ELECTRONIC SUPPORTING INFORMATION

Structural Resilience in Organic–Inorganic Stacked Assemblies: Sulfur-Mediated Self-Compensating Interaction and Metal Identity Masking in Group 10 Dithiocarbamate Cocrystals with Tetracyanobenzene

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S1. X-ray diffraction studies

Table S1. Crystal data and refinement details for cocrystals (**1**–**4**)·TCB.

Compound	**1**·TCB	**2**·TCB	**3**·TCB	**4**·TCB
Identification code	M377	M314	KMV-729	M247
CCDC number	2482470	2482471	2482472	2482473
Empirical formula	$C_{20}H_{22}N_6NiS_4$	$C_{20}H_{22}N_6PdS_4$	$C_{20}H_{22}N_6PtS_4$	$C_{24}H_{26}N_6NiS_4$
Formula weight	533.38	581.07	669.76	585.46
Temperature/K	100(2)	100(2)	100(2)	100(2)
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	P-1
a/Å	15.52120(10)	15.5498(2)	15.5679(2)	7.92840(10)
b/Å	22.63540(10)	22.9143(3)	22.9237(3)	15.8277(2)
c/Å	20.6603(2)	20.5914(3)	20.6209(2)	21.3669(2)
α/°	90	90	90	95.6690(10)
β/°	95.9790(10)	95.8330(10)	95.6680(10)	92.1450(10)
γ/°	90	90	90	98.3620(10)
Volume/Å^3	7219.07(9)	7298.99(17)	7323.08(15)	2636.16(5)
Z	12	12	12	4
ρ_{calc}g/cm^3	1.472	1.586	1.822	1.475
μ/mm^{-1}	4.570	9.524	14.114	4.226
F(000)	3312.0	3528.0	3912.0	1216.0
Crystal size/mm^3	0.14×0.06×0.04	0.14×0.1×0.08	0.15×0.11×0.07	0.16×0.14×0.05
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	Cu Kα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.726 to 160.272	6.894 to 152.462	5.704 to 139.698	4.162 to 160.43
Index ranges	–19 ≤ h ≤ 18 –28 ≤ k ≤ 27 –26 ≤ l ≤ 26	–19 ≤ h ≤ 18 –28 ≤ k ≤ 28 –18 ≤ l ≤ 25	–18 ≤ h ≤ 15 –27 ≤ k ≤ 26 –24 ≤ l ≤ 24	–10 ≤ h ≤ 9 –20 ≤ k ≤ 20 –27 ≤ l ≤ 26
Reflections collected	59517	35342	51642	97166
Independent reflections	15144 [R_{int} = 0.0338, R_{sigma} = 0.0306]	14974 [R_{int} = 0.0326, R_{sigma} = 0.0331]	13501 [R_{int} = 0.0464, R_{sigma} = 0.0327]	11103 [R_{int} = 0.0704, R_{sigma} = 0.0293]
Data/restraints/parameters	15144/0/853	14974/0/853	13501/0/853	11103/0/634
Goodness-of-fit on F^2	1.052	1.067	1.028	1.061
Final R indexes [I>=2σ (I)]	R_1 = 0.0342, wR_2 = 0.0919	R_1 = 0.0402, wR_2 = 0.1058	R_1 = 0.0423, wR_2 = 0.0948	R_1 = 0.0341, wR_2 = 0.0893
Final R indexes [all data]	R_1 = 0.0430, wR_2 = 0.0963	R_1 = 0.0527, wR_2 = 0.1186	R_1 = 0.0500, wR_2 = 0.0983	R_1 = 0.0421, wR_2 = 0.0922
Largest diff. peak/hole / e Å^{-3}	0.30/–0.39	1.18/–0.95	1.60/–2.36	0.59/–0.43

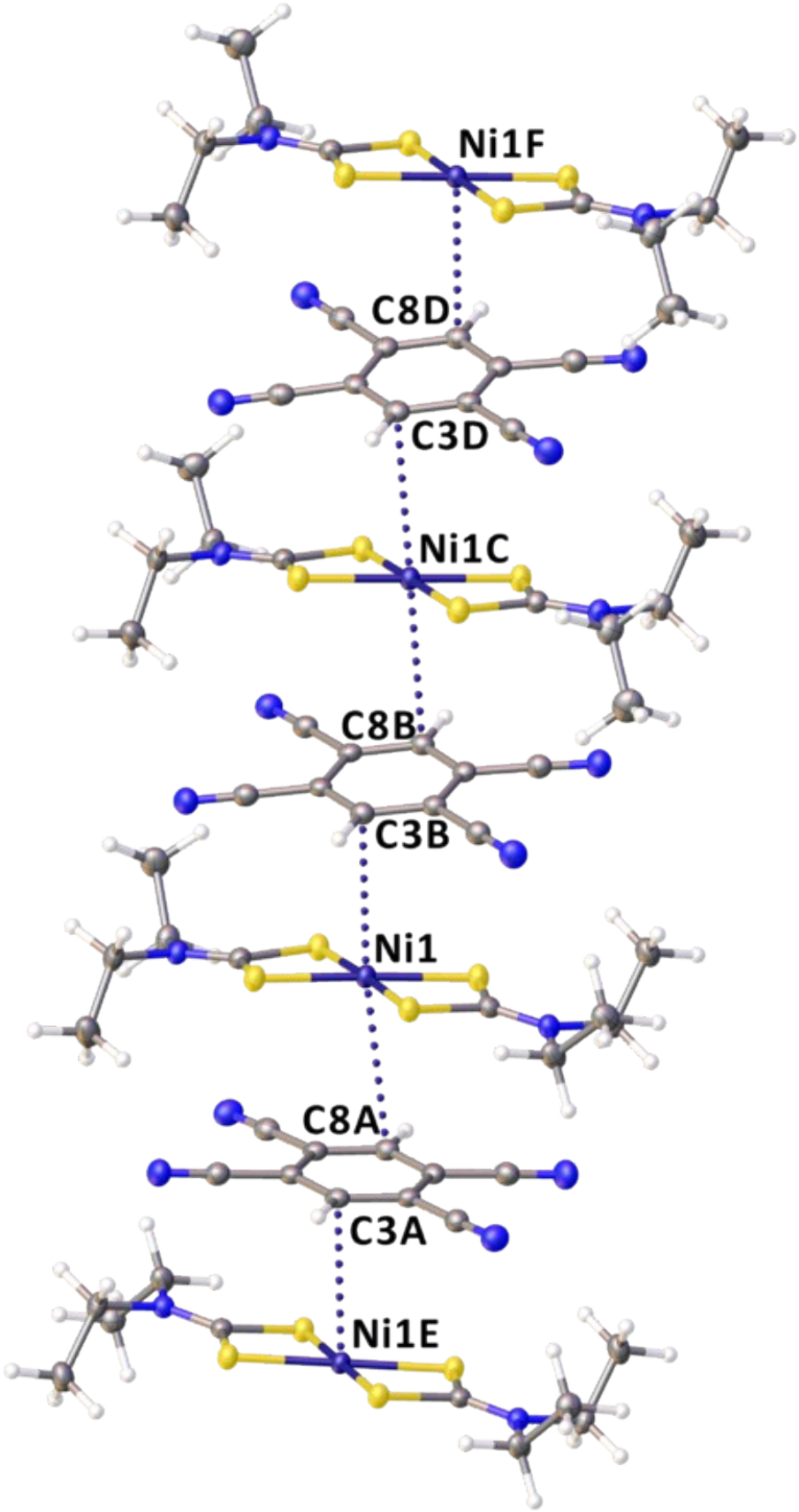

Figure S1. Fragment of molecular packing of **1**·TCB, demonstrating alternating stacking of **1** and TCB, only intermolecular Ni···C short contacts are highlighted by dotted lines.

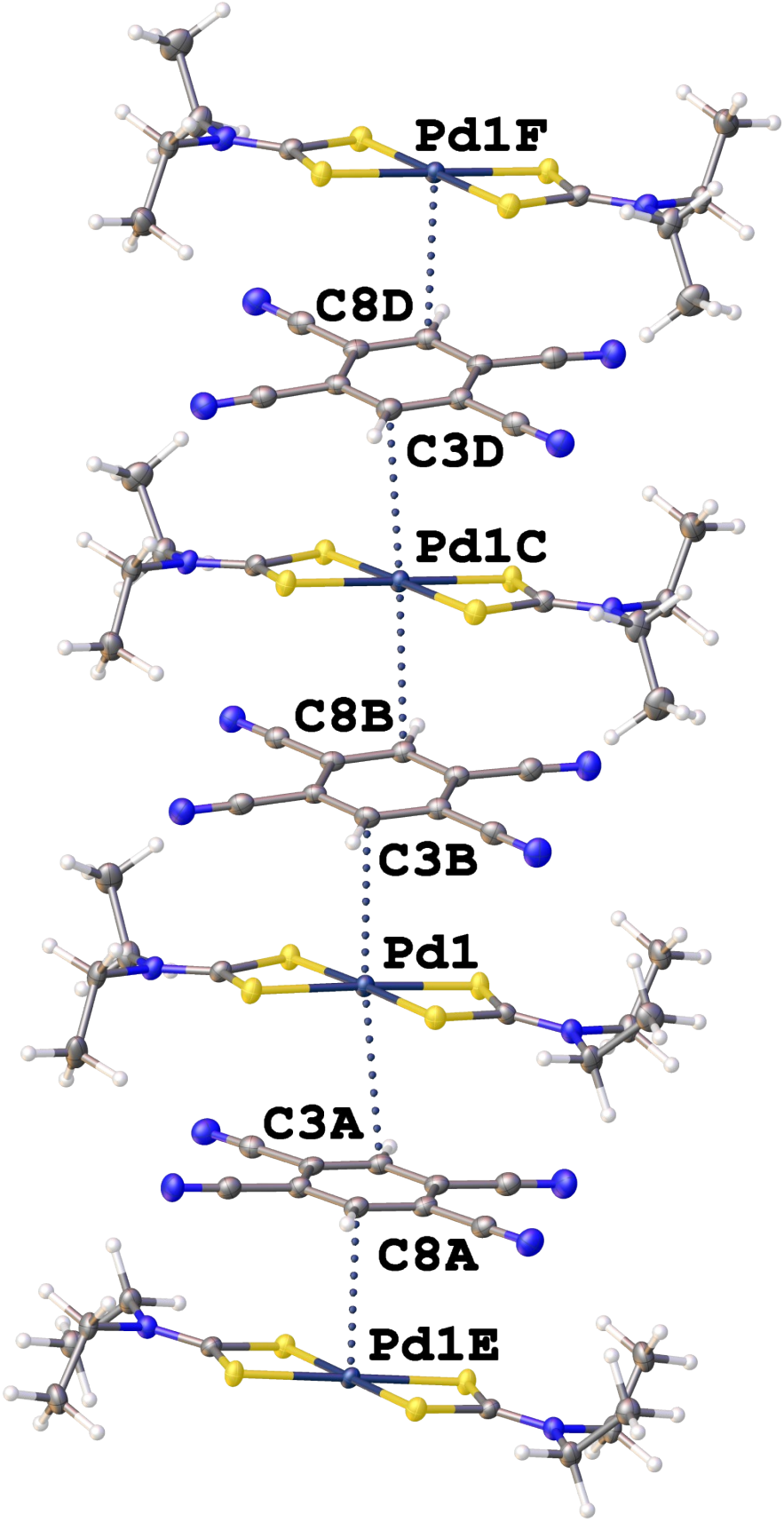

Figure S2. Fragment of molecular packing of **2**·TCB, demonstrating alternating stacking of **2** and TCB, only intermolecular Ni···C short contacts are highlighted by dotted lines.

