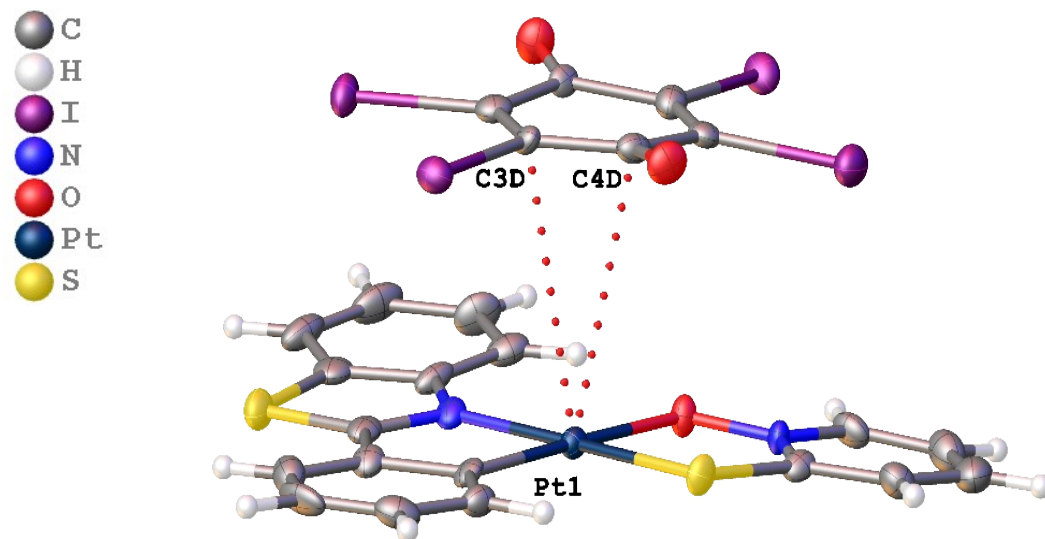


**Figure S14**. Molecular structure of **1**·QI with C···Pt contacts in dotted lines.
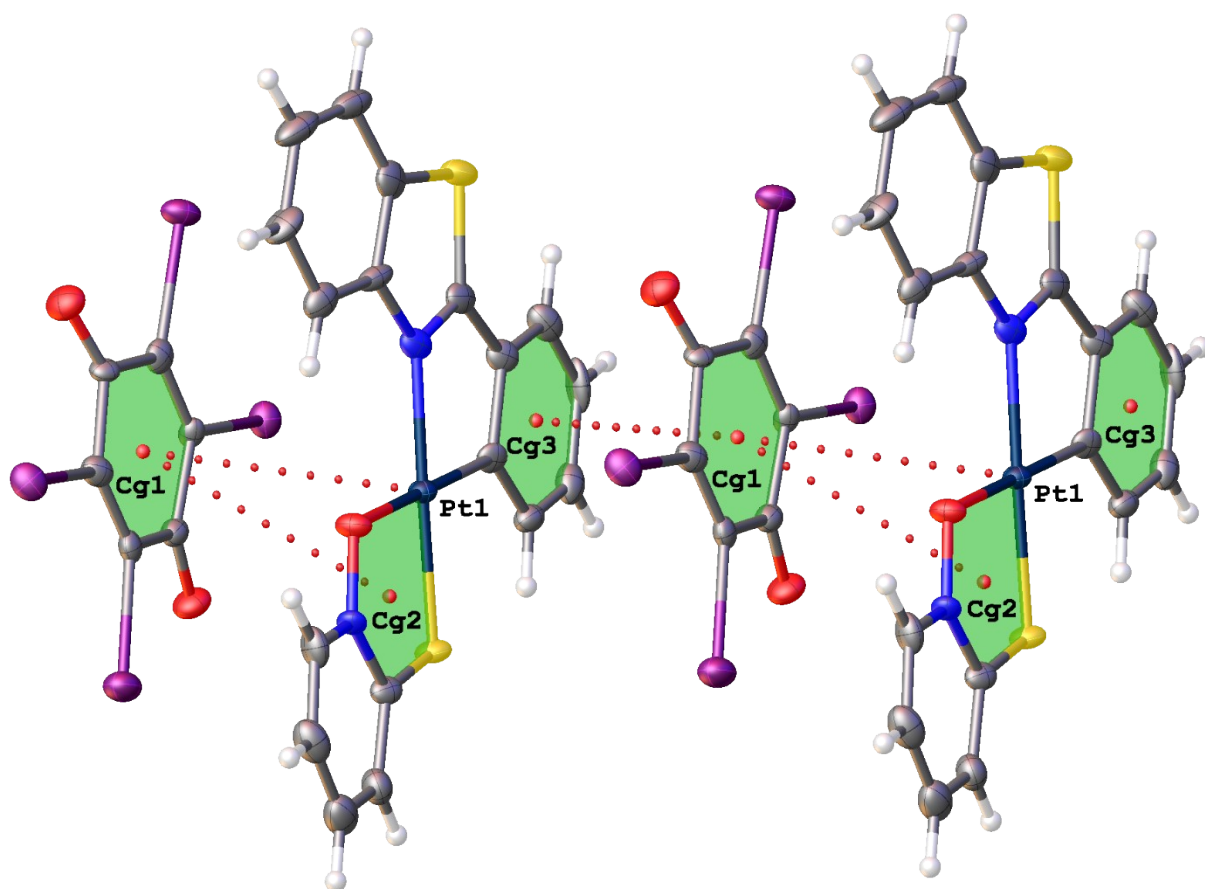
**Figure S15**. Fragment of crystal packing of **1**·QI (Cg···Pt and π-π interactions are dotted line).
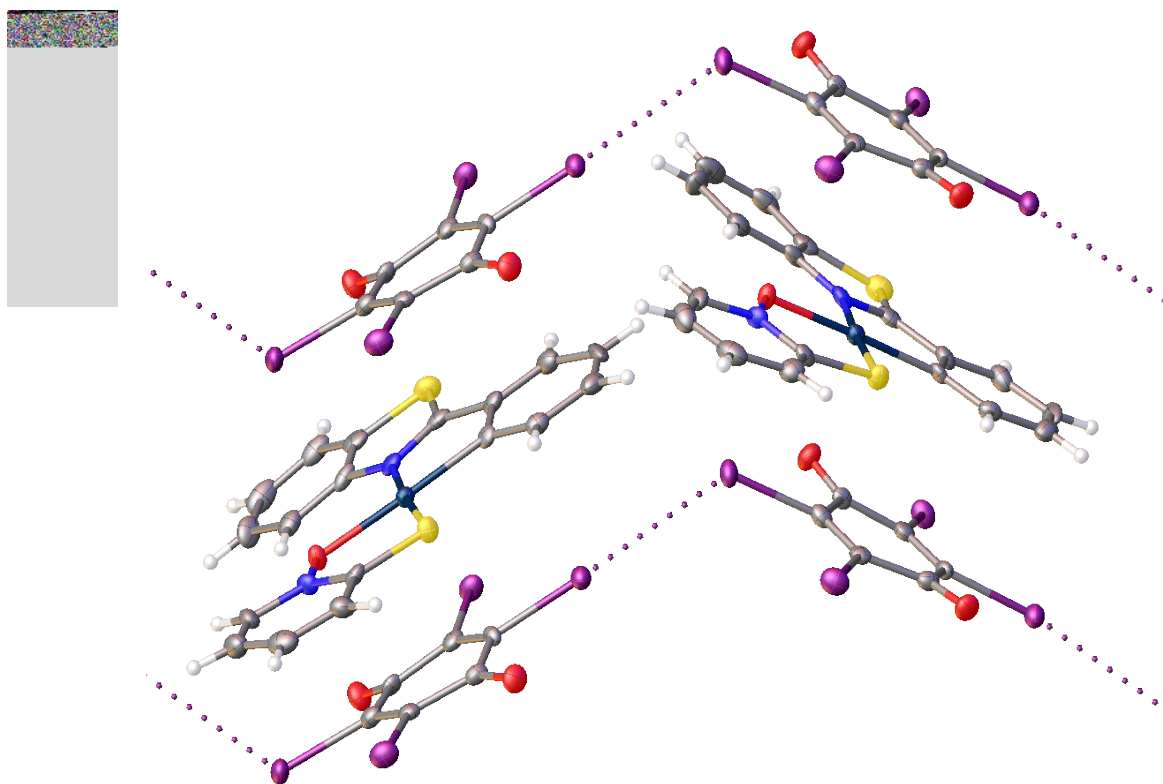
**Figure S16.** HaB between QI molecules in the structure of **1**·QI.
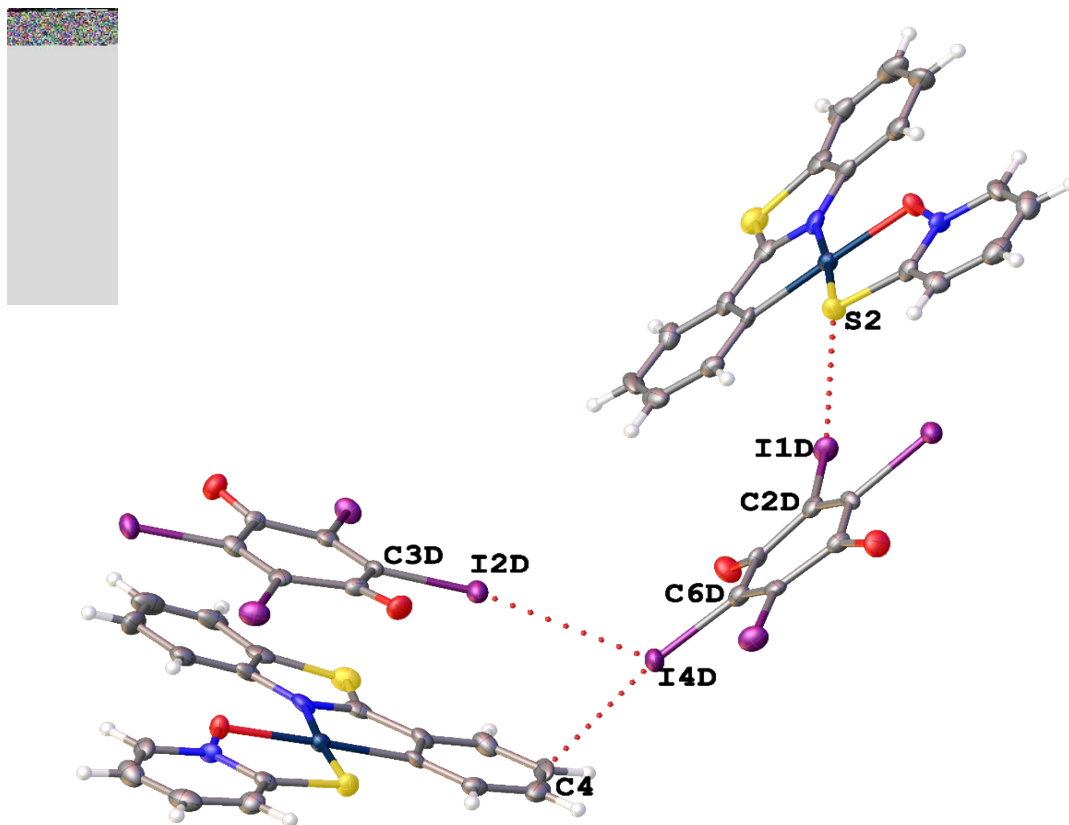
**Figure S17**. Fragment of the crystal structure of **1**·QI; HaBs are given in dotted lines.

# S2.    THERMOGRAVIMETRIC ANALYSIS
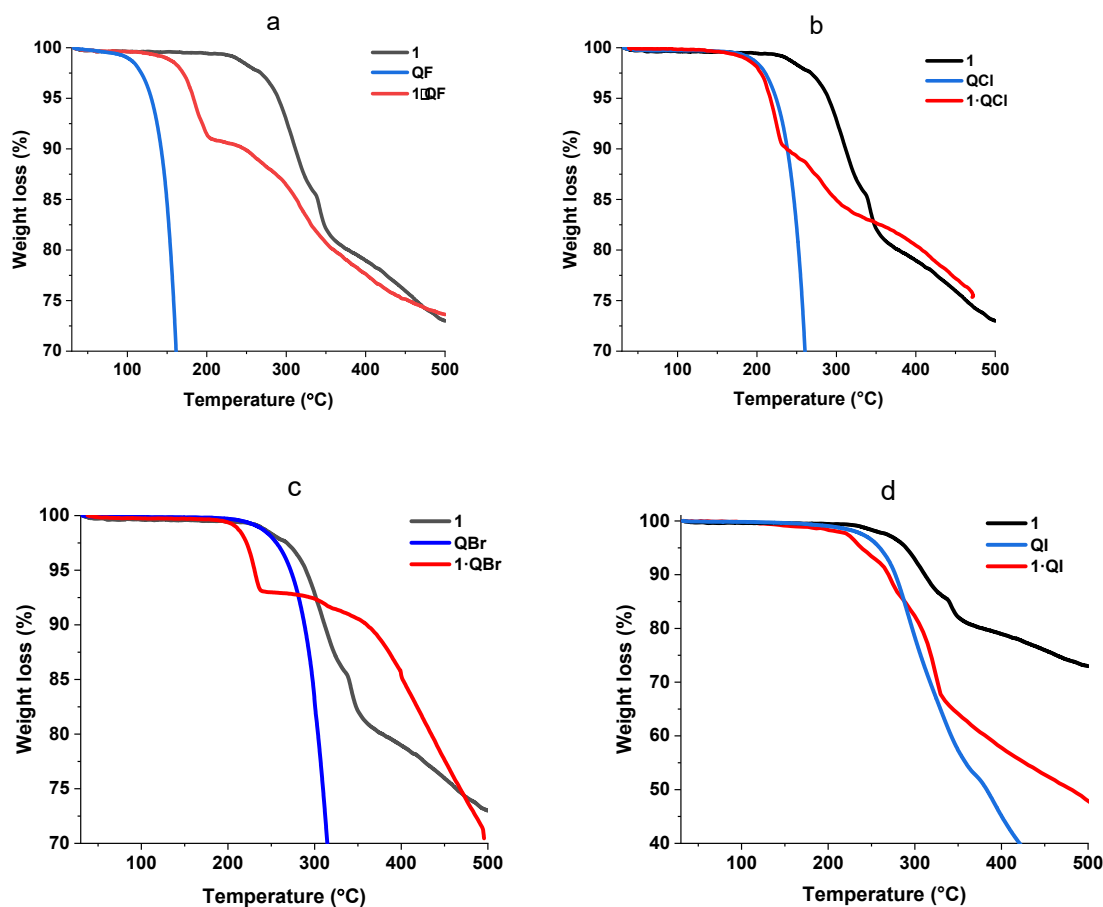


**Figure S18**. TGA curves of crystal samples of **1** (black), **QX** (blue) and **1·QX** (red).

*Thermal properties*. The thermal behavior of **1**·QX is different from that of **1**. On the thermogravimetric (TG) curves, for **1**·QX, the first mass-loss was observed at 166 °C (8% weight loss, **1**·QF), 204 °C (8% weight loss, **1**·QCl), 351 °C (8% weight loss, **1**·QBr), and 273 °C (29% weight loss, **1**·QI) (**Figure S18**). The parent complex **1** exhibits highest thermal stability among measured **1**·QX and it starts to decompose at 275 °C (8% weight loss).

