ELECTRONIC SUPPLEMENTARY MATERIALS

A New Look at the Chalcogen Bond: π-Hole-based Chalcogen (Se, Te) Bonding Which Does Not Include a σ-Hole Interaction

Eugene A. Katlenok,*[1] Maxim L. Kuznetsov,[2] Nikolay A. Semenov,[3] Nadezhda A. Bokach,[1] Vadim Yu. Kukushkin*[1,4]

[1]*Institute of Chemistry, Saint Petersburg State University, Universitetskaya Nab. 7/9, 199034 Saint Petersburg, Russian Federation; e-mail: v.kukushkin@spbu.ru*

[2]*Centro de Química Estrutural, Institute of Molecular Sciences, Departamento de Engenharia Química, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal*

[3]*Institute of Organic Chemistry, Siberian Branch, Russian Academy of Sciences, 9 Lavrentiev Avenue, 630090 Novosibirsk, Russian Federation*

[4]*Laboratory of Crystal Engineering of Functional Materials, South Ural State University, 76, Lenin Av., 454080 Chelyabinsk, Russian Federation*

Contents

1. Crystal data and structure refinement

Table S1. Crystal data and structure refinement for **1**·3TeDA·THF, **1**·3SeDA·CH$_2$Cl$_2$, **2**·2SeDA·2H$_2$O·CH$_2$Cl$_2$, and **3**·2SeDA.

Identification code	**1**·3TeDA·THF	**1**·3SeDA·CH$_2$Cl$_2$	**2**·2SeDA·2H$_2$O·CH$_2$Cl$_2$	**3**·2SeDA
Empirical formula	C$_{50}$H$_{34}$N$_{18}$OPt$_2$S$_4$Te$_3$	C$_{47}$H$_{28}$Cl$_2$N$_{18}$Pt$_2$S$_4$Se$_3$	C$_{45}$H$_{30}$Cl$_2$N$_{12}$O$_2$Pt$_2$S$_4$Se$_2$	C$_{26}$H$_{12}$N$_{10}$OPtS$_2$Se$_2$
Formula weight	1804.17	1671.07	1518.05	897.59
Temperature/K	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P2$_1$/c	P2$_1$/c	I2/a	P2$_1$/c
a/Å	9.88596(10)	9.95820(10)	14.3494(2)	17.42591(13)
b/Å	26.2733(3)	26.3182(2)	16.1541(2)	7.83162(7)
c/Å	20.9857(2)	20.9412(2)	20.5667(2)	20.84877(19)
α/°	90	90	90	90
β/°	98.3721(10)	96.3630(10)	95.2320(10)	100.6242(8)
γ/°	90	90	90	90
Volume/Å^3	5392.67(10)	5454.50(9)	4747.53(10)	2796.52(4)
Z	4	4	4	4
ρ$_{calc}$g/cm^3	2.222	2.035	2.124	2.132
μ/mm^{-1}	24.041	14.521	15.748	14.12
F(000)	3376	3168	2888	1696
Crystal size/mm^3	0.08 × 0.06 × 0.05	0.13 × 0.11 × 0.08	0.06 × 0.04 × 0.03	0.1 × 0.08 × 0.07
Radiation	Cu Kα (λ = 1.54184)	CuKα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.426 to 139.998	5.414 to 139.94	6.97 to 154.008	5.16 to 139.998
Index ranges	-9 ≤ h ≤ 12, -32 ≤ k ≤ 31, -24 ≤ l ≤ 25	-12 ≤ h ≤ 12, -32 ≤ k ≤ 32, -24 ≤ l ≤ 25	-18 ≤ h ≤ 18, -10 ≤ k ≤ 20, -23 ≤ l ≤ 25	-18 ≤ h ≤ 21, -9 ≤ k ≤ 9, -25 ≤ l ≤ 25
Reflections collected	38723	22131	15496	32290
Independent reflections	10127 [R$_{int}$ = 0.0406, R$_{sigma}$ = 0.0342]	22131 [R$_{int}$ = n/a, R$_{sigma}$ = 0.0263]	4801 [R$_{int}$ = 0.0270, R$_{sigma}$ = 0.0254]	5307 [R$_{int}$ = 0.0473, R$_{sigma}$ = 0.0292]
Data/restraints/parameters	10127/0/705	22131/0/688	4801/0/315	5307/0/379
Goodness-of-fit on F^2	1.015	1.05	1.026	1.039
Final R indexes [I>=2σ (I)]	R$_1$ = 0.0278, wR$_2$ = 0.0660	R$_1$ = 0.0564, wR$_2$ = 0.1581	R$_1$ = 0.0256, wR$_2$ = 0.0671	R$_1$ = 0.0223, wR$_2$ = 0.0516
Final R indexes [all data]	R$_1$ = 0.0317, wR$_2$ = 0.0678	R$_1$ = 0.0641, wR$_2$ = 0.1647	R$_1$ = 0.0271, wR$_2$ = 0.0680	R$_1$ = 0.0250, wR$_2$ = 0.0526
Largest diff. peak/hole / e Å^{-3}	1.57/-0.99	1.41/-3.56	1.30/-1.12	1.08/-0.94
CCDC Nos	2218816	2218817	2218818	2218819

*1.1. Structural features of **1**·3SeDA·CH₂Cl₂ and **1**·3TeDA·THF*
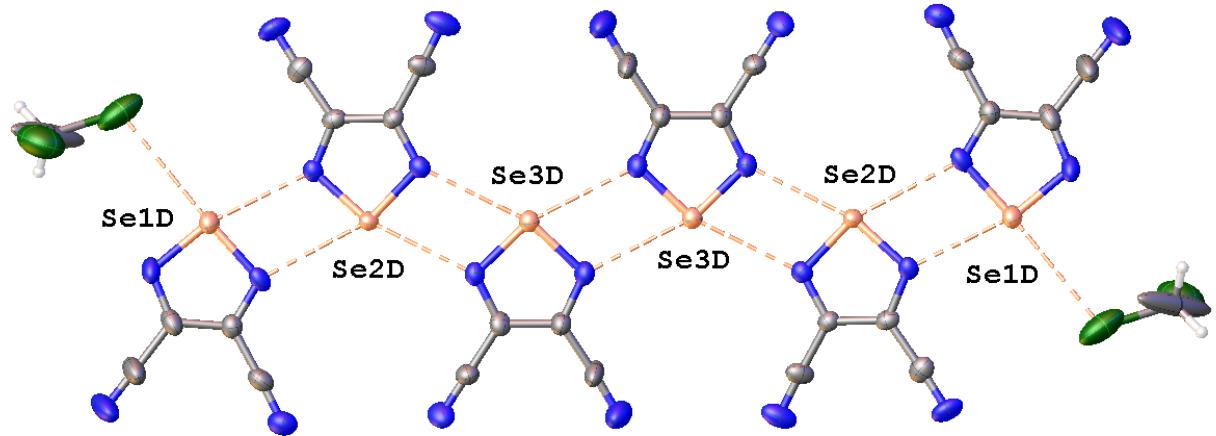
Figure S1. View of the supramolecular heterooctamer in the crystal structure of **1**·3SeDA·CH₂Cl₂.
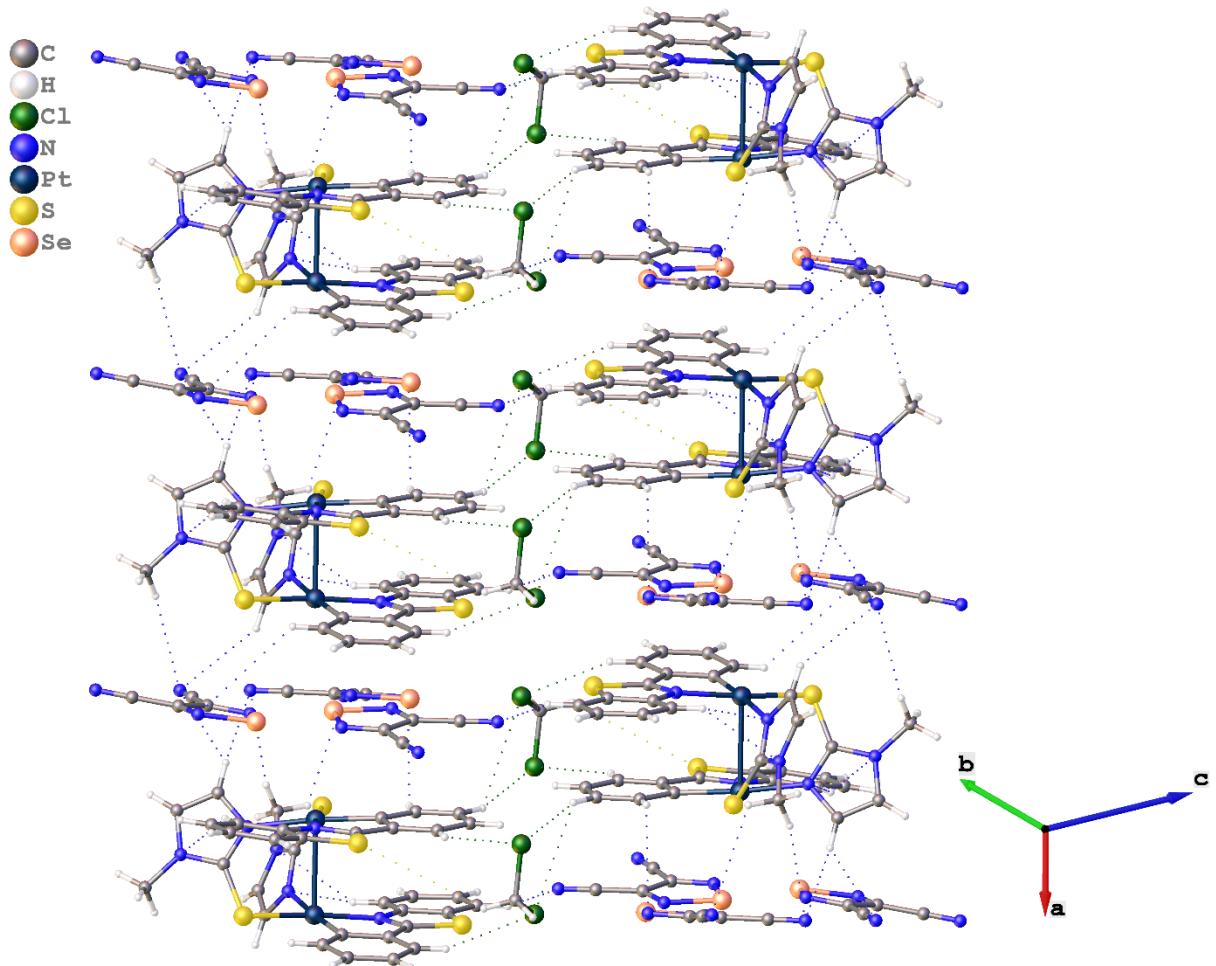
Figure S2. A fragment of the crystal packing of **1**·3SeDA·CH₂Cl₂ illustrating the occurred 3D-network.

Table S2. Parameters of short intermolecular contacts (other than HBs) in the crystal structure of $1 \cdot 3SeDA \cdot CH_2Cl_2$.

Contact	Distance, Å (Nc[a])	Angle, °	Other parameters and comments
Se1D···Cl2S	3.379(5) (0.93)	N1D–Se1D–Cl2S 174.6(3) Se1D–Cl2S–C1S 109.0(8)	Se···Cl ChB with C_4N_4Se-1 donor
Se1D···N5D	2.751(7) (0.80)	N1D–Se1D–N5D 165.7(3)	Se···N ChB with SeDA-1 donor
Se2D···N2D	2.941(8) (0.85)	N6D–Se2D–N2D 161.0(3)	Se···N ChB with SeDA-2 donor
Se2D···N9D	2.822(6) (0.82)	N5D–Se2D–N9D 164.4(3)	Se···N ChB with SeDA-2 donor
Se3D···N6D	2.898(8) (0.84)	N6D–Se3D–N10D 162.9(3)	Se···N ChB with SeDA-3 donor
Se3D···N10D	2.883(7) (0.84)	N9D–Se3D–N10D 163.1(3)	Se···N ChB with SeDA-3 donor
Pt1···Se2D	3.6473(10) (1.00)	$(C_2N_2Se)_{plane\ centroid}$–Se2D–Pt1D 100.97(13)	π-(Se)-hole···Pt contact, supported by π–π stacking between SeDA and bt ligand (C_3Nplane) (interplane distance 3.308(5)Å)
Se2D···Pt2	3.5070(9) (0.96)	$(C_2N_2Se)_{plane\ centroid}$–Se2D–Pt2 101.17(13)	π-(Se)-hole···Pt contact, supported by π–π stacking between SeDA and bt ligand (C_3Nplane) (interplane distance 3.284(5) Å)
Se3D–C_6H_4plane	3.299(4)		π-(Se)-hole···C_6H_4plane contact between SeDA-3 and C_6H_4 from bt ligand

[a]Normalized contact (Nc) is defined as the ratio between the separation observed in the crystal and $\sum_{vdW}$ of interacting atoms: Nc = d/$\sum_{vdW}$; $\sum_{vdW}$(Se+Pt) = 3.65 Å, $\sum_{vdW}$(Se+N) = 3.45 Å, $\sum_{vdW}$(Se+Cl) = 3.65 Å, $\sum_{vdW}$(Se+S) = 3.70 Å, $\sum_{vdW}$(Se+C) = 3.60 Å.

Table S3. Parameters of short intermolecular contacts (other than HBs) in the crystal structure of

1·3TeDA·THF.

Contact	Distance, Å (Nc[a])	Angle, °	Other parameters and comments
Te3D···O1S	2.744(4) (0.77)	N9D–Te1D– O1S 159.05(14)	Te···O ChB with TeDA-3 donor
Te3D···N5D	2.694(4) (0.75)	N1D–Te3D– N10D 153.16(4)	Te···N ChB with TeDA-3 donor
Te1D···N9D	2.729(4) (0.76)	N9D–Te2D– N2D 152.44(13)	Te···N ChB with TeDA-1 donor
Te1D···N5D	2.671(4) (0.74)	N5D–Te2D– N1D 151.80(14)	Te···N ChB with TeDA-1 donor
Te2D···N2D	2.651(4) (0.73)	N2D–Te2D– N6D 150.98(13)	Te···N ChB with TeDA-2 donor
Te2D···N6D	2.726(4) (0.76)	N6D–Te2D– N10D 150.77(13)	Te···N ChB with TeDA-2 donor
Te1D···Pt1	3.3767(4) (0.89)	$(C_2N_2Te)_{plane\ centroid}$–Te1D– Pt1 93.99(6)	π-(Te)-hole···Pt contact, supported by π-π stacking between TeDA and bt ligand (C_3Nplane) (interplane distance 3.242(3)Å)
Te1D···Pt2	3.5636(4) (0.94)	$(C_2N_2Te)_{plane\ centroid}$–Te1D– Pt2 92.36(6)	π-(Te)-hole···Pt contact, supported by π-π stacking between TeDA and bt ligand (C_3Nplane) (interplane distance 3.295(3) Å)
Te3D–C_6H_{4plane}	3.316(2)		π-(Te)-hole···C_6H_{4plane} contact between TeDA-3 and C_6H_4 from bt ligand

[a]The Normalized contact (Nc) is defined as the ratio between the separation observed in the crystal and $\sum_{vdW}$ of interacting atoms: Nc = d/$\sum_{vdW}$; $\sum_{vdW}$(Se+Pt) = 3.81 Å, $\sum_{vdW}$(Te+N) = 3.61 Å, $\sum_{vdW}$(Te+O) = 3.58 Å.

*1.2. Structural features of **2**·2SeDA·2H$_2$O·CH$_2$Cl$_2$*

Table S4. Parameters of short intermolecular contacts (other than HBs) in the crystal structure of **2**·2SeDA·2H$_2$O·CH$_2$Cl$_2$.