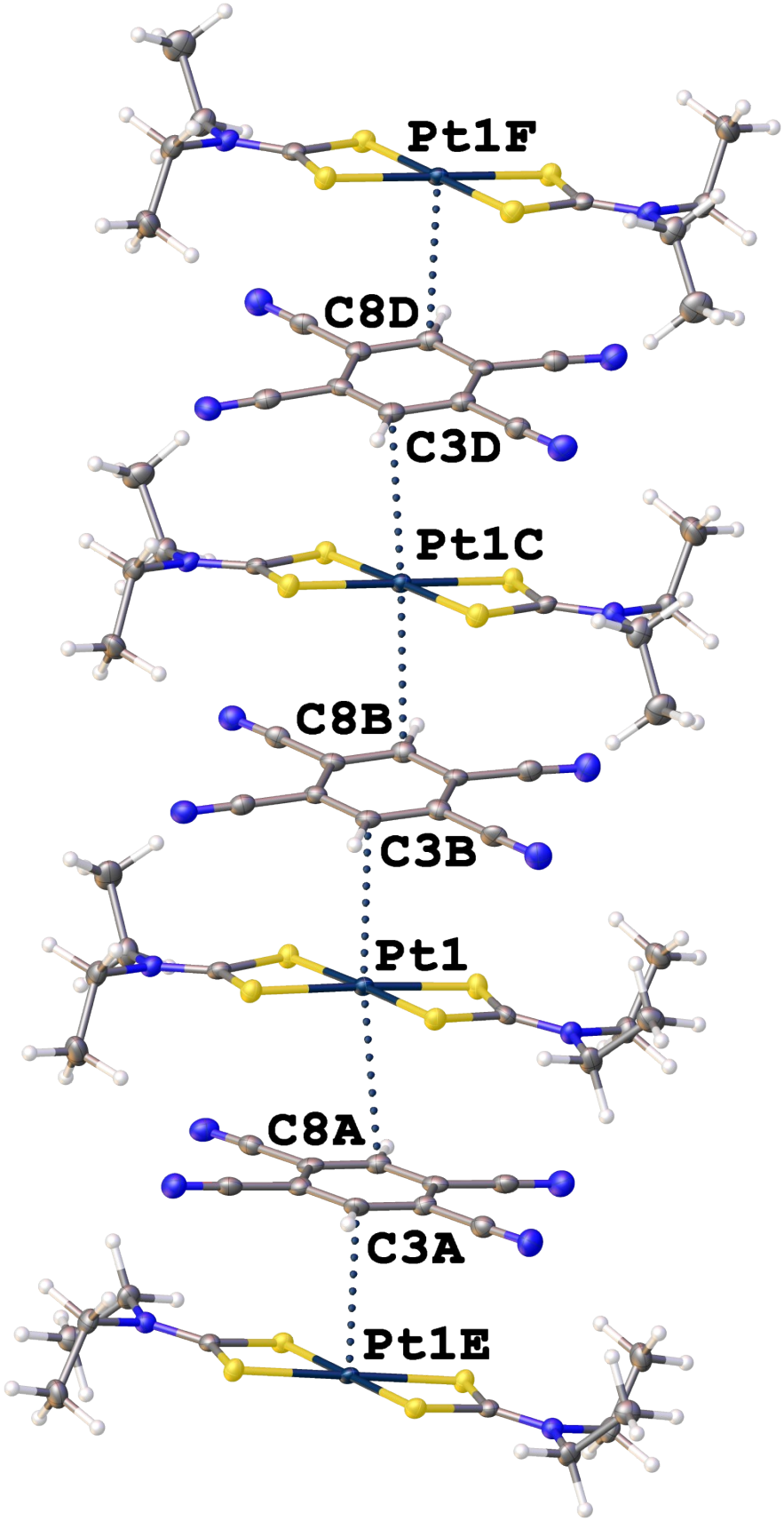

Figure S3. Fragment of molecular packing of **3**·TCB, demonstrating alternating stacking of **3** and TCB, only intermolecular Ni···C short contacts are highlighted by dotted lines.

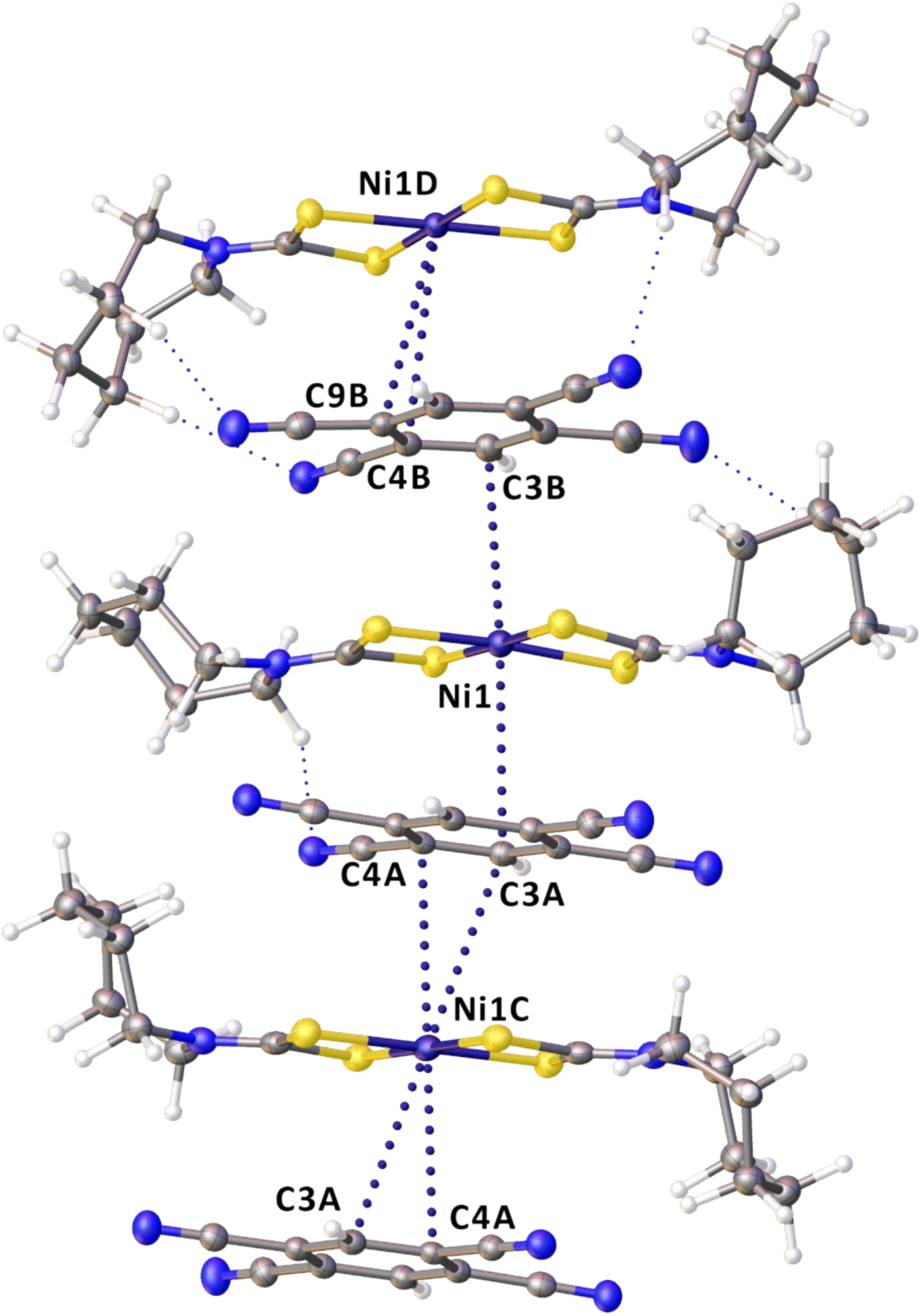

Figure S4. Fragment of molecular packing of **4**·TCB, demonstrating alternating stacking of **4** and TCB, only intermolecular Ni···C short contacts are highlighted by dotted lines.

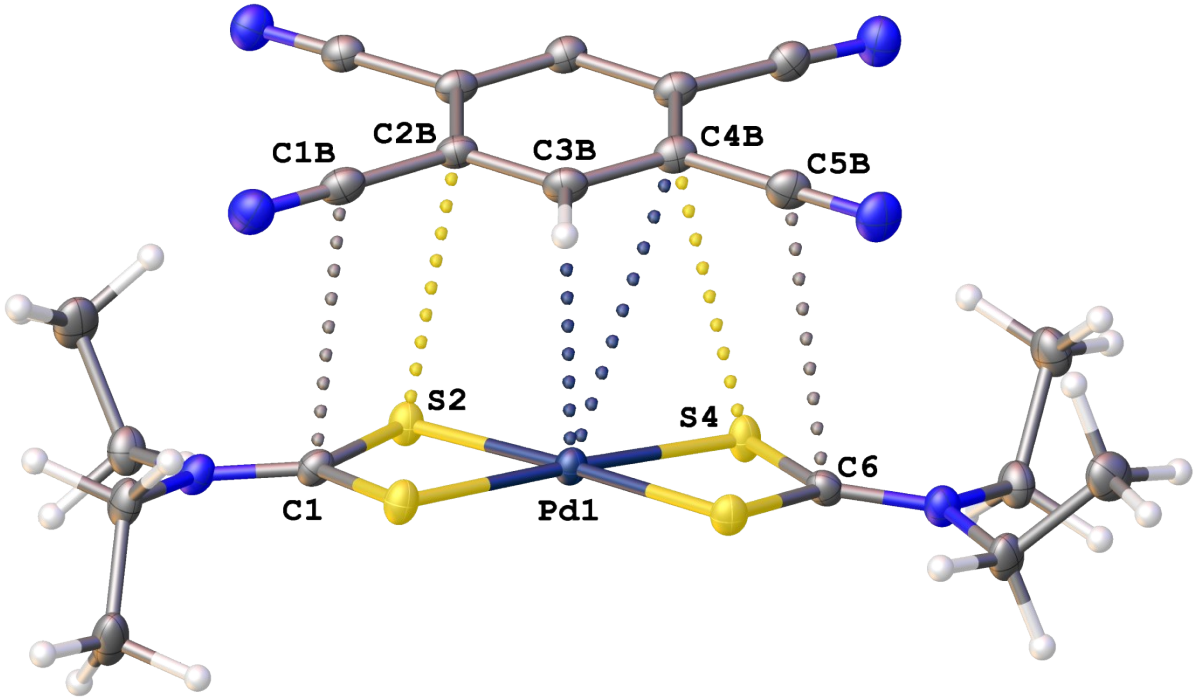

Figure S5. Noncovalent stacking in the molecular structure **2**·TCB, short contacts are depictured by dotted lines.