## S3.    SOLID-STATE $^{195}$Pt NMR SPECTRA
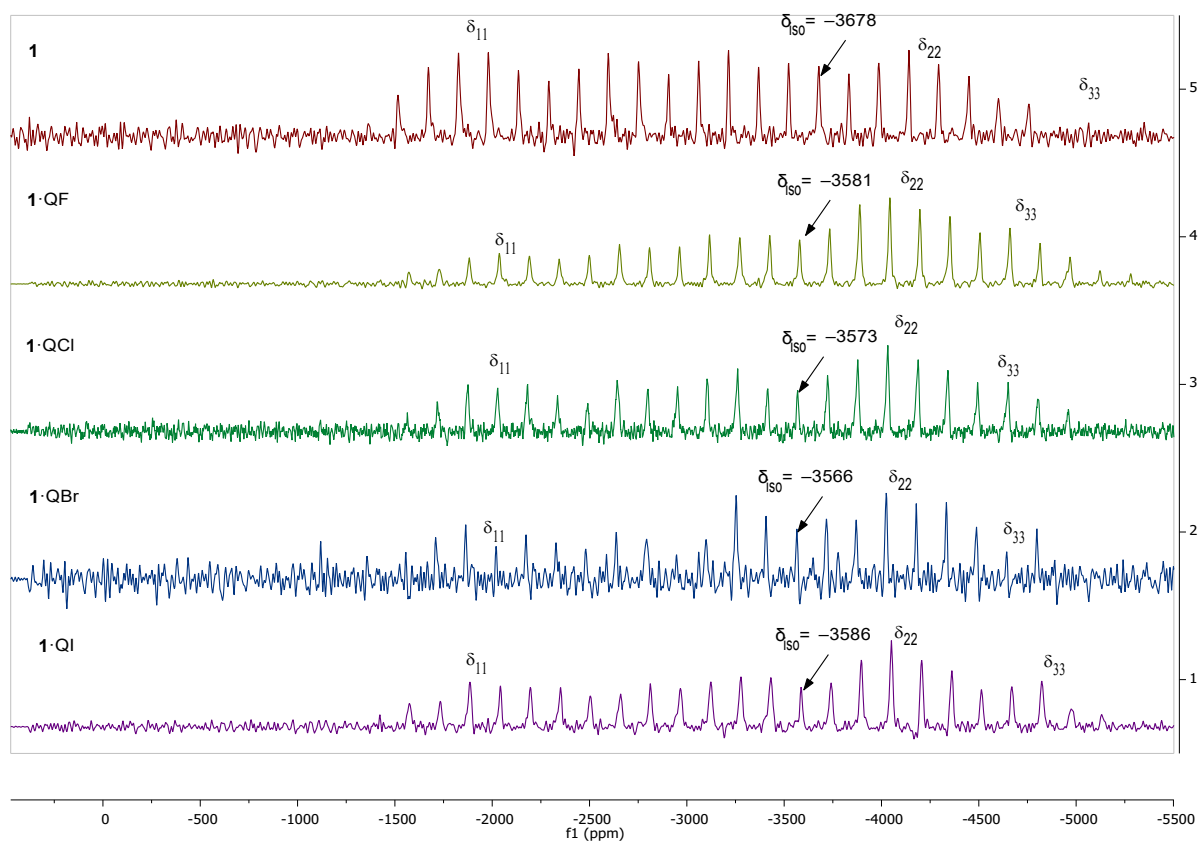


**Figure S19**. $^{195}$Pt solid-state NMR overlayed spectra for **1**, **1**·QF, **1**·QCl, **1**·QBr and **1**·QI (MAS rotation frequency 13.3 kHz).
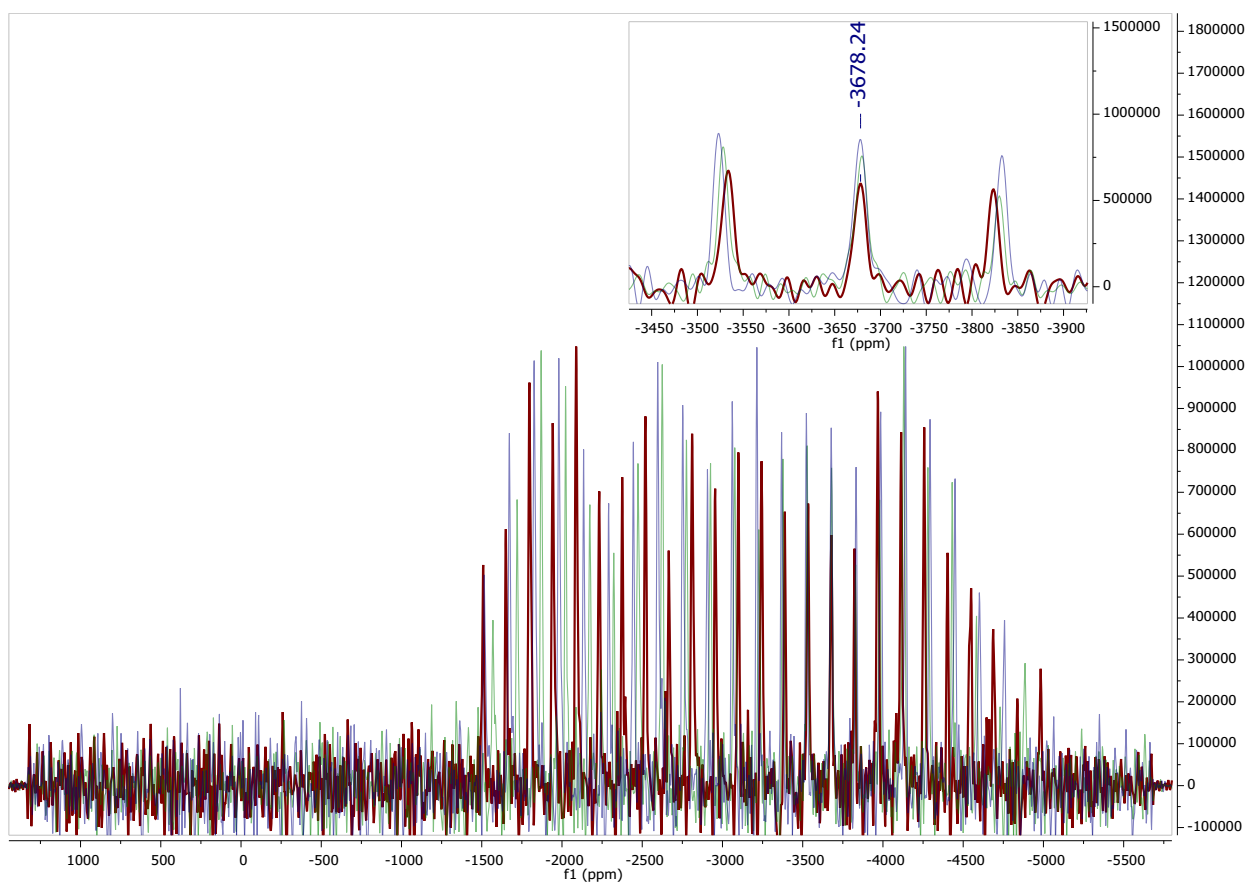
**Figure S20.** $^{195}$Pt solid-state NMR overlayed spectra for **1** at 12.5 kHz (red) 13.0 kHz (green) and 13.3 kHz (blue) MAS rotation frequency (inset: enlarged part of spectra to determine $\delta_{iso}$).
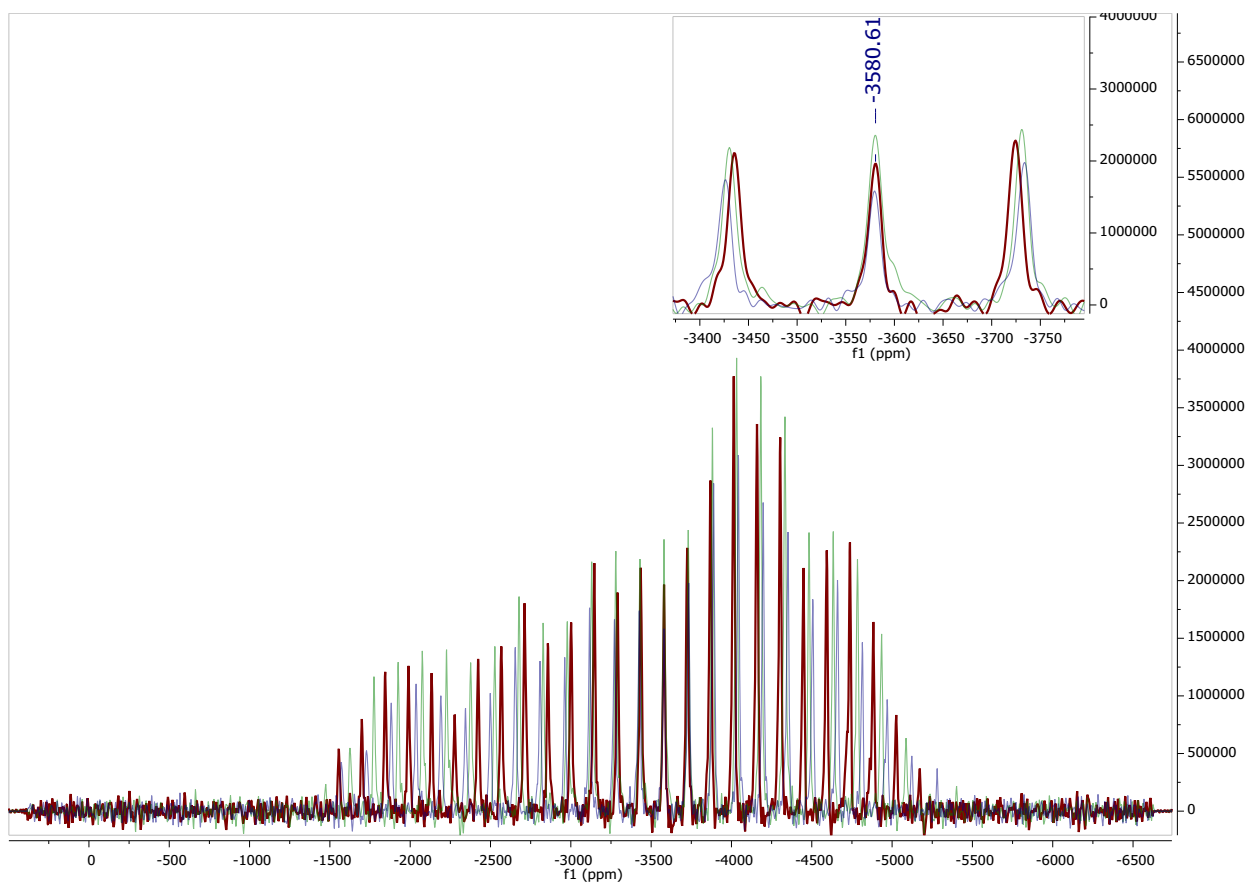
**Figure S21**. $^{195}$Pt solid-state NMR overlayed spectra for **1**·QF at 12.5 kHz (red) 13.0 kHz (green) and 13.3 kHz (blue) MAS rotation frequency (inset: enlarged part of spectra to determine $\delta_{iso}$).
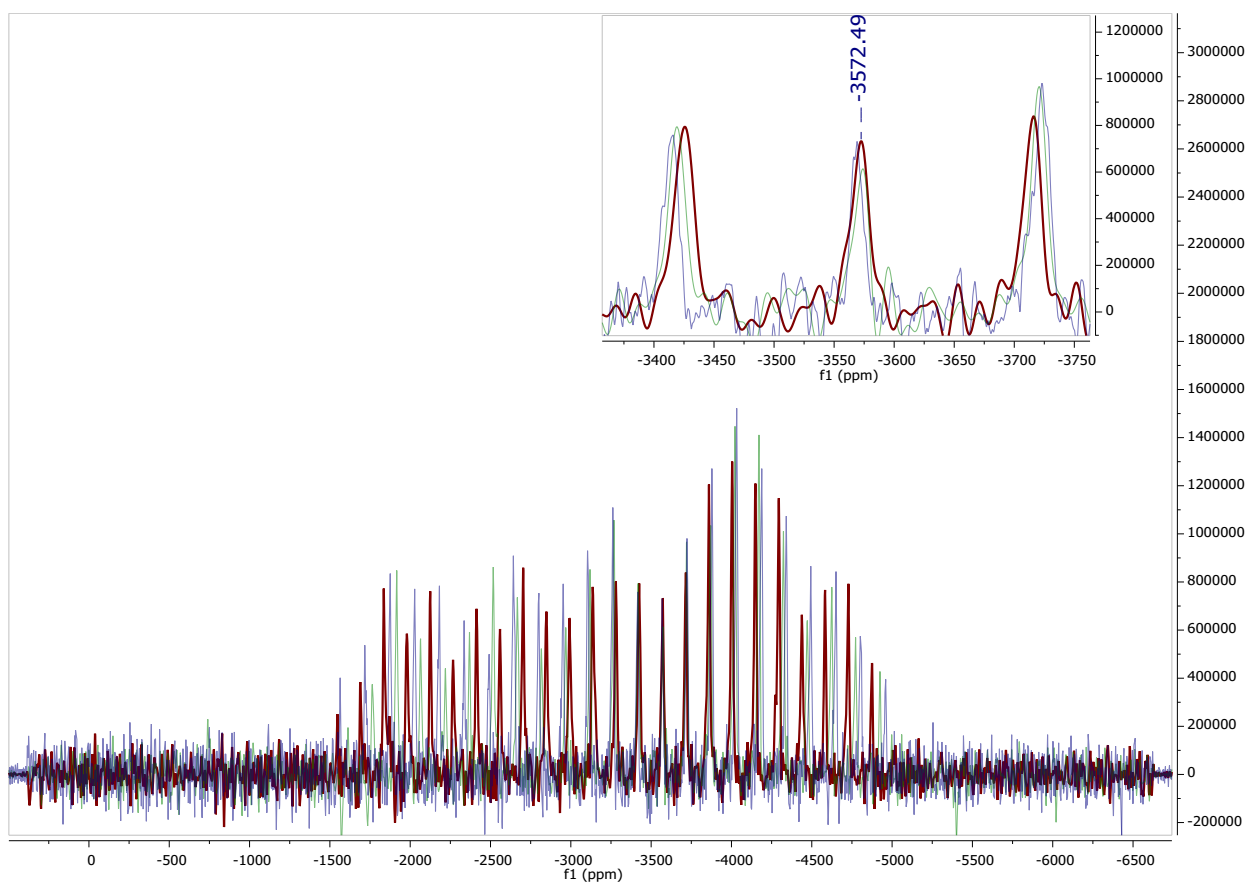
**Figure S22**. $^{195}$Pt solid-state NMR overlayed spectra for **1**·QCl at 12.5 kHz (red) 13.0 kHz (green) and 13.3 kHz (blue) MAS rotation frequency (inset: enlarged part of spectra to determine $\delta_{iso}$).
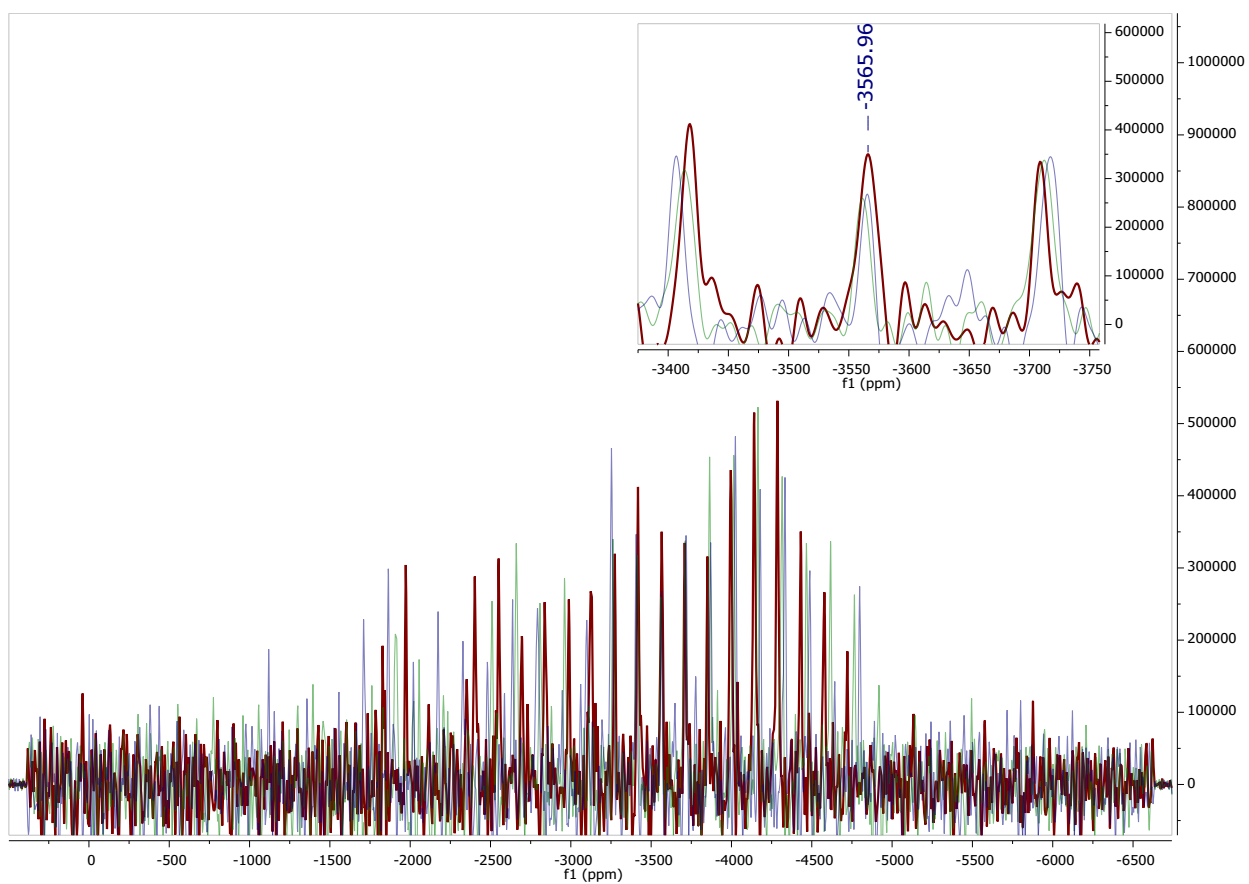
**Figure S23**. [195]Pt solid-state NMR overlayed spectra for **1**·QBr at 12.5 kHz (red) 13.0 kHz (green) and 13.3 kHz (blue) MAS rotation frequency (inset: enlarged part of spectra to determine $\delta_{iso}$).
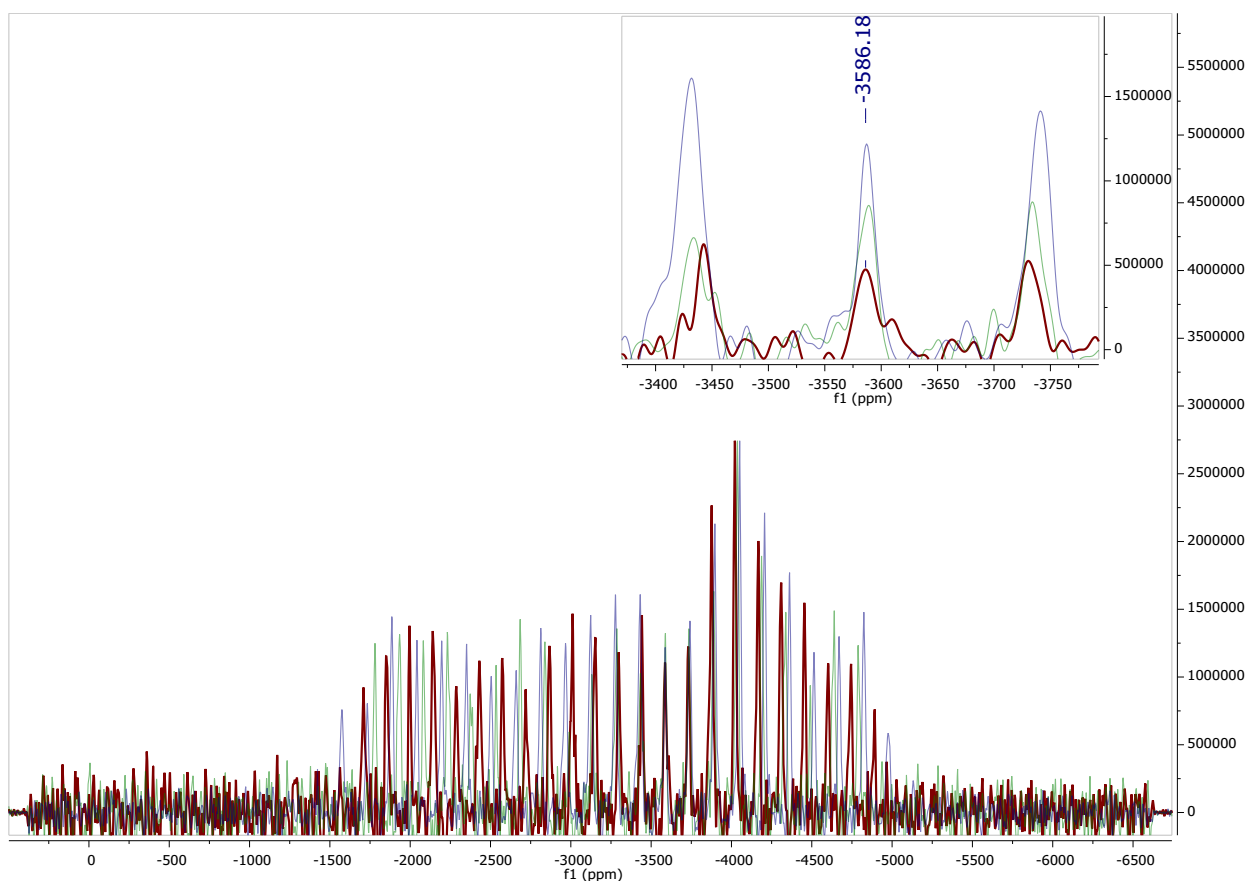
**Figure S24**. $^{195}Pt$ solid-state NMR overlayed spectra for **1**·QI at 12.5 kHz (red) 13.0 kHz (green) and 13.3 kHz (blue) MAS rotation frequency (inset: enlarged part of spectra to determine $\delta_{iso}$).