Contact	Distance, Å (Nc[a])	Angle, °	Other parameters and comments
Se1D···N1D	2.916(3) (0.85)	N1D–Se1D–N2D 165.26(12)	Se···N ChB
Se1D···O1S	2.758(5) (0.81)	O1S–Se1D–N1D 172.85(13)	Se···O ChB
Pt1···Se1D	3.3661(6) (0.92)	(C$_2$N$_2$Se)$_{plane\ centroid}$–Se1D–Pt1D 104.19(6)	πh(Se)···Pt contact, supported by π–π stacking between C$_2$N$_2$Se and *o*-C$_6$H$_4$ from bt ligand (interplane distance 3.387(3)Å)
C$_2$N$_2$Se$_{plane}$– C$_6$H$_4$$_{plane}$	interplane distance 3.419(3)		π–π stacking between C$_2$N$_2$Se and C$_6$H$_4$ from bt ligand, accompanied by the Se···(C,S) contact (interatomic distances ca. 3.70 Å)

[a]Normalized contact (Nc) is defined as the ratio between the separation observed in the crystal and $\sum_{vdW}$ of interacting atoms: Nc = d/$\sum_{vdW}$; $\sum_{vdW}$(Se+Pt) = 3.65 Å, $\sum_{vdW}$(Se+N) = 3.45 Å, $\sum_{vdW}$(Se+O) = 3.42 Å, $\sum_{vdW}$(Se+S) = 3.70 Å, $\sum_{vdW}$(Se+C) = 3.60 Å.
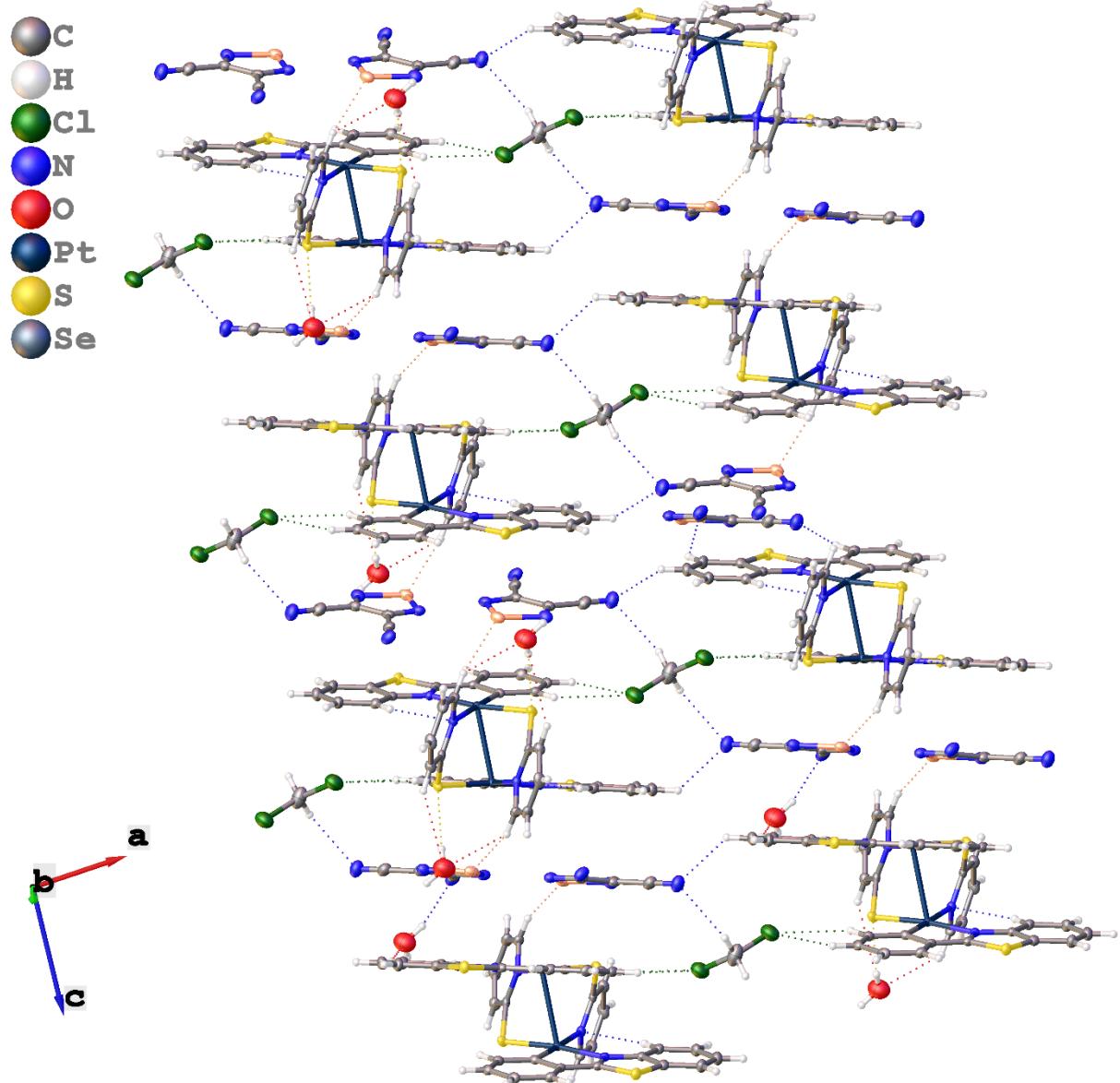
Figure S3. A fragment of the crystal packing of **1**·3SeDA·CH_2Cl_2 illustrating the occurrence of
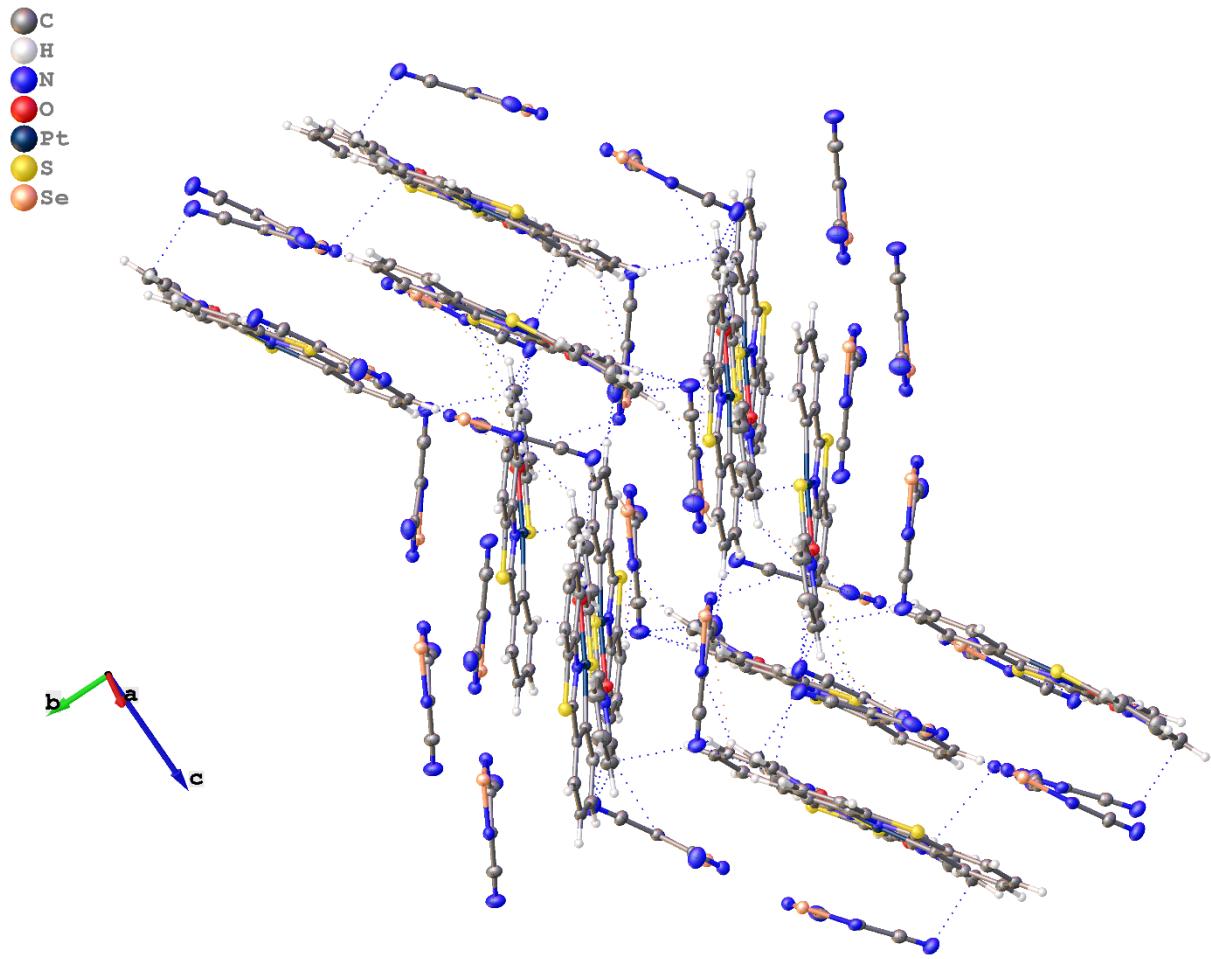
the 3D-network.

Figure S4. A fragment of the crystal packing of **3**·2SeDA illustrating the occurrence of the 3D-network.
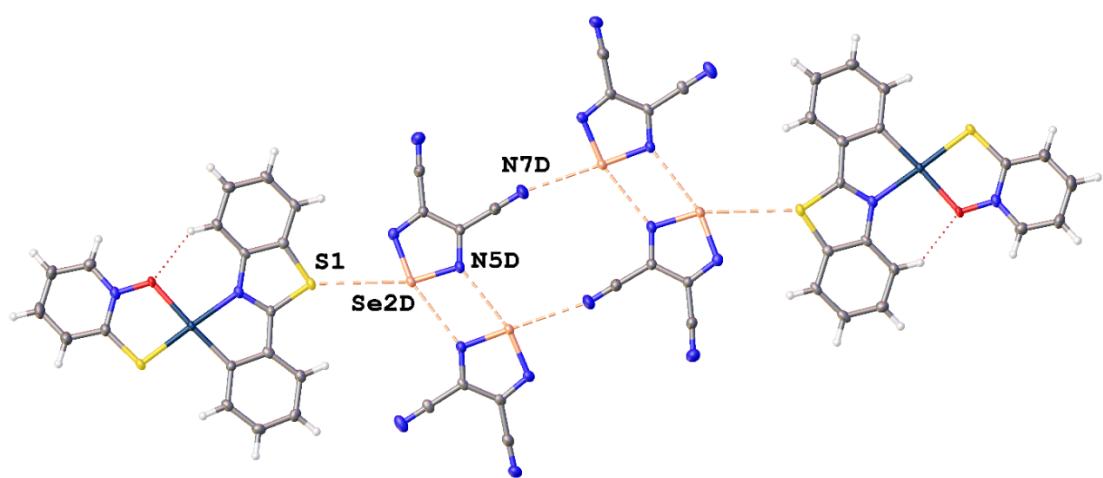

Figure S5. View of the supramolecular heterohexamer in the crystal structure of **3**·2SeDA.

Table S5. Parameters of short intermolecular contacts (other than HBs) in the crystal structure of

3·2SeDA.

Contact	Distance, Å (Nc^a)	Angle, °	Other parameters and comments
Se1D···N5D	2.813(3) (0.82)	N1D–Se1D–N5D 162.56(10)	Se···N ChB
Se2D···N2D	2.911(3) (0.84)	N6D–Se2D–N2D 162.85(10)	Se···N ChB
Se1D···N7D	2.965(3) (0.86)	N2D–Se1D–N7D 177.86(11)	Se···N ChB
Se2D···S1	3.5301(8) (0.95)	N5D–Se2D–S1 164.17(10)	Se···S ChB
Se2D···Pt1	3.3737(4) (0.92)	(C$_2$N$_2$Se)$_{plane\ centroid}$–Se2D–Pt1 89.24(5)	π-(Se)-hole···Pt contact, supported by π–π stacking between SeDA and OPyt ligand (S2–C5D distance 3.321(3) Å)

^{a}The Normalized contact (Nc) is defined as the ratio between the separation observed in the crystal and $\sum_{vdW}$ of interacting atoms: Nc = d/$\sum_{vdW}$; $\sum_{vdW}$(Se+Pt) = 3.65 Å, $\sum_{vdW}$(Se+N) = 3.45 Å, $\sum_{vdW}$(Se+S) = 3.70 Å.

Table S6. Pt–Pt bond lengths.

Complex	Pt–Pt, Å
1	2.9327(4)
	2.9202(4)
2	2.8764(4)
1·3TeDA·THF	2.9572(3)
1·3SeDA·CH$_2$Cl$_2$	2.9463(4)
2·4SeDA·H$_2$O	2.9064(8)

2. Computational details

*2.1. Calculations of interaction energy for the Pt···Ch contact in [**1**·TeDA]*

Apart from the Te···Pt bonding, in structure [**1**·TeDA], a short contact (Å) and corresponding BCP were detected between Te and an H atom of one of the imidazolethiole ligands (Figure S8,a). Therefore, the $\Sigma E_{int}^{SM} - E_{int}(C \cdots C/S)^{SM}$ difference for this structures is the sum of interaction energies of the Te···Pt and H···Te bonds, $E_{int}(Te \cdots Pt)$ and $E_{int}(H \cdots Te)$, respectively. The $E_{int}(H \cdots Te)$ value of –1.2 kcal/mol was calculated using the formula of Espinosa, Molins and Lecomte[1] ($E_{int}(H \cdots Te)^{EML} \approx 0.5V_b$). The interaction energy for the separate Te···Pt bond given in Table 4 was calculated as $E_{int}(Te \cdots Pt)^{SM} = \Sigma E_{int}^{SM} - E_{int}(C \cdots C/S)^{SM} - E_{int}(H \cdots Te)^{EML}$.

2.2. MEP and geometric parameters of optimized clusters

Wave-function calculations for the QTAIM, IGMH and NOCV analyses were carried out at the DFT PBE0-D3BJ/ZORA-def2-TZVP level of theory for the clusters (a) and (b) (Figure S12a. c) using crystallographic coordinates.
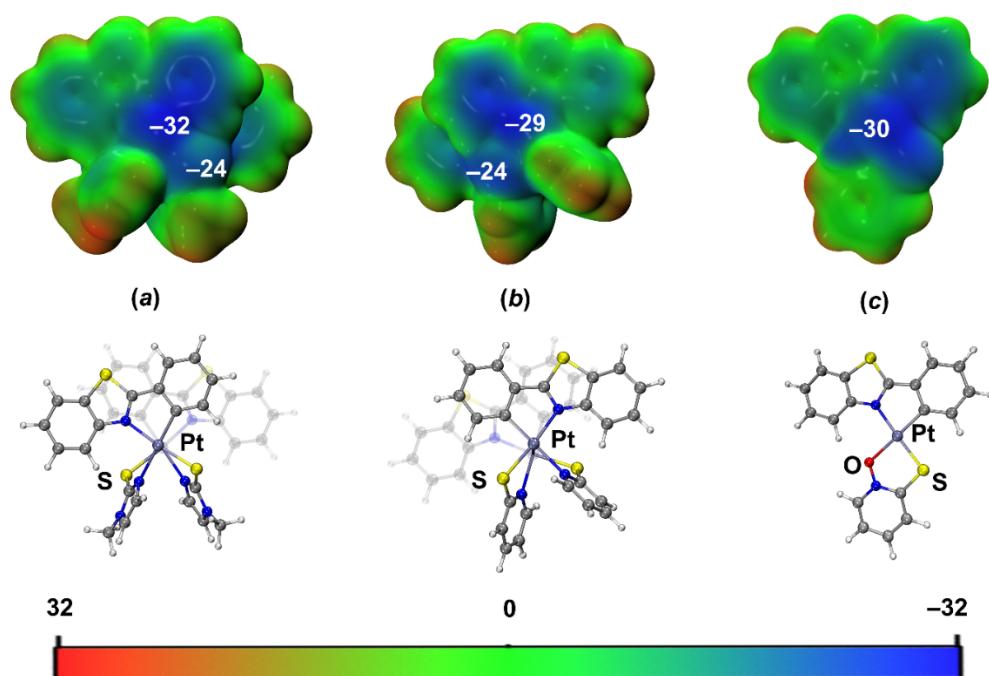
Figure S6. MEP distribution in **1**–**3** calculated for the optimized structures at the PBE0-D3BJ/ZORA-def2-TZVP level of theory (MEP values in kcal/mol).

