Supporting Information

Phosphine oxide-donor based tricarbonylrhenium(I) complexes from phosphine/phosphine oxide and dihydroxybenzoquinones

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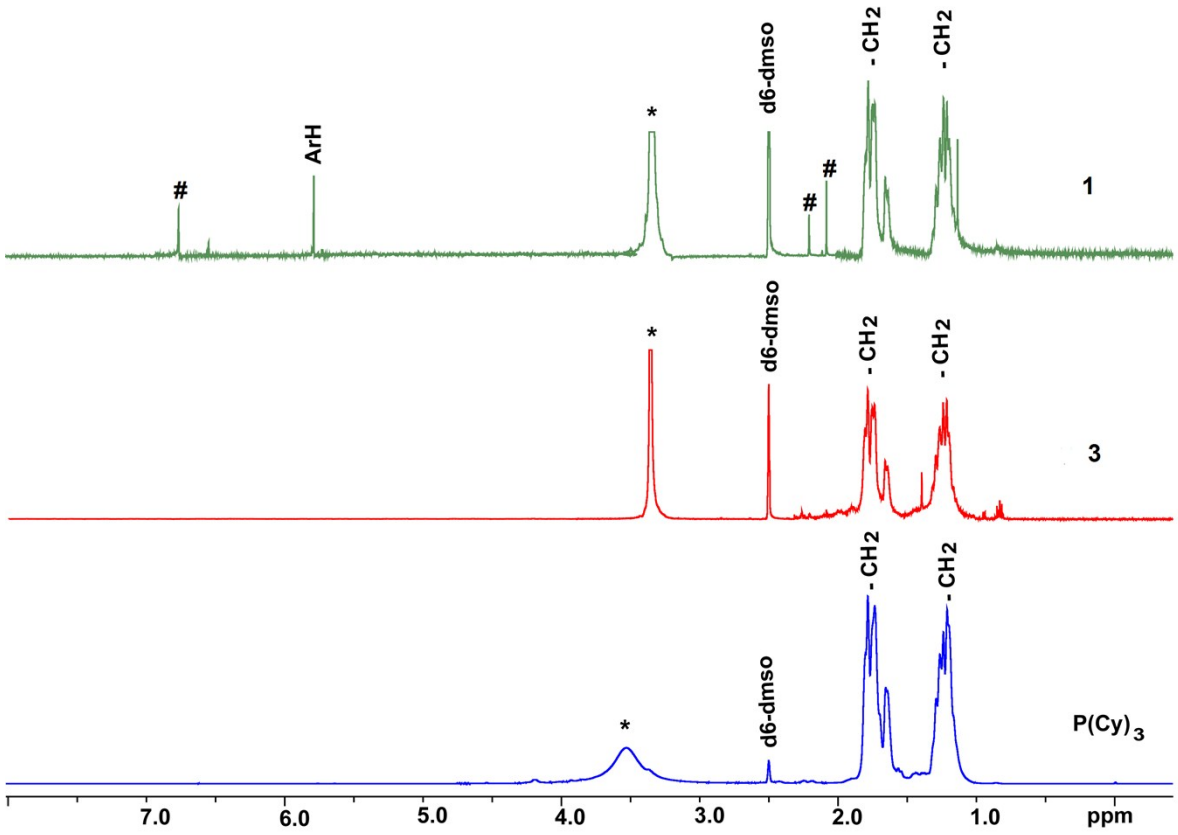


Figure S1. ^{1}H NMR spectra of free ligand, **3** and **1** in dmso–d_6 (# indicates mesitylene, and *indicates solvent water peaks).