Analysis of the $^{195}Pt$ MAS-NMR spectra, measured at different spinning rates (12.5, 13.0, and 13.3 kHz), allowed the assignment of the isotropic $^{195}Pt$ chemical shifts ($\delta_{iso}$). We found that $\delta_{iso}$ in the cocrystals are low-field shifted and $\Delta\delta_{iso}$ is in the range 92–112 ppm (**Table 2**, **Figures S19–24**). To interpret the obtained NMR data, we performed theoretical calculations of the magnetic shielding tensor and magnetically induced currents for the bimolecular models [**1**·QX] and also for the parent complex **1** (**Table S3**). As a whole, the calculated isotropic shift correlates well with the experimentally observed one. However, we found a discrepancy of the $\delta_{iso}$ between the theoretical and experimental data (**Table S3**), most likely because all noncovalent interactions were not considered in the bimolecular model.

The disc-like shaped orientations of the calculated magnetic shielding tensors are nearly the same for all systems. The $\sigma_{11}$ axis of the tensor is directed perpendicularly to the molecular plane, while the $\sigma_{33}$ axis is oriented toward the C∩N and N∩O chelated rings (**Figure S5**). The directions of the $\sigma_{11}$ and $\sigma_{33}$ tensors are most susceptible to all structural changes accompanied the generation of the adducts.

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Next, the skew parameter ($\kappa$) increases from –0.53 to –0.47 ongoing from **1·QF** to **1·QI**. The $\kappa$ value for **1·QI** is practically the same as in the parent complex **1** (–0.48). According to refs[1-3], the changes in the $\kappa$ values are associated with the deshielding effect oriented perpendicularly to the complex square-plane. The occurrence of intermolecular contacts between **1** and QX is also affected by the local environment around the Pt-atom, as reflected by a significant change in $\Omega$ on pairing of the coformers (3727 ppm for **1**; 2620 **1·QF**; 2604 **1·QCl**; 2644 **1·QBr**; 2935 **1·QI**). Usually, strengthening of noncovalent interactions leads to a higher polarization of the electronic density of the system and this effect is accompanied by appropriate changes in density of the magnetically induced current (MIC) within the overall system.[4, 5] Hence, visualization of MIC and quantitative estimate of the density along chemical bonds under study are useful parameters to understand reasons of the observed chemical shift. The analysis of MIC for the Pt–C, Pt–N, Pt–S, and N–C (in *pbt*-ligand) bonds revealed that the noncovalent interaction of **1** with any one of QX leads to an increase in diatropic and paratropic currents by 0.45–0.12 nT/A within the chelated rings. This effect increases in the series from [**1·QI**] to [**1·QF**] (**Table S3**). Such trend in the MIC density values is probably due to the polarization of electronic density from **1** toward QX.

Thus, we can conclude that the induction of ring currents in the QX molecule affects the MIC ring currents of **1**, resulting in changes in the tensor components in the adducts. This is attributed to the formation of the [**1·QX**] adducts.

**Table S3**. Calculated Solid-State [195]Pt NMR Parameters of **1** and **1·QX** (X = F, Cl, Br, I)

|  | $\delta_{11}$, ppm | $\delta_{22}$, ppm | $\delta_{33}$, ppm | $\delta_{iso}$, ppm | $\Omega$, ppm | $\kappa$ |
|---|---|---|---|---|---|---|
| **1** | –3387 | –4500 | –5028 | –4305 | 1641 | –0.36 |
| **1·QF** | –2673 | –4957 | –5053 | –4228 | 2380 | –0.92 |
| **1·QCl** | –2496 | –4859 | –5238 | –4198 | 2742 | –0.72 |
| **1·QBr** | –2502 | –4871 | –5247 | –4207 | 2745 | –0.73 |
| **1·QI** | –2583 | –4992 | –5207 | –4261 | 2624 | –0.84 |

# S4.   CALCULATION DETAILS



**1·(QX)**$_{\text{big}}$                    **(1·QX)**
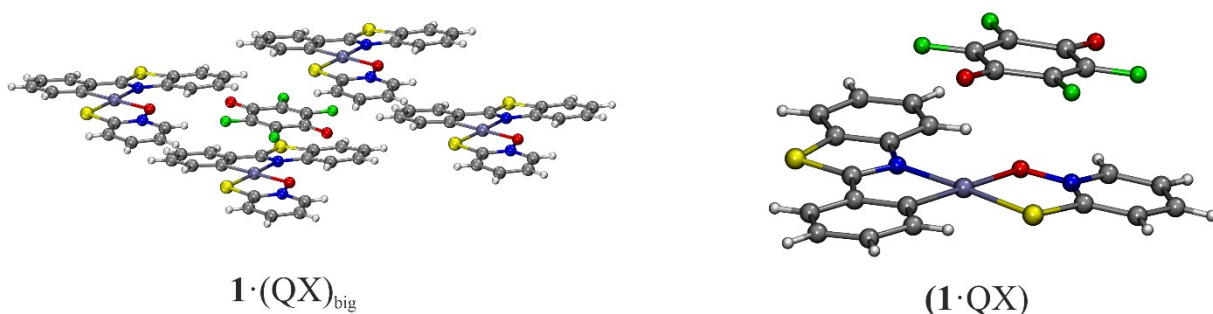
**Figure S25**. Clusters used in calculations.

**Table S4.** Electron density ($\rho_b$), its Laplacian ($\nabla^2\rho_b$), potential and kinetic energy densities ($V_b$ and $G_b$), second eigenvalue of the Hessian matrix ($\lambda_2$), electron localization function at BCPs (in a.u.), and IBSI.

| Contact | Clusters | $\rho_b$ | $\nabla^2\rho_b$ | $V_b$ | $G_b$ | $H_b$ | $\lambda_2$ | ELF |
|---------|----------|----------|---------|-------|-------|-------|-------------|-----|
| C1D···Pt | **[1·QF]** | 0.0109 | 0.0279 | –0.0055 | 0.0062 | –0.0007 | –0.0016 | 0.058 |
| C1D···Pt | **(1·QF)** | 0.0106 | 0.0298 | –0.0052 | 0.0063 | 0.0011 | –0.0029 | 0.051 |
| C1D···Pt | **(1·QF)**$_{\text{big}}$ | 0.0108 | 0.0275 | –0.0054 | 0.0062 | 0.0007 | -0.0018 | 0.0567 |
| C3D···Pt | **[1·QCl]** | 0.0084 | 0.0217 | –0.0040 | 0.0047 | –0.0007 | –0.0020 | 0.042 |
| C3D···Pt | **(1·QCl)** | 0.0076 | 0.0206 | –0.0034 | 0.0043 | –0.0009 | –0.0015 | 0.037 |
| C3D···Pt | **(1·QCl)**$_{\text{big}}$ | 0.0086 | 0.0214 | –0.0038 | 0.0042 | –0.0006 | –0.0022 | 0.044 |
| C3D···Pt | **[1·QBr]** | 0.0070 | 0.0187 | –0.0032 | 0.0039 | –0.0007 | –0.0011 | 0.033 |
| C3D···Pt | **(1·QBr)** | 0.0066 | 0.0158 | –0.0031 | 0.0035 | –0.0004 | –0.0017 | 0.035 |
| C3D···Pt | **(1·QBr)**$_{\text{big}}$ | 0.0071 | 0.0188 | –0.0030 | 0.0037 | –0.0006 | –0.0009 | 0.030 |
| C3D···Pt1 | **[1·QI]** | 0.0065 | 0.0175 | –0.0175 | 0.0037 | 0.0007 | –0.0009 | 0.030 |
| C3D···Pt | **(1·QI)** | 0.0059 | 0.0154 | –0.0026 | 0.0032 | 0.0006 | –0.0014 | 0.0288 |

| C3D···Pt | (**1**·QI)big | 0.0060 | 0.0156 | −0.0027 | 0.0030 | 0.0005 | | | −0.0014 | 0.0287 |

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**Table S5.** Contact distance ($d$) in Å, ratio between the distance and Alvarez $\Sigma_{vdW}$ ($R_r$), electron density ($\rho_b$), its Laplacian ($\nabla^2\rho_b$), potential and kinetic energy densities ($V_b$ and $G_b$), second eigenvalue of the Hessian matrix ($\lambda_2$), elliptical bond index ($\varepsilon$) (in a.u.), electron localization function at BCPs, and IBSI and dg$_{pair}$ at the PBE0-D3BJ/ZORA-def2-TZVP and PBE-D3BJ/ZORA-def2-TZVP (in parentheses for [**1**·QF]) levels of theory.

[**1**·QF]

| Contact | d | R | $\rho_b$ | $\nabla^2\rho_b$ | $V_b$ | $G_b$ | H(r) | $\varepsilon$ | $\lambda_2$ | ELF | IBSI | dg$_{pair}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C6D···Pt1 | 3.369 | 0.91 | 0.0115 (0.0115) | 0.0286 (0.0270) | −0.0058 (−0.0053) | 0.0065 (0.0061) | 0.0007 (0.0007) | 4.5504 (2.0725) | −0.0014 (-0.0022) | 0.0628 (0.0705) | 0.0140 | 0.0646 |
| C1D···Pt1 | 3.323 | 0.82 | | | | | | | | | 0.0150 | 0.0672 |
| C2D···Pt1 | 3.632 | 0.89 | | | | | | | | | 0.0081 | 0.0433 |
| C3D···Pt1 | 3.965 | 0.98 | | | | | | | | | 0.0041 | 0.0263 |
| C4D···Pt1 | 4.025 | 0.99 | | | | | | | | | 0.0039 | 0.0255 |
| C5D···Pt1 | 3.739 | 0.92 | | | | | | | | | 0.0068 | 0.0385 |
| C4D···O1 | 3.075 | 0.91 | 0.0071 (0.070) | 0.0275 (0.0265) | −0.0040 (−0.0039) | 0.0054 (0.0052) | 0.0014 (0.0014) | 0.3732 (0.2408) | −0.0029 (−0.0030) | 0.0185 (0.0191) | 0.0092 | 0.0352 |
| C18···O2D | 3.161 | 0.97 | 0.0057 (0.0050) | 0.0230 (0.0197) | −0.0030 (−0.0025) | 0.0044 (0.0037) | 0.0014 (0.0012) | 0.4963 (0.6043) | −0.0025 (−0.021) | 0.0139 (0.0129) | 0.0066 | 0.0269 |
| C12···F2D | 3.289 | 1.02 | 0.0041 (0.0049) | 0.0166 (0.0190) | −0.0021 (−0.0025) | 0.0031 (0.0036) | 0.0010 (0.0011) | 0.5716 (0.2386) | −0.0017 (−0.0026) | 0.0095 (0.0123) | 0.0042 | 0.0183 |
| C13···F1D | 3.204 | 0.99 | 0.0048 (0.0050) | 0.0223 (0.0240) | −0.0027 (−0.0029) | 0.0042 (0.0044) | 0.0014 (0.0016) | 3.9902 (7.579) | −0.0005 (−0.004) | 0.0085 (0.0092) | 0.0051 | 0.0212 |
| C14···F3D | 3.282 | 1.02 | | | | | | | | | 0.0040 | 0.0173 |
| N1···C2D | 3.255 | 0.95 | | | | | | | | | 0.0069 | 0.0296 |

[**1**·QCl]

| Contact | d | R | $\rho_b$ | $\nabla^2\rho_b$ | $V_b$ | $G_b$ | H(r) | $\varepsilon$ | $\lambda_2$ | ELF | IBSI | dg$_{pair}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C3D···Pt1 | 3.562 | 0.88 | 0.0084 | 0.0217 | -0.0040 | 0.0047 | 0.0007 | 1.3753 | -0.0020 | 0.0423 | 0.0096 | 0.0494 |
| C1D···Pt1 | 3.797 | 0.94 | | | | | | | | | 0.0058 | 0.0339 |
| C2D···Pt1 | 3.651 | 0.90 | | | | | | | | | 0.0080 | 0.0432 |
| C4D···Pt1 | 3.612 | 0.89 | | | | | | | | | 0.0079 | 0.0420 |
| C5D···Pt1 | 3.837 | 0.95 | | | | | | | | | 0.0051 | 0.0308 |
| C6D···Pt1 | 3.914 | 0.96 | | | | | | | | | 0.0048 | 0.0301 |
| C12···O2D | 3.530 | 1.08 | 0.0027 | 0.0106 | -0.0012 | 0.0019 | 0.0007 | 0.5485 | -0.0010 | 0.0064 | 0.0030 | 0.0149 |
| C18···Cl3D | 3.480 | 0.97 | 0.0058 | 0.0204 | -0.0028 | 0.0039 | 0.0012 | 1.5291 | -0.0015 | 0.0185 | 0.0062 | 0.0307 |

| Contact | d | R | $\rho_b$ | $\nabla^2\rho_b$ | $V_b$ | $G_b$ | $H(r)$ | $\varepsilon$ | $\lambda_2$ | ELF | IBSI | dg$_{pair}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C6···Cl1D | 3.658 | 1.02 | 0.0049 | 0.0177 | -0.0022 | 0.0033 | 0.0011 | 2.4562 | -0.0006 | 0.0144 | 0.0046 | 0.0250 |
| C13···Cl3D | 3.606 | 1.01 | | | | | | | | | 0.0062 | 0.0307 |
| N1···Cl2D | 3.491 | 1.00 | 0.0054 | 0.0220 | -0.0027 | 0.0041 | 0.0014 | 0.8435 | -0.0016 | 0.0135 | 0.0052 | 0.0255 |
| C7···C2D | 3.583 | 0.99 | | | | | | | | | 0.0051 | 0.0268 |
| S2···C6D | 3.515 | 0.96 | 0.0067 | 0.0201 | -0.0030 | 0.0040 | 0.0010 | 0.3813 | -0.0021 | 0.0274 | 0.0084 | 0.0421 |

[**1**·QBr]

| Contact | d | R | $\rho_b$ | $\nabla^2\rho_b$ | $V_b$ | $G_b$ | $H(r)$ | $\varepsilon$ | $\lambda_2$ | ELF | IBSI | dg$_{pair}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C1D···Pt1 | 3.652 | 0.90 | 0.0079 | 0.0206 | -0.0037 | 0.0044 | 0.0007 | 1.4355 | -0.0018 | 0.0397 | 0.0073 | 0.0396 |
| C2D···Pt1 | 3.600 | 0.87 | | | | | | | | | 0.0088 | 0.0461 |
| C3D···Pt1 | 3.663 | 0.90 | | | | | | | | | 0.0078 | 0.0423 |
| C4D···Pt1 | 3.785 | 0.93 | | | | | | | | | 0.0060 | 0.0344 |
| C5D···Pt1 | 3.937 | 0.97 | | | | | | | | | 0.0046 | 0.0289 |
| C6D···Pt1 | 3.885 | 0.96 | | | | | | | | | 0.0046 | 0.0286 |
| C2···O2D | 3.697 | 1.13 | 0.0023 | 0.0084 | -0.0009 | 0.0015 | 0.0006 | 0.8781 | -0.0004 | 0.0056 | 0.0021 | 0.0116 |
| C12···O1D | 3.567 | 1.09 | 0.0026 | 0.0102 | -0.0011 | 0.0018 | 0.0007 | 0.7196 | -0.0009 | 0.0059 | 0.0027 | 0.0142 |
| C18···Br4D | 3.586 | 0.99 | 0.0060 | 0.0189 | -0.0028 | 0.0038 | 0.0009 | 0.9221 | -0.0019 | 0.0226 | 0.0066 | 0.0345 |
| C1···Br2D | 3.713 | 1.02 | 0.0052 | 0.0173 | -0.0024 | 0.0033 | 0.0010 | 8.6088 | -0.0003 | 0.0175 | 0.0054 | 0.0304 |
| C13···Br1D | 3.646 | 1.00 | | | | | | | | | 0.0058 | 0.0314 |
| C7···Br1D | 3.742 | 1.03 | | | | | | | | | 0.0049 | 0.0276 |
| C6···Br2D | 3.720 | 1.02 | | | | | | | | | 0.0051 | 0.0285 |
| N1···Br1D | 3.612 | 1.03 | 0.0054 | 0.0204 | -0.0026 | 0.0039 | 0.0012 | 1.6101 | -0.0010 | 0.0147 | 0.0055 | 0.0292 |
| N2···Br4D | 3.599 | 1.02 | | | | | | | | | 0.0050 | 0.0263 |
| S2···C4D | 3.684 | 1.01 | 0.0067 | 0.0200 | -0.0030 | 0.0040 | 0.0010 | 0.5042 | -0.0020 | 0.0282 | 0.0058 | 0.0318 |
| S2···Br3D | 3.884 | 1.04 | | | | | | | | | 0.0063 | 0.0386 |