Approaches to characterize the positive area of ChDA

Analysis of the literature focused on ChDA indicates that there is no single terminology for characterization of the positive area ($V_{s,max}$ of +45 (Se) and +51 (Te) kcal/mol; Figure S7) on ChDA. This region is characterized by different terms depending on the identity of interacting atom, geometry, and also molecular orbitals involved. Politzer and coauthors[2, 3] classified this

region as π-hole because the electron density depletion region is located at the position of the π* orbital of ChDA. Notably, the π* orbital of ChDA is delocalized over the entire molecule, but the Ch site makes a significant contribution to the formation of the π* orbital.[4]

According to Ibrahim and Telb,[5] this region can be perceived as a lp-hole, since the positive region is located on the opposite side to the electron lone pair. Anther terminology is based on the molecular orbitals involved. Kozuch and coauthors[6] suggested that interactions with a region of lower electron density (which are perpendicular to the planar fragments of the molecular framework) should be referred to as π-hole due to the interacting empty p-orbitals. Considering that electron density depletion region is located at the π* orbital of ChDA, the π-hole terminology perhaps is the most accurate (or the most common) to describe the interaction occurred between of the platinum complex with ChDA and we use this terminology in our report.
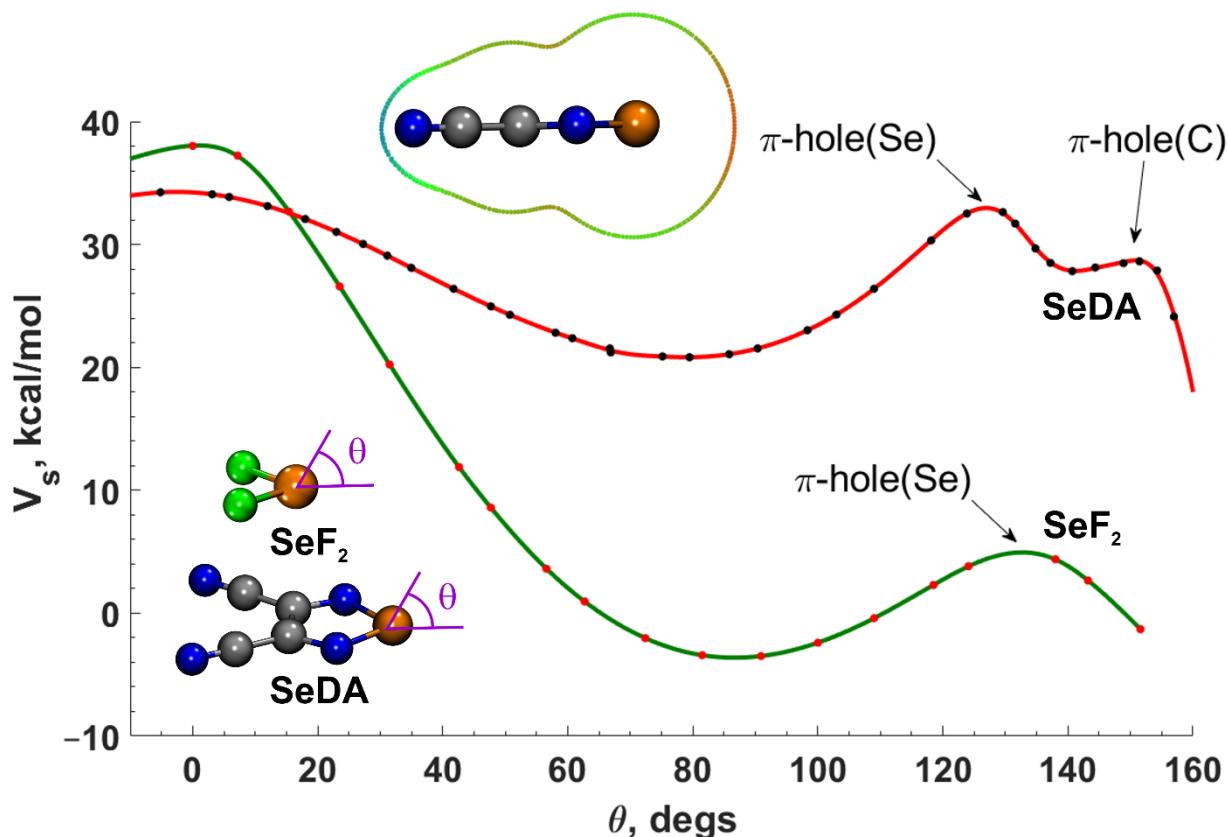
Figure S7. Dependence of the MEP value *vs.* angle θ for SeDA and SeF$_2$ (0.001 a.u. isosurface of the electron density). Inset: MEP plot around the SeDA molecule in the plane passing via the Se atom and the middle point of the C–C bond of the diazole cycle (blue-green-red color scale –35 < V$_s$ < 55 kcal/mol).
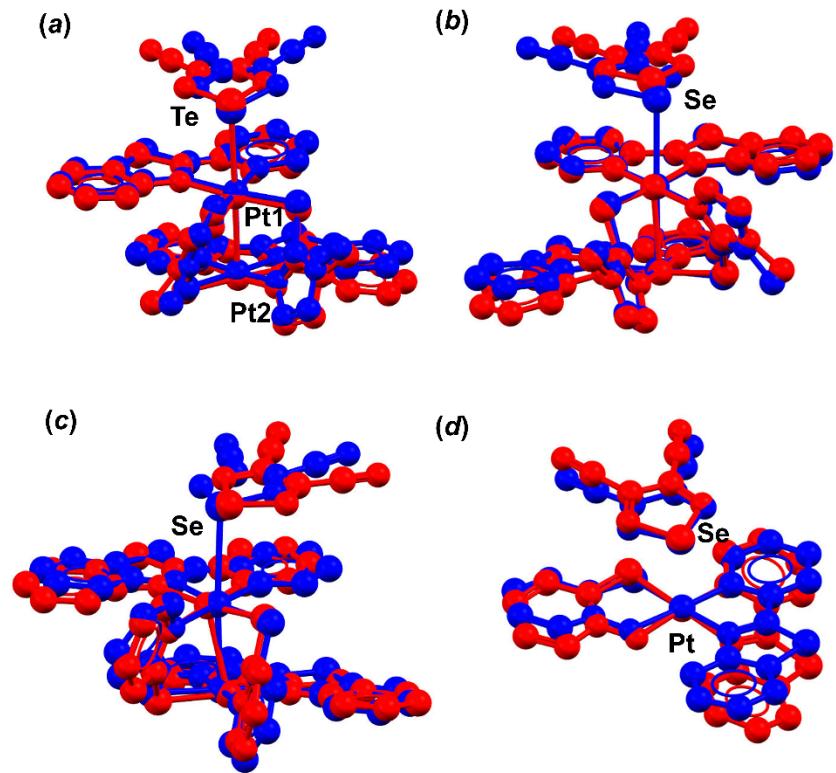
Figure S8 Overlay images for (a) [**1**·TeDA]; (b) [**1**·SeDA]; (c) [**2**·SeDA]; (d) [**3**·SeDA] of X-ray geometry (blue) and its optimized (red) computational clusters.

Table S7. Geometric parameters of optimized clusters.

Clusters	d(Ch$\cdots$Pt), Å	$\angle$(M–M–Ch),°
[**1**·TeDA]	3.377	178
[**1**·SeDA]	3.507	166
[**2**·SeDA]	3.366	156
[**3**·SeDA]	3.374	–

(a)   (b)

(c)   (d)
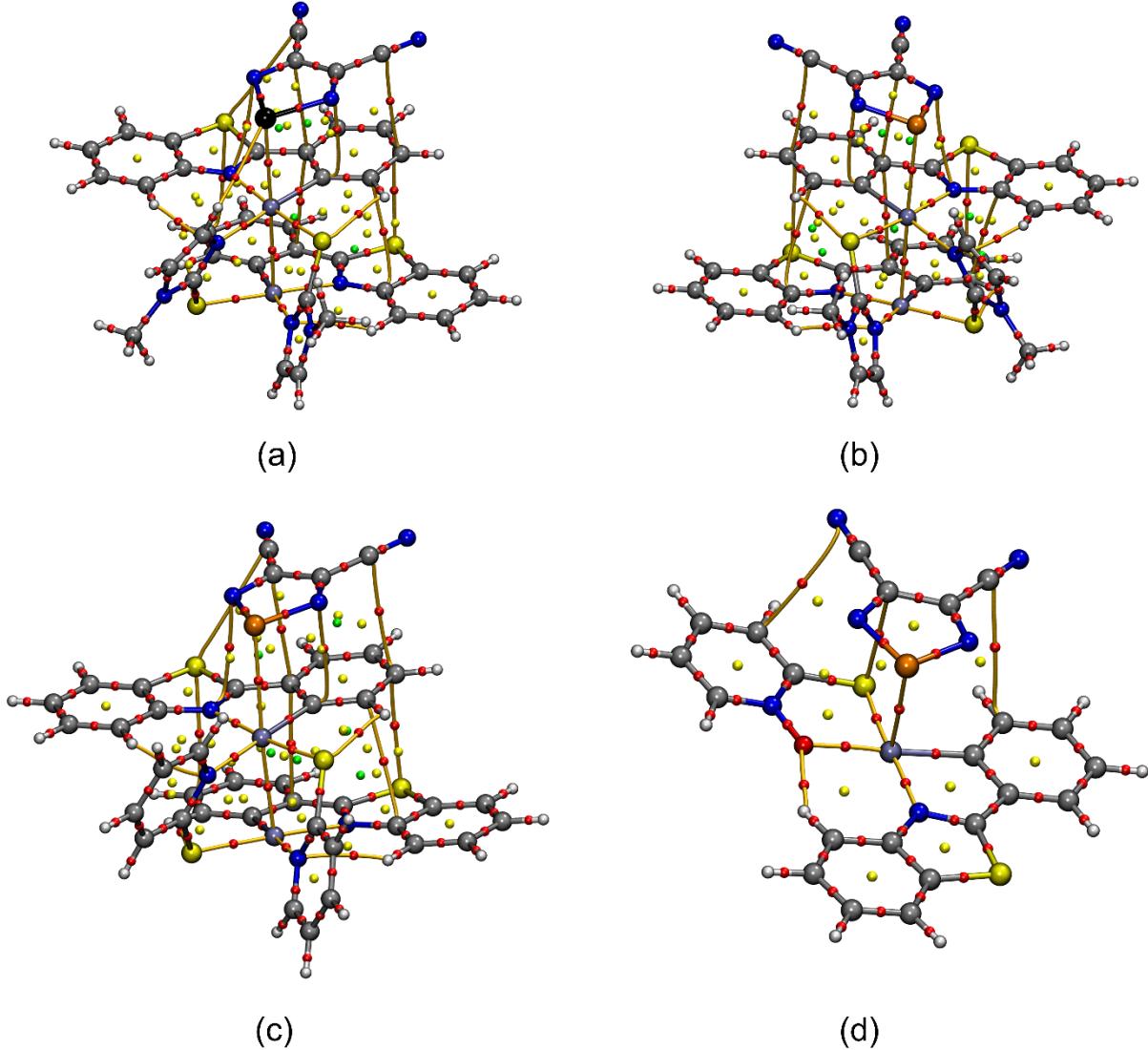
Figure S9. QTAIM distribution of bond, ring, and cage critical points (red, yellow, and green spheres, respectively) and bond paths for (a) [**1**·TeDA]; (b) [**1**·SeDA]; (c) [**2**·SeDA]; (d) [**3**·SeDA].

Table S8. Electron density (ρ_b), its Laplacian ($\nabla^2\rho_b$), potential and kinetic energy densities (V_b and G_b), second eigenvalue of the Hessian matrix (λ_2), elliptical bond index (ε), electron localization function at BCPs (in a.u.), and IBSI calculated at the PBE0-D3BJ/ZORA-def2-TZVP level of theory.

| Contact	Clusters	ρ_b	$\nabla^2\rho_b$	V_b	G_b	ε	λ_2	ELF	IBSI
Te···Pt	[**1**·TeDA]	0.0422	0.055	−0.0277	0.0207	0.03	−0.0293	0.33	0.0729
Se···Pt	[**1**·SeDA]	0.0344	0.0635	−0.0223	0.0191	0.05	−0.0247	0.23	0.0561
Se···Pt	[**2**·SeDA]	0.0277	0.0528	−0.0162	0.0147	0.07	−0.0184	0.20	0.0432
Se···Pt	[**3**·SeDA]	0.0196	0.0418	−0.0108	0.0106	0.02	−0.0126	0.13	0.0290
Pt···Pt	[**1**·TeDA]	0.0440	0.092	−0.038	0.0305	0.01	−0.0328	0.21	0.0752
Pt···Pt	[**1**·SeDA]	0.0442	0.0977	−0.0395	0.0319	0.01	−0.0329	0.20	0.0771
Pt···Pt	[**2**·SeDA]	0.0508	0.1148	−0.0504	0.0396	0.01	−0.0386	0.20	0.0930
NC···C	[**1**·TeDA]	0.0048	0.0159	−0.0021	0.003	0.89	−0.0011	0.02	0.0054

NC···C	[**1**·SeDA]	0.0047	0.0155	−0.0021	0.003	1.63	−0.0009	0.02	0.0052
NC···C	[**2**·SeDA]	0.0049	0.0164	−0.0022	0.0031	0.61	−0.0013	0.02	0.0055
NC···C	[**3**·SeDA]	0.0034	0.012	−0.0015	0.0022	0.37	−0.0011	0.01	0.0066
C···C	[**1**·TeDA]	0.0078	0.0248	−0.0039	0.0051	0.28	−0.0025	0.03	0.0092
C···C	[**1**·SeDA]	0.0078	0.0248	−0.0039	0.005	0.04	−0.0028	0.03	0.0089
C···C	[**2**·SeDA]	0.0080	0.0257	−0.0041	0.0053	0.44	−0.0024	0.03	0.0095
C···S	[**3**·SeDA]	0.0108	0.0296	−0.0052	0.0063	0.46	−0.0041	0.05	0.0144