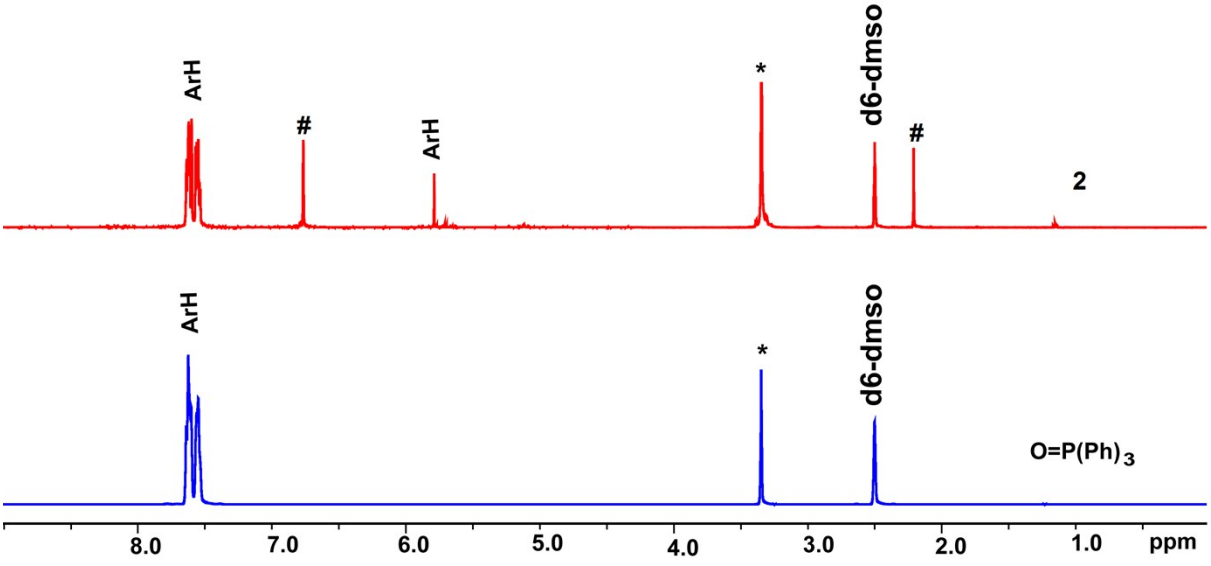


Figure S2. ^{1}H NMR spectra of free ligand and **2** in dmso–d_6 (# indicates mesitylene, and *indicates solvent water peaks).

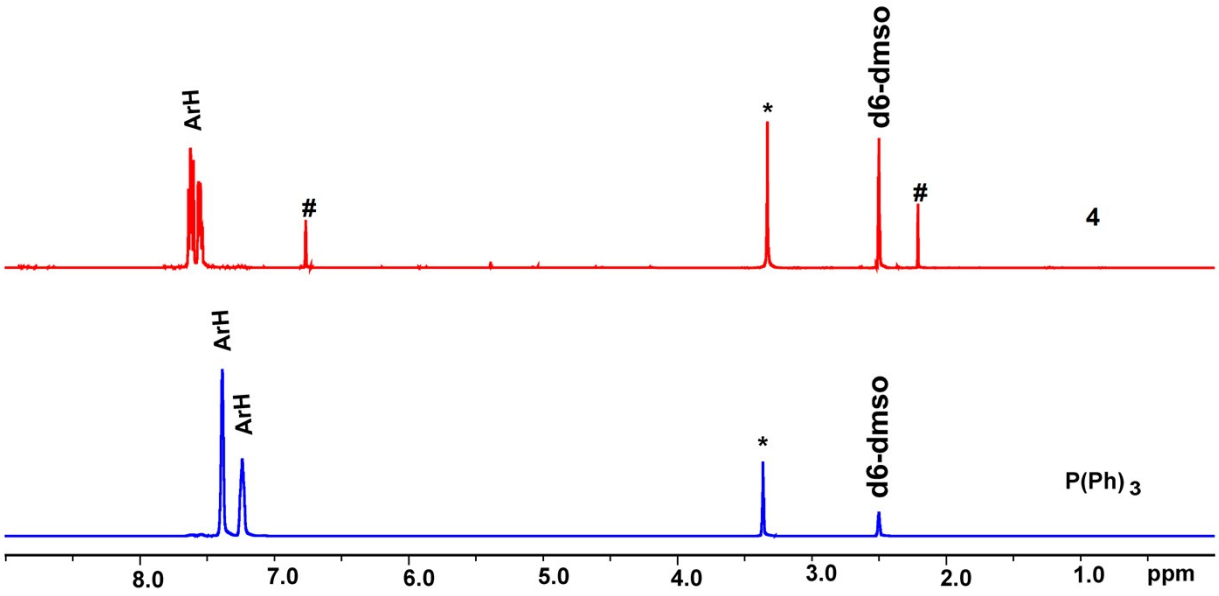


Figure S3. ^{1}H NMR spectra of free ligand and **4** in dmso–d_6 (# indicates mesitylene, and *indicates solvent water peaks).