[**1**·QI]

| Contact | d | R | $\rho_b$ | $\nabla^2\rho_b$ | $V_b$ | $G_b$ | $H(r)$ | $\varepsilon$ | $\lambda_2$ | ELF | IBSI | dg$_{pair}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| C3D···Pt1 | 3.764 | 0.93 | 0.0061 | 0.0167 | -0.0028 | 0.0035 | 0.0007 | 8.7805 | -0.0003 | 0.0271 | 0.0061 | 0.0348 |
| C5D···Pt1 | 3.703 | 0.91 | 0.0065 | 0.0175 | 0.0175 | 0.0037 | 0.0007 | 2.3199 | -0.0009 | 0.0299 | 0.0071 | 0.0369 |
| C1D···Pt1 | 3.862 | 0.95 | | | | | | | | | 0.0046 | 0.0281 |
| C2D···Pt1 | 3.879 | 0.96 | | | | | | | | | 0.0048 | 0.0291 |
| C4D···Pt1 | 3.636 | 0.90 | | | | | | | | | 0.0081 | 0.0433 |

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C6D⋯Pt1 | 3.794 | 0.93 | | | | | | | | 0.0057 | 0.0334 |
| C12⋯O1D | 3.279 | 1.00 | 0.0048 | 0.0184 | -0.0023 | 0.0034 | 0.0012 | 0.6982 | -0.0017 | 0.0125 | 0.0052 | 0.026 |
| C13⋯O1D | 3.445 | 1.05 | | | | | | | | | 0.0037 | 0.0176 |
| C2⋯I2D | 3.851 | 1.01 | 0.0056 | 0.0158 | -0.0024 | 0.0032 | 0.0008 | 2.2043 | -0.0009 | 0.0247 | 0.0058 | 0.0351 |
| C14⋯I3D | 3.694 | 0.97 | 0.0066 | 0.0187 | -0.0031 | 0.0039 | 0.0008 | 0.6408 | -0.0019 | 0.0284 | 0.0078 | 0.0435 |
| C18⋯I4D | 3.898 | 1.02 | 0.0046 | 0.0136 | -0.0020 | 0.0027 | 0.0007 | 0.8181 | -0.0014 | 0.0185 | 0.0053 | 0.0327 |
| C3⋯I2D | 3.916 | 1.03 | | | | | | | | | 0.0051 | 0.0319 |
| C7⋯I1D | 3.839 | 1.01 | | | | | | | | | 0.0057 | 0.0343 |
| C15⋯I3D | 3.902 | 1.02 | | | | | | | | | 0.0050 | 0.0307 |
| S1⋯I1D | 3.934 | 1.00 | 0.0065 | 0.0177 | -0.0027 | 0.0036 | 0.0009 | 0.4333 | -0.0025 | 0.0327 | 0.0079 | 0.0495 |
| S2⋯I3D | 4.098 | 1.04 | | | | | | | | | 0.0384 | 0.0056 |
| H12⋯I4D | 3.688 | 1.14 | 0.0026 | 0.0082 | -0.0011 | 0.0016 | 0.0005 | 2.4849 | -0.0004 | 0.0076 | 0.0023 | 0.0102 |
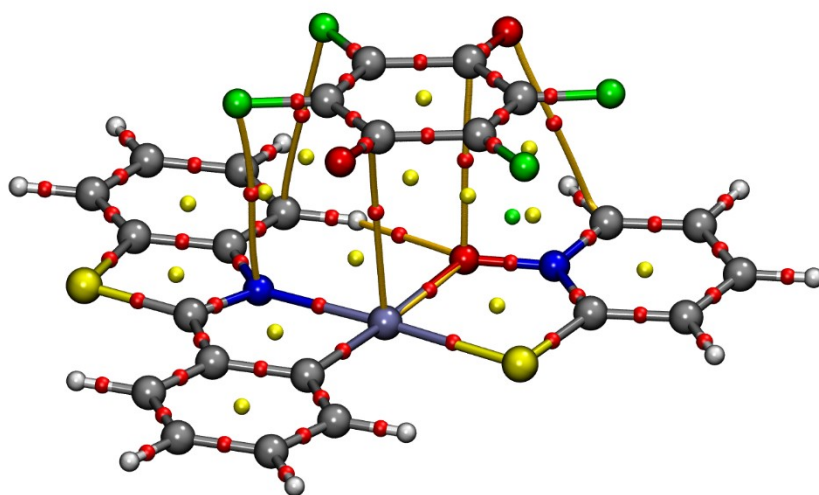


**Figure S26.** QTAIM distribution of bond, ring, and cage critical points (red, yellow, and green spheres, respectively) and bond paths for [**1**·QF].
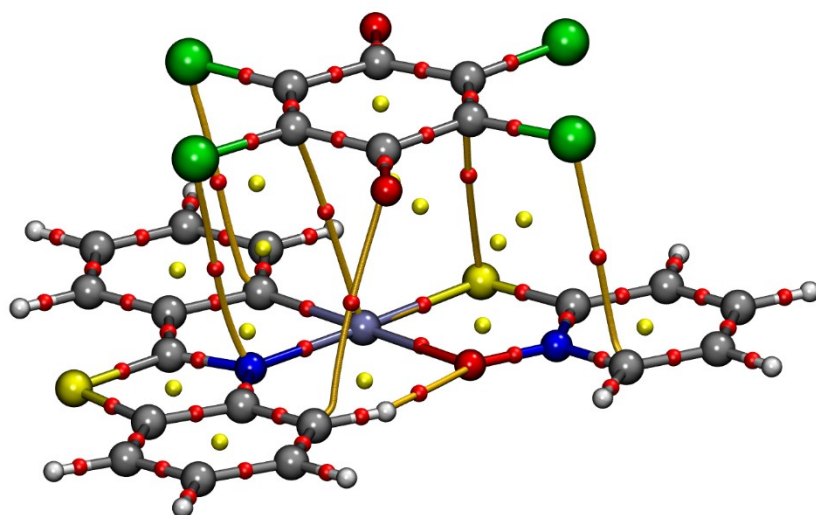
**Figure S27.** QTAIM distribution of bond, ring, and cage critical points (red, yellow, and green spheres, respectively) and bond paths for [**1**·QCl].
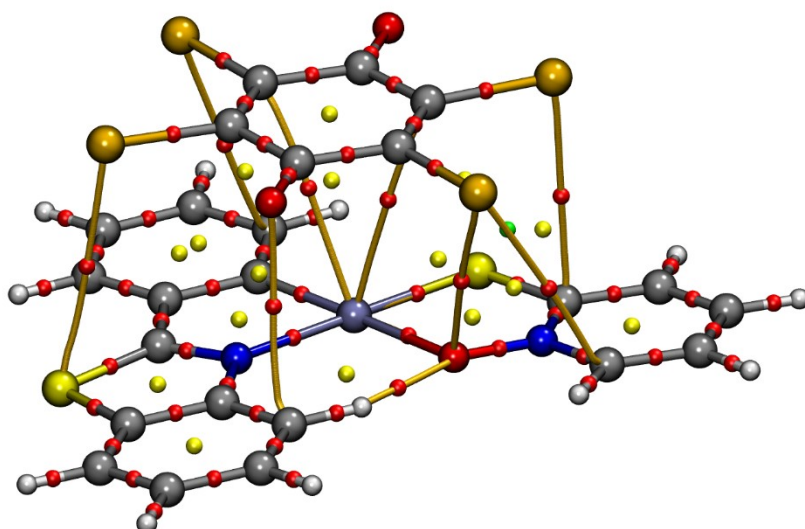


**Figure S28.** QTAIM distribution of bond, ring, and cage critical points (red, yellow, and green spheres, respectively) and bond paths for [**1**·QBr].
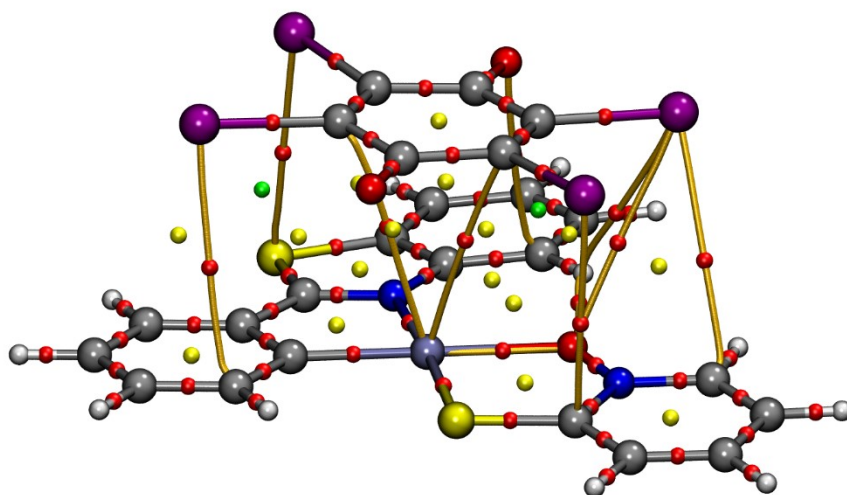
**Figure S29.** QTAIM distribution of bond, ring, and cage critical points (red, yellow, and green spheres, respectively) and bond paths for [**1**·QI].



(a)                                                                  (b)
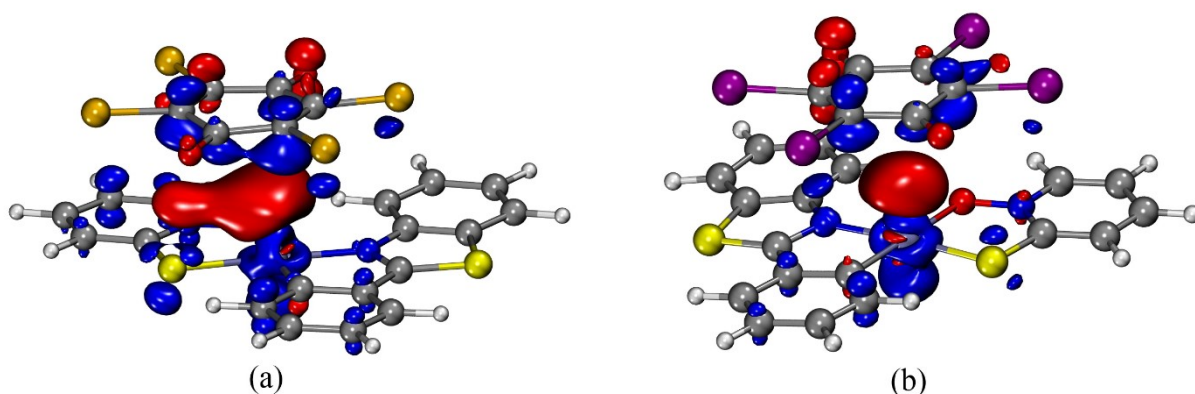
**Figure S30**. ETS-NOCV deformation densities for (a) [**1**·QBr] and (b) [**1**·QI] (isovalues 0.0005 and 0.005 a.u. , electrons transfer occurs from the decreased electron density regions (blue) to the increased electron density regions (red).

## Geometry optimization

Analysis of the X-ray diffraction data shows that adducts **1**·QX are arranged in stacks, where the quinone molecule interacts with the Pt complexes. To exclude the effect of crystal packing on the interactions between **1** and a quinone, the full geometry optimization of two cluster models of the cocrystals **1**·QX was carried out, *i.e.* bimolecular and trimolecular clusters, [**1**·QX] and [QX **1**·QX], respectively (**Figure S31**).
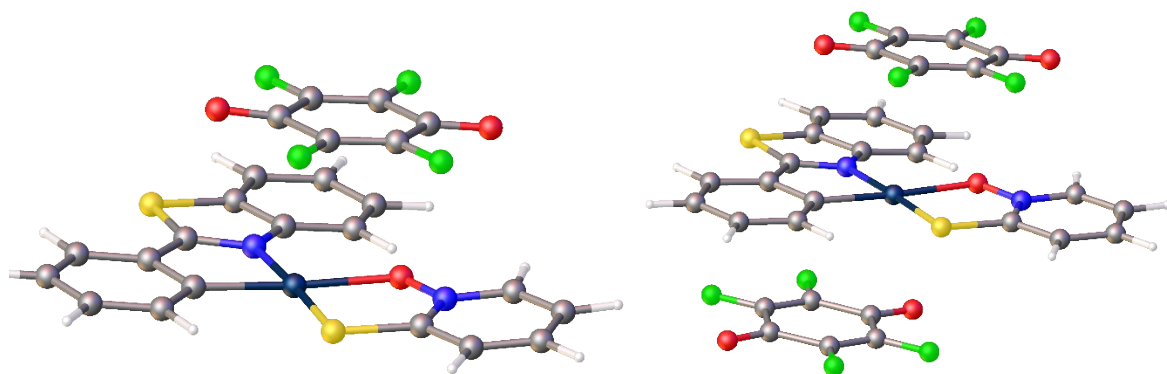
**Figure S31.** Schematic representation of of bimolecular (*left*) and trimolecular (*right*) model clusters used for the calculations.

To distinguish quinone molecules from each other depending on the position relative to the complex, we introduced the designations $QX^A$ and $QX^B$ (see **Figure S32**).
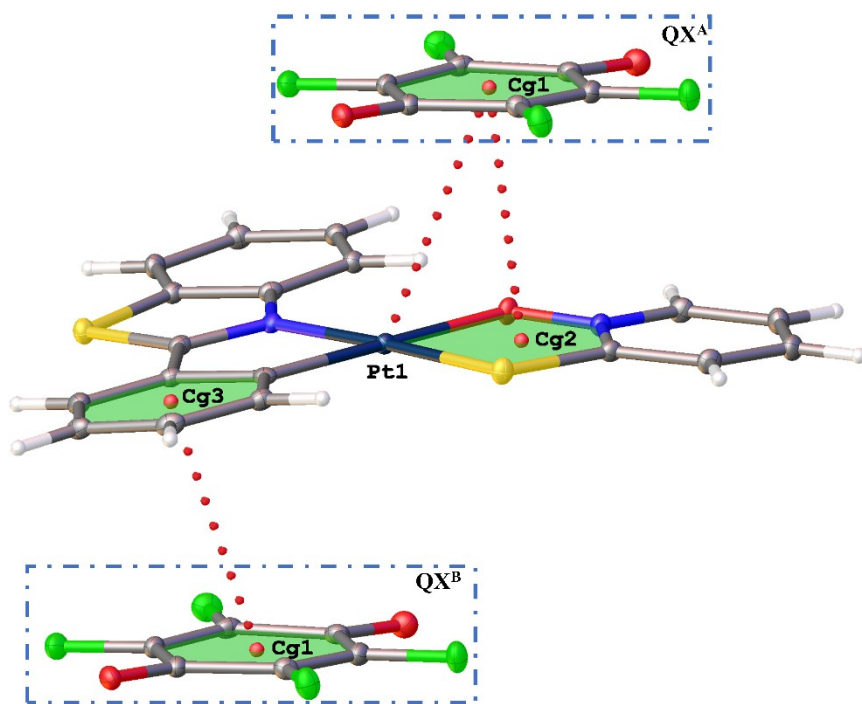


**Figure S32**. Schematic representation of $QX^A$ and $QX^B$.

Comparison of the structural parameters of the X-ray and optimized structures indicates that the optimized geometries for **1** and $QX^A$ of the bimolecular cluster models do not deviate significantly from the experimental structures (**Table S6**, **Figure S32**). At the same time, the optimization of trimolecular cluster resulted in the notable structural changes, *i.e.*, the $QX^B$ molecule is strongly shifted relative to the X-ray structure (**Table S6**, **Figure S32**). Thus, in the further theoretical studies, the bimolecular model was used.