2.3. ETS-NOCV/CDF
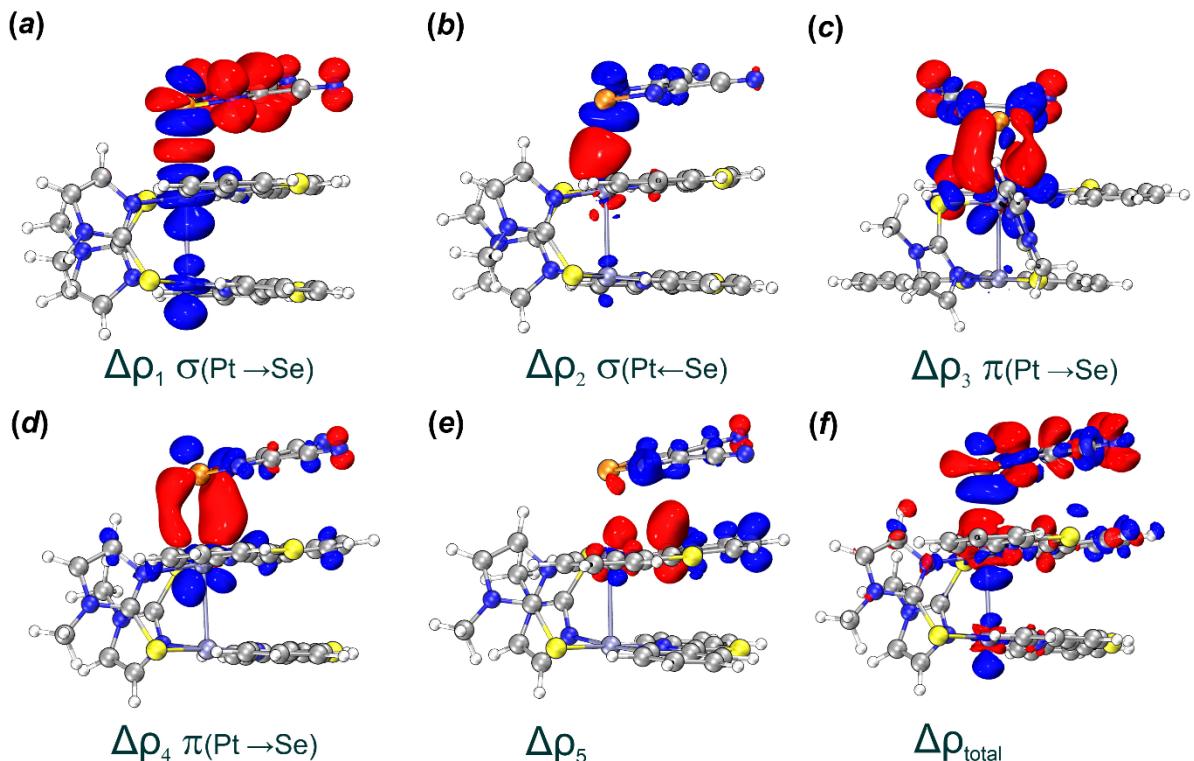
Figure S10. ETS–NOCV deformation densities for [**1**·SeDA]. Electron transfer occurs from regions of the electron density depletion (blue) to those of the electron density concentration (red) (isovalues 0.0005 (*a*, *d*, *e*), 0.001 (*b*), 0.0002 (*c*) and 0.002 (*f*) a.u.).
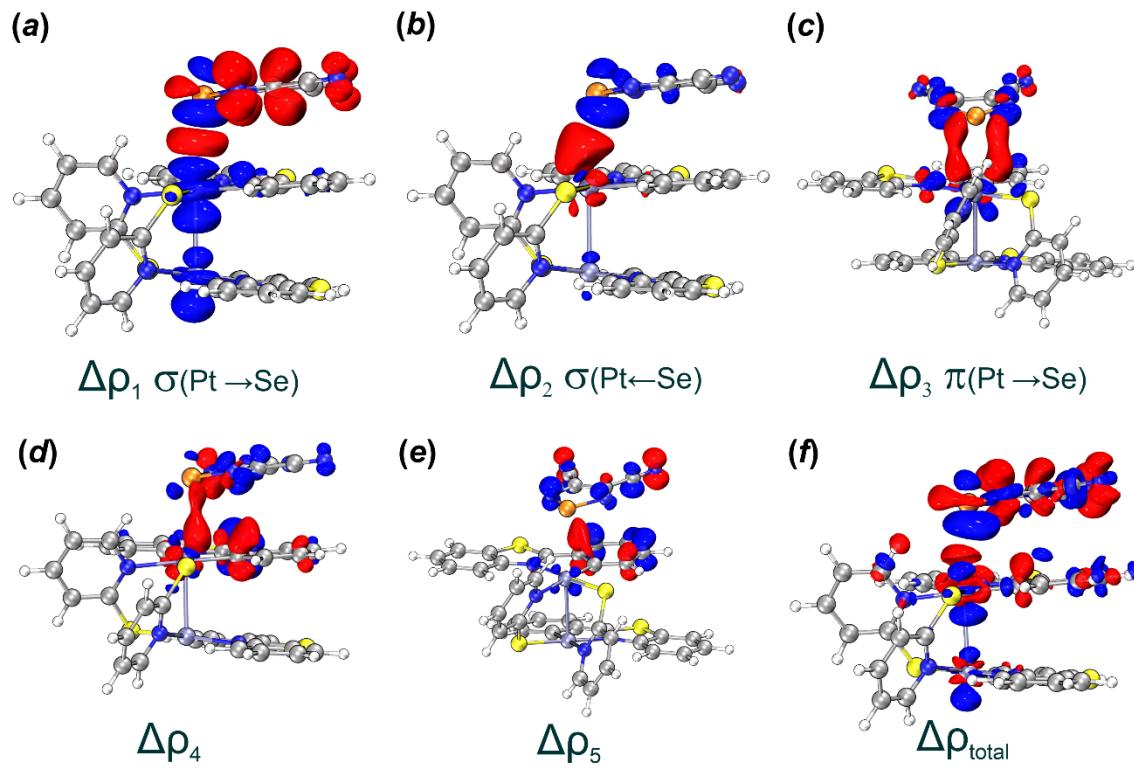
Figure S11. ETS–NOCV deformation densities for [**2**·SeDA]. Electron transfer occurs from regions of the electron density depletion (blue) to those of the electron density concentration (red) (isovalues 0.0005 (*a*, *d*, *e*), 0.001 (*b*), 0.0002 (*c*) and 0.002 (*f*) a.u.).
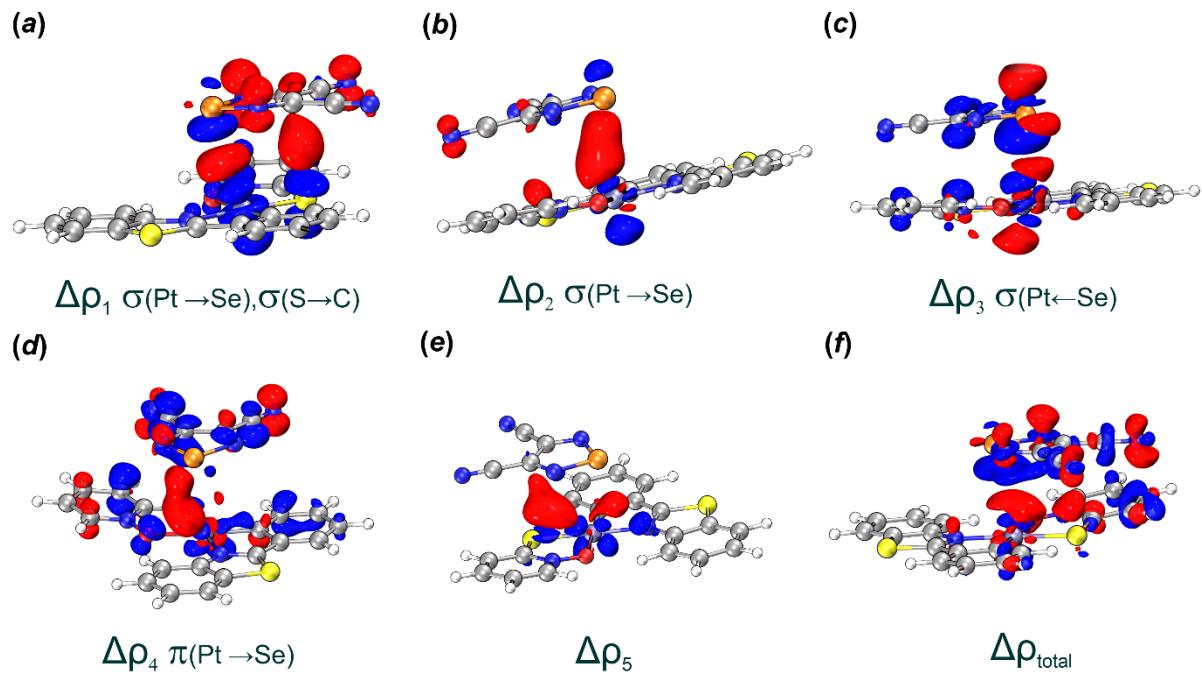

Figure S12. ETS–NOCV deformation densities for [**3**·SeDA]. Electron transfer occurs from regions of the electron density depletion (blue) to those of the electron density concentration (red) (isovalues 0.0005 (*a*, *d*, *e*), 0.001 (*b*), 0.0002 (*c*) and 0.002 (*f*) a.u.).
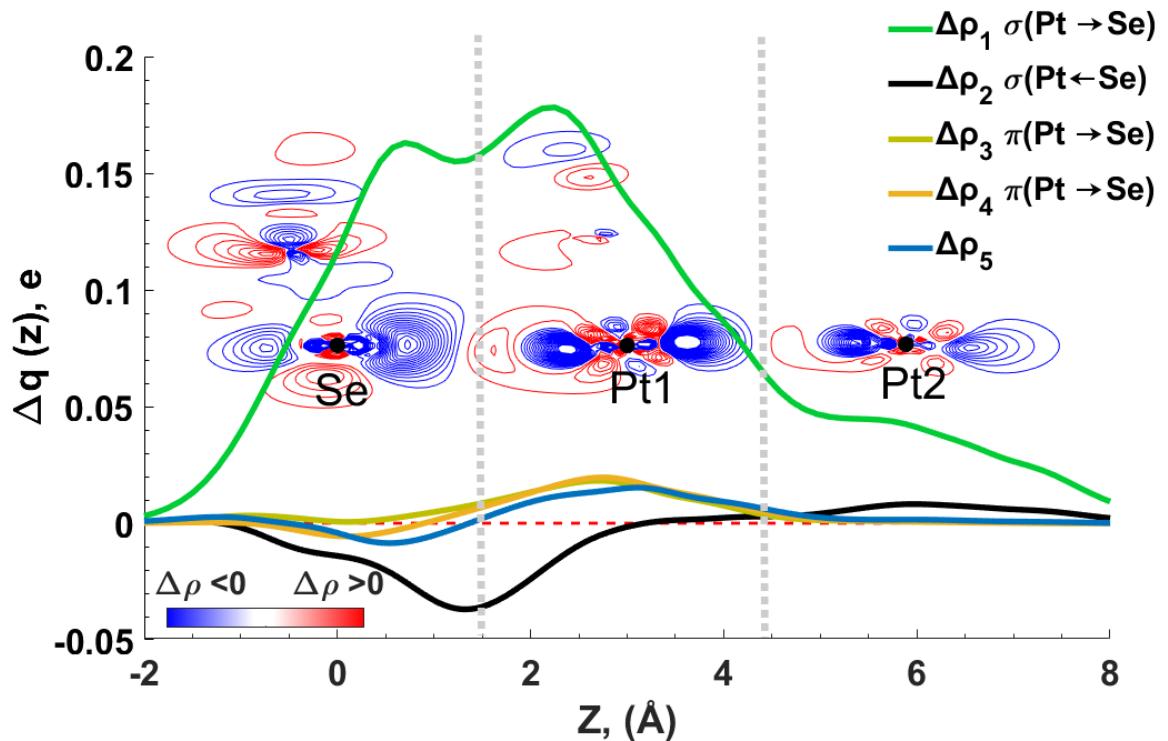
Figure S13. EDD contour plot (red – charge concentration, blue – charge depletion, range – 0.01 to 0.01 a.u., step 0.0005 a.u.) and CDF functions for the Se···Pt interaction in [**1**·SeDA] (black dots indicate positions of the atomic nuclei, grey vertical lines identify the boundaries between the Se, Pt2 and Pt1 atoms, which are placed along the *z* axis).
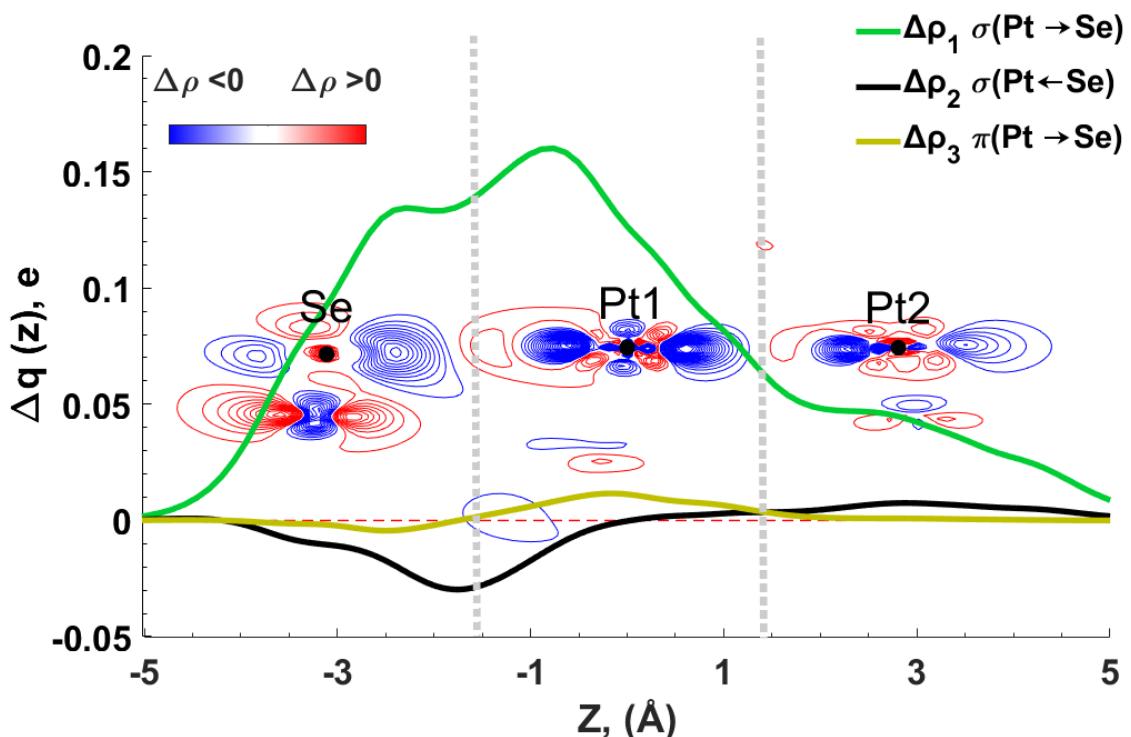
Figure S14. EDD contour plot (red – charge concentration, blue – charge depletion, range – 0.01 to 0.01 a.u., step 0.0005 a.u.) and CDF functions for the Se···Pt interaction in [**2**·SeDA] (black dots indicate positions of the atomic nuclei, grey vertical lines identify the boundaries between the Se, Pt2 and Pt1 atoms, which are placed along the *z* axis).
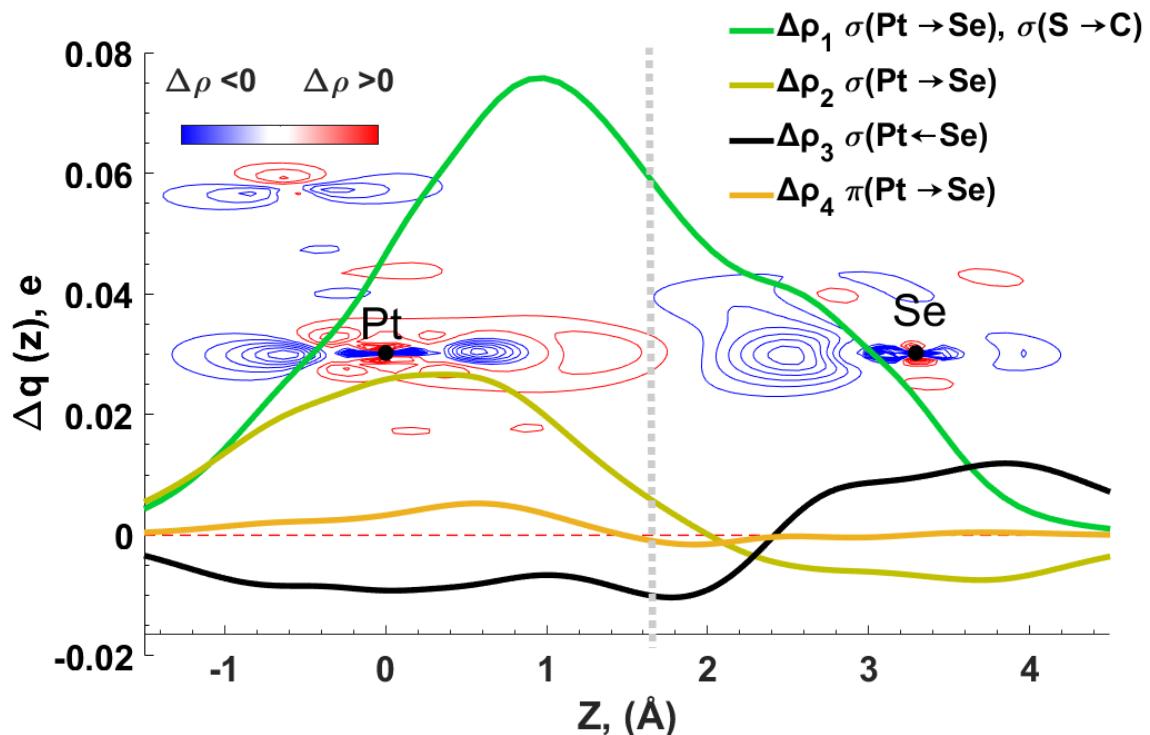
Figure S15. EDD contour plot (red – charge concentration, blue – charge depletion, range – 0.01 to 0.01 a.u., step 0.0005 a.u.) and CDF functions for the Se···Pt interaction in [**3**·SeDA] (black dots indicate positions of the atomic nuclei, grey vertical lines identify the boundaries between the Se and Pt1 atoms, which are placed along the z axis).
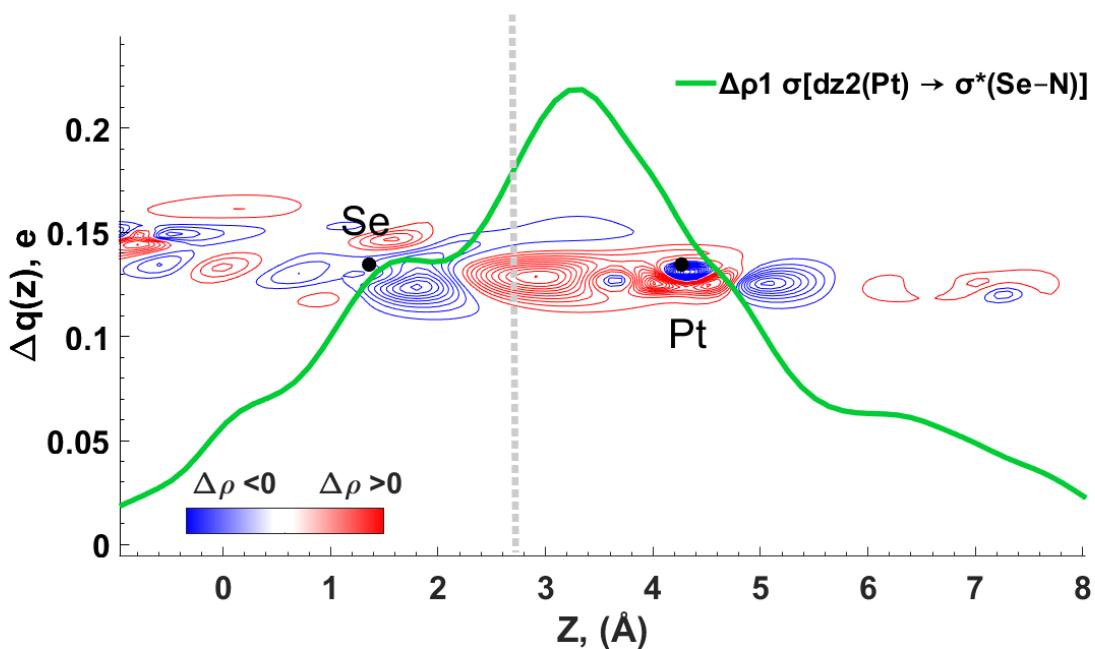
Figure S16. EDD contour plot (red – charge concentration, blue – charge depletion, range – 0.01 to 0.01 a.u., step 0.0005 a.u.) and CDF functions for the Se···Pt interaction in [**1**·SeDA]σ (black dots indicate positions of the atomic nuclei, grey vertical lines identify the boundaries between the Se and Pt1 atoms, which are placed along the z axis).

