Supporting Information

(η^4-Tetraphenylcyclobutadiene)-(η^5-pentaphenylcyclopentadienyl)-cobalt

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1. TABLES

Table S1. Experimental Details of the Structure determination.

Identification code	Compd **1**
Empirical formula	$C_{63}H_{45}Co$
Formula weight	860.92
Temperature	111(2) K
Crystal system	Monoclinic
Space group	*P* $2_1/n$
Unit cell dimensions	
a [Å]	9.8503(8)
b	13.5296(12)
c	33.179(2)
ß [°]	90.930(2)
Volume [$Å^3$]	4421.2(6)
Z	4
ρ_{calc} [g cm^{-3}]	1.293
μ [mm^{-1}]	0.431 mm-1
F(000)	1800
Crystal size	0.100 x 0.020 x 0.010
θ range	2.379 to 25.051°.
Index ranges	-10≤h≤11, -16≤k≤16, -39≤l≤38
Reflections collected	48011
Independent reflections [R_{int}]	7821 [0.0995]
Absorption correction	Semi-empirical from equivalents
T_{max}/ T_{min}	0.8620 / 0.8283
Data / parameters	7821 / 577
GOOF	1.013
R1/ wR2 [I>2σ(I)]	0.0487/ 0.0849
R1/wR2 (all data)	0.0867/ 0.0952
Largest diff. peak and hole [$eÅ^{-3}$]	0.268 and -0.371

Table S2. C–H…C(π) interactions in the [C_5Ph_5] ligand of **1**.

D–H…A	H…A [Å]	D-H-A
C26–H26…C11	2.571	111.6
C52–H52…C11	2.640	111.6
C22–H22…C31	2.628	119.2
C46–H46…C31	2.803	103.9
C42–H42…C51	2.670	115.2
C76–H76…C61	2.726	129.6
C72–H72…C81	2.776	118.7
C92–H92…C61	2.892	126.0
C76–H76…C81	2.797	129.2

Table S3. C–H…C(π) interactions in the [C_4Ph_4] ligand of **1**.

D–H…A	H…A [Å]	D-H-A [°]
C52–H52…C12	2.726	141.3
C26–H26…C16	2.836	140.6
C22–H22…C36	2.811	147.3
C76–H76…C62	2.776	137.5
C92–H92…C66	2.754	127.6
C72–H72…C86	2.689	148.2

Table S4. C–H…C(π) interactions between the [C_5Ph_5] and [C_4Ph_4] ligands of **1**.

D–H…A	H…A [Å]	D-H-A [°]
C16–H16…C71	2.748	130.6
C32–H32…C81	2.743	165.9
C46–H46…C91	2.778	126.0
C86–H86…C21	2.701	161.8
C62–H62…C51	2.861	122.3
C16–H16…C76	2.793	141.5
C26–H26…C72	2.684	125.8
C32–H32…C86	2.558	141.3
C46–H46…C96	2.818	150.9
C72–H72…C26	2.837	113.3
C62–H62…C56	2.803	95.5

Table S5. C–H…CT(π) interactions in **1**.

C–H…CT	H…CT [Å]	C–H—CT [°]	C…CT [Å]	C–H—(π-plane) [°]	Symm. Op.
C24–H24…CT(C81-C86)	2.91	173	3.856(3)	70	*1-x, -1-y, 1-z*
C35–H35…CT (C21-C26)	2.89	138	3.655(3)	47	*-x, -y, 1-z*
C46–H46…CT(C91-C96)	2.73	124	3.355(3)	42	*x, y, z*
C83–H83…CTC1-C5)	2.57	155	3.456(3)	73	*1+x, y, z*
C86–H86…CT(C21-C26)	2.97	158	3.870(3)	70	*x, y, z*