**Table S6**. Parameters of QX shifts.

| Entry | $r$, Å | | $\alpha$, º | |
|---|---|---|---|---|
| | QX$^A$ | QX$^B$ | QX$^A$ | QX$^B$ |
| [QF$^A$·**1**·QF$^B$]$_{XRD}$ | 1.578 | 2.972 | 25.7 | 56.0 |
| [**1**·QF$^A$] | 0.920 | – | 15.7 | – |
| [QF$^A$·**1**·QF$^B$] | 0.966 | 1.323 | 16.5 | 23.5 |
| [QCl$^A$·**1**·QCl$^B$]$_{XRD}$ | 1.222 | 2.811 | 18.0 | 38.3 |
| [**1**·QCl$^A$] | 0.461 | – | 7.7 | – |
| [QCl$^A$·**1**·QCl$^B$] | 0.468 | 0.094 | 7.8 | 1.6 |
| [QBr$^A$·**1**·QBr$^B$]$_{XRD}$ | 0.342 | 3.139 | 5.7 | 41.2 |
| [**1**·QBr$^A$] | 0.463 | – | 7.8 | – |
| [QBr$^A$·**1**·QBr$^B$] | 0.457 | 0.579 | 7.6 | 9.6 |
| [QI$^A$·**1**·QI$^B$]$_{XRD}$ | 1.566 | 2.623 | 23.5 | 36 |
| [**1**·QI$^A$] | 1.226 | – | 20.5 | – |
| [QI$^A$·**1**·QI$^B$] | 0.460 | 0.433 | 7.6 | 7.1 |
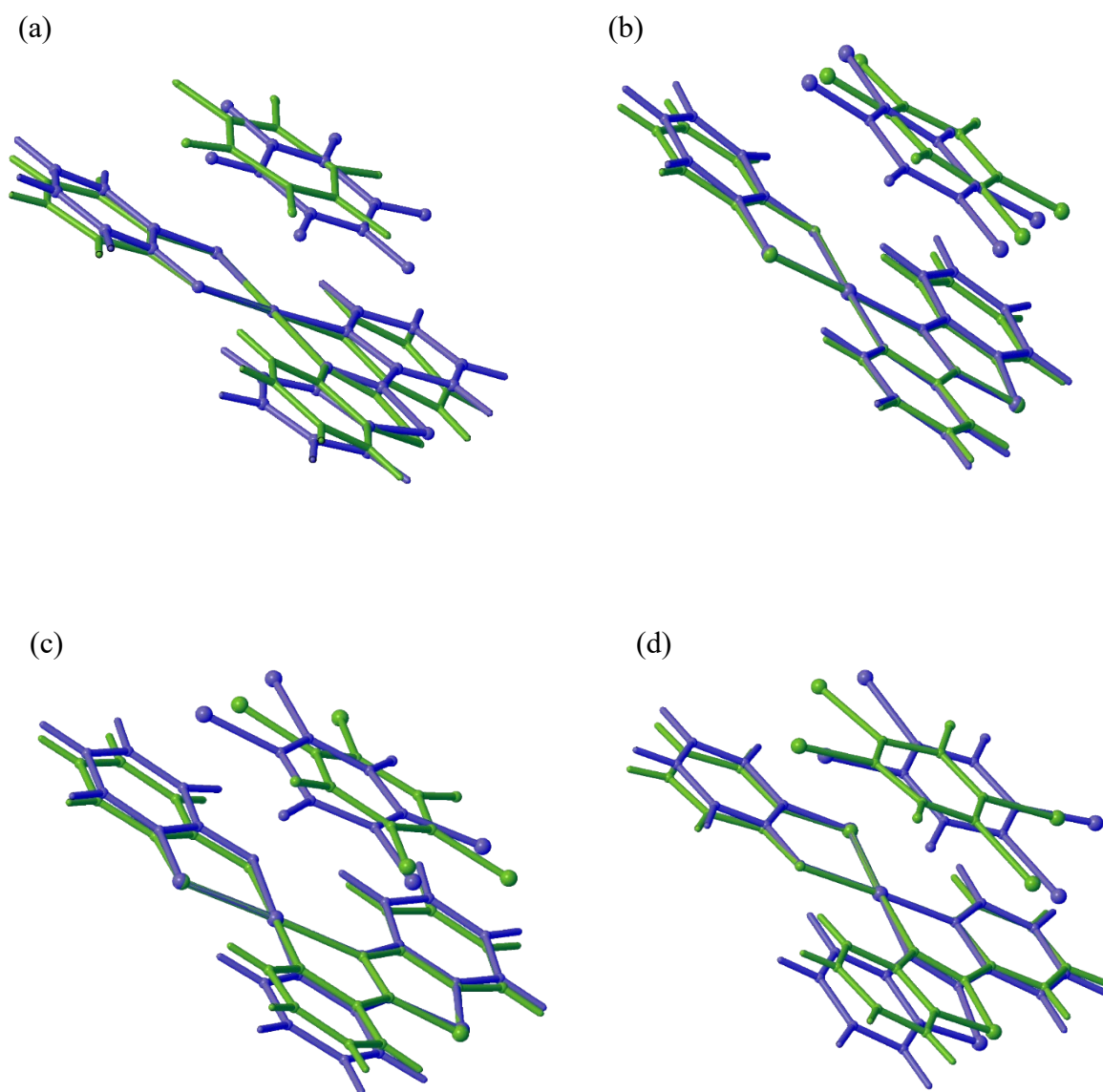
**Figure S33.** Overlayed images of **1**·QF (a) **1**·QCl (b), **1**·QBr (c) and **1**·QI (d) in X-ray (green) and optimized bimolecular (blue) geometries.
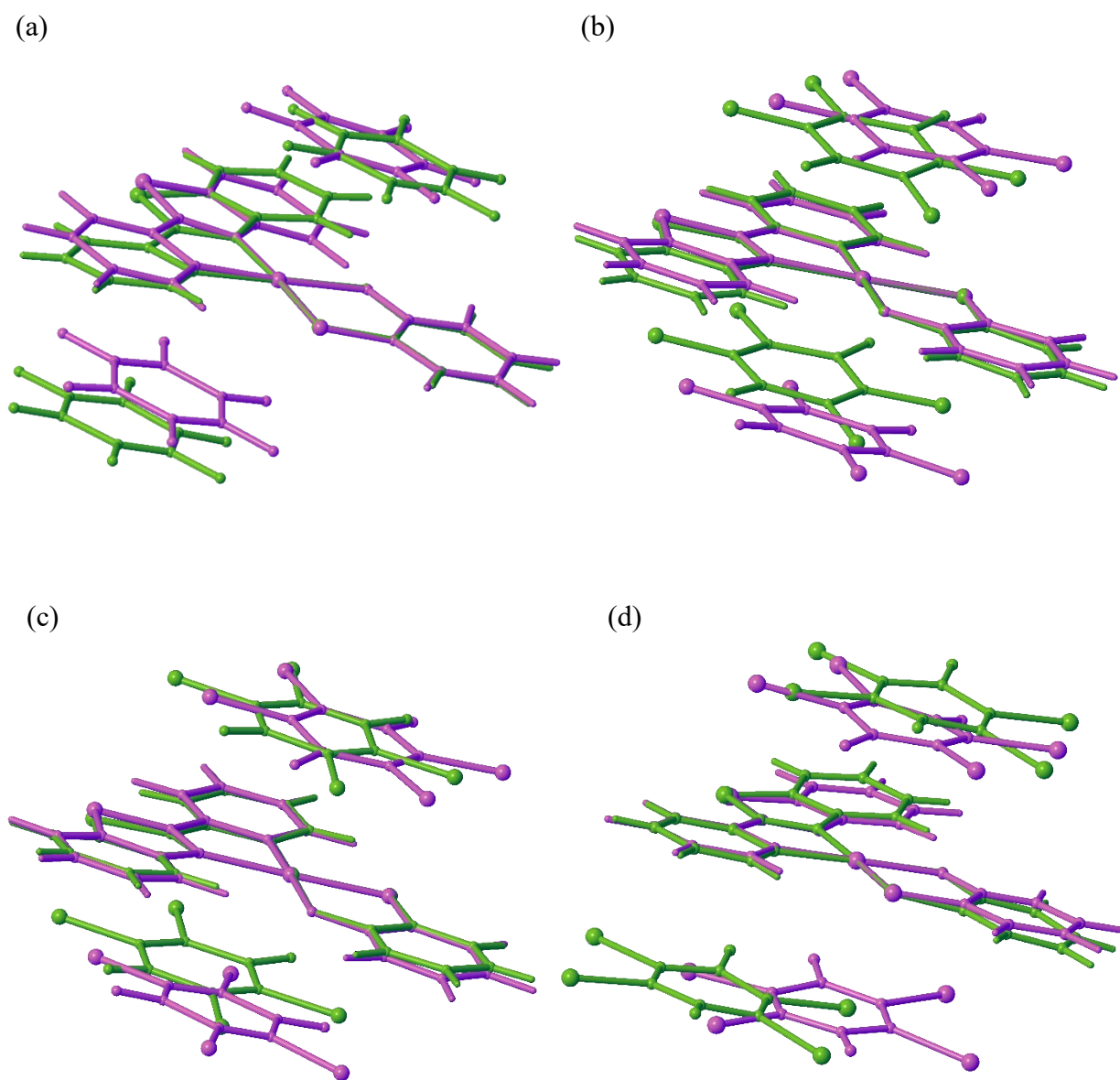
**Figure S34.** Overlayed images of **1**·QF (a) **1**·QCl (b), **1**·QBr (c) and **1**·QI (d) in X-ray (green) and optimized trimolecular model (purple) geometries.
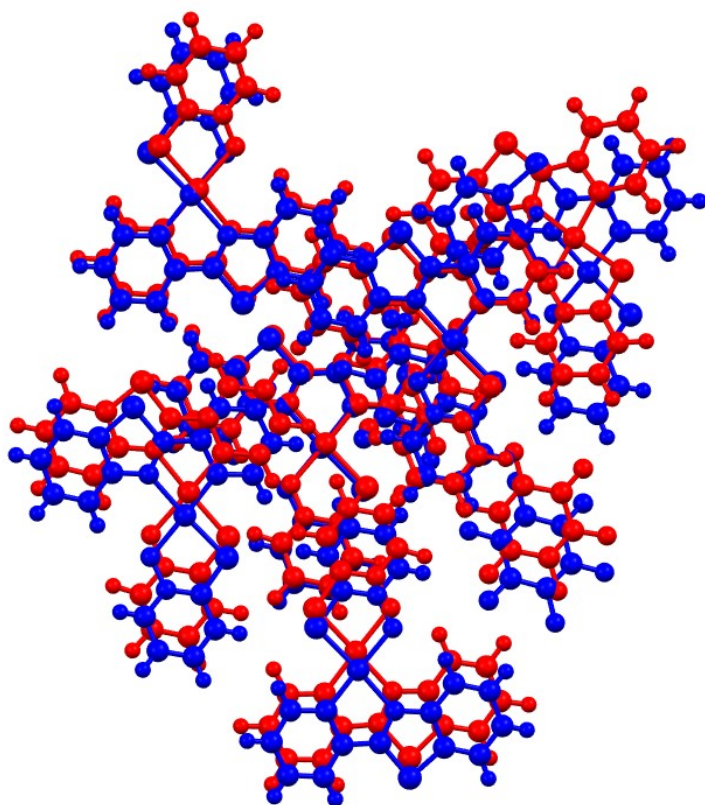
**Figure S35.** Overlayed images of the optimized and experimental X-ray geometries of **1**·QF (an octa-molecular cluster bearing 6 molecules of **1** and 2 molecules of QF).
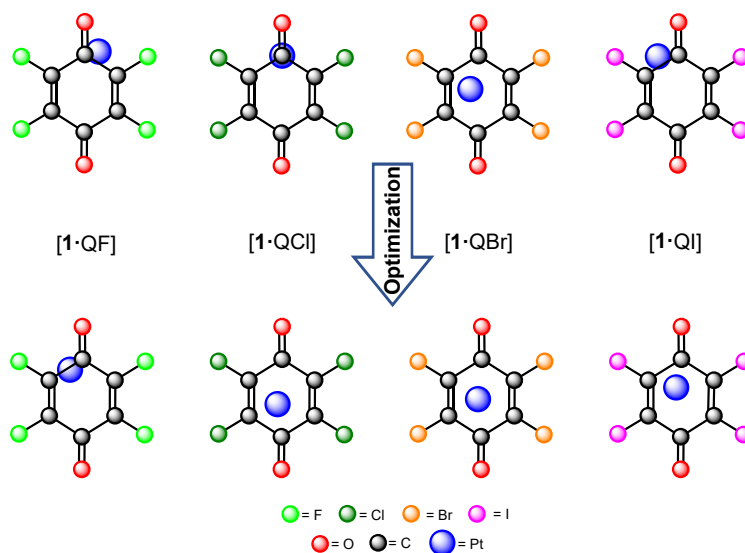


**Figure S36**. Projections of Pt centers (in blue) onto the mean-square planes of the closest QX rings in the cocrystals from the XRD data (top panel) and in the optimization of dimeric adducts (bottom panel) [**1**·QX].

(a)

(b)

(c)

(d)

Highest
contribution

Lowest
contribution
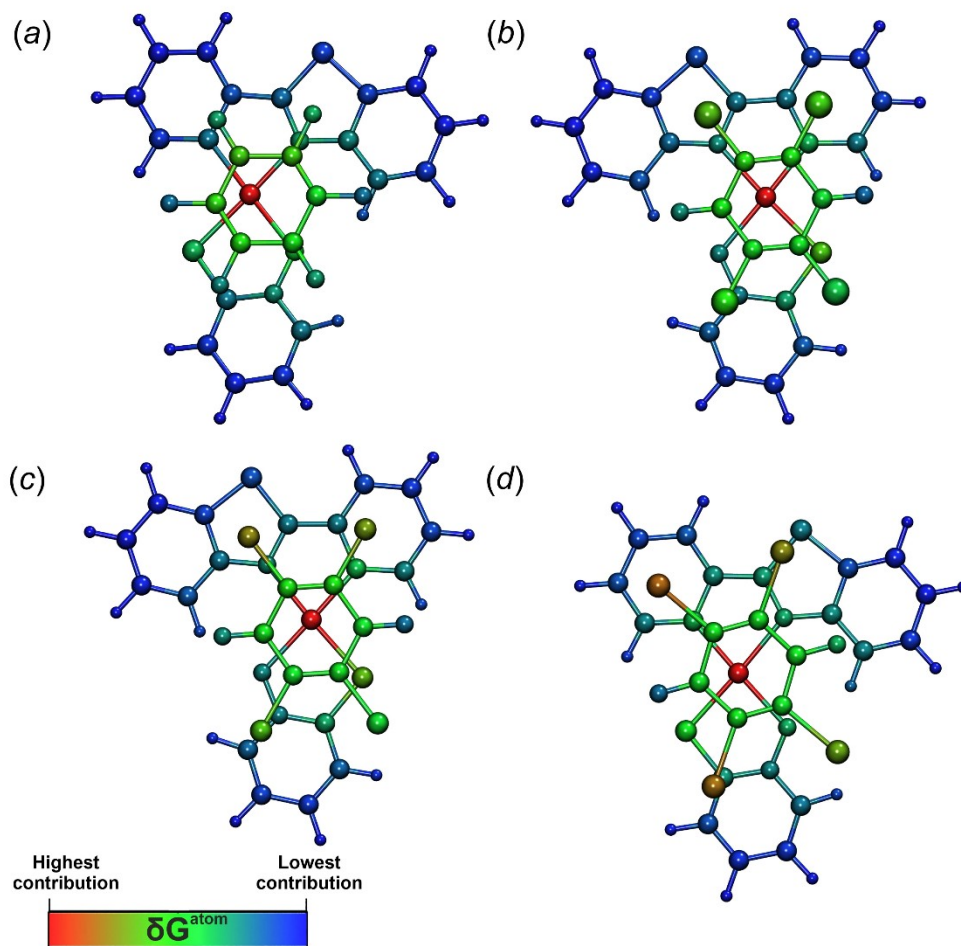
$\delta G^{atom}$

**Figure S37**. The $\delta G^{atom}$ colored [**1**·QX] structures.

**Table S7.** Geometrical parameters of the observed noncovalent interactions in the crystal and optimized structures.

| Structure | Contact | $d$(X⋯Y), Å | $\Sigma_{Wdv}^{Alvarez}$ (X⋯Y), Å | $R_r$ | QX–square plane angle, º | $d1$, Å | $d2$, Å | $d3$, Å | $r$, Å | $\alpha$, º |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | **X-ray** | | | | | | | |
| | Pt1⋯C1D | 3.320(3) | 4.06 | 0.82 | | | | | | |
| | Pt1⋯C2D | 3.426(3) | 4.06 | 0.84 | | | | | | |
| | Pt1⋯C3D | 4.002(3) | 4.06 | 0.99 | | | | | | |
| | Pt1⋯C4D | 4.421(3) | 4.06 | 1.09 | | | | | | |
| | Pt1⋯C5D | 4.308(3) | 4.06 | 1.06 | | | | | | |
| | Pt1⋯C6D | 3.837(3) | 4.06 | 0.95 | 4.62(15) | 3.6366(13) | 3.276(2) | 3.3522(17) | 1.578 | 25.7 |
| | C18⋯O2D | 3.326(5) | 3.27 | 0.99 | | | | | | |
| **1·QF** | O1⋯C4D | 3.262(4) | 3.27 | 1.00 | | | | | | |
| | N1⋯C2D | 3.615(4) | 3.43 | 1.05 | | | | | | |
| | C12⋯F2D | 3.205(4) | 3.23 | 0.99 | | | | | | |
| | C13⋯F1D | 3.386(3) | 3.23 | 1.05 | | | | | | |
| | C14⋯F3D | 3.531(4) | 3.23 | 1.09 | | | | | | |
| | | | **Optimized** | | | | | | | |
| | Pt1⋯C1D | 3.323 | 4.06 | 0.82 | 5.42 | 3.396 | 3.269 | 3.542 | 0.920 | 15.7 |
| | Pt1⋯C2D | 3.632 | 4.06 | 0.89 | | | | | | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Pt1···C3D | 3.966 | 4.06 | 0.98 | | | | | | |
| | Pt1···C4D | 4.025 | 4.06 | 0.99 | | | | | | |
| | Pt1···C5D | 3.739 | 4.06 | 0.92 | | | | | | |
| | Pt1···C6D | 3.369 | 4.06 | 0.83 | | | | | | |
| | C18···O2D | 3.161 | 3.27 | 0.97 | | | | | | |
| | O1···C4D | 3.075 | 3.27 | 0.94 | | | | | | |
| | N1···C2D | 3.255 | 3.43 | 0.95 | | | | | | |
| | C12···F2D | 3.289 | 3.23 | 1.02 | | | | | | |
| | C13···F1D | 3.204 | 3.23 | 0.99 | | | | | | |
| | C14···F3D | 3.282 | 3.23 | 1.02 | | | | | | |
| | **X-ray** | | | | | | | | | |
| **1·QCl** | Pt1···C1D | 3.504(9) | 4.06 | 0.86 | 5.45(41) | 3.627(4) | 3.449(6) | 3.896(5) | 1.222 | 18.0 |
| | Pt1···C2D | 3.634(10) | 4.06 | 0.90 | | | | | | |
| | Pt1···C3D | 4.071(9) | 4.06 | 1.00 | | | | | | |
| | Pt1···C4D | 4.328(10) | 4.06 | 1.06 | | | | | | |
| | Pt1···C5D | 4.079(8) | 4.06 | 1.00 | | | | | | |
| | Pt1···C6D | 3.735(10) | 4.06 | 0.92 | | | | | | |
| | C18···Cl3D | 3.347(9) | 3.59 | 0.93 | | | | | | |
| | C13···Cl2D | 3.542(10) | 3.59 | 0.99 | | | | | | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | C6···Cl1D | 3.569(9) | 3.59 | 0.99 | | | | | | |
| | N1···Cl2D | 3.915(9) | 3.48 | 1.13 | | | | | | |
| | C7···Cl2D | 4.142(10) | 3.59 | 1.15 | | | | | | |
| | S2···C6D | 3.987(11) | 3.66 | 1.09 | | | | | | |
| | **Optimized** | | | | | | | | | |
| | Pt1···C1D | 3.798 | 4.06 | 0.94 | | | | | | |
| | Pt1···C2D | 3.651 | 4.06 | 0.90 | | | | | | |
| | Pt1···C3D | 3.562 | 4.06 | 0.88 | | | | | | |
| | Pt1···C4D | 3.612 | 4.06 | 0.89 | | | | | | |
| | Pt1···C5D | 3.837 | 4.06 | 0.95 | | | | | | |
| | Pt1···C6D | 3.914 | 4.06 | 0.96 | 1.58 | 3.443 | 3.412 | 3.693 | 0.461 | 7.7 |
| | C18···Cl3D | 3.480 | 3.59 | 0.97 | | | | | | |
| | C13···Cl2D | 3.606 | 3.59 | 1.01 | | | | | | |
| | C6···Cl1D | 3.658 | 3.59 | 1.02 | | | | | | |
| | N1···Cl2D | 3.492 | 3.48 | 1.00 | | | | | | |
| | C7···Cl2D | 3.583 | 3.59 | 0.99 | | | | | | |
| | S2···C6D | 3.515 | 3.66 | 0.96 | | | | | | |
| | **X-ray** | | | | | | | | | |
| **1·QBr** | Pt1···C1D | 3.896(8) | 4.06 | 0.96 | 1.81(25) | 3.467(3) | 3.450(3) | 4.006(4) | 0.342 | 5.7 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | Pt1···C2D | 3.850(8) | 4.06 | 0.95 | | | | | | |
| | Pt1···C3D | 3.727(9) | 4.06 | 0.92 | | | | | | |
| | Pt1···C4D | 3.644(9) | 4.06 | 1.63 | | | | | | |
| | Pt1···C5D | 3.648(8) | 4.06 | 0.90 | | | | | | |
| | Pt1···C6D | 3.752(7) | 4.06 | 0.92 | | | | | | |
| | C2···O2D | 3.994(10) | 3.27 | 1.22 | | | | | | |
| | C12···O1D | 3.300(11) | 3.27 | 1.01 | | | | | | |
| | N1···Br1D | 3.839(7) | 3.52 | 1.09 | | | | | | |
| | N2···Br4D | 3.873(7) | 3.52 | 1.10 | | | | | | |
| | C13···Br1D | 3.974(8) | 3.63 | 1.09 | | | | | | |
| | C7···Br1D | 3.615(8) | 3.63 | 0.99 | | | | | | |
| | C1···Br2D | 3.748(8) | 3.63 | 1.03 | | | | | | |
| | C18···Br4D | 3.843(9) | 3.63 | 1.06 | | | | | | |
| | S2···Br3D | 3.8814(18) | 3.75 | 1.03 | | | | | | |
| | S2···C4D | 3.840(9) | 3.66 | 1.05 | | | | | | |
| **Optimized** | | | | | | | | | | |
| | Pt1···C1D | 3.652 | 4.06 | 0.90 | | | | | | |
| | Pt1···C2D | 3.600 | 4.06 | 0.87 | 0.60 | 3.470 | 3.438 | 3.718 | 0.463 | 7.8 |
| | Pt1···C3D | 3.663 | 4.06 | 0.90 | | | | | | |