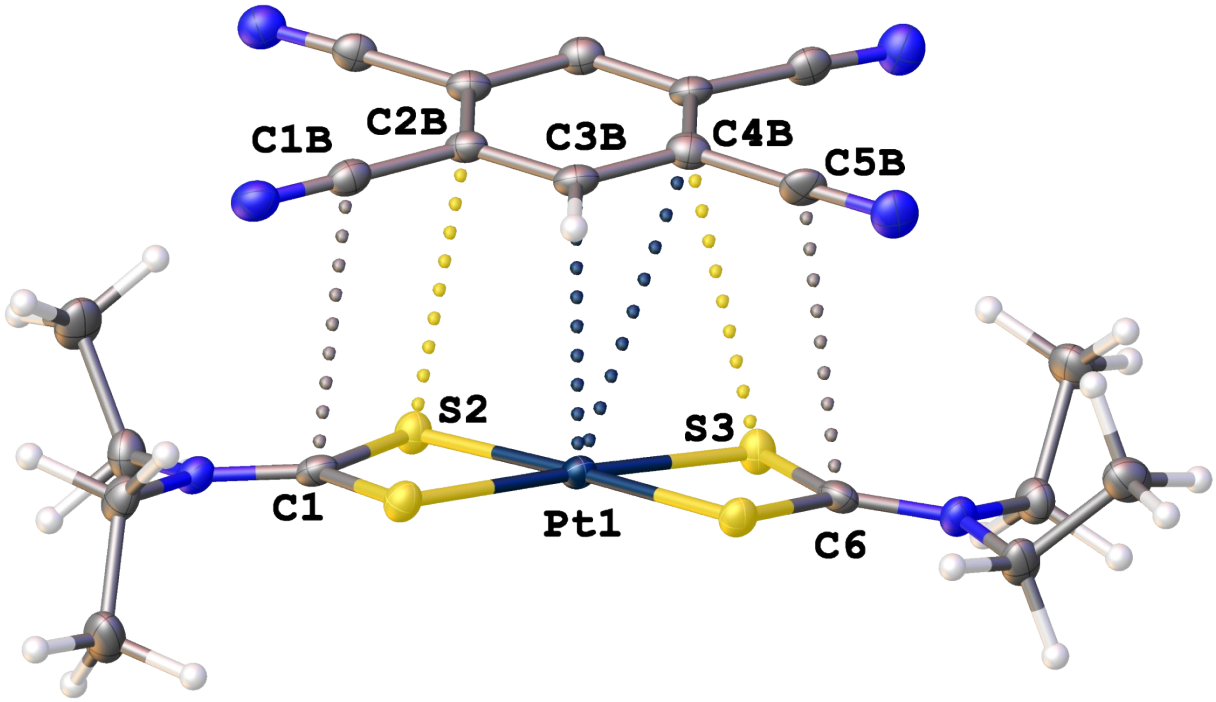

Figure S6. Noncovalent stacking in the molecular structure **3**·TCB, short contacts are depictured by dotted lines.

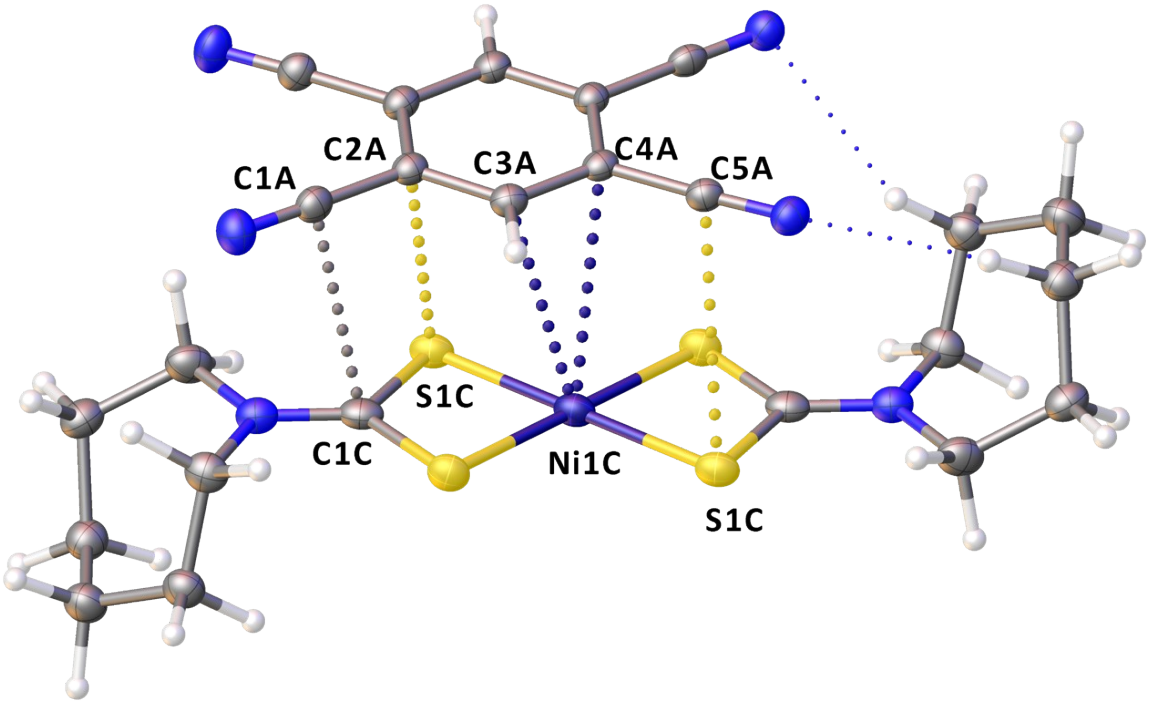

Figure S7. Noncovalent stacking in the molecular structure **4**·TCB, short contacts are depictured by dotted lines.

S2. Photophysical Properties and Measurements

To analyze the nature of the photoluminescence in **3**·TCB and the lack of this effect for other adducts as well as for **1**–**3**, the triplet excited states (T_1) were fully optimized for all these species. The excitation did not result in significant structural deviations (**Figure S8**). The photoluminescence emission in **3**·TCB is due to metal-to-ligand charge transfer (MLCT) between the Pt(dithiocarbamate) and TCB units. This is supported by the analysis of the spin density distribution of the fully optimized triplet excited state (T_1) of this adduct (the density being distributed among the **3** and TCB molecules, **Figure S9**, **A**) and of the HOMO and LUMO composition of the ground state of **3**·TCB (the HOMO is localized at the Pt center and the S atoms of the dithiocarbamate ligand while the LUMO is centered on the TCB molecule, **Figure S9**, **B**,**C**).

Comparison of the spin density distribution and the HOMO/LUMO composition for the excited and ground states of **3** and **3**·TCB (**Figure S9**) indicates that cocrystallization of **3** with TCB introduces a new charge transfer pathway. Indeed, in **3**, the excitation has the mixed MLCT/LC character and involve the metal centre and the dithiocarbamate ligands. In **3**·TCB, the excitation occurs at the TCB centred LUMO. The likely explanation of the luminescence active behaviour of **3**·TCB and the dark nature of **3** in such situation is the insertion of the TCB MOs between the LUMO of **3** and a MO responsible for the generation of the metal centred ^{3}MC state involved in the nonradiative pathways. As a result, the population of the Pt-centred ^{3}MC associated MO is hampered in **3**·TCB, and the importance of the nonradiative decay decreases. This mechanism was previously found for the tetramethylheptanedione phenylpyridine plane square Pt complexes and their adducts with the anticrown-Hg_3 cluster [*Inorg. Chem. Front.*, **2023**, *10*, 493–510].

Analysis of the adiabatic excitation energy (E_{ad}) between the S_0 and T_1 states of complexes **1**–**3** indicates very low E_{ad} value for the Ni complex **1** (0.18 eV) that is typical for the square planar Ni complexes, in particular, with soft ligands like dithiocarbamates, and makes the Ni species dark due to very efficient nonradiative pathway. The E_{ad} values increase from **1** (0.18 eV) to **2** (1.87 eV) and to **3** (2.30 eV). On the other hand, the SOC also increases from **1** to **3** along the same group of the periodic table. These effects lead to decrease of nonradiative decay and to enhancement of the radiative rate and intersystem crossing in this row corroborating with the non-emissive behaviour of the Pd and Ni species.

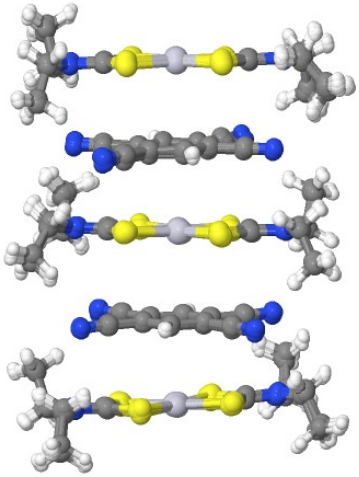

Figure S8. Superimposed equilibrium structures of the ground and excited (T_1) states of **3**·TCB.