2. FIGURES

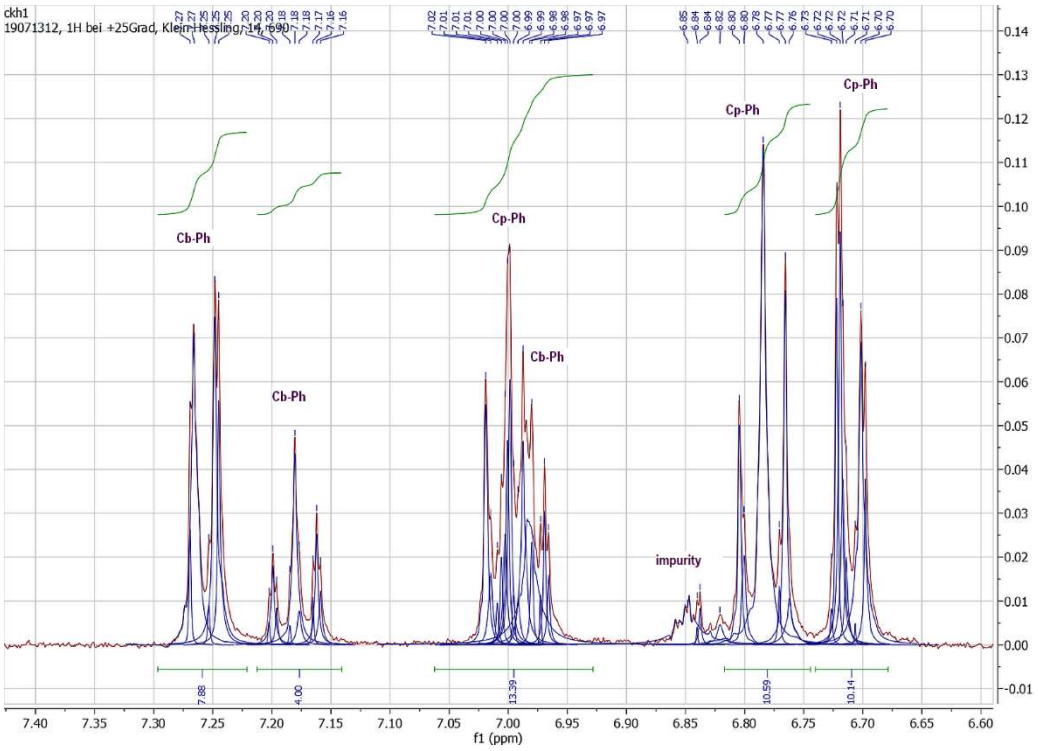

Figure S1. ^{1}H-NMR spectrum (400 MHz) of **1** in CD_2Cl_2, phenyl region.