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| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Pt1···C4D | 3.785 | 4.06 | 0.93 | | | | | | |
| | Pt1···C5D | 3.937 | 4.06 | 0.97 | | | | | | |
| | Pt1···C6D | 3.885 | 4.06 | 0.96 | | | | | | |
| | C2···O2D | 3.697 | 3.27 | 1.13 | | | | | | |
| | C12···O1D | 3.567 | 3.27 | 1.09 | | | | | | |
| | N1···Br1D | 3.612 | 3.52 | 1.03 | | | | | | |
| | N2···Br4D | 3.599 | 3.52 | 1.02 | | | | | | |
| | C13···Br1D | 3.646 | 3.63 | 1.00 | | | | | | |
| | C7···Br1D | 3.742 | 3.63 | 1.03 | | | | | | |
| | C1···Br2D | 3.713 | 3.63 | 1.02 | | | | | | |
| | C18···Br4D | 3.586 | 3.63 | 0.99 | | | | | | |
| | S2···Br3D | 3.884 | 3.75 | 1.04 | | | | | | |
| | S2···C4D | 3.684 | 3.66 | 1.01 | | | | | | |
| **1·QI** | **X-ray** | | | | | | | | | |
| | Pt1···C1D | 4.698(12) | 4.06 | 1.16 | | | | | | |
| | Pt1···C2D | 4.206(11) | 4.06 | 1.04 | | | | | | |
| | Pt1···C3D | 3.717(10) | 4.06 | 0.92 | 3.1(3) | 3.928(4) | 3.602(8) | 4.392(6) | 1.566 | 23.5 |
| | Pt1···C4D | 3.707(11) | 4.06 | 0.91 | | | | | | |
| | Pt1···C5D | 4.103(10) | 4.06 | 1.01 | | | | | | |

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Pt1···C6D | 4.561(11) | 4.06 | 1.12 | | | | | | |
| | C12···O1D | 3.753(15) | 3.27 | 1.15 | | | | | | |
| | C13···O1D | 4.285(15) | 3.27 | 1.31 | | | | | | |
| | C7···I1D | 4.082(11) | 3.81 | 1.07 | | | | | | |
| | C18···I4D | 4.614(12) | 3.81 | 1.21 | | | | | | |
| | C3···I2D | 4.304(11) | 3.81 | 1.13 | | | | | | |
| | C14···I3D | 3.672(11) | 3.81 | 0.96 | | | | | | |
| | C15···I3D | 3.869(12) | 3.81 | 1.02 | | | | | | |
| | H12···I4D | 4.1904(7) | 3.24 | 1.29 | | | | | | |
| | S1···I1D | 3.946(3) | 3.93 | 1.00 | | | | | | |
| | S2···I3D | 4.427(3) | 3.93 | 1.13 | | | | | | |
| | **Optimized** | | | | | | | | | |
| | Pt1···C1D | 3.862 | 4.06 | 0.95 | | | | | | |
| | Pt1···C2D | 3.879 | 4.06 | 0.96 | 3.62 | | | | | |
| | Pt1···C3D | 3.764 | 4.06 | 0.93 | | | | | | |
| | Pt1···C4D | 3.636 | 4.06 | 0.90 | | 3.497 | 3.275 | 4.145 | 1.226 | 20.5 |
| | Pt1···C5D | 3.703 | 4.06 | 0.91 | | | | | | |
| | Pt1···C6D | 3.794 | 4.06 | 0.93 | | | | | | |
| | C12···O1D | 3.279 | 3.27 | 1.00 | | | | | | |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | C13···O1D | 3.447 | 3.27 | 1.05 | | | | | |
| | O1···I4D | 3.764 | 3.54 | 1.06 | | | | | |
| | C7···I1D | 3.839 | 3.81 | 1.10 | | | | | |
| | C18···I4D | 3.898 | 3.81 | 1.02 | | | | | |
| | C3···I2D | 3.916 | 3.81 | 1.03 | | | | | |
| | C14···I3D | 3.694 | 3.81 | 0.97 | | | | | |
| | C15···I3D | 3.902 | 3.81 | 1.02 | | | | | |
| | H12···I4D | 3.688 | 3.24 | 1.14 | | | | | |
| | S1···I1D | 3.934 | 3.93 | 1.00 | | | | | |
| | S2···I3D | 4.098 | 3.93 | 1.04 | | | | | |

# S5. CARTESIAN COORDINATES FOR THE STUDIED MOLECULES

## Optimized geometries

Cartesian coordinate for [**1**·QF] (in Å)

| | | | |
|---|---|---|---|
| Pt | 0.000000 | 2.100980 | 0.000000 |
| S | 4.086866 | 3.926284 | 0.052870 |
| S | -2.233801 | 1.874314 | 0.003797 |
| O | 0.000000 | 0.000000 | 0.000000 |
| N | 2.029577 | 2.399726 | -0.048736 |
| N | -1.197814 | -0.576811 | 0.026121 |
| C | 2.384449 | 3.664884 | 0.063313 |
| C | 1.344083 | 4.642106 | 0.164002 |
| C | 3.072230 | 0.168600 | -0.320241 |
| H | 2.118317 | -0.339845 | -0.361132 |
| C | 0.050459 | 4.072862 | 0.115987 |
| C | 5.492746 | 0.156639 | -0.360142 |
| H | 6.416124 | -0.404715 | -0.433046 |
| C | 3.110426 | 1.550918 | -0.169660 |
| C | 4.269470 | -0.513134 | -0.412315 |
| H | 4.257994 | -1.590405 | -0.524787 |
| C | 1.555854 | 6.012719 | 0.295268 |
| H | 2.565369 | 6.409225 | 0.335283 |
| C | -1.217789 | -1.925709 | 0.076979 |
| H | -0.239499 | -2.381110 | 0.103831 |
| C | -3.554567 | -0.523483 | 0.054004 |
| H | -4.458619 | 0.070805 | 0.052211 |
| C | 5.542727 | 1.531116 | -0.218541 |
| H | 6.490080 | 2.054084 | -0.180658 |
| C | 4.342858 | 2.218782 | -0.125709 |
| C | 0.470415 | 6.858858 | 0.378519 |
| H | 0.615167 | 7.926860 | 0.483432 |
| C | -2.397330 | -2.610909 | 0.111181 |
| H | -2.377908 | -3.690320 | 0.159490 |
| C | -0.813889 | 6.324097 | 0.329695 |
| H | -1.670110 | 6.986405 | 0.396964 |
| C | -1.021265 | 4.959421 | 0.201948 |
| H | -2.039050 | 4.587437 | 0.176058 |
| C | -2.333923 | 0.162341 | 0.024045 |
| C | -3.595034 | -1.892251 | 0.096059 |

| | | | |
|---|---|---|---|
| H | -4.546301 | -2.408235 | 0.124874 |
| F | 3.037774 | 1.969246 | 3.006076 |
| F | -1.968869 | -0.231592 | 3.261444 |
| F | 2.718578 | -0.745130 | 2.819054 |
| F | -1.652709 | 2.480740 | 3.449229 |
| O | 0.853583 | 3.487544 | 3.425596 |
| O | 0.224057 | -1.749962 | 2.884222 |
| C | -0.783571 | 0.345458 | 3.207013 |
| C | 1.853594 | 1.397440 | 3.043418 |
| C | 0.363642 | -0.555132 | 3.002417 |
| C | -0.636537 | 1.670718 | 3.280731 |
| C | 1.698835 | 0.075339 | 2.956006 |
| C | 0.702375 | 2.307510 | 3.241357 |
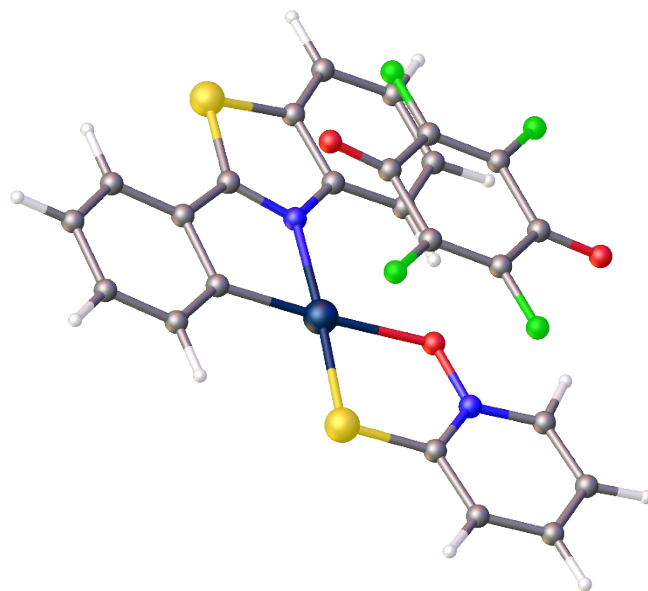
## Cartesian coordinate for [**1**·QCl] (in Å)

| | | | |
|---|---|---|---|
| Pt | 0.000000 | 0.000000 | 0.000000 |
| S | 0.000000 | 2.242416 | 0.000000 |
| S | 1.431305 | -4.242444 | 0.034989 |
| N | 0.098885 | -2.051497 | 0.001737 |
| C | 2.406759 | -1.580268 | 0.036161 |
| O | -2.082756 | 0.207406 | -0.020784 |
| C | -3.023746 | -4.013255 | -0.172229 |
| H | -4.099145 | -3.902756 | -0.240054 |
| C | 1.960489 | -0.238289 | 0.004865 |
| C | 3.756952 | -1.922414 | 0.025685 |
| H | 4.057690 | -2.965160 | 0.046596 |
| C | -1.690830 | 2.511211 | -0.069275 |
| C | 1.328862 | -2.522594 | 0.035731 |
| N | -2.536742 | 1.451406 | -0.063032 |
| C | 4.295064 | 0.405709 | -0.057970 |
| H | 5.038220 | 1.194140 | -0.104186 |
| C | -4.443259 | 2.845487 | -0.178552 |
| H | -5.519941 | 2.931534 | -0.220004 |
| C | -3.876642 | 1.605361 | -0.113304 |
| H | -4.425602 | 0.675494 | -0.107701 |
| C | -2.253095 | 3.792336 | -0.141075 |
| H | -1.571517 | 4.632414 | -0.155366 |
| C | 2.950662 | 0.742587 | -0.043518 |
| H | 2.677754 | 1.790799 | -0.084376 |
| C | 4.707142 | -0.923534 | -0.021226 |

| | | | |
|---|---|---|---|
| H | 5.761491 | -1.170534 | -0.033400 |
| C | -2.468612 | -5.293908 | -0.146767 |
| H | -3.115981 | -6.161289 | -0.188764 |
| C | -0.852552 | -3.049816 | -0.043939 |
| C | -2.231295 | -2.884347 | -0.121088 |
| H | -2.649204 | -1.887805 | -0.153476 |
| C | -0.300683 | -4.339017 | -0.028381 |
| C | -3.610642 | 3.967521 | -0.195674 |
| H | -4.030322 | 4.963690 | -0.253651 |
| C | -1.099537 | -5.471049 | -0.076059 |
| H | -0.664437 | -6.462532 | -0.063091 |
| Cl | -0.603880 | 3.467238 | -3.554001 |
| Cl | 2.834988 | -0.677783 | -3.482489 |
| Cl | 0.381876 | -2.712108 | -3.415147 |
| C | 1.006645 | 1.302710 | -3.422133 |
| C | 0.184524 | -1.023545 | -3.407335 |
| O | 1.930137 | 2.071738 | -3.407403 |
| C | -1.431923 | 0.926277 | -3.437632 |
| Cl | -3.056165 | 1.432809 | -3.490980 |
| C | 1.217890 | -0.170191 | -3.438181 |
| C | -1.220958 | -0.543735 | -3.356245 |
| O | -2.147632 | -1.307172 | -3.278489 |
| C | -0.402864 | 1.782840 | -3.461281 |
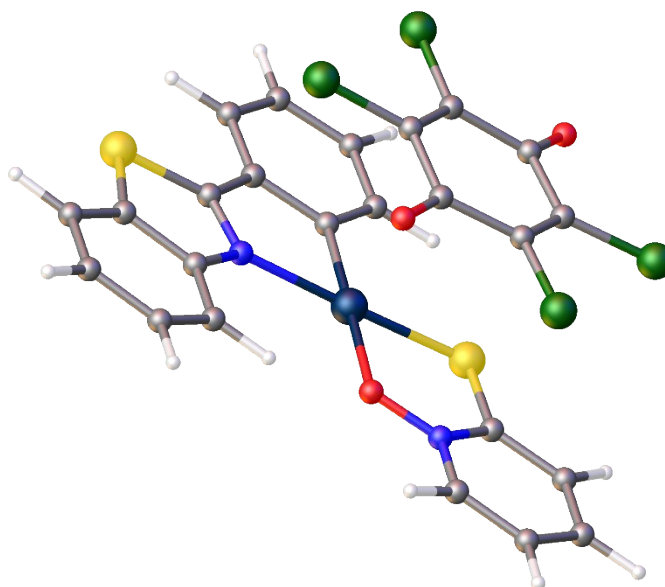
## Cartesian coordinate for [**1**·QBr] (in Å)

| | | | |
|---|---|---|---|
| Pt | 0.000000 | 0.000000 | 0.000000 |
| S | -0.082223 | -4.244611 | 1.423191 |
| S | 0.000000 | 2.242416 | 0.000000 |
| O | 0.009144 | 0.207190 | -2.081960 |
| N | 0.022140 | 1.451162 | -2.537369 |
| C | 0.140254 | -2.881619 | -2.234108 |
| H | 0.188127 | -1.884798 | -2.649872 |
| N | -0.010682 | -2.051597 | 0.095421 |
| C | 0.075678 | 3.792931 | -2.256016 |
| H | 0.095512 | 4.633445 | -1.575230 |
| C | 0.033589 | 2.511268 | -1.691849 |
| C | 0.033038 | 0.736838 | 2.952513 |
| H | 0.091233 | 1.784785 | 2.681918 |
| C | 0.035149 | 1.604899 | -3.878040 |
| H | 0.028042 | 0.674595 | -4.426218 |
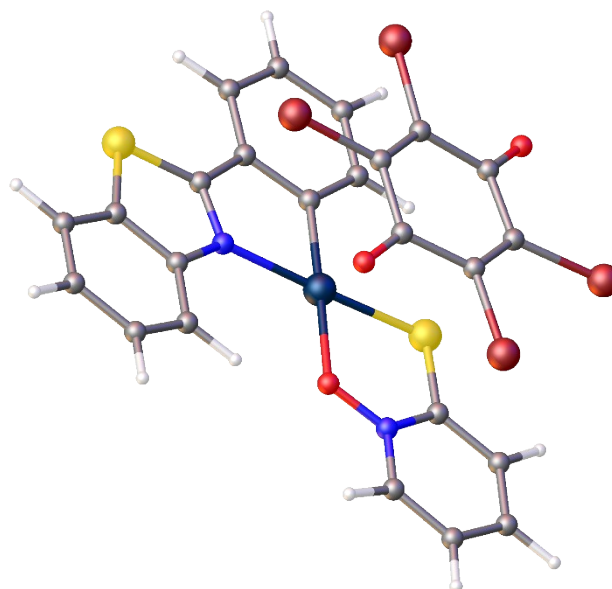
```
C     0.026038   0.397398   4.296251
H     0.073727   1.183717   5.041547
C     0.002699  -4.338701  -0.307932
C    -0.081478  -1.928664   3.752940
H    -0.119727  -2.971605   4.051331
C    -0.069039  -1.584056   2.403405
C    -0.064283  -2.524525   1.324008
C    -0.016079  -0.241648   1.959890
C     0.038006  -3.048750  -0.857200
C     0.197308  -4.009829  -3.027348
H     0.285737  -3.897772  -4.101086
C     0.055784  -5.469840  -1.107692
H     0.027841  -6.461833  -0.674386
C     0.152183  -5.291125  -2.475071
H     0.199399  -6.157800  -3.123055
C     0.091300   3.967995  -3.614615
H     0.123897   4.964737  -4.035658
C    -0.034186  -0.931985   4.705470
H    -0.039814  -1.180745   5.759493
C     0.066548   2.845654  -4.446406
H     0.076732   2.931829  -5.523835
Br    3.556769   1.588478  -3.201738
Br    3.505128  -2.866049   0.254333
Br    3.525186  -0.785769   2.934757
Br    3.574633   3.669181  -0.522700
O     3.352798   2.027248   1.959647
O     3.294546  -1.216809  -2.224176
C     3.411583   1.289524   1.012695
C     3.470911   0.993149  -1.436075
C     3.473175   1.815218  -0.381566
C     3.454822  -1.008696   0.116156
C     3.387662  -0.484469  -1.273984
C     3.464724  -0.190412   1.175415
```