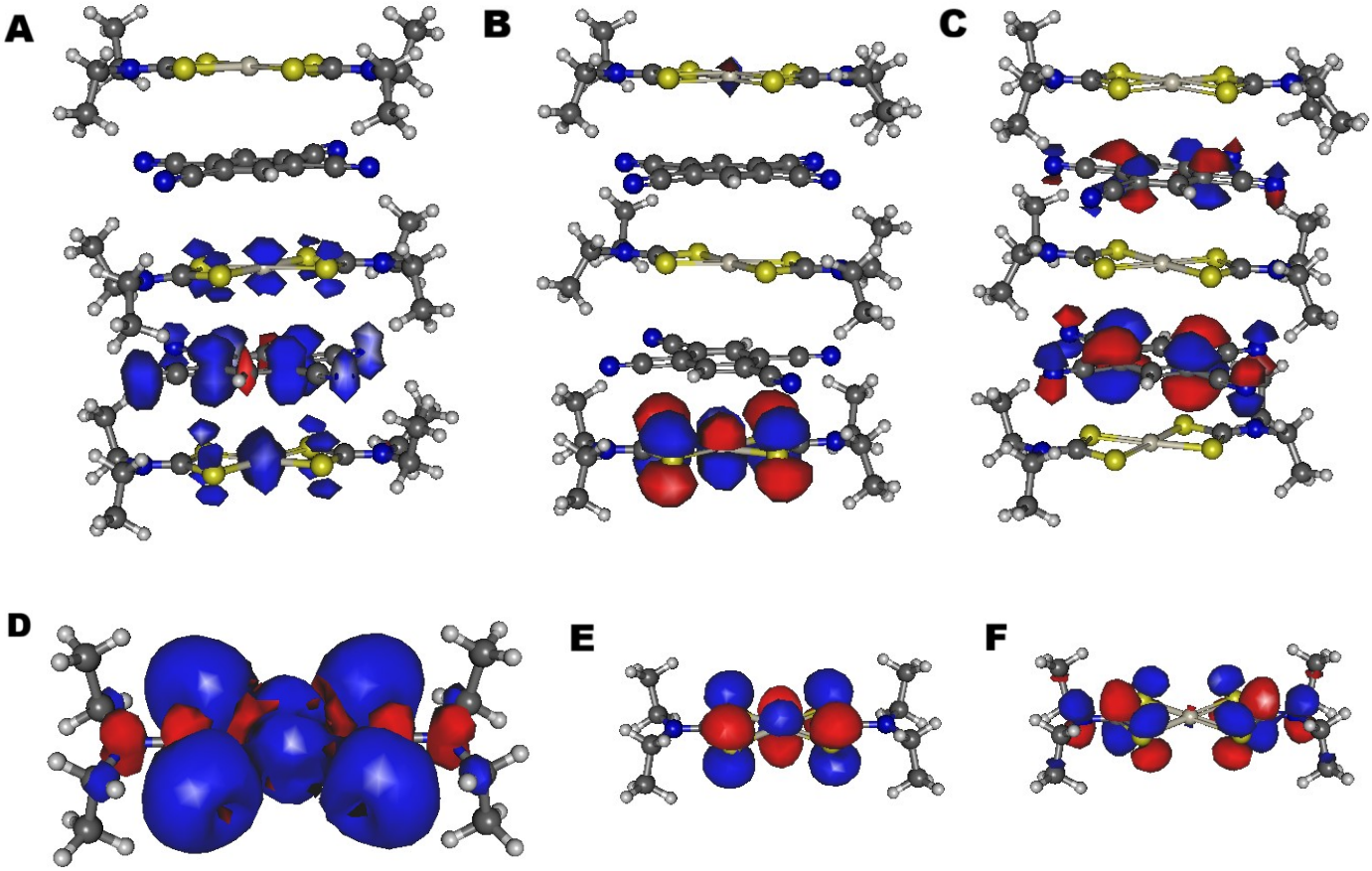

Figure S9. Plots of the spin density distribution in the fully optimized triplet spin state (**A, D**), the HOMO (**B, E**) and LUMO (**C, F**) in the ground state of **3**·TCB (**A**, **B**, **C**) and **3** (**D**, **E**, **F**).

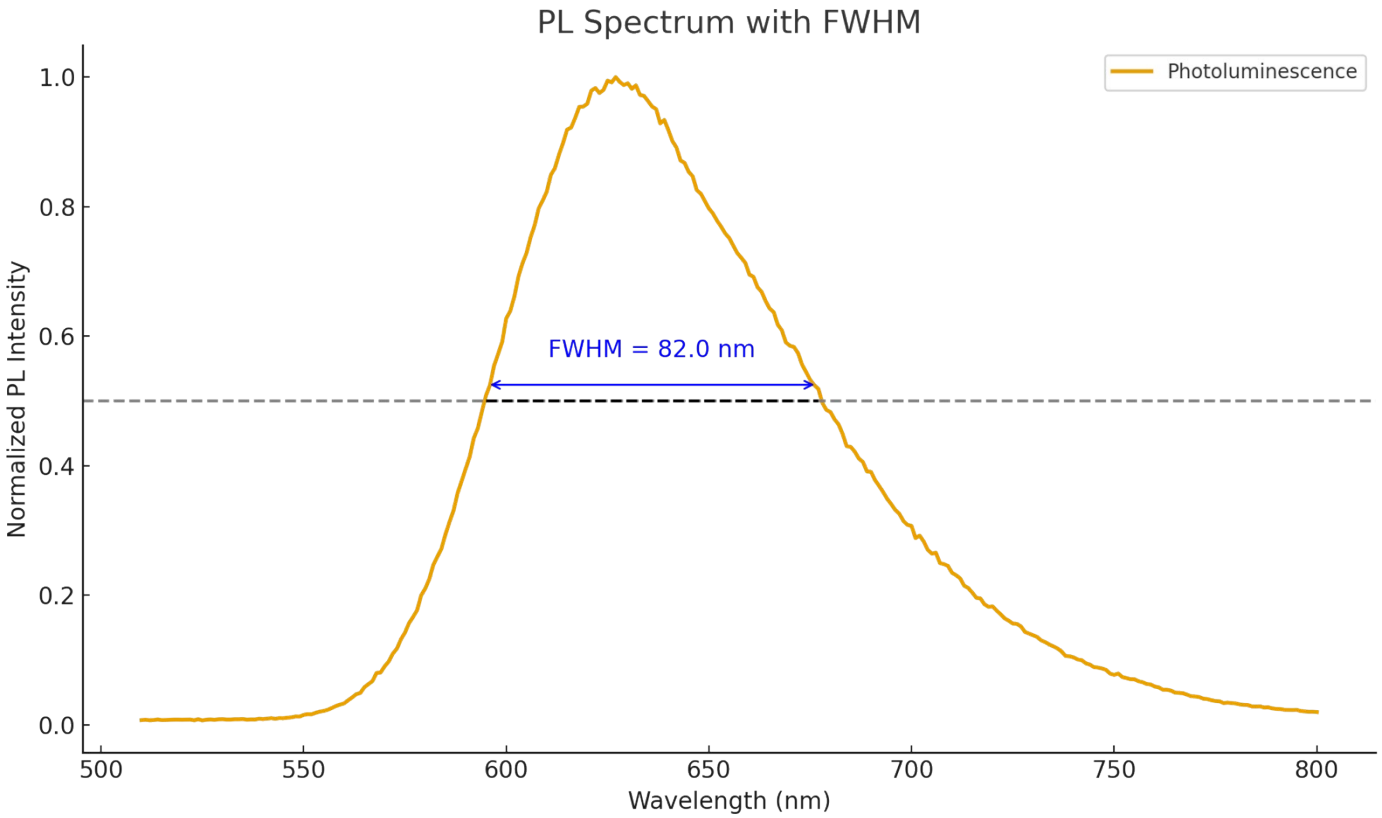

Figure S10. Photoluminescence spectrum of **3**·TCB.