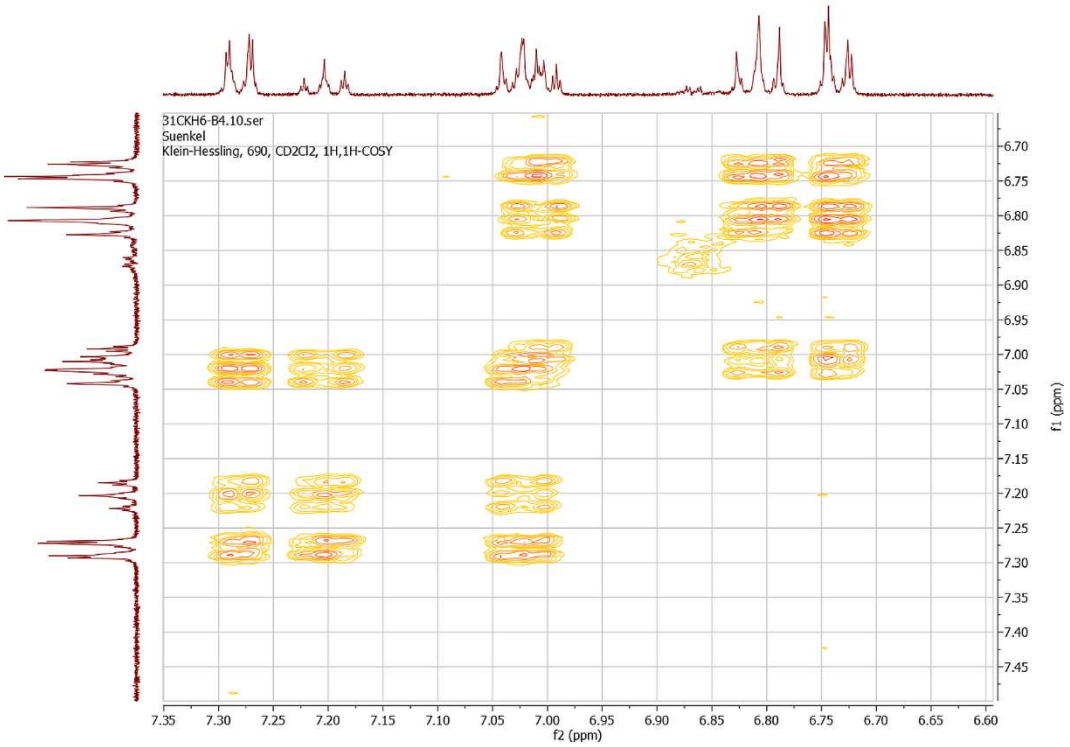

Figure S2. ^{1}H-^{1}H-COSY spectrum (400 Mhz) of **1** in CD_2Cl_2, phenyl region.

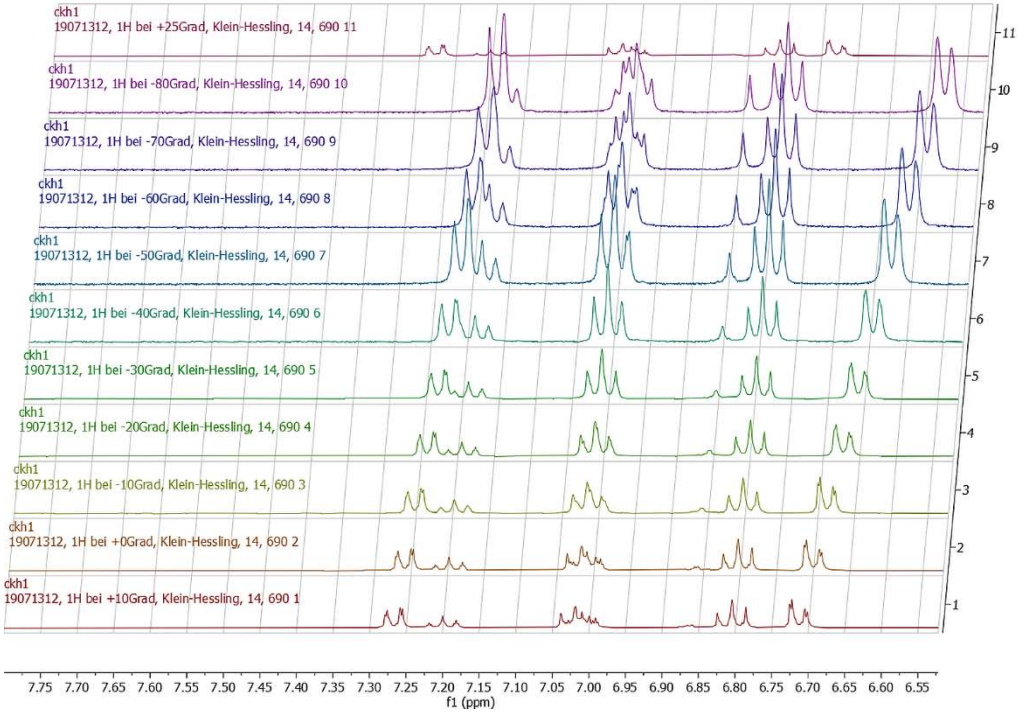

Figure S3. VT-^{1}H-NMR spectra (400 MHz) of **1** in CD_2Cl_2, phenyl region.