## Cartesian coordinate for [**1**·QI] (in Å)

```
Pt    0.000000   0.000000   0.000000
S     2.225312   0.222252   0.154052
S    -4.020781  -1.834305  -0.711511
O     0.000000   2.093451   0.000000
N     1.191710   2.668446   0.075137
```



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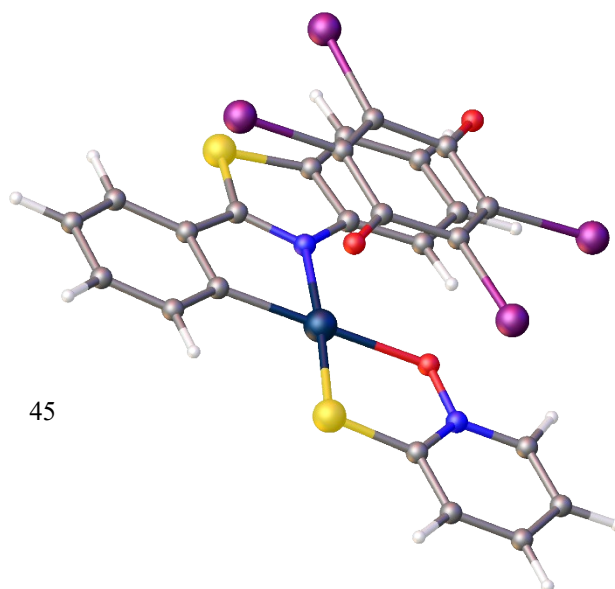
| | | | |
|---|---|---|---|
| C | -0.041593 | -1.973283 | -0.025669 |
| C | -3.086065 | 1.934315 | -0.254518 |
| H | -2.156535 | 2.446224 | -0.046708 |
| N | -2.020520 | -0.302116 | -0.232803 |
| C | -0.441441 | -4.774483 | -0.126978 |
| H | -0.579770 | -5.848089 | -0.160119 |
| C | -1.317084 | -2.549990 | -0.234994 |
| C | 2.327485 | 1.931059 | 0.141292 |
| C | -1.519013 | -3.927470 | -0.283164 |
| H | -2.515503 | -4.329335 | -0.436273 |
| C | 1.021805 | -2.862489 | 0.129861 |
| H | 2.023363 | -2.486802 | 0.304716 |
| C | 0.825011 | -4.233362 | 0.077752 |
| H | 1.674138 | -4.895692 | 0.206861 |
| C | 3.546029 | 2.618938 | 0.216276 |
| H | 4.448104 | 2.023872 | 0.268819 |
| C | 1.212616 | 4.018370 | 0.092247 |
| H | 0.234400 | 4.471715 | 0.038747 |
| C | -5.471823 | 1.939122 | -0.663487 |
| H | -6.392722 | 2.499098 | -0.770854 |
| C | -2.352853 | -1.570352 | -0.371321 |
| C | -4.278003 | 2.613629 | -0.402343 |
| H | -4.288376 | 3.692447 | -0.305988 |
| C | 2.388802 | 4.706199 | 0.170124 |
| H | 2.368831 | 5.786777 | 0.181592 |
| C | -4.301584 | -0.123477 | -0.631580 |
| C | -5.496911 | 0.562158 | -0.781726 |
| H | -6.421938 | 0.035494 | -0.980085 |
| C | -3.099056 | 0.548376 | -0.369149 |
| C | 3.586199 | 3.987928 | 0.232055 |
| H | 4.535426 | 4.505020 | 0.292720 |
| I | -0.484970 | -3.296450 | 3.647330 |
| I | -1.050499 | 3.680409 | 3.247471 |
| I | -3.738644 | -1.634889 | 3.207491 |
| I | 2.198353 | 2.031927 | 3.831217 |
| O | 1.596054 | -1.000171 | 3.699784 |
| O | -3.083644 | 1.376282 | 2.976745 |
| C | -0.772285 | 1.625285 | 3.340161 |
| C | 0.528168 | -0.462297 | 3.567299 |
| C | -2.025805 | 0.835342 | 3.180187 |
| C | -1.919849 | -0.643085 | 3.308700 |

C    -0.736177   -1.249738   3.473023

C     0.409291    1.027218   3.534181

Cartesian coordinate for [**1·(QF)₂**] (in Å)

| | | | |
|---|---|---|---|
| Pt | 0.000000 | 0.000000 | 0.000000 |
| S | 0.000000 | 2.246287 | 0.000000 |
| S | -1.393005 | -4.242669 | -0.270894 |
| O | 2.068810 | 0.205188 | 0.222859 |
| N | -0.101068 | -2.048634 | 0.017122 |
| N | 2.517121 | 1.452530 | 0.334522 |
| C | -1.936376 | -0.239548 | -0.304878 |
| C | -1.303472 | -2.525572 | -0.247948 |
| C | -2.366551 | -1.583501 | -0.426478 |
| C | 2.163567 | -2.868012 | 0.596430 |
| H | 2.559758 | -1.869332 | 0.719855 |
| C | -2.916654 | 0.742589 | -0.436186 |
| H | -2.652616 | 1.790650 | -0.354758 |
| C | 0.827970 | -3.041929 | 0.251277 |
| C | 2.939520 | -3.993869 | 0.784332 |
| H | 3.982087 | -3.879694 | 1.054382 |
| C | 1.676283 | 2.511038 | 0.255995 |
| C | 2.230182 | 3.790994 | 0.373566 |
| H | 1.554547 | 4.633699 | 0.312369 |
| C | 0.294503 | -4.332053 | 0.121773 |
| C | -4.241792 | 0.404784 | -0.660317 |
| H | -4.983336 | 1.191395 | -0.740940 |
| C | 3.847758 | 1.600633 | 0.502849 |
| H | 4.396661 | 0.671436 | 0.521904 |
| C | -3.696700 | -1.924132 | -0.661923 |
| H | -3.989140 | -2.965685 | -0.743489 |
| C | 1.077306 | -5.460122 | 0.309362 |
| H | 0.659827 | -6.453642 | 0.205438 |
| C | 2.407160 | -5.276045 | 0.638602 |
| H | 3.041207 | -6.140580 | 0.792129 |
| C | -4.639006 | -0.924363 | -0.774514 |
| H | -5.679621 | -1.170653 | -0.942269 |
| C | 3.577750 | 3.961994 | 0.554883 |
| H | 3.992766 | 4.957901 | 0.643691 |
| C | 4.406752 | 2.840160 | 0.618758 |
| H | 5.476095 | 2.925205 | 0.749551 |
| F | 1.097726 | -3.183234 | -2.889538 |
| F | 3.635009 | -2.299697 | -2.341326 |
| F | 2.222709 | 2.173410 | -2.981645 |

| | | | |
|---|---|---|---|
| F | -0.316664 | 1.293543 | -3.519465 |
| O | -0.786653 | -1.363483 | -3.498083 |
| O | 4.103319 | 0.348451 | -2.371136 |
| C | 1.413150 | -1.906365 | -2.885597 |
| C | 2.648167 | -1.477126 | -2.621917 |
| C | 1.903972 | 0.894987 | -2.982475 |
| C | 2.988928 | -0.038484 | -2.630564 |
| C | 0.661425 | 0.471982 | -3.227315 |
| C | 0.316043 | -0.969607 | -3.216956 |
| F | -3.368830 | -2.934058 | 2.636233 |
| F | -0.706178 | -3.291999 | 3.145743 |
| F | -0.125696 | 1.401791 | 3.416614 |
| F | -2.788591 | 1.762764 | 2.889842 |
| O | -4.344916 | -0.423479 | 2.595836 |
| O | 0.831134 | -1.115308 | 3.535473 |
| C | -2.550698 | -1.920561 | 2.824533 |
| C | -1.251406 | -2.095285 | 3.073521 |
| C | -0.944238 | 0.393740 | 3.213459 |
| C | -0.338441 | -0.953154 | 3.290201 |
| C | -2.245881 | 0.567855 | 2.970300 |
| C | -3.161416 | -0.573692 | 2.768861 |
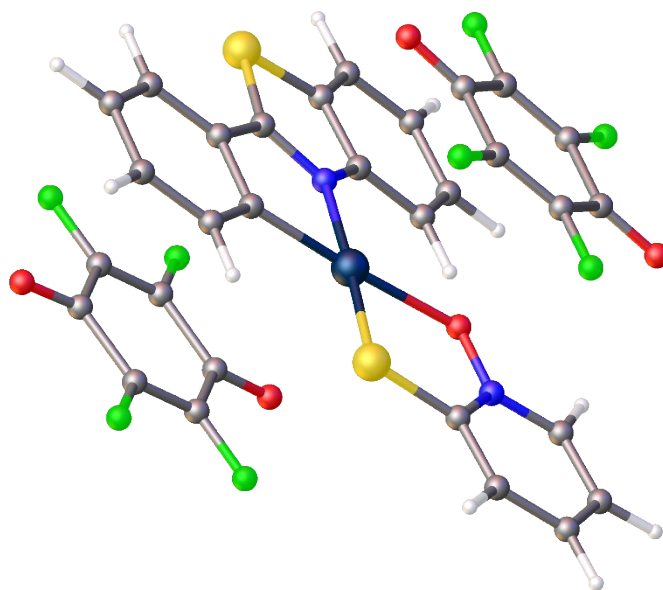
## Cartesian coordinate for [**1·(QCl)₂**] (in Å)

| | | | |
|---|---|---|---|
| Pt | -0.003009 | -0.001594 | -0.009122 |
| S | -2.230494 | -0.262501 | 0.025764 |
| S | 4.038342 | 1.912517 | -0.209882 |
| N | 2.023543 | 0.334704 | -0.077184 |
| C | 1.286375 | 2.572026 | -0.045586 |
| O | 0.036837 | -2.091278 | -0.009053 |
| C | 4.329906 | -2.542859 | -0.240625 |
| H | 4.345313 | -3.625681 | -0.252262 |
| C | 0.005324 | 1.974510 | -0.006251 |
| C | 1.467687 | 3.952466 | -0.045671 |
| H | 2.467823 | 4.372988 | -0.073242 |
| C | -2.297440 | -1.975216 | 0.012244 |
| C | 2.347775 | 1.611976 | -0.099875 |
| N | -1.146485 | -2.689468 | 0.008541 |
| C | -0.908608 | 4.215842 | 0.019637 |
| H | -1.779150 | 4.861856 | 0.041884 |
| C | -2.305295 | -4.748382 | 0.020183 |

| | | | |
|---|---|---|---|
| H | -2.265015 | -5.828474 | 0.025659 |
| C | -1.139489 | -4.038665 | 0.016585 |
| H | -0.150760 | -4.472138 | 0.010724 |
| C | -3.504394 | -2.684620 | 0.009439 |
| H | -4.419171 | -2.107150 | 0.006514 |
| C | -1.085596 | 2.841052 | 0.024209 |
| H | -2.094816 | 2.446951 | 0.050896 |
| C | 0.363590 | 4.779266 | -0.012409 |
| H | 0.485707 | 5.855311 | -0.012845 |
| C | 5.534517 | -1.841192 | -0.308695 |
| H | 6.469607 | -2.384288 | -0.370211 |
| C | 3.123450 | -0.496969 | -0.147597 |
| C | 3.118968 | -1.886970 | -0.159387 |
| H | 2.181105 | -2.421438 | -0.109147 |
| C | 4.336192 | 0.202336 | -0.220765 |
| C | -3.517693 | -4.054536 | 0.014301 |
| H | -4.458208 | -4.590507 | 0.012248 |
| C | 5.551529 | -0.459225 | -0.300789 |
| H | 6.483668 | 0.088931 | -0.355538 |
| Cl | -3.487930 | -1.059031 | -3.439367 |
| Cl | 0.308197 | 2.761237 | -3.521853 |
| Cl | 2.569486 | 0.513390 | -3.517721 |
| C | -1.484792 | 0.752449 | -3.393722 |
| C | 0.909236 | 0.155970 | -3.450284 |
| O | -2.337633 | 1.598588 | -3.366381 |
| C | -0.876936 | -1.639569 | -3.395335 |
| Cl | -1.227463 | -3.305368 | -3.407734 |
| C | -0.039801 | 1.103019 | -3.455536 |
| C | 0.567810 | -1.287886 | -3.363651 |
| O | 1.418630 | -2.135262 | -3.289989 |
| C | -1.828550 | -0.697157 | -3.402906 |
| Cl | -2.540654 | -1.779121 | 3.541520 |
| Cl | 0.063439 | 2.938513 | 3.549782 |
| Cl | 2.845190 | 1.400216 | 3.311860 |
| C | -1.116241 | 0.514192 | 3.478969 |
| C | 1.345314 | 0.601151 | 3.341861 |
| O | -2.167049 | 1.091305 | 3.561283 |
| C | 0.119478 | -1.616402 | 3.313695 |
| Cl | 0.239754 | -3.311594 | 3.247226 |
| C | 0.177073 | 1.250082 | 3.446011 |
| C | 1.408135 | -0.878627 | 3.227697 |
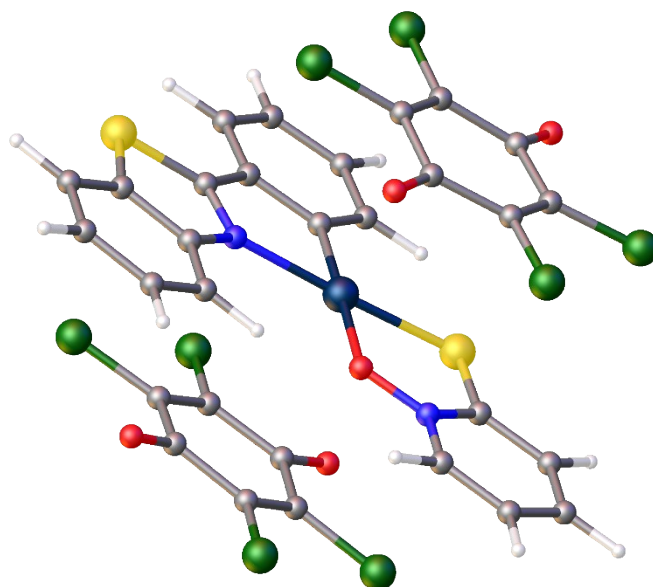
O     2.454086   -1.456861   3.088854

C     -1.048737   -0.973030   3.434890

## Cartesian coordinate for [**1·(QBr)₂**] (in Å)
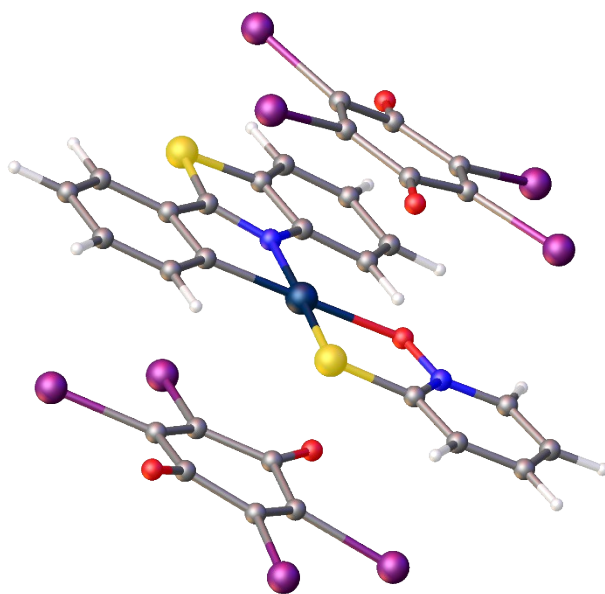


Pt    0.033934    2.449488   -0.026550

S     -3.999926   4.336122   -0.481744

S     2.232419    2.192656    0.326261

O     0.039937    0.376405   -0.283050

N     1.219467   -0.215883   -0.158757

C     -3.021970   0.555639   -0.636824

H     -2.086582   0.028002   -0.516455

N     -1.972075   2.778229   -0.326353

C     3.538494   -0.211386    0.267385

H     4.423449    0.359832    0.513643

C     2.334944    0.492940    0.139165

C     1.029086    5.268295    0.532862

H     2.025917    4.874305    0.692704

C     1.247489   -1.549935   -0.353469

H     0.285850   -1.979413   -0.591074

C     0.822692    6.631852    0.671378

H     1.659250    7.269992    0.933600

C     -4.261195   2.632869   -0.677721

C     -1.498253   6.376683    0.153413

H     -2.487963   6.796082    0.004417

C     -1.290364   5.005669    0.025494

C     -2.319244   4.048875   -0.255298

C     -0.019117   4.410688    0.203462

C     -3.047435   1.942872   -0.551022

C     -4.211678   -0.106203   -0.860470

H     -4.212066   -1.187380   -0.925422

C     -5.453925   1.965790   -0.907781

H     -6.386162   2.506578   -1.011089

C     -5.414870   0.587380   -1.000412

H     -6.332537   0.040475   -1.179172

C     3.586472   -1.567278    0.077493

H     4.524437   -2.098605    0.176560

C     -0.435475   7.194454    0.478387

H     -0.579784   8.262498    0.584302

C     2.412705   -2.252931   -0.245409

H     2.400933   -3.321422   -0.408014
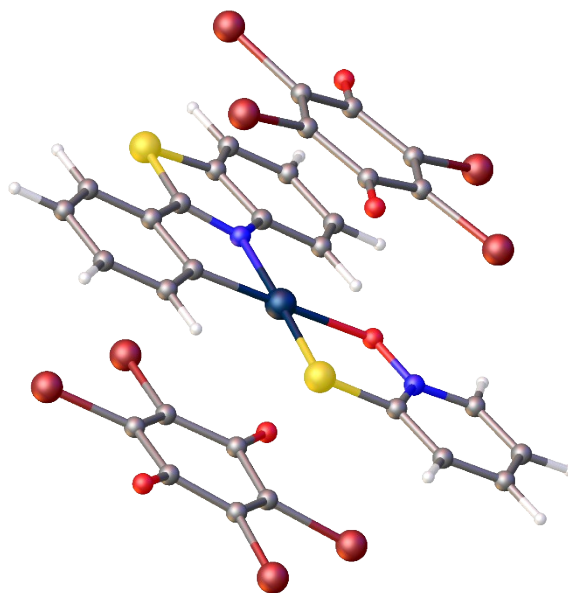
| | | | |
|---|---|---|---|
| Br | -1.045516 | -0.033036 | -3.806495 |
| Br | -2.169361 | 5.496874 | -3.692241 |
| Br | 1.102768 | 6.151239 | -3.125161 |
| Br | 2.258923 | 0.636891 | -3.422184 |
| O | 2.605576 | 3.575970 | -3.095147 |
| O | -2.553089 | 2.537393 | -3.746820 |
| C | 1.436882 | 3.341941 | -3.247687 |
| C | -0.363053 | 1.687146 | -3.599752 |
| C | 0.937595 | 1.949991 | -3.430242 |
| C | -0.872594 | 4.168924 | -3.520906 |
| C | -1.378611 | 2.775661 | -3.630212 |
| C | 0.422851 | 4.432354 | -3.310321 |
| Br | 0.764847 | -1.399341 | 3.207648 |
| Br | -3.299280 | 2.504090 | 3.016314 |
| Br | -1.019686 | 4.913523 | 3.726825 |
| Br | 3.044960 | 1.008425 | 3.925916 |
| O | 1.685651 | 3.663028 | 3.844444 |
| O | -1.865917 | -0.093127 | 2.693088 |
| C | 0.867712 | 2.804805 | 3.647496 |
| C | 0.349908 | 0.416911 | 3.298849 |
| C | 1.251135 | 1.365046 | 3.576759 |
| C | -1.477854 | 2.169482 | 3.217993 |
| C | -1.075613 | 0.750190 | 3.028014 |
| C | -0.580510 | 3.121795 | 3.501105 |