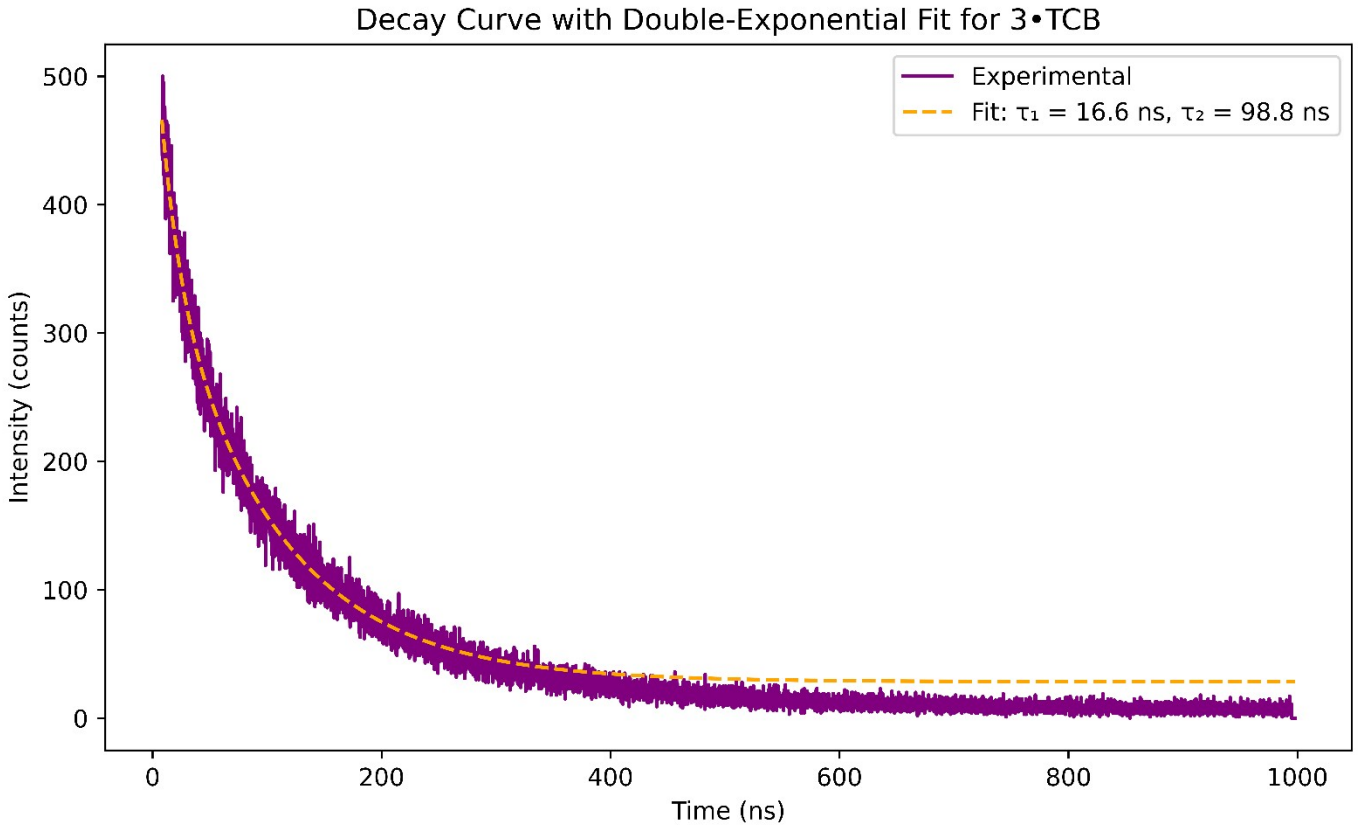

Figure S11. Measurement of lifetimes for **3**·TCB

S3. Calculation details

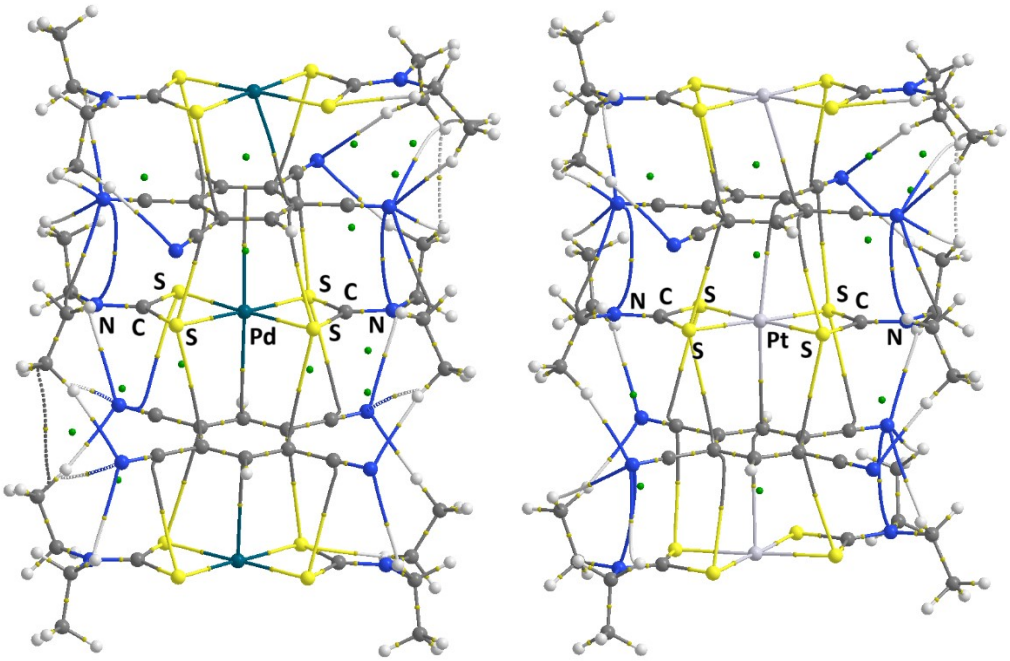

Figure S12. Bond paths with bond (yellow) and cage (green) critical points in the optimized structures of **2**·TCB (left) and **3**·TCB (right).

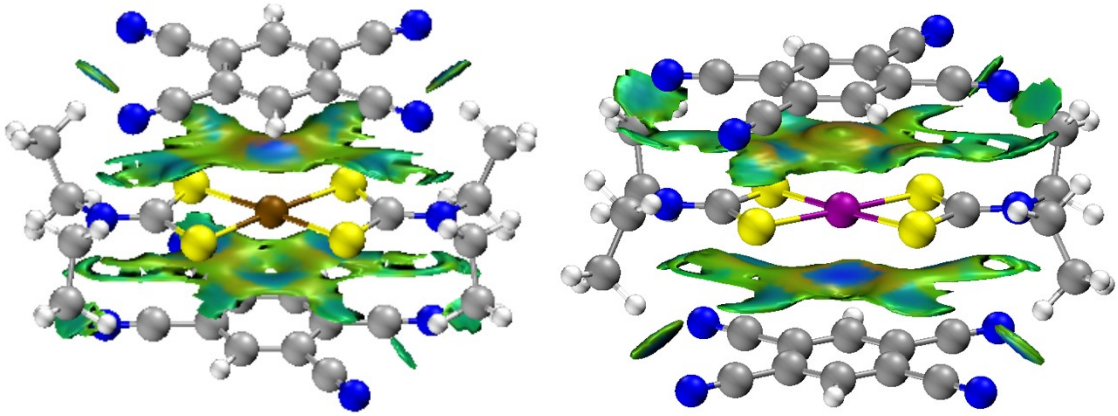

Figure S13. The sign(λ_2)ρ(r) function mapped on the δg^{inter} isosurface (δg^{inter} = 0.005 au and blue-cyan-green-yellow-red colour scale −0.015 < sign(λ_2)ρ(r) < 0.015) for the optimized structures **2**·TCB (left) and **3**·TCB (right).

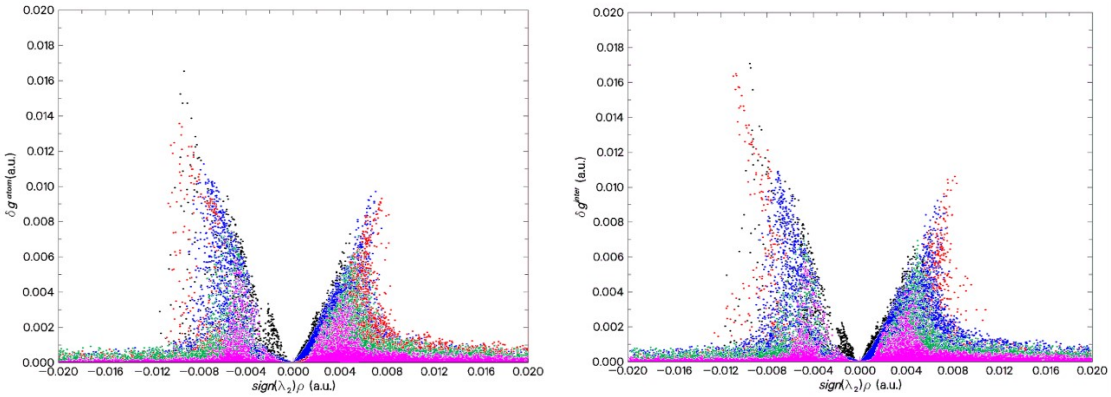

Figure S14. Scatter map of the IGMH δg^{atom} signatures for the metal (red), sulfur (blue), thiocarbamate carbon (green), nitrogen (pink) atoms and ethyl groups (black) in the optimized structures of **2**·TCB (left) and **3**·TCB (right).

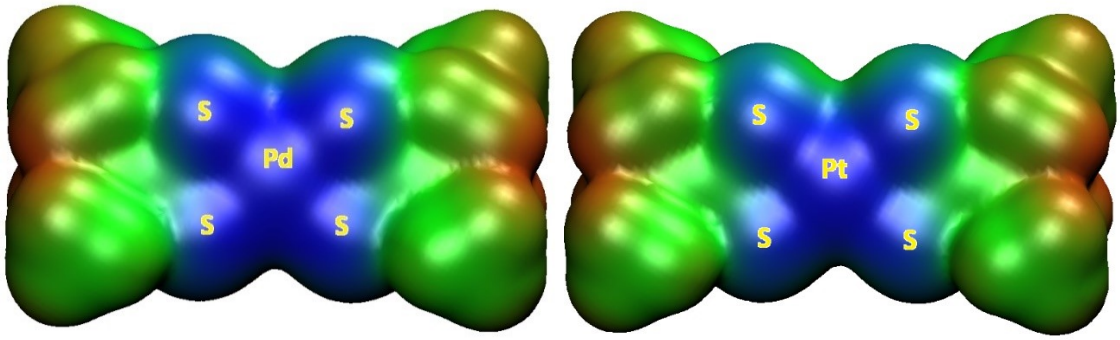

Figure S15. Distribution of ESP in the optimized structures of **2** and **3** (electron density isosurfaces 0.002 au, blue-cyan-green-yellow-red colour scale from –0.05 to 0.05).

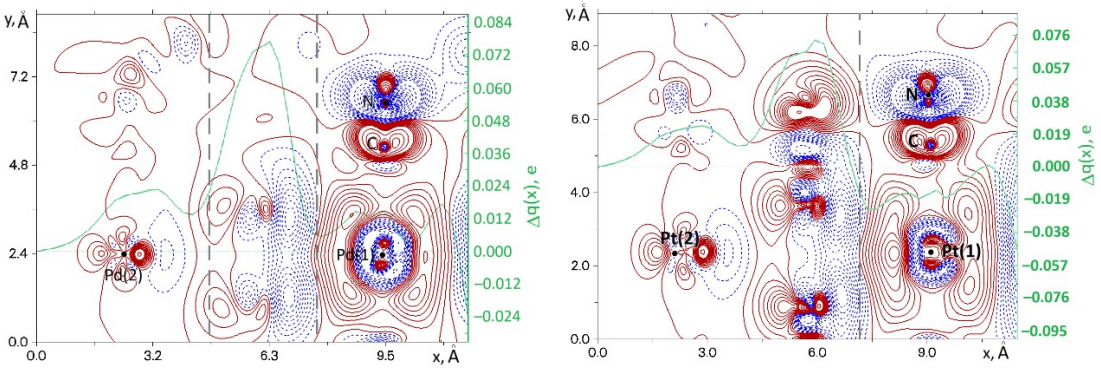

Figure S16. EDD contour plots for the M(1)M(2)N(1) plane (isovalues from –0.01 to 0.01 au, red solid contours – charge concentration, blue dashed contours – charge depletion) and CDF function along the M(1)M(2) axis in the optimized structures **2**·TCB (left) and **3**·TCB (right) (the gray vertical lines identifies the boundary between two molecules).