3. Cartesian coordinates for the studied molecules

Optimized geometries

*Cartesian coordinate for 1 (in Å)*

```
Pt  8.98115936952892   10.22477292723849    5.37399906226541
Pt  6.03631320474285   10.28225766274412    5.40631057592790
S   6.10089353839408    9.90194107074395    7.67510267126854
S   9.18390831991478   14.66143418445319    6.00691628871118
S   8.88735500844339    8.23176001505016    4.22671559744231
S   5.90188556016938   12.61448176023159    1.57558870743911
N   5.87810111497743   10.80433495722188    3.40906692649215
N   9.16486083165124   12.09567122800622    6.24130702285079
N   7.18422595587562    6.21104308795936    4.87193769442972
N   6.28930148065299    8.19208439959585    5.17713035549511
N   8.68652871554546    9.08122801635977    7.13171686357915
N   7.74735948516609    8.07880789155306    8.84383567957018
C   5.84958233527972   12.25404998486364    5.60802015231947
C   5.80770042033314   12.97138298914796    4.38227857989104
C   5.81237860920049   13.02949728577265    6.77769591549643
H   5.87411943085939   12.53780206941709    7.74743557431187
C   9.20225774918494   11.31753977268652    3.72444519808193
C   9.26552374005539   12.71892647649809    3.94986100286966
C   5.71537318838808   14.41912496791302    6.72358758232792
H   5.68508043999389   14.98543658017293    7.65461296820059
C   9.12077318880867   12.57386611833686    7.53629841299858
C   5.91800589309177   10.10683470180071    2.21771177106986
C   5.85845623347181   12.11351924034602    3.22964767542884
C   9.10886818515616   13.98452458248568    7.60615549215159
C   9.04039599528748   14.66170011478498    8.82281933025237
H   9.02263462122406   15.74935655185939    8.85565950387718
C   9.10469549534549   11.83186874081181    8.72278130799985
H   9.15289266848115   10.75042248101522    8.67699223890803
C   7.40119655603938    7.55472196848491    4.79772313226594
C   5.72560982160316   14.36909113355512    4.32149392036170
H   5.70432586391409   14.87665295849427    3.35627954324013
C   9.02642233675994    7.57321806638935    8.73673545791989
H   9.41040058910902    6.82903987840743    9.42306907731754
C   9.03893145918057   12.50569878671195    9.93420268378732
H   9.02126412811596   11.93267114421576   10.85954939154023
C   5.89471447399998    6.00326670986060    5.31593536953951
H   5.48514322212805    5.00994662401105    5.44954828987271
C   9.24291425009704   10.90645299910517    2.38277775380381
H   9.16539936663815    9.84636761524715    2.14583318770324
C   5.91204086968519    8.71899308186221    2.03794783110677
H   5.84822633566053    8.06901204929071    2.90241783813732
C   9.20820551755536   13.06505856460339    5.34412813352122
C   5.95110007219382   10.94800812893074    1.08357155841019
C   9.59065735390111    8.19437052355589    7.65890786249529
H  10.57425661758985    8.06991119204089    7.22359189152240
C   6.03896394716827    9.05566796778956   -0.36872453436285
H   6.09426740840628    8.62961843977289   -1.36887792793021
C   5.35815447175885    7.24336890927663    5.51609175261699
H   4.37695772794026    7.52395714470296    5.87801987621555
C   5.67068834890011   15.09848075397798    5.50023335424175
H   5.60354516723760   16.18455921241033    5.47359566478984
C   5.97656996027622    8.20949643431932    0.74872249873317
H   5.97703640912902    7.13057551009283    0.60430501025481
C   8.15435329799706    5.19606817999937    4.54984761235296
H   8.10925961617522    4.91827131251217    3.48954791922610
H   7.97281455403305    4.30864426156451    5.16309375862398
H   9.15340309603251    5.59136783708323    4.76176851253878
C   6.01835811940940   10.43653865960825   -0.21157175856359
H   6.05240645156474   11.10111011995153   -1.07271319882446
C   9.37108902259402   13.65255689246163    2.91006432641967
H   9.40809116174711   14.71988723775107    3.13173287586494
C   8.99713264474829   13.90707428544073    9.98921901423282
H   8.94028776786108   14.41027937220797   10.95278080143345
C   7.56385902001240    8.99542886978776    7.85183717733555
C   9.36263718395432   11.82956513993255    1.34501342247095
H   9.39449136491313   11.47019018914079    0.31629826663776
C   6.75691200594815    7.70659088671575    9.82138882815044
H   6.90974455936194    6.66514090752825   10.11899257602537
H   5.76528118932885    7.81848094096971    9.37039350638136
H   6.80780355502223    8.34770026388880   10.71010473918233
```
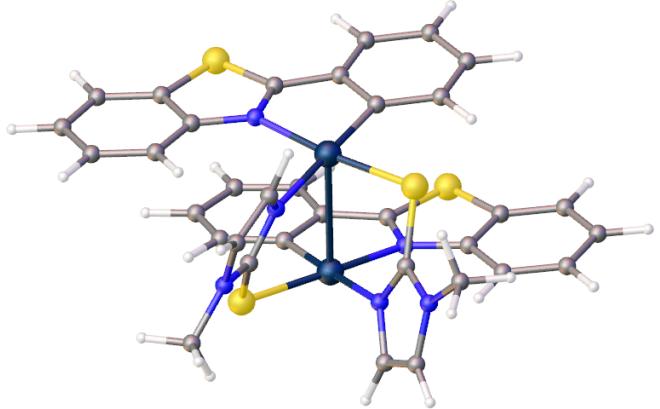
| C | 9.42818035479032 | 13.20496654806639 | 1.59827252106388 |
| H | 9.51294198029420 | 13.91440243920976 | 0.77711733068650 |

*Cartesian coordinate for **2** (in Å)*

Pt	2.14681929988971	5.19963126229465	11.56677900474681
S	4.89587751985478	6.44921034458565	9.68698242579281
S	4.40395978798268	1.50209191462885	12.75900162712820
N	3.56372013287805	3.90877061266672	12.37814389545727
N	3.22491177683261	7.04589281202999	11.74948337187799
C	1.14571944074902	3.48828036978855	11.41013930186430
C	5.52827763470767	5.23852625865407	13.15921960920502
H	5.04477120115081	6.19409005631952	12.99964626879822
C	2.80005461403522	7.85318787218460	12.73962965724
H	1.91799973291938	7.50280471641038	13.27217217381687
C	1.88510576847566	2.33444864779483	11.77930678172980
C	3.20052154003799	2.64241006337117	12.27002309378424
C	5.47827010442598	2.81531174356420	13.13772132288318
C	6.82291890548139	5.16815138979716	13.65344891383029
H	7.35805044837764	6.09136182476729	13.86794319067538
C	6.78000234854438	2.74373411808899	13.63216511931096
H	7.25326198747813	1.78180621158035	13.81944522955715
C	4.28198574598989	7.41488616992679	10.99172735177480
C	-0.15422173224622	3.26537494709635	10.92912891289295
H	-0.75968596203372	4.11164076593935	10.60887383832529
C	3.43314247080792	9.03271742362016	13.08135671062410
H	3.05350483607280	9.63793923963923	13.90021149455096
C	4.97514681423289	8.60885201890447	11.29402178042009
H	5.82438488994821	8.88064564426033	10.67150575506535
C	0.07589871027631	0.85617106267331	11.19933865819378
H	-0.34330613583381	-0.14422465693609	11.10925139382223
C	4.84379144088259	4.05057038466603	12.87802957405377
C	1.36846097306949	1.03609923673861	11.66883606189181
H	1.97848891314853	0.17719001691006	11.95079937626102
C	-0.67910214384634	1.97789109969746	10.83521540755005
H	-1.69341760200806	1.84459173460314	10.45884399582605
C	7.45124891193846	3.93477378270529	13.88171782327956
H	8.46929140505388	3.90782497201010	14.26588656707767
C	4.56200079801976	9.40789211235794	12.34072891715387
H	5.09768787805914	10.32787765257193	12.57126402480931
Pt	3.14791204365229	5.19526405130659	8.90764117025490
S	0.40145174396551	6.45516766766847	10.78452349002161
S	0.88266625958176	1.49954247502306	7.72509022205672
N	1.72818389123422	3.90536001776246	8.09964385469669
N	2.07334473115111	7.04336050105545	8.72023062364429
C	4.14533957129749	3.48217287472034	9.06869528486522
C	-0.23335199330654	5.23736715306975	7.31520335047397
H	0.25211938851481	6.19229373619598	7.47206094713201
C	2.49946738850752	7.84730284727774	7.72792974709356
H	3.38102232710978	7.49405415155618	7.19640504732266
C	3.40345258218605	2.32898346106678	8.70250534137291
C	2.08870362758288	2.63849563560093	8.21090851463120
C	-0.18884384189740	2.81411714104983	7.34311387321491
C	-1.52836247587260	5.16853976126695	6.82129884360355
H	-2.06145667132337	6.09236638125710	6.60440040975478
C	-1.49074515622094	2.74410462798548	6.84888690233112
H	-1.96610446537548	1.78272912688563	6.66410939764269
C	1.01689285457307	7.41608905725297	9.47704505971315
C	5.44461212484651	3.25769972773478	9.55077181521389
H	6.05182450480787	4.10347952823442	9.86898844530032
C	1.86817323584085	9.02683754794791	7.38290044485694
H	2.24870919097023	9.62924843581101	6.56239247557281
C	0.32558650658708	8.61031649928204	9.17149124445105
H	-0.52320985711029	8.88515584153129	9.79327061466009
C	5.20923296194722	0.84829387318897	9.28699032930779
H	5.62619272708087	-0.15277671199669	9.37996057920124
C	0.44835451018576	4.04865532588008	7.59955456886489
C	3.91724132976878	1.02980130317262	8.81652586853559
H	3.30538654237388	0.17148516228592	8.53672518628966
C	5.96657185657531	1.96930802727380	9.64842986994157
H	6.98040080505075	1.83475097412470	10.02567750109089
C	-2.15942110648400	3.93595861524568	6.59632102928665
H	-3.17755237969324	3.91023478985332	6.21230534423695
C	0.73987491112850	9.40576115058100	8.12251112685423
H	0.20557381516965	10.32590141593574	7.88939011882040
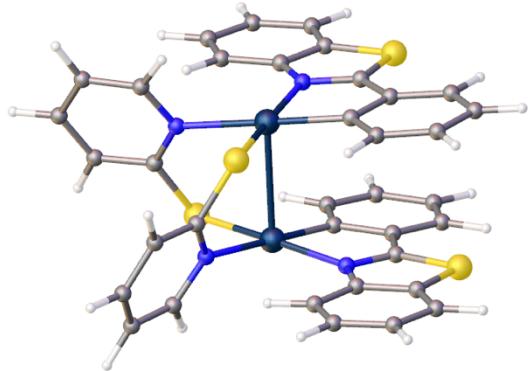
Cartesian coordinate for *3* (in Å)

```
Pt  2.17025712036107    5.42388330010266    5.44622044765857
S   1.70795197560401    3.48788313684309    6.49951368036642
S   4.30489254294749    9.12412103400521    4.08234069173766
O   0.26389428877037    5.17602746871481    4.62170913789370
N  -0.40024997269498    4.10412065972007    4.98442120666884
N   2.66853175423062    7.18429443767397    4.52480192500705
C   4.64123927237775    6.86613863473848    5.78599116160712
C  -1.63529258319139    3.93228873689767    4.45150828025939
H  -1.93331070892881    4.72410795664884    3.77115211637848
C   2.28089706742761   10.07250098290463    2.34643273628869
H   2.87033306641273   10.94420664228974    2.06901315216159
C   3.96453005762367    5.68810067847160    6.21079683433498
C  -1.89492635696483    1.88932084982454    5.66712074983844
H  -2.47989769144203    1.01345067115630    5.93944578081943
C  -0.63809215129911    2.07905808044324    6.20088823440394
H  -0.20314345785286    1.36800264623622    6.89942677108067
C   4.65656597864069    4.86955498643515    7.11776766417636
H   4.19688785210433    3.95153432995066    7.48205076912787
C   1.01673573004478    9.86059654975315    1.80746633875233
H   0.61140385057179   10.57876612099044    1.09700888858793
C   3.86482700770548    7.63753641838701    4.85647488410149
C   0.13757704490065    3.20590341426380    5.86226597370916
C   0.26102429907314    8.73382967020162    2.16753382413439
H  -0.72552937527625    8.59195050039191    1.72959384153097
C   0.74547245768095    7.79670482895124    3.07033046312332
H   0.17533272298376    6.91795327229699    3.36270873589968
C   2.77104080829966    9.13318185447242    3.25255438602427
C  -2.40678824335937    2.84088977464530    4.76913207255572
H  -3.39114757275094    2.73777831056560    4.32100710584545
C   2.01687269447520    7.99819797410356    3.61991846815631
C   5.93068196579248    5.20598388686265    7.56907094496305
H   6.43749206762904    4.54652519199038    8.27337720055535
C   5.92308397065201    7.20814900216034    6.23857137001714
H   6.40392093336989    8.12170238883331    5.88670544929546
C   6.57205823538907    6.37381050066937    7.13609052887794
H   7.56737334869225    6.62244510740382    7.49928908406072
```
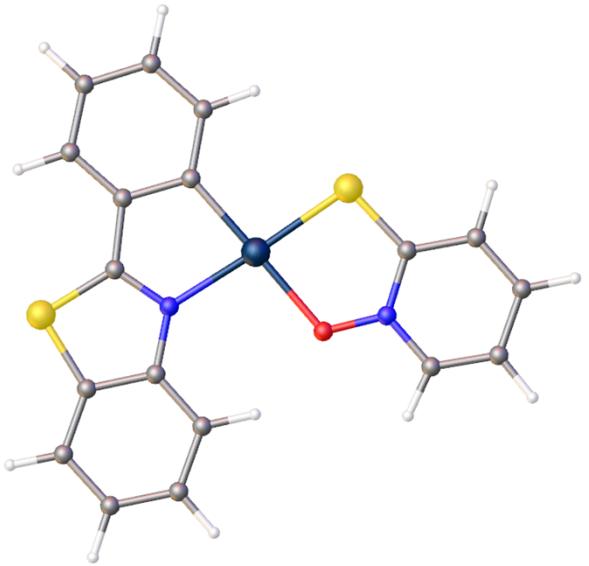
Cartesian coordinate for SeDA (in Å)

```
C  -4.04351316848341   -1.44071744283260   -18.70901409304277
C  -3.26314427647961   -0.60314190237007   -17.82439396773952
C  -4.08813233290198   -2.86292943936305   -18.59673422172011
C  -2.46779357113749   -1.12367133769676   -16.75962293396816
N  -4.72177855443991   -0.82544525212958   -19.63742828906329
N  -3.31857247504280    0.68063620968670   -18.04677751866981
N  -4.10527804949522   -4.00687738031934   -18.48248976921670
N  -1.83541826084158   -1.57108273736120   -15.90998666426330
Se -4.40355831117798    0.91924228238592   -19.44274054231619
```
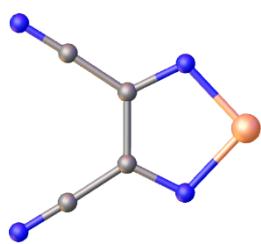
Cartesian coordinate for TeDA (in Å)

```
C  -4.04904230028160   -1.44123717808878   -18.71671060774761
C  -3.26094775962535   -0.59400256927070   -17.82141340956593
C  -4.06361943472294   -2.86544946930511   -18.56501101727771
C  -2.47629413093078   -1.16205789683470   -16.76630487618908
N  -4.74461042650576   -0.88848676179223   -19.66157703985354
N  -3.27577306541549    0.69177152539508   -17.99102300877943
N  -4.06250144699181   -4.00718419665821   -18.42679807511767
N  -1.85238559315225   -1.63796289452315   -15.92552176409678
Te -4.46201484237400    1.07062244107781   -19.53482820137200
```
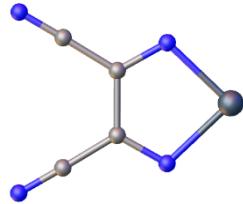
Cartesian coordinate for [*1*·TeDA] (in Å)

```
Pt   0.000000000    0.000000000    2.896409000
Pt   0.000000000    0.000000000    0.000000000
S   -2.300234000    0.233604000    0.073142000
S    0.417039000    4.461144000    3.148758000
```