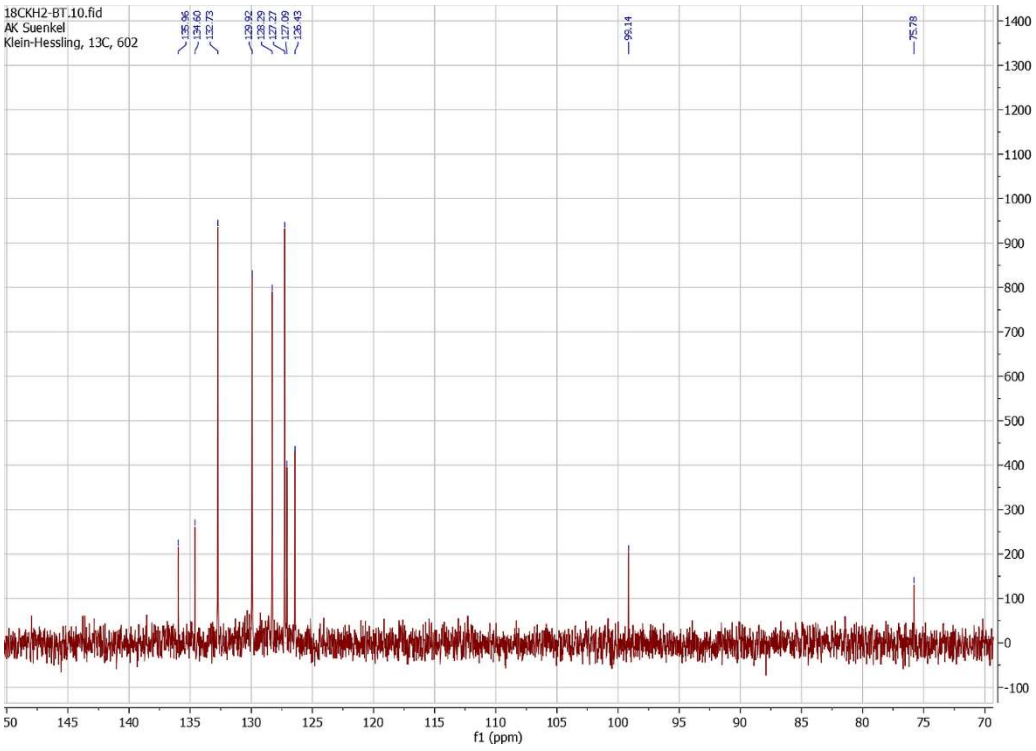

Figure S4. $^{13}C\{^{1}H\}$-NMR spectrum (100 MHz) of **1** in CD_2Cl_2, 150 > δ > 70ppm.