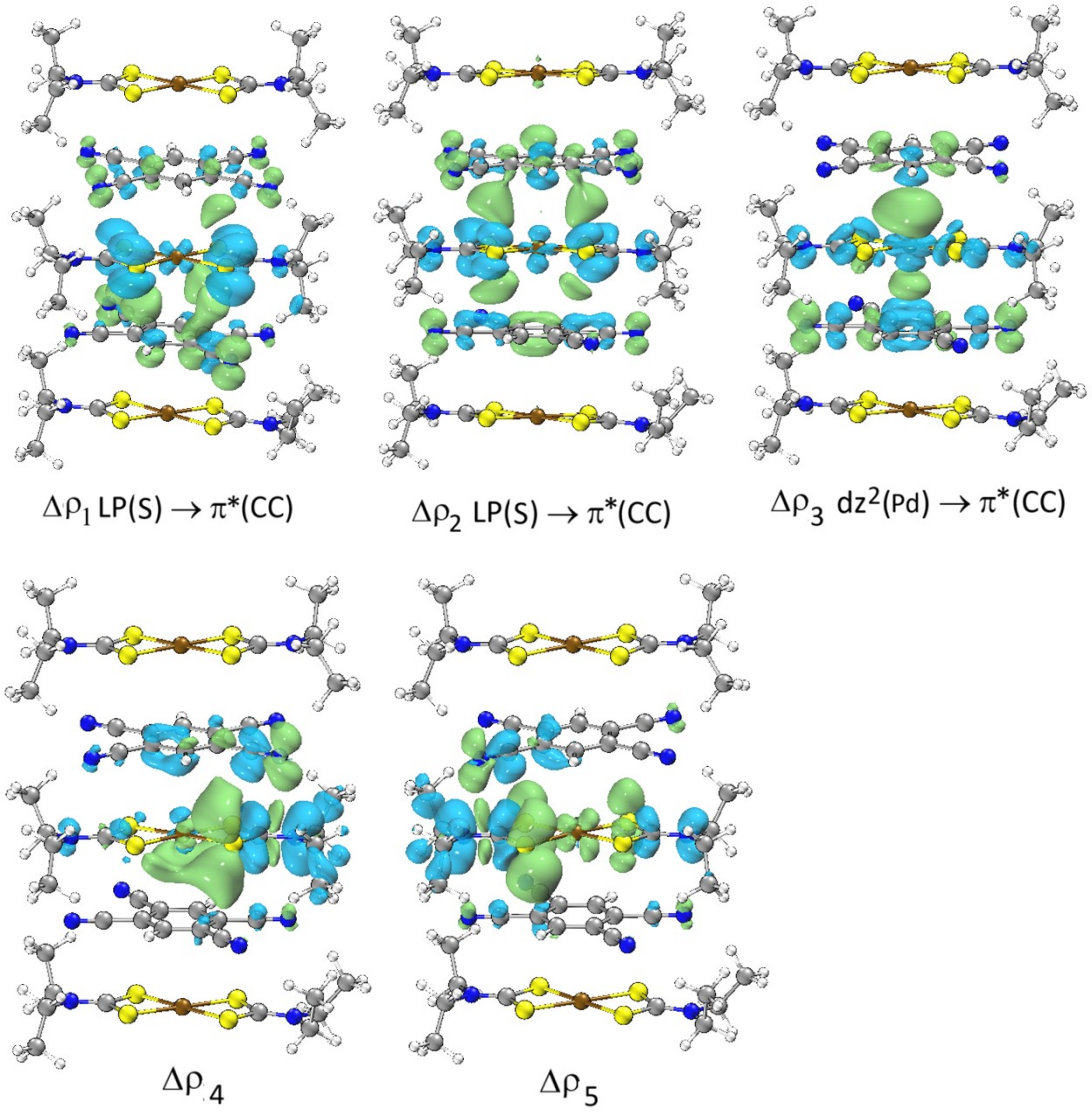

Figure S17. ETS-NOCV deformation densities for the optimized structure **2**·TCB (electron transfer occurs from the zones of the charge density depletion (cyan) to those of the charge density concentration (green), isovalues ±0.0001 au).

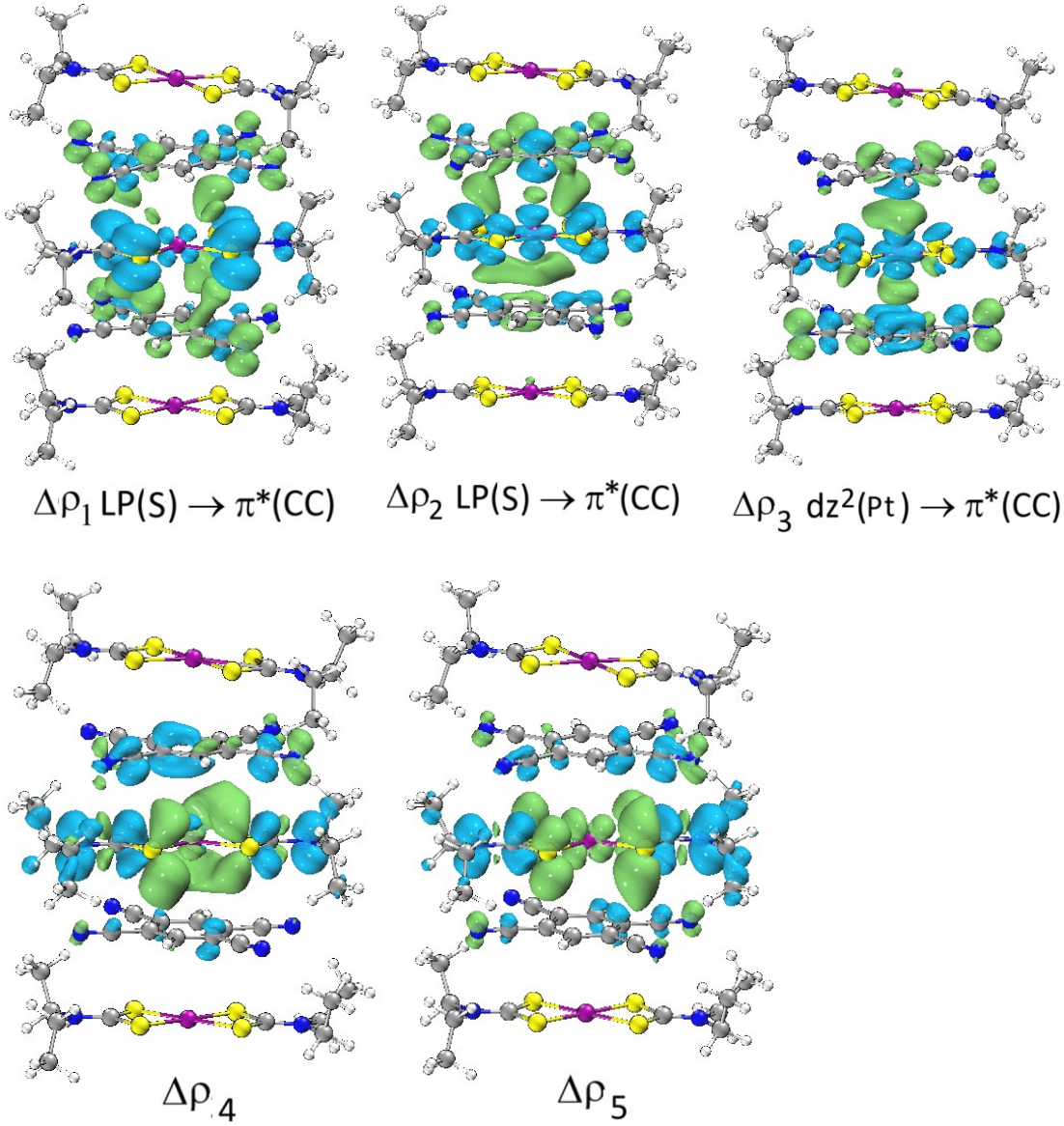

Figure S18. ETS-NOCV deformation densities for the optimized structure **3**·TCB (electron transfer occurs from the zones of the charge density depletion (cyan) to those of the charge density concentration (green), isovalues ±0.0001 au).

Table S2. 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) (in au) and intrinsic bond strength index (IBSI) at BCPs in the optimized structures of **1**·TCB and **2**·TCB.

Structure	Contacts	ρ_b	$\nabla^2\rho_b$	V_b	G_b	λ_2	IBSI
1·TCB	Ni···C	0.0068	0.0185	–0.0035	0.0041	–0.0010	0.0082
		0.0065	0.0179	–0.0033	0.0039	–0.0004	0.0076
	S···C	0.0086	0.0241	–0.0041	0.0051	–0.0021	0.0091
		0.0074	0.0215	–0.0034	0.0044	–0.0017	0.0078
		0.0065	0.0180	–0.0028	0.0036	–0.0005	
		0.0079	0.0220	–0.0036	0.0045	–0.0022	0.0073
		0.0072	0.0210	–0.0034	0.0043	–0.0015	0.0070
		0.0085	0.0236	–0.0040	0.0050	–0.0020	0.0084
		0.0080	0.0216	–0.0036	0.0045	–0.0021	0.0074
		0.0064	0.0174	–0.0027	0.0035	–0.0010	
	N···H	0.0061	0.0231	–0.0033	0.0045	–0.0031	0.0067
		0.0054	0.0221	–0.0031	0.0043	–0.0020	0.0055
		0.0054	0.0201	–0.0028	0.0039	–0.0033	0.0055
		0.0057	0.0226	–0.0032	0.0044	–0.0025	0.0058
		0.0068	0.0229	–0.0034	0.0045	–0.0050	0.0094
		0.0069	0.0234	–0.0035	0.0047	–0.0051	0.0095
		0.0056	0.0207	–0.0029	0.0040	–0.0036	0.0058
		0.0053	0.0212	–0.0029	0.0041	–0.0021	0.0049
		0.0050	0.0208	–0.0028	0.0040	–0.0018	0.0048
		0.0064	0.0237	–0.0034	0.0047	–0.0036	0.0072
2·TCB	Pd···(C=C)	0.0070	0.0201	–0.0035	0.0043	–0.0003	
	Pd···C	0.0098	0.0260	–0.0053	0.0059	–0.0029	
	S···C	0.0080	0.0228	–0.0038	0.0047	–0.0018	
		0.0067	0.0196	–0.0030	0.0040	–0.0011	
		0.0070	0.0199	–0.0031	0.0041	–0.0016	

		0.0074	0.0210	–0.0034	0.0043	–0.0019	
		0.0069	0.0217	–0.0033	0.0043	–0.0026	
		0.0059	0.0176	–0.0026	0.0035	–0.0014	
	S···N	0.0070	0.0225	–0.0033	0.0045	–0.0022	
	N···C	0.0045	0.0192	–0.0025	0.0036	–0.0007	
		0.0050	0.0211	–0.0029	0.0041	–0.0009	
	N···H	0.0060	0.0221	–0.0032	0.0043	–0.0037	
		0.0050	0.0192	–0.0027	0.0037	–0.0032	
		0.0093	0.0315	–0.0048	0.0064	–0.0077	
		0.0054	0.0198	–0.0027	0.0038	–0.0033	
		0.0057	0.0195	–0.0028	0.0038	–0.0039	
		0.0047	0.0177	–0.0024	0.0034	–0.0030	
		0.0094	0.0319	–0.0049	0.0064	–0.0078	
3·TCB	Pt···C	0.0080	0.0226	–0.0042	0.0049	–0.0006	
		0.0108	0.0280	–0.0059	0.0065	–0.0028	
	S···C	0.0071	0.0220	–0.0034	0.0044	–0.0026	
		0.0067	0.0193	–0.0030	0.0039	–0.0015	
		0.0079	0.0225	–0.0038	0.0047	–0.0017	
		0.0071	0.0203	–0.0032	0.0042	–0.0018	
		0.0074	0.0210	–0.0034	0.0043	–0.0019	
		0.0071	0.0217	–0.0033	0.0044	–0.0025	
		0.0059	0.0176	–0.0027	0.0035	–0.0013	
	N···C	0.0042	0.0180	–0.0023	0.0034	–0.0006	
		0.0050	0.0209	–0.0028	0.0040	–0.0009	
	N···H	0.0064	0.0234	–0.0034	0.0046	–0.0040	
		0.0059	0.0214	–0.0031	0.0042	–0.0043	
		0.0094	0.0317	–0.0049	0.0064	–0.0078	
		0.0053	0.0195	–0.0027	0.0038	–0.0032	
		0.0061	0.0206	–0.0030	0.0041	–0.0042	

		0.0047 0.0096	0.0177 0.0326	–0.0024 –0.0050	0.0034 0.0066	–0.0031 –0.0082	

Table S3. Highest atomic pair and overall atomic contributions (%) in the interaction of complexes **1** or **2** with two TCB molecules (X-ray structures).