|			
S	0.675990000	-2.211664000	2.827328000
S	4.293467000	1.277287000	-0.276358000
N	2.067283000	0.000017000	-0.129046000
N	-0.403176000	2.028301000	3.016096000
N	-0.524267000	-4.050950000	1.220504000
N	-0.334978000	-2.082681000	0.263073000
N	-1.977749000	-0.733624000	2.637193000
N	-3.870124000	-1.304338000	1.678388000
C	0.313993000	1.971733000	-0.143089000
C	1.679468000	2.344122000	-0.197457000
C	-0.626397000	3.007259000	-0.205550000
H	-1.689250000	2.778592000	-0.162942000
C	1.872882000	0.692721000	3.031896000
C	1.971921000	2.104779000	3.079958000
C	-0.221407000	4.335552000	-0.330825000
H	-0.976655000	5.117073000	-0.401874000
C	-1.555615000	2.784762000	3.066406000
C	3.033064000	-0.983447000	-0.181487000
C	2.576083000	1.219854000	-0.178388000
C	-1.295686000	4.171945000	3.122846000
C	-2.324913000	5.111717000	3.160518000
H	-2.106206000	6.177001000	3.197456000
C	-2.880601000	2.334444000	3.089524000
H	-3.088461000	1.271149000	3.081583000
C	-0.095769000	-2.769263000	1.384770000
C	2.091272000	3.679791000	-0.311062000
H	3.150912000	3.925919000	-0.374230000
C	-3.883181000	-1.850950000	2.942893000
H	-4.719815000	-2.430366000	3.312535000
C	-3.904260000	3.270380000	3.133220000
H	-4.937259000	2.927654000	3.149256000
C	-1.057975000	-4.169760000	-0.044049000
H	-1.462887000	-5.103223000	-0.414182000
C	3.072028000	-0.027510000	3.092819000
H	3.054686000	-1.114699000	3.054479000
C	2.848632000	-2.370764000	-0.198952000
H	1.846111000	-2.781329000	-0.182432000
C	0.694391000	2.764982000	3.059372000
C	4.342927000	-0.459055000	-0.247202000
C	-2.694967000	-1.502687000	3.519201000
H	-2.310589000	-1.764047000	4.496860000
C	5.263190000	-2.661018000	-0.282918000
H	6.121617000	-3.329169000	-0.315253000
C	-0.949132000	-2.935885000	-0.619318000
H	-1.280917000	-2.609003000	-1.596528000
C	1.133752000	4.679688000	-0.384290000
H	1.432969000	5.718758000	-0.501280000
C	3.965322000	-3.193245000	-0.247364000
H	3.829595000	-4.273176000	-0.258946000
C	-0.432605000	-5.093069000	2.213642000
H	0.519202000	-5.632254000	2.139832000
H	-1.258601000	-5.797125000	2.080792000
H	-0.496764000	-4.635230000	3.205922000
C	5.464470000	-1.286267000	-0.289599000
H	6.466758000	-0.864922000	-0.332986000
C	3.201919000	2.769652000	3.187048000
H	3.236725000	3.857182000	3.245926000
C	-3.634304000	4.647170000	3.158534000
H	-4.456530000	5.359539000	3.187546000
C	-2.697075000	-0.633150000	1.515054000
C	4.296220000	0.629301000	3.211156000
H	5.210344000	0.041370000	3.281554000
C	-4.910038000	-1.417008000	0.685090000
H	-5.440120000	-2.364103000	0.817842000
H	-4.448430000	-1.390714000	-0.307152000
H	-5.623922000	-0.588151000	0.758890000
C	4.369569000	2.025752000	3.259345000
H	5.330737000	2.522168000	3.371628000
Te	0.055437000	-0.057228000	-2.994379000
N	-0.724765000	1.696397000	-3.386440000
N	1.826034000	0.758650000	-3.188258000
N	-0.212666000	5.061879000	-3.898178000
C	0.275889000	2.547843000	-3.490790000
N	3.692764000	3.618329000	-3.505989000
C	1.632686000	2.048446000	-3.383992000
C	2.769066000	2.918645000	-3.467715000
C	0.003317000	3.937415000	-3.717528000
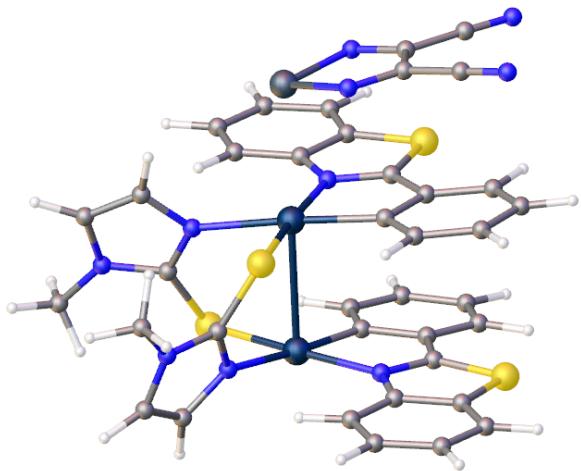
*Cartesian coordinate for [**1**·SeDA] (in Å)*

Pt	0.000000000	0.000000000	0.000000000
Pt	-0.035299000	0.090484000	-2.909989000
S	0.924374000	-2.113671000	-0.105056000
S	1.599410000	1.707647000	-2.823806000
S	-3.201757000	3.128290000	0.378589000
S	-4.165694000	-1.645061000	-3.103123000
N	-1.625642000	-1.218611000	-3.109307000
N	-1.002640000	1.807411000	0.187238000
N	1.974368000	0.733133000	-0.264450000
N	1.523090000	-1.327351000	-2.686041000
C	-1.517040000	1.414339000	-3.062070000
N	3.782208000	1.544868000	-1.209701000
C	-2.313994000	1.656133000	0.249730000
C	-0.615970000	3.130190000	0.245763000
C	-2.813986000	0.840264000	-3.122970000
C	-1.871990000	-0.685835000	0.158713000
N	2.928904000	-2.775300000	-1.822442000
C	2.454979000	1.289146000	-1.381658000
C	-2.792743000	-0.597542000	-3.116811000
C	-2.861192000	0.325585000	0.253151000
C	-1.756599000	-2.593865000	-3.104037000
C	0.685141000	3.645605000	0.241769000
H	1.530357000	2.969011000	0.202569000
C	3.015482000	0.612130000	0.621167000
H	2.885697000	0.157756000	1.595187000
C	-1.460057000	2.816015000	-3.046106000
H	-0.494094000	3.312782000	-2.970312000
C	-3.983546000	1.610786000	-3.167920000
H	-4.960053000	1.126365000	-3.201574000
C	2.483605000	-1.605344000	-3.625295000
H	2.473212000	-1.130239000	-4.598257000
C	-4.226625000	0.035437000	0.384548000
H	-4.953992000	0.841735000	0.478422000
C	1.809995000	-2.034513000	-1.589948000
C	-0.737650000	-3.552949000	-3.132743000
H	0.296144000	-3.234553000	-3.192207000
C	-2.324782000	-2.011359000	0.190430000
H	-1.608600000	-2.826950000	0.110368000
C	0.860432000	5.020986000	0.298122000
H	1.869958000	5.428073000	0.292791000
C	-3.102825000	-3.020460000	-3.082223000
C	-3.448040000	-4.370637000	-3.044938000
H	-4.491167000	-4.679407000	-3.017412000
C	3.357941000	-2.518816000	-3.107963000
H	4.232075000	-2.999069000	-3.529314000
C	-1.710262000	4.018334000	0.338838000
C	-3.680569000	-2.305001000	0.332521000
H	-3.996621000	-3.346492000	0.377949000
C	-4.636973000	-1.288564000	0.432695000
H	-5.689399000	-1.532987000	0.559137000
C	-1.080976000	-4.897059000	-3.098235000
H	-0.291974000	-5.646757000	-3.115493000
C	-2.421599000	-5.307464000	-3.044275000
H	-2.662802000	-6.368270000	-3.010907000
C	-2.619688000	3.588140000	-3.103413000
H	-2.535293000	4.674757000	-3.088175000
C	4.144900000	1.128943000	0.053691000
H	5.156100000	1.232408000	0.426531000
C	-3.885926000	2.994634000	-3.163693000
H	-4.782953000	3.609928000	-3.198397000
C	-0.235455000	5.894895000	0.363843000
H	-0.069385000	6.969823000	0.403916000
C	3.543416000	-3.670990000	-0.875013000
H	3.372862000	-3.282977000	0.134531000
H	4.618226000	-3.726606000	-1.069153000
H	3.111938000	-4.677432000	-0.936874000
C	4.646063000	2.138019000	-2.199355000
H	4.288197000	1.846958000	-3.192501000
H	5.667912000	1.775645000	-2.056248000
H	4.637554000	3.232822000	-2.134497000
C	-1.533789000	5.400344000	0.391250000
H	-2.389280000	6.069567000	0.458195000
Se	0.000000000	0.000000000	2.985451000
N	-0.930804000	-1.472121000	3.310322000
N	-1.383516000	1.082940000	3.218439000
C	-2.439094000	0.315042000	3.426394000
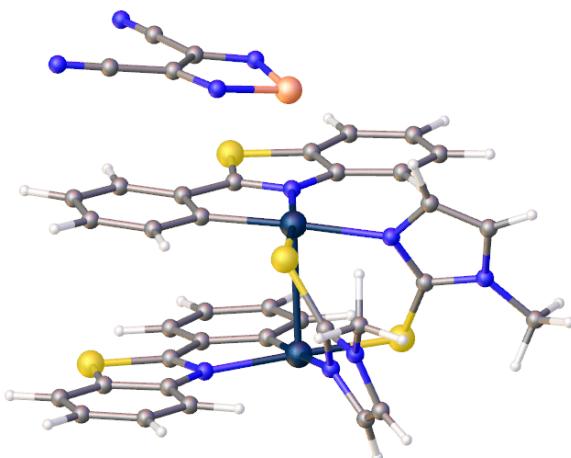
N	-4.787365000	1.376572000	3.669147000
C	-2.187939000	-1.102478000	3.478792000
C	-3.734539000	0.902126000	3.571027000
N	-4.047232000	-2.853924000	3.897814000
C	-3.209039000	-2.076585000	3.708496000

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

Pt	0.000000000	0.000000000	0.000000000
S	-0.005063000	2.286750000	2.598081000
S	-4.470383000	0.324998000	-0.325859000
N	-1.932185000	0.737034000	-0.227752000
N	1.098387000	1.849482000	0.172389000
C	-0.993730000	-1.728166000	-0.112419000
C	-1.827802000	3.224977000	-0.397460000
H	-0.745014000	3.259797000	-0.396737000
C	1.914991000	2.171336000	-0.845653000
H	1.957961000	1.449135000	-1.657300000
C	-2.401667000	-1.592895000	-0.184578000
C	-2.840458000	-0.223822000	-0.226535000
C	-3.902051000	1.967006000	-0.368104000
C	-2.580113000	4.387610000	-0.480779000
H	-2.069809000	5.347452000	-0.534924000
C	-4.658458000	3.135831000	-0.448492000
H	-5.745483000	3.096068000	-0.478044000
C	1.040623000	2.654697000	1.253985000
C	-0.482707000	-3.032693000	-0.110420000
H	0.591687000	-3.193443000	-0.049162000
C	2.664286000	3.332847000	-0.879128000
H	3.298698000	3.546922000	-1.735162000
C	1.776513000	3.854515000	1.285794000
H	1.709122000	4.480707000	2.172116000
C	-2.721870000	-3.977214000	-0.254371000
H	-3.371189000	-4.846849000	-0.326272000
C	-2.490686000	1.994783000	-0.322347000
C	-3.260863000	-2.699570000	-0.247394000
H	-4.339095000	-2.556066000	-0.315226000
C	-1.332713000	-4.134891000	-0.187578000
H	-0.904953000	-5.136429000	-0.205982000
C	-3.982907000	4.348903000	-0.497546000
H	-4.549107000	5.276261000	-0.559323000
C	2.579948000	4.200509000	0.214765000
H	3.153822000	5.125716000	0.236412000
Pt	0.000000000	0.000000000	2.808247000
S	2.046744000	-1.026963000	0.126502000
S	-1.778394000	-4.094351000	3.308742000
N	-0.236668000	-2.045344000	3.089261000
N	2.144596000	0.087825000	2.605273000
C	-1.985572000	-0.069473000	3.004133000
C	2.019138000	-3.111663000	3.210181000
H	2.556737000	-2.173287000	3.159204000
C	2.817210000	0.611872000	3.648656000
H	2.208884000	0.997535000	4.464483000
C	-2.518129000	-1.376710000	3.122793000
C	-1.509287000	-2.401208000	3.146732000
C	-0.060773000	-4.356472000	3.297059000
C	2.698423000	-4.317423000	3.307923000
H	3.786692000	-4.312814000	3.322264000
C	0.621976000	-5.568652000	3.391005000
H	0.080469000	-6.509150000	3.470409000
C	2.829416000	-0.353362000	1.526221000
C	-2.902725000	0.989491000	3.032176000
H	-2.553108000	2.015463000	2.933970000
C	4.196553000	0.667211000	3.709344000
H	4.682340000	1.092470000	4.583496000
C	4.240278000	-0.331176000	1.531032000
H	4.763292000	-0.697573000	0.650778000
C	-4.771979000	-0.548062000	3.288596000
H	-5.839118000	-0.717411000	3.413742000
C	0.619859000	-3.123622000	3.186298000
C	-3.892656000	-1.620204000	3.252182000
H	-4.264157000	-2.639766000	3.352842000
C	-4.268814000	0.753031000	3.181672000
H	-4.953891000	1.598819000	3.223571000
C	2.010946000	-5.537922000	3.389003000
H	2.568622000	-6.469726000	3.460564000
C	4.924057000	0.165891000	2.623386000
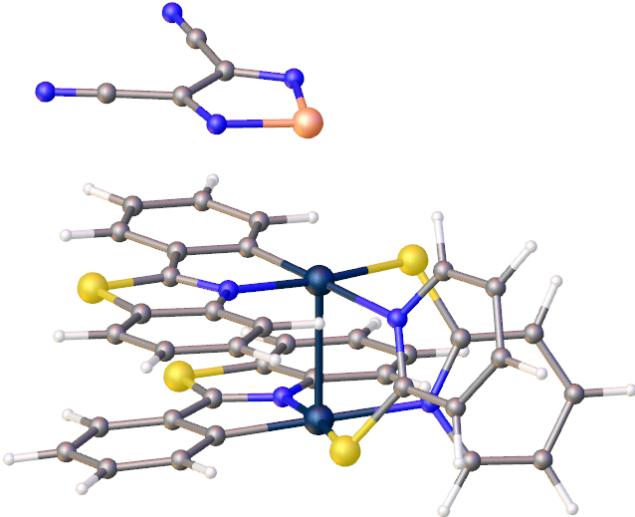
H	6.012959000	0.184865000	2.625972000
Se	-0.180692000	-0.250915000	-3.111707000
N	-1.951503000	-0.235313000	-3.230110000
N	-0.054602000	-2.003888000	-3.347898000
N	-4.857086000	-2.079856000	-3.433356000
N	-1.735585000	-5.006756000	-3.704736000
C	-1.283183000	-2.472847000	-3.430328000
C	-2.337984000	-1.488375000	-3.364901000
C	-3.730222000	-1.810893000	-3.415280000
C	-1.522712000	-3.874831000	-3.580601000