## Cartesian coordinate for [**1·(QI)₂**] (in Å)

| | | | |
|---|---|---|---|
| Pt | 0.311453 | -0.391877 | -0.082367 |
| S | -1.916454 | -0.177342 | -0.228514 |
| S | 4.406378 | -2.192679 | -0.034014 |
| O | 0.269467 | 1.642623 | 0.388114 |
| N | -0.930699 | 2.204358 | 0.419263 |
| C | 0.398019 | -2.318207 | -0.512802 |
| C | 3.350366 | 1.532307 | 0.496570 |
| H | 2.398637 | 2.042894 | 0.462594 |
| N | 2.340025 | -0.680257 | 0.030129 |
| C | 0.864023 | -5.052508 | -1.069362 |
| H | 1.027415 | -6.101324 | -1.284249 |
| C | 1.693587 | -2.884847 | -0.487493 |
| C | -2.049236 | 1.492000 | 0.136739 |
| C | 1.927237 | -4.230235 | -0.758165 |

| | | | |
|---|---|---|---|
| H | 2.937276 | -4.626156 | -0.727005 |
| C | -0.650335 | -3.178834 | -0.836581 |
| H | -1.666733 | -2.805800 | -0.884728 |
| C | -0.420347 | -4.518179 | -1.109887 |
| H | -1.258396 | -5.158379 | -1.362024 |
| C | -3.275057 | 2.167665 | 0.161105 |
| H | -4.161860 | 1.593467 | -0.070490 |
| C | -0.977452 | 3.512681 | 0.743290 |
| H | -0.012059 | 3.948435 | 0.951041 |
| C | 5.757803 | 1.534640 | 0.747944 |
| H | 6.670137 | 2.089244 | 0.930222 |
| C | 2.712720 | -1.927588 | -0.174410 |
| C | 4.533596 | 2.204891 | 0.722303 |
| H | 4.511943 | 3.276564 | 0.878064 |
| C | -2.164651 | 4.185953 | 0.783671 |
| H | -2.166062 | 5.234389 | 1.046409 |
| C | 4.637327 | -0.507078 | 0.304778 |
| C | 5.823995 | 0.170289 | 0.536344 |
| H | 6.772455 | -0.351821 | 0.549046 |
| C | 3.403780 | 0.158799 | 0.290495 |
| C | -3.341346 | 3.498768 | 0.479277 |
| H | -4.296586 | 4.007684 | 0.495991 |
| I | -1.573735 | -4.117777 | 2.856770 |
| I | 1.340959 | 2.174038 | 3.888307 |
| I | 2.072562 | -3.693505 | 3.152311 |
| I | -2.320201 | 1.695142 | 3.943453 |
| O | -2.747429 | -1.276739 | 3.220663 |
| O | 2.506877 | -0.627549 | 3.300579 |
| C | 0.386054 | 0.361418 | 3.565935 |
| C | -1.553120 | -1.141998 | 3.293273 |
| C | 1.313573 | -0.787221 | 3.344367 |
| C | 0.702334 | -2.139865 | 3.214290 |
| C | -0.626692 | -2.300321 | 3.147637 |
| C | -0.941456 | 0.190223 | 3.571186 |
| I | 1.188817 | -2.655230 | -4.276812 |
| I | -0.821050 | 3.914597 | -2.947589 |
| I | 3.620253 | -0.004450 | -3.451991 |
| I | -3.262956 | 1.255961 | -3.721705 |
| O | -1.589865 | -1.351526 | -3.838386 |
| O | 1.882926 | 2.430709 | -2.627694 |
| C | -0.338960 | 1.913093 | -3.211166 |

| | | | |
|---|---|---|---|
| C | -0.789339 | -0.465606 | -3.689635 |
| C | 1.110567 | 1.604471 | -3.042607 |
| C | 1.561171 | 0.241664 | -3.440189 |
| C | 0.679885 | -0.722735 | -3.739518 |
| C | -1.224955 | 0.950156 | -3.493608 |

## Cartesian coordinate for 1 (in Å)

| | | | |
|---|---|---|---|
| Pt | 2.141438669 | 5.440252825 | 5.475395509 |
| S | 1.662350368 | 3.539538592 | 6.563184049 |
| S | 4.316401298 | 9.087482667 | 4.055496974 |
| O | 0.239739306 | 5.195750783 | 4.638125659 |
| N | -0.413882123 | 4.103800437 | 5.003306375 |
| N | 2.658388253 | 7.186326682 | 4.528810266 |
| C | 4.633437952 | 6.849391596 | 5.767610541 |
| C | -1.626749834 | 3.905464264 | 4.443366076 |
| H | -1.920641463 | 4.678724234 | 3.749034543 |
| C | 2.300730266 | 10.061224984 | 2.349045166 |
| H | 2.900656368 | 10.915764459 | 2.061863997 |
| C | 3.949941860 | 5.695412972 | 6.218995332 |
| C | -1.876064357 | 1.883360732 | 5.669762815 |
| H | -2.448665637 | 1.003626602 | 5.934801354 |
| C | -0.644408019 | 2.099663536 | 6.228247239 |
| H | -0.215802559 | 1.405920619 | 6.939480771 |
| C | 4.642260383 | 4.882867037 | 7.118260795 |
| H | 4.179216956 | 3.980386612 | 7.500868286 |
| C | 1.032884309 | 9.874200541 | 1.830918243 |
| H | 0.634065664 | 10.593934844 | 1.126510150 |
| C | 3.861920858 | 7.621049501 | 4.842064368 |
| C | 0.116200562 | 3.229982648 | 5.896782988 |
| C | 0.264335258 | 8.770410149 | 2.204759552 |
| H | -0.726150466 | 8.647290224 | 1.783295307 |
| C | 0.739510074 | 7.832329125 | 3.099931866 |
| H | 0.153595583 | 6.973280581 | 3.397612277 |
| C | 2.780862187 | 9.121186543 | 3.247778574 |
| C | -2.380459366 | 2.810561403 | 4.753022801 |
| H | -3.345589972 | 2.684226185 | 4.282968835 |
| C | 2.014656165 | 8.009456365 | 3.628228329 |
| C | 5.923255046 | 5.202875876 | 7.538681561 |
| H | 6.431028161 | 4.547773697 | 8.238432023 |
| C | 5.921605021 | 7.175151685 | 6.188554979 |

| H | 6.409439405 | 8.070578296 | 5.816109535 |
|---|---|---|---|
| C | 6.570821548 | 6.347651747 | 7.080053800 |
| H | 7.572172279 | 6.583600956 | 7.418339064 |
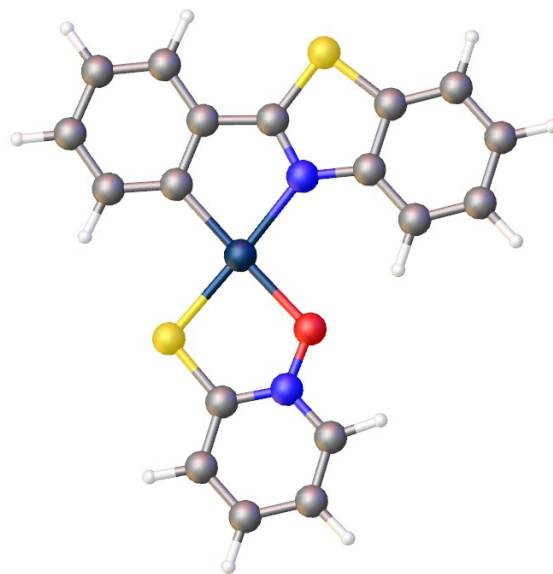
## Cartesian coordinate for QF (in Å)

| F | 1.032450000 | 5.806982000 | -1.522971000 |
|---|---|---|---|
| F | 1.151448000 | 3.610013000 | 0.111953000 |
| O | 3.147063000 | 7.473305000 | -1.582492000 |
| C | 2.078169000 | 5.544312000 | -0.773473000 |
| C | 2.136010000 | 4.474233000 | 0.023096000 |
| C | 3.198389000 | 6.509283000 | -0.863335000 |
| F | 5.488856000 | 4.894609000 | 1.522959000 |
| F | 5.369858000 | 7.091578000 | -0.111965000 |
| O | 3.374245000 | 3.228285000 | 1.582477000 |
| C | 4.443129000 | 5.157291000 | 0.773477000 |
| C | 4.385288000 | 6.227370000 | -0.023092000 |
| C | 3.322895000 | 4.192339000 | 0.863366000 |
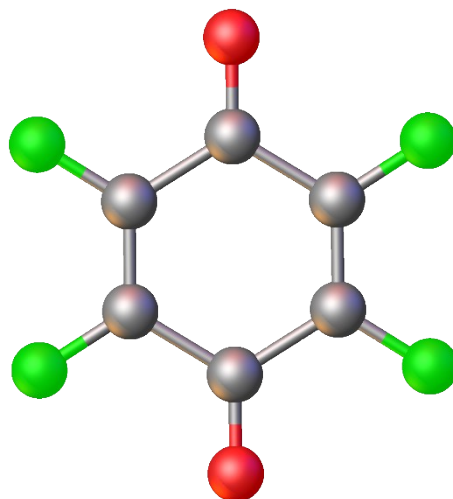


## Cartesian coordinate for QCl (in Å)

| Cl | 1.274016000 | 7.477191000 | 2.239551000 |
|---|---|---|---|
| Cl | 3.541111000 | 5.305604000 | 1.668837000 |
| Cl | -2.514914000 | 3.723196000 | 1.471937000 |
| Cl | -0.247824000 | 1.551460000 | 0.901968000 |
| O | -1.369529000 | 6.317605000 | 2.045279000 |
| O | 2.395764000 | 2.710882000 | 1.096793000 |
| C | 1.882684000 | 4.942805000 | 1.631602000 |
| C | 0.929704000 | 5.855572000 | 1.871561000 |
| C | -0.515371000 | 5.499433000 | 1.829870000 |
| C | 1.541613000 | 3.529139000 | 1.311779000 |
| C | -0.856444000 | 4.085929000 | 1.509634000 |
| C | 0.096486000 | 3.173041000 | 1.269902000 |
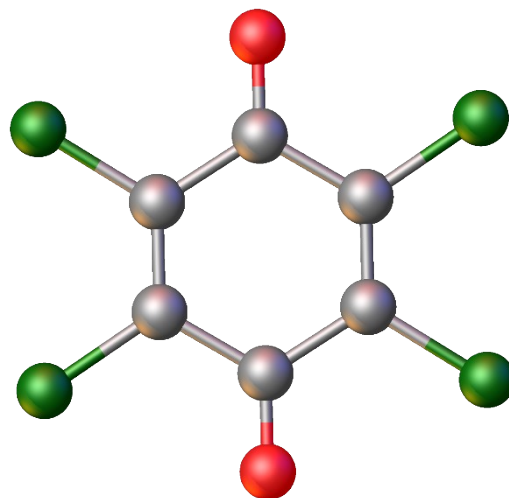


## Cartesian coordinate for QBr (in Å)

| Br | 1.290986000 | 7.636166000 | 2.275684000 |
|---|---|---|---|
| Br | 3.703714000 | 5.325254000 | 1.668806000 |
| Br | -2.677555000 | 3.703492000 | 1.471959000 |
| Br | -0.264657000 | 1.392580000 | 0.865446000 |
| O | -1.370163000 | 6.317920000 | 2.045192000 |
| O | 2.396351000 | 2.710642000 | 1.096634000 |

| | | | |
|---|---|---|---|
| C | 1.882289000 | 4.943974000 | 1.631944000 |
| C | 0.930792000 | 5.855302000 | 1.871627000 |
| C | -0.515768000 | 5.499625000 | 1.830222000 |
| C | 1.541959000 | 3.528906000 | 1.311836000 |
| C | -0.856085000 | 4.084665000 | 1.509447000 |
| C | 0.095432000 | 3.173330000 | 1.269915000 |
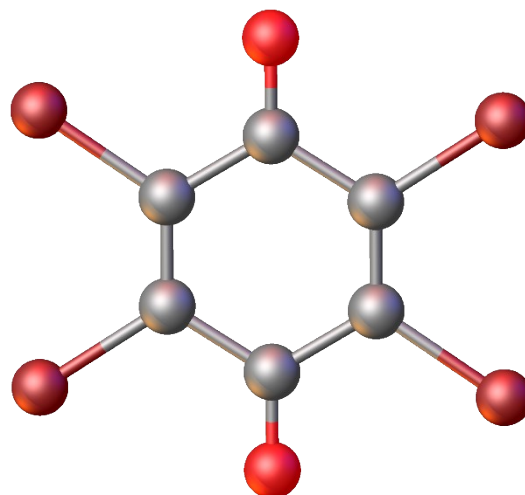
## Cartesian coordinate for QI (in Å)

| | | | |
|---|---|---|---|
| I | 11.34789831724660 | -1.51945984134358 | 9.27608749240645 |
| I | 5.18415393181739 | -4.83124322234611 | 8.74637706517489 |
| I | 9.51337464524704 | -2.69146625330675 | 12.25469596693273 |
| I | 7.02147755503089 | -3.66391253692769 | 5.76750176345664 |
| O | 9.58602154491685 | -2.33888640554971 | 6.87186980466656 |
| O | 6.94648151045126 | -4.01269425730527 | 11.15050487518255 |
| C | 7.00781011589777 | -3.84612892327232 | 8.80272810943721 |
| C | 8.98622438107133 | -2.71901738107558 | 7.84437360722771 |
| C | 8.85792825234695 | -2.93117085985107 | 10.30219901031118 |
| C | 7.54683263484628 | -3.63317705179889 | 10.17808567653792 |
| C | 7.67552462938688 | -3.42208804283625 | 7.72023018144272 |
| C | 9.52497248174071 | -2.50605522438677 | 9.21964644722342 |
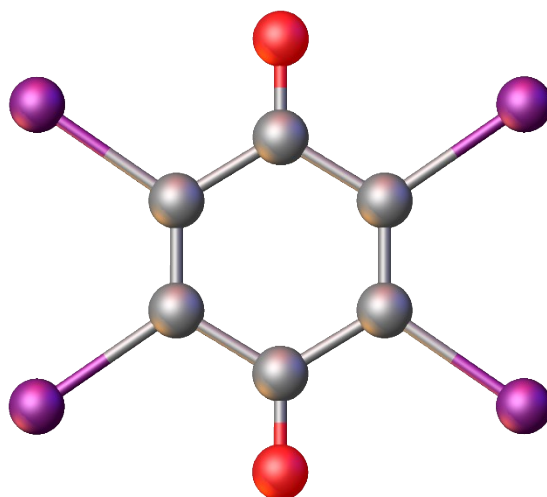
## References

1.    B. E. G. Lucier, A. R. Reidel and R. W. Schurko, Multinuclear solid-state NMR of square-planar platinum complexes — Cisplatin and related systems, *Canadian Journal of Chemistry*, 2011, **89**, 919-937.

2.    M.-H. Thibault, B. E. G. Lucier, R. W. Schurko and F.-G. Fontaine, Synthesis and solid-state characterization of platinum complexes with hexadentate amino- and iminophosphine ligands, *Dalton Transactions*, 2009, DOI: 10.1039/B907737E, 7701-7716.

3.    B. A. Demko and R. E. Wasylishen, Comparing Main Group and Transition-Metal Square-Planar Complexes of the Diselenoimidodiphosphinate Anion: A Solid-State NMR Investigation of M[N(iPr2PSe)2]2 (M = Se, Te; Pd, Pt), *Inorganic Chemistry*, 2008, **47**, 2786-2797.

4.    E. Kuzniak, J. Hooper, M. Srebro-Hooper, J. Kobylarczyk, M. Dziurka, B. Musielak, D. Pinkowicz, J. Raya, S. Ferlay and R. Podgajny, A concerted evolution of supramolecular interactions in a {cation; metal complex; π-acid; solvent} anion-π system, *Inorganic Chemistry Frontiers*, 2020, **7**, 1851-1863.

5.    D. Sundholm, H. Fliegl and R. J. F. Berger, Calculations of magnetically induced current densities: theory and applications, *WIREs Computational Molecular Science*, 2016, **6**, 639-678.