Atomic pair percentage contributions				Overall atomic percentage contribution			
Contact	%	Contact	%	Atom	%	Atom	%
1·TCB							
Ni···C	1.60	N···H	0.94	Ni	14.73	S	7.60
Ni···C	1.47	Ni···C	0.94	S	8.28	C	5.84
Ni···C	1.06	S···C	0.93	S	7.92	C	5.42
Ni···C	1.04	S···C	0.91	S	7.85	H	3.20
2·TCB							
Pd···C	2.05	N···H	0.98	Pd	13.87	S	8.12
Pd···C	1.82	S···C	0.98	S	8.87	C	6.02
Pd···C	1.13	S···C	0.97	S	8.47	C	5.56
Pd···C	1.06	S···C	0.93	S	8.38	H	3.23

Table S4. Cartesian atomic coordinates (in Å) of the calculated equilibrium structures of **1**·TCB, **2**·TCB, and **3**·TCB.

1·TCB			
Ni	6.561236	0.089617	0.103435
S	6.537996	1.641768	1.688569
S	6.675946	1.944647	-1.143141
S	6.507653	-1.705035	1.411985
S	6.695037	-1.537494	-1.432915
N	6.768998	-3.899028	-0.119294
N	7.007473	4.037077	0.528276
C	6.762172	2.739895	0.383322
C	6.671641	-2.577909	-0.062391
C	7.197471	4.894145	-0.639769
H	7.796941	4.328403	-1.371288
H	7.806294	5.748672	-0.306513
C	6.972740	-4.604515	-1.378786
H	7.710956	-5.400242	-1.184610
H	7.436335	-3.898952	-2.084032
C	7.130210	4.643863	1.849796
H	8.077487	5.209742	1.860187

H	7.237509	3.823432	2.573515
C	6.687657	-4.704413	1.093817
H	6.246845	-5.671694	0.809188
H	5.970409	-4.217732	1.771291
C	5.961104	5.535891	2.230201
H	5.888387	6.418253	1.576482
H	6.096975	5.897255	3.260878
H	5.013260	4.980380	2.176910
C	5.903463	5.365779	-1.281993
H	6.131200	6.019836	-2.137380
H	5.275360	5.927284	-0.576208
H	5.316980	4.517489	-1.657866
C	5.692587	-5.180722	-1.957557
H	5.922049	-5.764990	-2.861363
H	4.988947	-4.386524	-2.239610
H	5.186561	-5.846679	-1.241903
C	8.037464	-4.888690	1.766595
H	8.761873	-5.373672	1.093736
H	7.931464	-5.519512	2.662074
H	8.446211	-3.915894	2.077246
Ni	-6.574113	-0.186821	0.071668
S	-6.647315	1.777394	-0.959793
S	-6.706419	1.194438	1.831627
N	-6.976265	3.714880	0.874833
C	-6.797091	2.422814	0.628844
C	-7.007777	4.678664	-0.221424
H	-6.261945	4.363847	-0.967060
H	-6.660862	5.639887	0.185850
C	-7.261424	4.217291	2.214483
H	-7.532994	3.352515	2.837028
H	-8.161030	4.851538	2.134705
C	-8.385767	4.814697	-0.847913
H	-8.362446	5.566663	-1.650949
H	-9.137015	5.132456	-0.108135
H	-8.705736	3.856421	-1.282629
C	-6.114619	4.990350	2.840185
H	-5.227198	4.358174	2.980393
H	-6.423542	5.368783	3.826313
H	-5.822358	5.858984	2.229834
S	-6.525613	-2.206657	1.042090
S	-6.499515	-1.494681	-1.722727
N	-6.467156	-4.061730	-0.923498
C	-6.494516	-2.782186	-0.580384
C	-6.508124	-5.125811	0.071984
H	-7.023579	-4.732572	0.960978
H	-7.141148	-5.927505	-0.342102
C	-6.389135	-4.456902	-2.325772
H	-5.767161	-3.716009	-2.849271
H	-5.839322	-5.409325	-2.362237
C	-5.131507	-5.652745	0.438719
H	-5.229400	-6.504926	1.128137
H	-4.576411	-5.991144	-0.449408

H	-4.533868	-4.879377	0.938821
C	-7.757816	-4.580423	-2.973573
H	-8.277055	-3.610841	-2.957650
H	-7.653394	-4.897991	-4.022019
H	-8.386078	-5.321601	-2.455160
Ni	0.018606	0.010438	-0.066930
S	0.259418	-1.047909	1.887681
S	0.115186	-2.105479	-0.757691
S	-0.209763	1.067497	-2.022544
S	-0.090512	2.125541	0.624013
N	0.354470	-3.700500	1.398954
N	-0.314377	3.719965	-1.535528
C	-0.219918	2.494617	-1.052325
C	0.257676	-2.474753	0.917441
C	0.389797	-3.947466	2.836555
H	-0.122911	-4.906193	3.006133
H	-0.223632	-3.174877	3.322544
C	0.441785	-4.856090	0.509777
H	1.094381	-5.587439	1.010504
H	0.969218	-4.536397	-0.401258
C	-0.318929	3.967545	-2.973814
H	0.311117	3.199437	-3.445643
H	0.190525	4.930232	-3.130410
C	-0.426861	4.875986	-0.648939
H	-0.967261	4.553075	0.253289
H	-1.077518	5.600348	-1.162176
C	1.796821	-3.958361	3.407905
H	2.434504	-4.701129	2.906932
H	1.759296	-4.195068	4.482002
H	2.270925	-2.973685	3.286918
C	-0.912148	-5.456850	0.173423
H	-0.771393	-6.362639	-0.435636
H	-1.524525	-4.750319	-0.404892
H	-1.471246	-5.730676	1.080613
C	-1.711389	3.968393	-3.579334
H	-1.649569	4.211814	-4.650801
H	-2.369191	4.700969	-3.089818
H	-2.177324	2.977787	-3.476331
C	0.915255	5.489060	-0.289430
H	1.521648	4.790786	0.304867
H	0.755432	6.396976	0.311583
H	1.490830	5.761765	-1.186575
N	3.198062	-3.004005	-3.304953
N	3.336018	3.360185	1.491555
N	2.969673	3.771624	-2.453236
N	3.492625	-3.566888	0.583702
C	3.235066	-2.096169	-2.586955
C	3.197188	0.315549	-2.244720
H	3.109031	0.456117	-3.321484
C	3.275761	-0.966370	-1.712866
C	3.373230	-1.144028	-0.315444
C	3.326171	2.400518	0.844450

C	3.085753	2.727245	-1.966002
C	3.397577	-0.039248	0.534123
H	3.479770	-0.179729	1.610620
C	3.208540	1.422688	-1.396441
C	3.310094	1.248917	-0.002056
C	3.440306	-2.473829	0.204623
N	-3.308724	-3.285668	-1.621283
N	-3.196065	3.154357	3.074395
N	-3.528385	3.645763	-0.819370
N	-2.857277	-3.629599	2.342833
C	-3.289410	-2.321386	-0.980231
C	-3.152523	-1.304947	1.247753
C	-3.266927	1.087716	1.520782
C	-3.392438	0.118049	-0.705379
H	-3.490749	0.234583	-1.783536
C	-3.470569	2.559293	-0.422039
C	-3.232228	2.233159	2.373915
C	-3.273762	-1.157644	-0.149536
C	-3.154319	-0.183625	2.074551
H	-3.052907	-0.302403	3.152703
C	-3.000733	-2.596630	1.839158
C	-3.383508	1.240227	0.122445
2·TCB			
Pd	-0.097787	0.044297	-0.736755
S	-0.266091	-1.608890	-2.374890
S	-0.225484	1.987643	-2.012151
S	0.015633	-1.995807	0.448779
S	0.011879	1.807414	0.834703
N	-0.158441	-4.062218	-1.282602
N	-0.228160	4.175009	-0.458844
C	-0.153033	2.857270	-0.528038
C	-0.136431	-2.753977	-1.093116
C	-0.195026	-4.620759	-2.630804
H	0.321403	-5.591274	-2.584484
H	0.415517	-3.971686	-3.276769
C	-0.166583	-5.000888	-0.165923
H	-0.899986	-5.783485	-0.417232
H	-0.563071	-4.471251	0.712870
C	-0.279586	4.881236	0.815661
H	-0.628945	4.168764	1.576799
H	-1.065454	5.647304	0.720270
C	1.200024	-5.593572	0.128081
H	1.906211	-4.824364	0.467793
H	1.629481	-6.087823	-0.757139
H	1.111859	-6.345711	0.926467
C	-0.301254	4.982903	-1.674025
H	0.324977	4.495503	-2.436620
H	0.181595	5.943619	-1.440435
C	-1.603738	-4.777234	-3.177443
H	-1.566946	-5.247346	-4.171780
H	-2.090154	-3.796404	-3.279050
H	-2.228392	-5.397554	-2.518281