*Cartesian coordinate for [**3**·SeDA] (in Å)*

Pt	2.082298000	0.556024000	11.169880000
S	4.244792000	0.602024000	10.547971000
S	-2.361727000	1.196076000	11.148711000
O	2.793690000	-0.568984000	12.791701000
N	0.086550000	0.589194000	11.664207000
N	4.066717000	-0.891912000	12.756131000
C	-0.695186000	2.370834000	8.541851000
H	-1.777073000	2.504793000	8.573636000
C	-0.671538000	1.193393000	10.765095000
C	-2.019670000	0.319584000	12.618338000
C	-0.123558000	-0.612920000	13.829490000
H	0.948276000	-0.785997000	13.899421000
C	-0.030791000	1.737268000	9.601461000
C	-0.632748000	0.081346000	12.726014000
C	-2.911110000	-0.122120000	13.594915000
H	-3.979101000	0.066877000	13.506288000
C	0.034899000	2.814140000	7.449675000
H	-0.464729000	3.301515000	6.614943000
C	1.377131000	1.535066000	9.608175000
C	-1.015450000	-1.052848000	14.798805000
H	-0.638039000	-1.592679000	15.665511000
C	1.421571000	2.619547000	7.428728000
H	1.999171000	2.952374000	6.567129000
C	2.080434000	1.997094000	8.486838000
H	3.159251000	1.862878000	8.420344000
C	5.835701000	-2.107215000	13.780792000
H	6.162290000	-2.773512000	14.574435000
C	4.519253000	-1.717881000	13.730585000
H	3.754693000	-2.025769000	14.436887000
C	-2.393772000	-0.811946000	14.686292000
H	-3.068999000	-1.167092000	15.462509000
C	4.890590000	-0.415935000	11.779809000
C	6.719894000	-1.638921000	12.796513000
H	7.764950000	-1.940020000	12.800040000
C	6.243135000	-0.801117000	11.810443000
H	6.886603000	-0.435622000	11.014197000
Se	1.261770000	-2.467382000	10.151793000
N	1.435560000	-1.714381000	8.551203000
N	2.998974000	-2.822515000	10.306014000
N	6.156866000	-2.493669000	8.969338000
N	3.604862000	-0.572604000	6.113505000
C	3.587923000	-2.318672000	9.248662000
C	2.713281000	-1.696329000	8.269418000
C	5.007880000	-2.414348000	9.093211000
C	3.193289000	-1.077538000	7.070896000
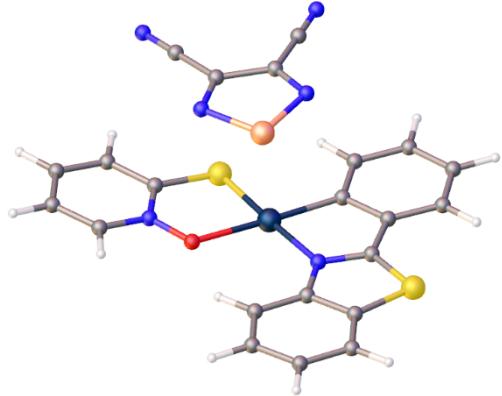
*Cartesian coordinate for [**1**·SeDA]$_\sigma$ (in Å)*

Pt	-0.45531719357297	-0.55481193098488	4.26628195140136
Pt	-0.62861331882767	-0.87194641685794	7.15992267421354
S	-1.65773259097356	-2.52007257470230	4.05258100887048
S	-1.99231604613848	0.98091783664298	7.21456616968048
S	3.12528004807572	2.13828147315151	4.26579960782264
S	3.17725182167580	-3.24022924037962	7.29302244921078
N	0.73556765043685	-2.42432086784215	7.23467038773612
N	0.77805481424324	1.09549911962218	4.35539942495233
N	-2.33333376046284	0.40144782963975	4.53765055160157
N	-2.36578128171924	-1.98061125921616	6.66386626977475
C	1.02632684909157	0.18045446243934	7.51958723193230
N	-4.09714163028910	1.27634607679701	5.50855190364344
C	2.05725069290285	0.78449494431423	4.28043275750363
C	0.55947553922114	2.45721721064626	4.38144920553287

|			
C	2.21715915013647	-0.59086750251361	7.54385964966783
C	1.30965162696017	-1.46788354176006	4.06302623602089
N	-3.93167810083848	-2.97260492867992	5.48731879162767
C	-2.81581697200044	0.85616442549197	5.69844220176737
C	1.97968864028231	-1.99795557526146	7.36838476064254
C	2.42735402836834	-0.59948316932213	4.13577715641482
C	0.65785747363166	-3.79300720217492	7.06613270464426
C	-0.66635932922562	3.13122723842112	4.39520633771761
H	-1.58925237950848	2.56551530503461	4.37866117678770
C	-3.32807291987589	0.51567780547645	3.59911587168703
H	-3.18099976319513	0.19811235359017	2.57435822792060
C	1.18269592675321	1.56789416996575	7.65516547238785
H	0.30701506407425	2.21338575532128	7.61322532781514
C	3.48846419449512	-0.01952221054541	7.68971874338472
H	4.37806769571049	-0.65041406082365	7.68595195087523
C	-3.45712007913262	-2.16724098430373	7.47353903699120
H	-3.45800547612607	-1.83244260160680	8.50328647231567
C	3.74569230484724	-1.06277732021251	4.04509710140435
H	4.57928698691095	-0.36317951693913	4.11307838410983
C	-2.66948596233945	-2.46380930633673	5.45612445939403
C	-0.49437708955665	-4.57562397354624	6.92785635759014
H	-1.46950468078050	-4.10513526805049	6.97404774195293
C	1.58150706386386	-2.83143709193181	3.88885163597675
H	0.75953057375863	-3.54439873549331	3.84852365645062
C	-0.66734720353103	4.51852838395983	4.40801102405611
H	-1.61815925400035	5.04835014955523	4.41505071045733
C	1.92315494829868	-4.42056827698129	7.05467295511629
C	2.06177603771621	-5.79571621450477	6.87159281723421
H	3.04548175837717	-6.26098276817742	6.85818830690249
C	-4.43560014820296	-2.79933772466728	6.75916030984344
H	-5.42701217071135	-3.13566679115530	7.03543092489884
C	1.75650900123631	3.20533976938127	4.35334091484549
C	2.89271890583217	-3.29592796090926	3.78521461046335
H	3.06918060975150	-4.36288701820704	3.64975241544191
C	3.97966945703542	-2.41908516161008	3.86361638335173
H	4.99804660220887	-2.79549428809662	3.78759968799812
C	-0.35649684902226	-5.94461929217425	6.74741695064655
H	-1.24886102383264	-6.55782664518988	6.63550569838320
C	0.90757111101021	-6.55271805300262	6.70964963446503
H	0.98717830288669	-7.62820305895962	6.56222709903164
C	2.44399835284574	2.14145998286719	7.80903201980820
H	2.52715891992349	3.22396679584444	7.90445203510461
C	-4.42753024049486	1.07428367909672	4.18514989340501
H	-5.39736566958063	1.34319265569290	3.78586286350002
C	3.60275954288499	1.35589529318500	7.82667458583993
H	4.58131600688712	1.81929123726753	7.93686396169247
C	0.52974374467843	5.25040671141760	4.40176913805962
H	0.49971141819586	6.33828751416778	4.40636759780448
C	-4.61586324629710	-3.57382119101272	4.36986602494728
H	-4.21754090018918	-3.14115993558082	3.44654741415592
H	-5.68682158315524	-3.36288733354192	4.43978775155424
H	-4.46154601071339	-4.65923535430732	4.34212256688451
C	-4.95496149671560	1.82151232052364	6.53058117339870
H	-4.62601870635677	1.43299887223448	7.49986574679769
H	-5.98819620197420	1.51413208741613	6.34447194807093
H	-4.90149920465186	2.91654342882474	6.55665889554916
C	1.75632951637283	4.59926636129348	4.36871024445448
H	2.68942103712112	5.15792353497476	4.33834121569836
Se	-0.50154390759086	-0.39522628239734	1.35834282358399
N	0.56699352114694	1.04257967924980	1.51711152070896
N	-0.75637266696558	-0.03562326171114	-0.42200893119556
C	-0.09649140832340	1.04336468416317	-0.72606726511765
N	-0.15195874749579	2.05489769167623	-3.11401964947122
C	0.65764199131470	1.64431790229711	0.36652188774519
C	-0.12996771660510	1.59732289613922	-2.05006369286629
N	2.09453028450112	3.79033561774573	0.15256764518179
C	1.45294517730786	2.83045372214312	0.24657557114560
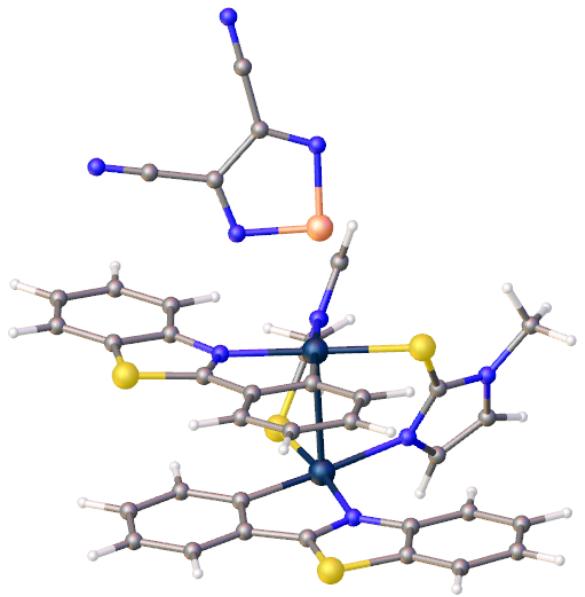
4. NMR data
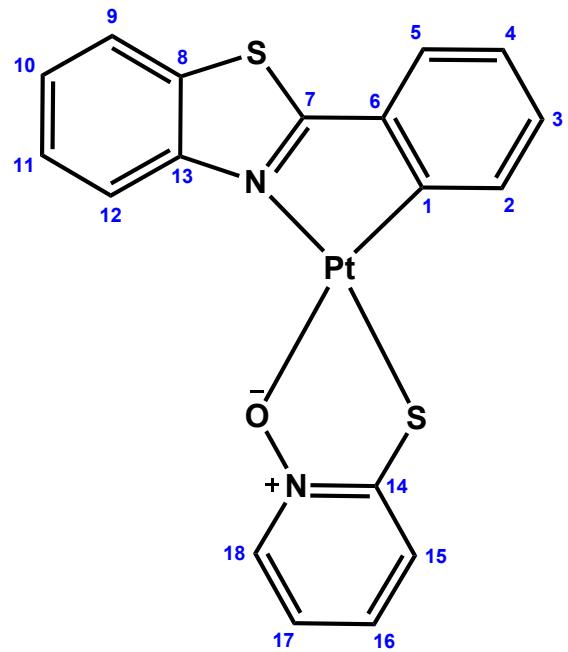
**Figure S17.** Complex numbering scheme as key for the attribution of the NMR spectra.
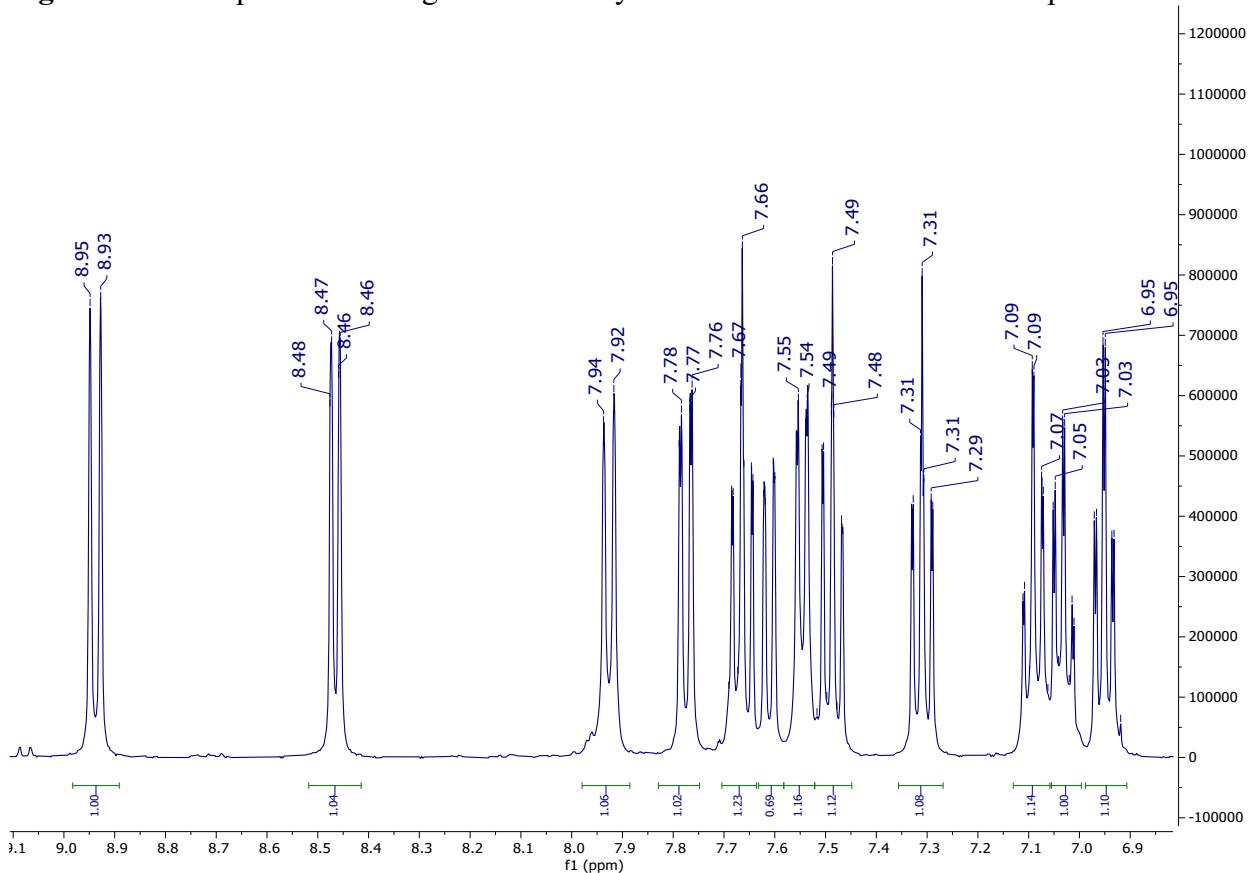
**Figure S18.** ^{1}H NMR spectrum of **3** in CD_2Cl_2.
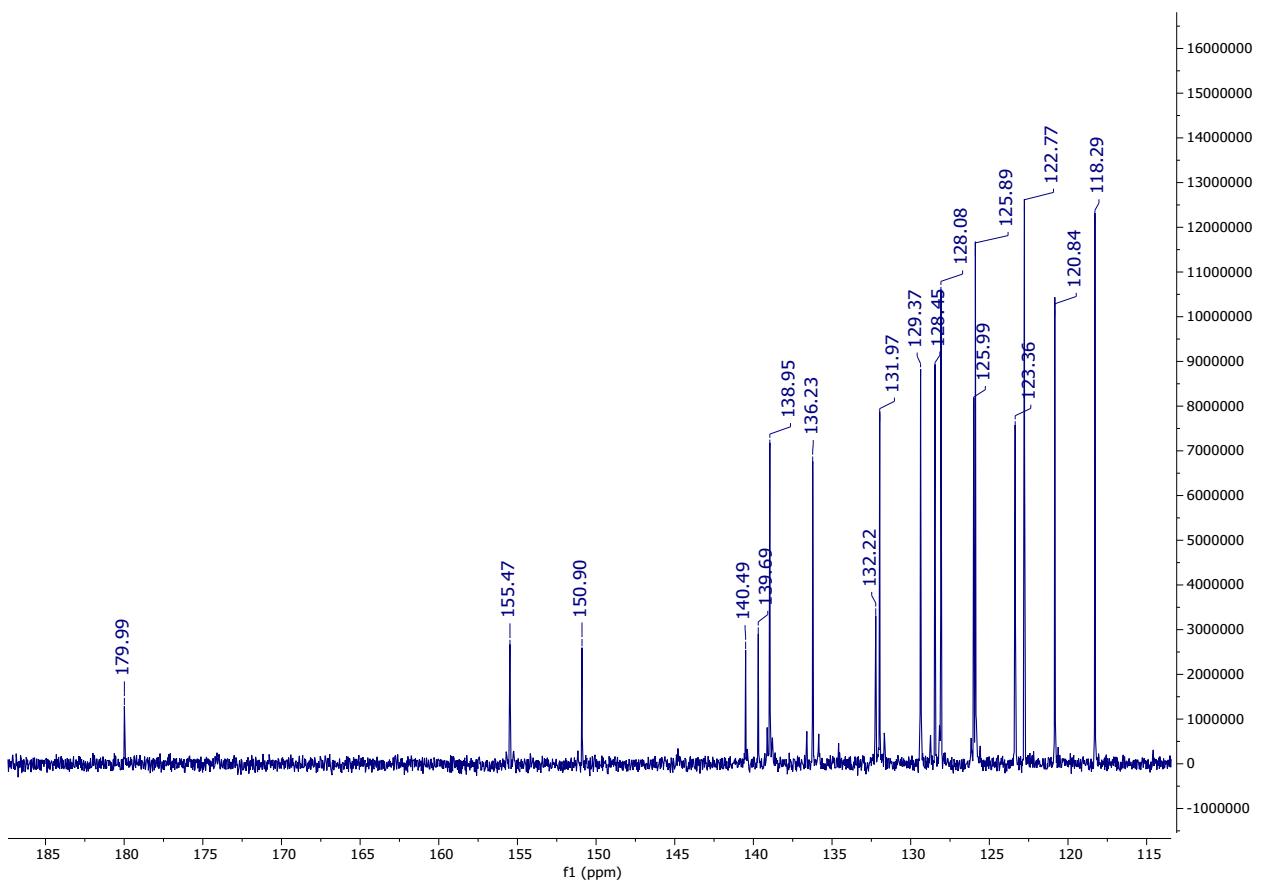
**Figure S19.** ^{13}C NMR spectrum of **3** in CD_2Cl_2.
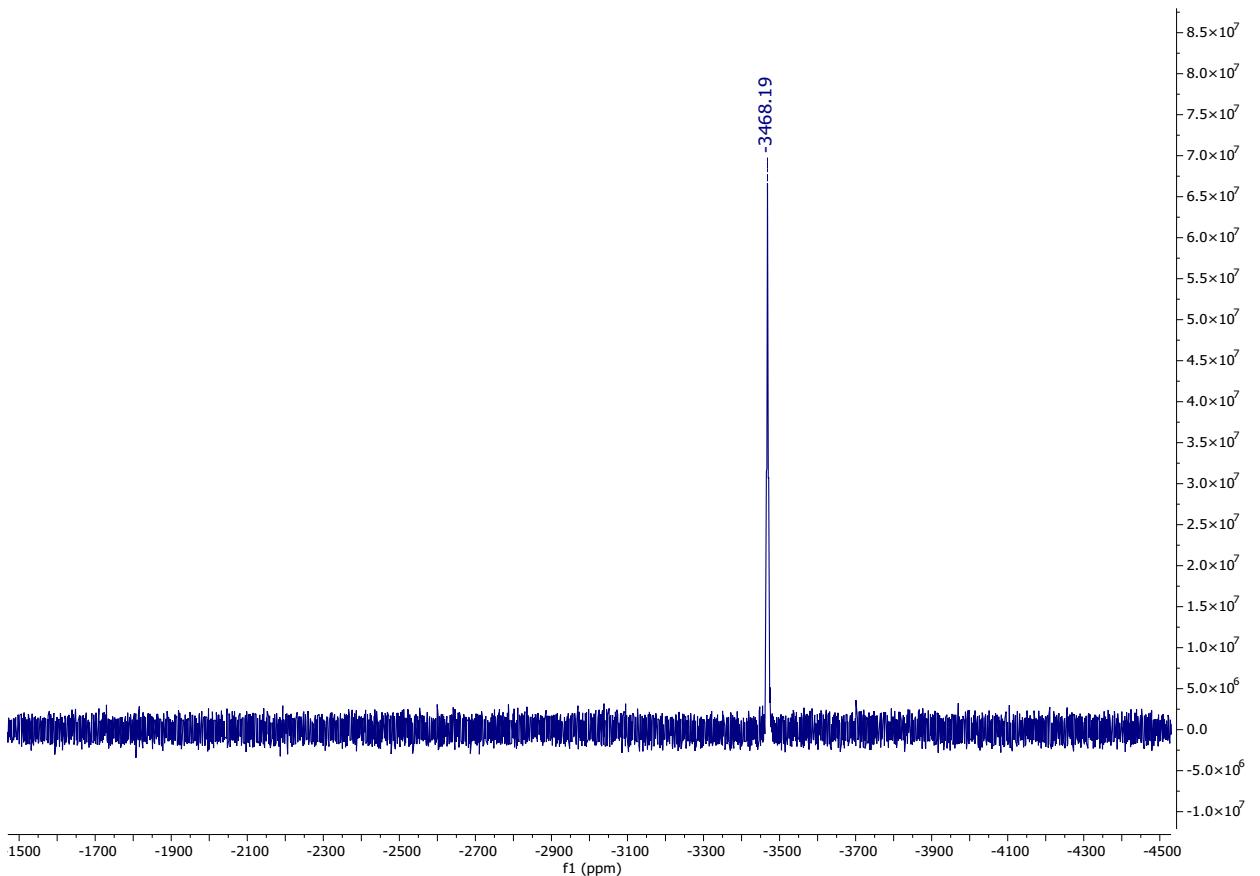