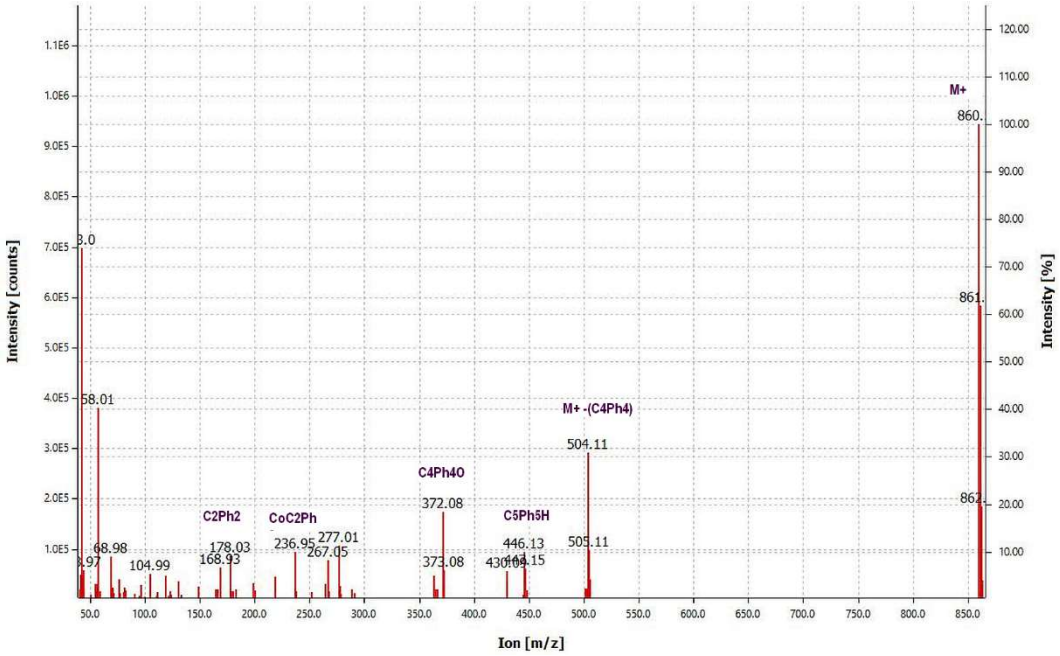

Figure S5. DEI-mass spectrum of **1**.

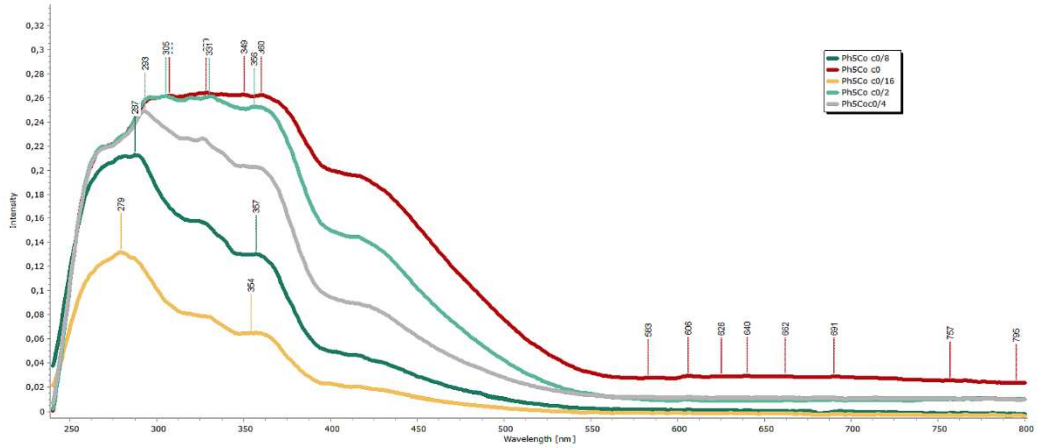

Figure S6. UV-Vis spectra of **1** in CH_2Cl_2, at five concentrations.

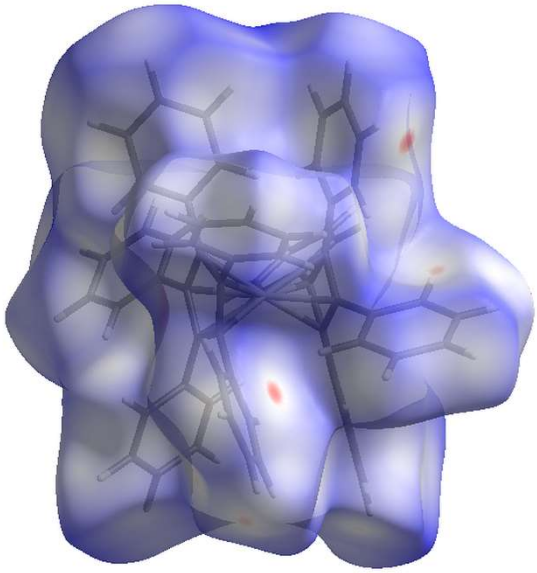

Figure S7. Hirshfeld surface of **1**.