C	1.050338	5.493820	1.216308
H	1.435340	6.175583	0.442327
H	1.809517	4.722268	1.401566
H	0.925356	6.073493	2.143313
C	-1.720550	5.191327	-2.174974
H	-1.708267	5.863340	-3.046361
H	-2.359737	5.639996	-1.400058
H	-2.178275	4.241607	-2.486391
Pd	6.816296	-0.031984	0.200386
S	6.954904	1.765161	1.680342
S	6.666524	1.891124	-1.163682
N	6.876077	4.111666	0.376405
C	6.832606	2.786527	0.299426
C	6.997251	4.771866	1.672768
H	6.399194	4.199571	2.398230
H	6.515811	5.756392	1.578910
C	6.919913	4.957454	-0.810555
H	7.140400	4.307635	-1.669928
H	7.782564	5.635484	-0.691465
C	8.439245	4.909069	2.133198
H	9.039621	5.490769	1.416429
H	8.902097	3.918695	2.253725
H	8.476715	5.426450	3.103629
C	5.646371	5.748511	-1.050833
H	5.780200	6.396953	-1.929929
H	5.397460	6.396750	-0.196366
H	4.789734	5.088617	-1.243905
S	6.647863	-1.921459	-1.207312
S	6.947109	-1.864718	1.639701
N	6.776792	-4.176307	0.282946
C	6.787170	-2.850648	0.236807
C	6.715608	-4.992089	-0.923032
H	7.066501	-4.373536	-1.762613
H	7.446881	-5.807705	-0.795446
C	6.867364	-4.876112	1.559708
H	6.318845	-4.284029	2.307526
H	6.318682	-5.823165	1.447711
C	5.329930	-5.545782	-1.206913
H	4.938741	-6.121951	-0.354251
H	4.617878	-4.741380	-1.433914
H	5.371318	-6.216540	-2.078482
C	8.303079	-5.118024	1.994585
H	8.321719	-5.664054	2.949793
H	8.855441	-5.714909	1.252085
H	8.829425	-4.162383	2.134502
N	2.960080	-3.205956	-2.295312
N	2.975460	3.687970	-1.701723
C	3.243730	-1.068597	-0.864405
C	3.488946	1.219698	0.725448
N	3.711306	3.371501	2.146443
N	3.684814	-3.542279	1.572928
C	3.095415	-2.245119	-1.663493

C	3.615248	2.399991	1.523393
C	3.254978	1.336286	-0.660471
C	3.592464	-2.482949	1.114316
C	3.126560	0.191825	-1.447645
H	2.926954	0.283234	-2.514890
C	3.606403	-0.042101	1.308247
H	3.808513	-0.133710	2.375039
C	3.476507	-1.186316	0.522665
C	3.109186	2.631274	-1.247902
Pd	-6.725532	-0.043690	0.583547
S	-6.951997	1.731627	-0.930775
S	-6.488681	-1.820752	2.101645
S	-6.805421	-1.984489	-0.739575
S	-6.621589	1.897724	1.903085
N	-6.555918	-4.180238	0.801535
N	-7.033055	4.088063	0.362159
C	-6.609286	-2.856484	0.734294
C	-6.879875	2.770700	0.438970
C	-7.062075	4.924917	1.555623
H	-7.017164	4.252873	2.424244
H	-8.048101	5.421804	1.585807
C	-6.613062	-4.995814	-0.405101
H	-5.991012	-5.885340	-0.223200
H	-6.125618	-4.433046	-1.214993
C	-6.454146	-4.875285	2.080391
H	-7.046310	-5.799844	1.986523
H	-6.949276	-4.252030	2.840860
C	-5.983697	4.968512	-1.734842
H	-5.505840	4.018564	-2.011338
H	-5.253031	5.569308	-1.175608
H	-6.232829	5.498968	-2.666465
C	-5.942601	5.948876	1.618626
H	-6.019059	6.692440	0.810487
H	-4.960933	5.459770	1.544924
H	-5.998822	6.492249	2.573960
C	-5.024028	-5.183921	2.488649
H	-4.461080	-4.262495	2.691347
H	-4.491617	-5.743301	1.704734
H	-5.023064	-5.789777	3.407380
C	-7.252927	4.734131	-0.930557
H	-7.767425	5.684703	-0.721151
H	-7.953594	4.104571	-1.503496
C	-8.033595	-5.375633	-0.787733
H	-8.027940	-6.002223	-1.692384
H	-8.628261	-4.474164	-0.997049
H	-8.531337	-5.943036	0.014116
C	-3.383565	-1.477526	-0.112914
N	-3.418421	3.861034	0.517419
N	-2.781310	-2.412135	3.225970
N	-3.390434	-4.049907	-0.397871
C	-3.417987	1.294454	0.195004
N	-3.859437	2.249958	-3.156726

C	-3.567680	0.725610	-1.086006
C	-2.986828	-1.739129	2.306180
C	-3.241707	0.478155	1.311886
H	-3.119063	0.926390	2.296914
C	-3.427117	2.713384	0.365535
C	-3.554611	-0.661911	-1.229913
H	-3.678306	-1.108571	-2.215281
C	-3.214657	-0.906517	1.166268
C	-3.732075	1.563593	-2.232672
C	-3.382921	-2.898768	-0.269513
3·TCB			
Pt	-0.005730	0.056886	0.318664
S	0.054413	1.636861	-1.430795
S	-0.033521	-1.433805	2.113837
S	0.002088	-2.087242	-0.657397
S	-0.006618	2.136586	1.371089
N	0.134375	4.150051	-0.405622
N	-0.021395	-3.991976	1.269976
C	0.065979	2.848142	-0.196343
C	-0.020420	-2.709668	0.953577
C	0.141602	-5.030481	0.258381
H	0.843558	-5.769498	0.676593
H	0.645360	-4.576481	-0.607935
C	-0.162109	-4.414724	2.660870
H	-0.659392	-5.396063	2.642886
H	-0.862169	-3.719854	3.149267
C	0.089817	5.084470	0.716704
H	-0.611819	4.677524	1.460905
H	-0.362188	6.012019	0.334690
C	0.314803	4.710554	-1.740000
H	0.729328	3.918320	-2.380026
H	1.096293	5.482417	-1.654236
C	1.454241	5.351043	1.329844
H	1.361799	6.111351	2.120040
H	2.168524	5.717181	0.577525
H	1.873281	4.441172	1.782421
C	1.159348	-4.486693	3.406591
H	0.987306	-4.852677	4.430043
H	1.622551	-3.491581	3.470677
H	1.871884	-5.159197	2.907362
C	-0.962543	5.277654	-2.332882
H	-1.413452	6.038202	-1.676861
H	-1.709791	4.493038	-2.512909
H	-0.738777	5.757344	-3.297641
C	-1.168051	-5.678560	-0.153566
H	-1.833318	-4.958676	-0.648849
H	-1.703523	-6.102728	0.710034
H	-0.967886	-6.496847	-0.861541
Pt	-6.749228	0.036493	0.022515
S	-6.658063	1.442451	1.898324
S	-6.601758	2.214883	-0.842840
N	-6.454781	4.028982	1.151073

C	-6.268817	5.075625	0.152921
H	-5.690917	4.646737	-0.679818
H	-5.631637	5.847479	0.611158
C	-6.557607	2.757927	0.791559
C	-6.518697	4.420236	2.554489
H	-7.202595	3.723215	3.063881
H	-6.989306	5.415688	2.587681
C	-7.582985	5.655982	-0.341116
H	-8.169143	6.092367	0.482805
H	-8.189354	4.876102	-0.824965
H	-7.391862	6.449589	-1.078989
C	-5.163769	4.434811	3.241487
H	-5.275841	4.780359	4.280363
H	-4.453620	5.096183	2.724573
H	-4.730895	3.424484	3.258047
S	-6.804919	-1.390167	-1.841922
S	-6.846883	-2.129693	0.907184
N	-6.850289	-3.977395	-1.058958
C	-6.911950	-5.026879	-0.047330
H	-7.500366	-4.641490	0.800015
H	-7.485534	-5.858787	-0.485961
C	-6.838937	-2.697898	-0.716563
C	-6.800076	-4.379438	-2.459222
H	-6.197837	-3.635112	-3.000897
H	-6.239912	-5.325611	-2.504572
C	-5.543053	-5.493263	0.419220
H	-4.924044	-5.832848	-0.424540
H	-5.004855	-4.683957	0.932899
H	-5.657902	-6.329003	1.126186
C	-8.181644	-4.513757	-3.076920
H	-8.097747	-4.832653	-4.126786
H	-8.793296	-5.258538	-2.544168
H	-8.708716	-3.548487	-3.051435
N	-3.287341	-3.038822	2.068625
C	-3.388590	1.024310	-1.464208
N	-3.613758	-3.765623	-1.837042
N	-3.199291	3.792798	0.636024
N	-3.452439	2.939095	-3.203530
C	-3.523890	-2.682326	-1.437414
C	-3.433871	-1.335174	-0.968495
C	-3.368557	-1.054182	0.410253
C	-3.324033	1.310288	-0.083362
C	-3.258290	2.674952	0.338104
C	-3.333497	-2.135974	1.344607
C	-3.442034	-0.295822	-1.898068
H	-3.505907	-0.519276	-2.962473
C	-3.307006	0.271935	0.845992
H	-3.249654	0.493510	1.910756
C	-3.421064	2.084846	-2.422326
Pt	6.736679	-0.067051	-0.226044
S	6.796756	1.893464	1.055287
S	6.676717	-1.825508	1.326866

S	6.772751	1.690743	-1.780001
S	6.673110	-2.028346	-1.512793
N	6.609221	-4.215615	0.071175
N	6.975848	4.081237	-0.508903
C	7.115558	4.757752	-1.792777
H	7.177623	3.978089	-2.565231
H	8.088789	5.280072	-1.786330
C	6.855595	2.761947	-0.430347
C	6.646947	-2.894706	-0.026373
C	6.656473	-5.067819	-1.112229
H	7.241159	-5.960279	-0.836349
H	7.230213	-4.534396	-1.885821
C	6.539734	-4.867114	1.373201
H	5.951070	-5.787767	1.242438
H	5.958482	-4.217334	2.044352
C	7.045530	4.889360	0.706993
H	7.558077	5.824279	0.432519
H	7.696936	4.359642	1.421857
C	5.283575	-5.456259	-1.633548
H	4.741858	-4.581984	-2.019927
H	4.668302	-5.917486	-0.846332
H	5.390763	-6.178467	-2.456993
C	5.988351	5.725797	-2.105413
H	5.963936	6.570914	-1.400148
H	5.014692	5.216996	-2.067408
H	6.133885	6.141753	-3.113839
C	5.694361	5.175215	1.343177
H	5.207829	4.248927	1.678719
H	5.016195	5.683819	0.644043
H	5.833069	5.817377	2.226134
C	7.912582	-5.159486	1.954863
H	7.812285	-5.667297	2.925963
H	8.470764	-4.224554	2.111340
H	8.502730	-5.810613	1.291275
N	3.399576	3.723200	-1.013967
C	3.389386	1.218181	-0.368309
N	3.113350	-2.864037	-2.937774
C	3.413710	0.821666	0.983966
N	3.324940	-4.008136	0.890524
C	3.301310	-1.092187	-1.060932
C	3.342150	-1.490382	0.291626
C	3.403045	2.603825	-0.718240
C	3.329048	-2.880259	0.626325
N	3.479909	2.606740	2.856106
C	3.333506	0.262471	-1.381647
H	3.309015	0.578402	-2.423700
C	3.394451	-0.535253	1.304738
H	3.420000	-0.849493	2.347066
C	3.454166	1.803267	2.022340
C	3.206346	-2.069975	-2.099822