Figure S20. ^{195}Pt NMR spectrum of **3** in CD_2Cl_2.
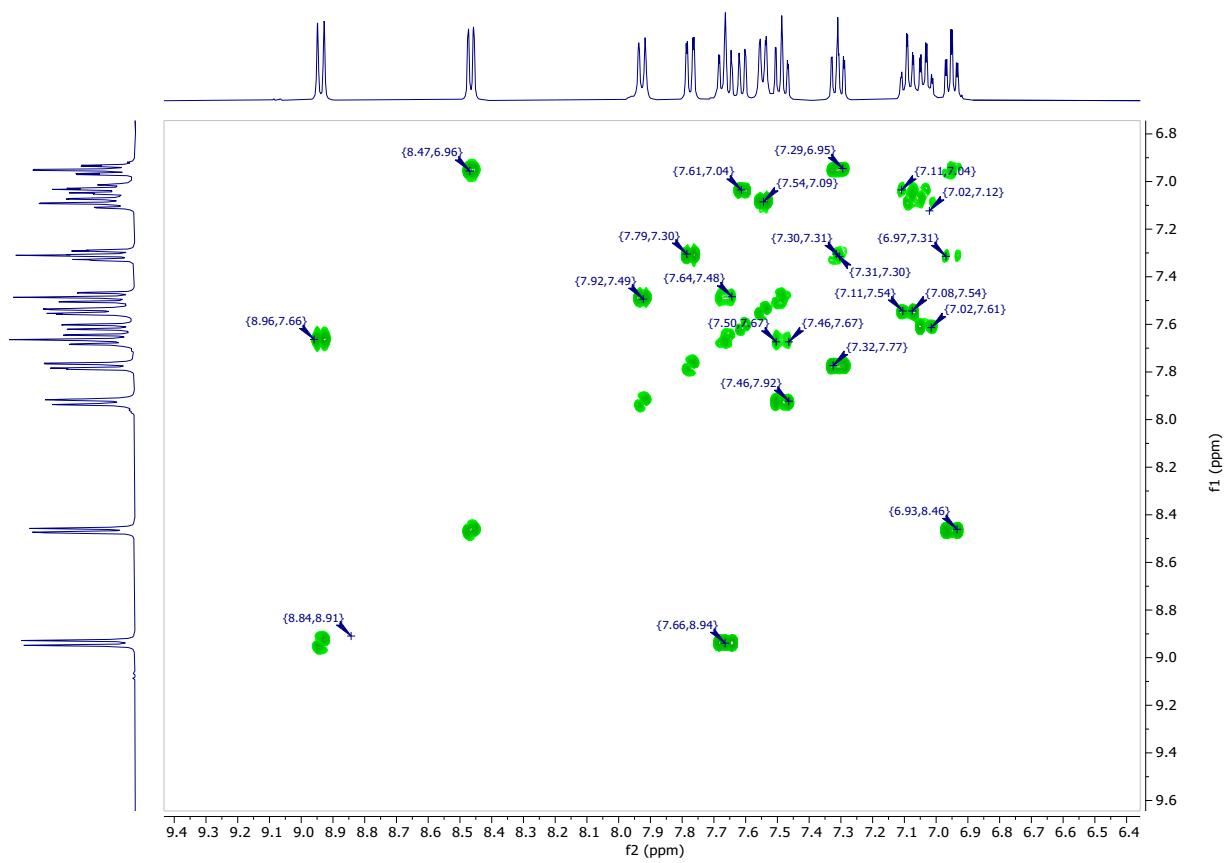
Figure S21. The ^{1}H-^{1}H COSY spectrum for **3** in CD_2Cl_2.


**Figure S22.** The ^{1}H-^{13}C HSQC spectrum for **3** in CD_2Cl_2.
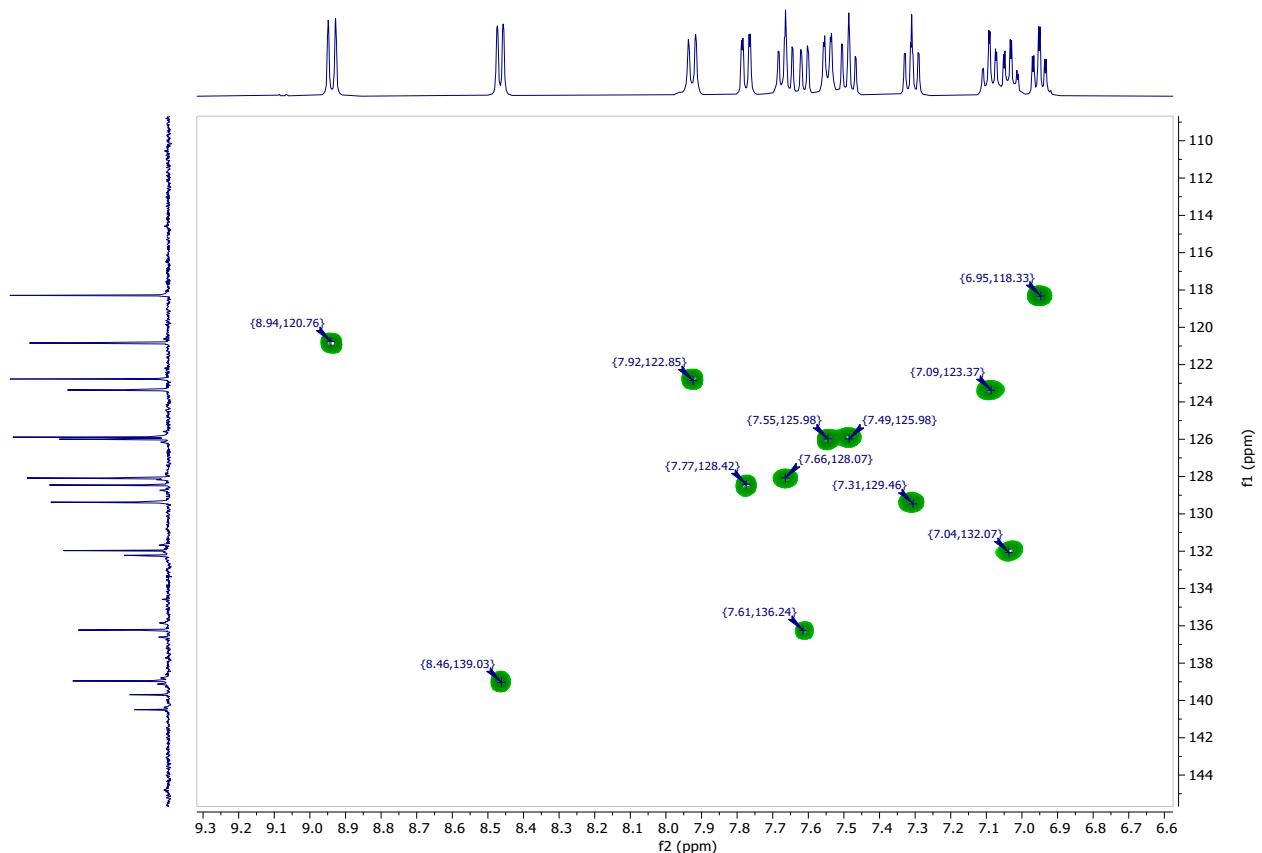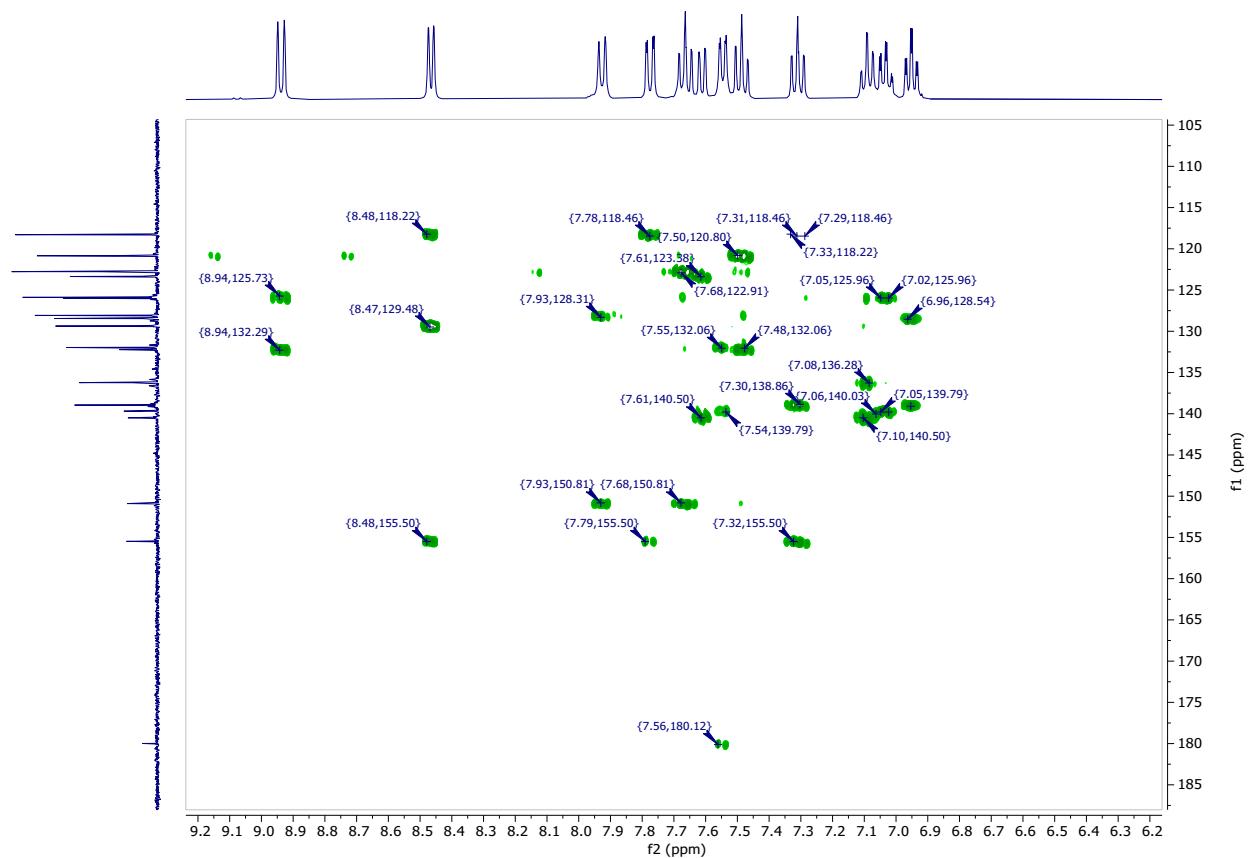
Figure S23. The ^{1}H-^{13}C HMBC spectrum for **3** in CD_2Cl_2.

5. References

1. E. Espinosa, E. Molins and C. Lecomte, Hydrogen bond strengths revealed by topological analyses of experimentally observed electron densities, *Chem. Phys. Lett.*, 1998, **285**, 170-173.
2. P. Politzer, J. S. Murray and T. Clark, The π-hole revisited, *Physical Chemistry Chemical Physics*, 2021, **23**, 16458-16468.
3. P. Politzer and J. Murray, An Overview of Strengths and Directionalities of Noncovalent Interactions: σ-Holes and π-Holes, *Crystals*, 2019, **9**, 165.
4. A. F. Cozzolino, I. Vargas-Baca, S. Mansour and A. H. Mahmoudkhani, The Nature of the Supramolecular Association of 1,2,5-Chalcogenadiazoles, *Journal of the American Chemical Society*, 2005, **127**, 3184-3190.
5. M. A. A. Ibrahim and E. M. Z. Telb, σ-Hole and Lone-Pair Hole Interactions in Chalcogen-Containing Complexes: A Comparative Study, *ACS Omega*, 2020, **5**, 21631-21640.
6. N. Tarannam, R. Shukla and S. Kozuch, Yet another perspective on hole interactions, *Physical Chemistry Chemical Physics*, 2021, **23**, 19948-19963.