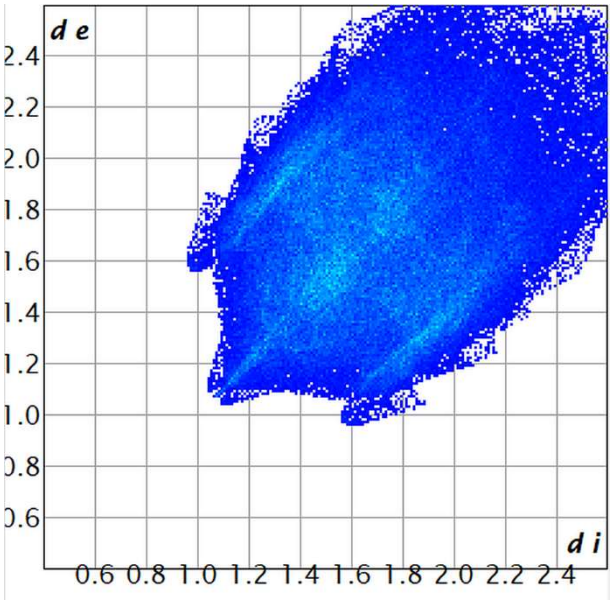

Figure S8. *CrystalExplorer* fingerprint plot of **1**.

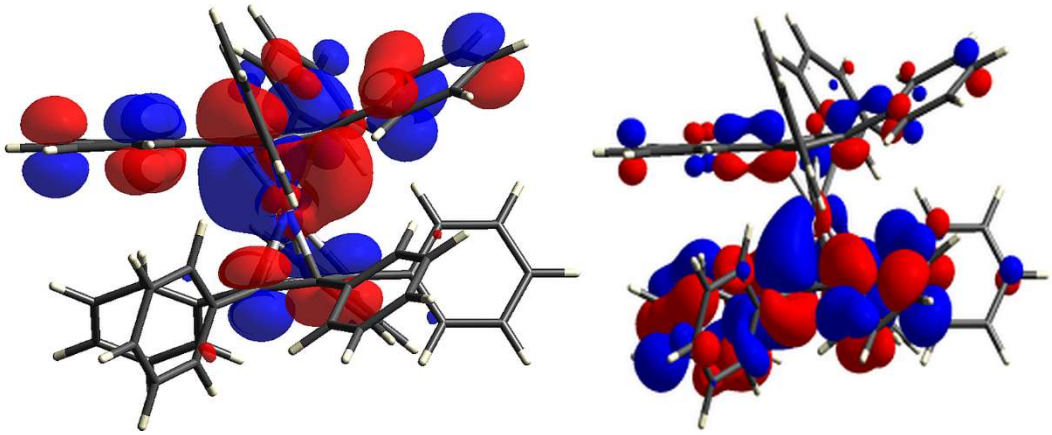

Figure S9. HOMO (left) and LUMO of **1**, as calculated by *CrystalExplorer*.

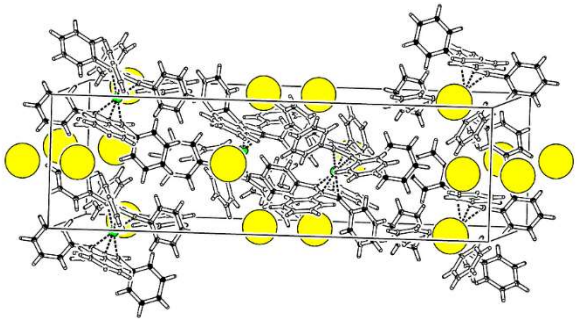

Figure S10. PLATON cavity plot for the unit cell of **1**.