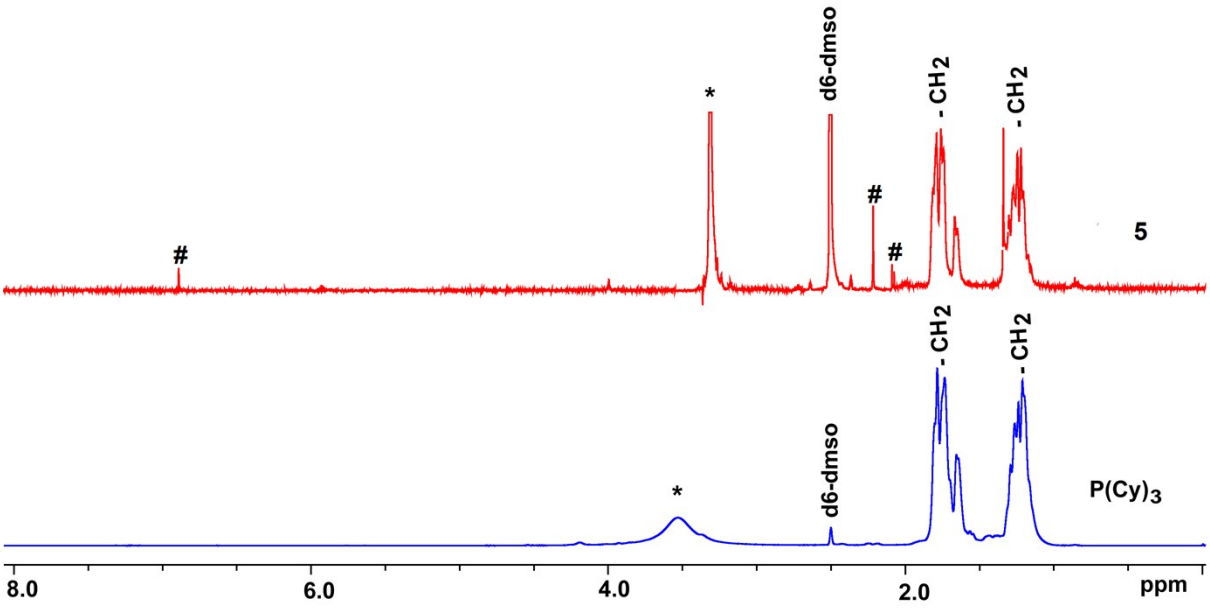


Figure S4. ^{1}H NMR spectra of free ligand and **5** in dmso–d_6 (# indicates mesitylene, and *indicates solvent water peaks).

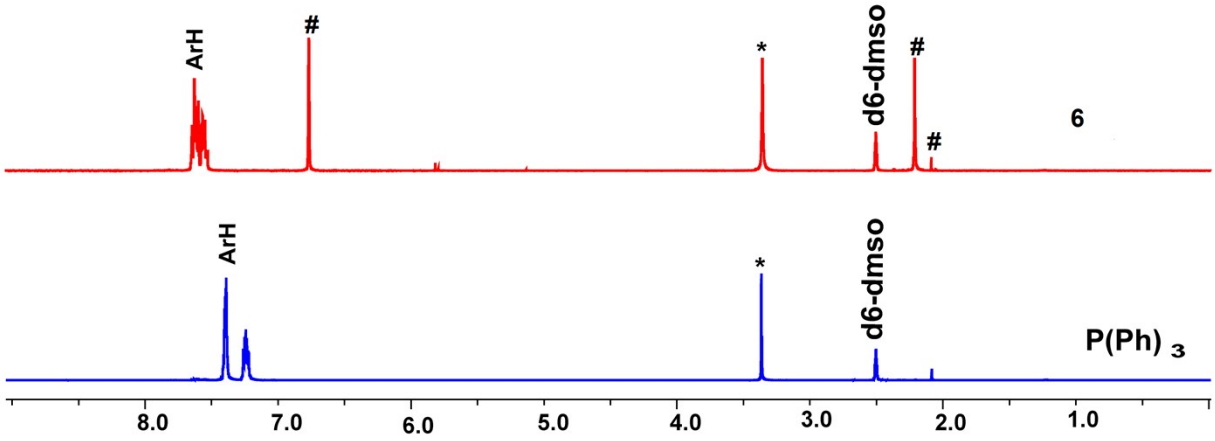


Figure S5. ^{1}H NMR spectra of free ligand and **6** in dmso–d_6 (# indicates mesitylene, and *indicates solvent water peaks).

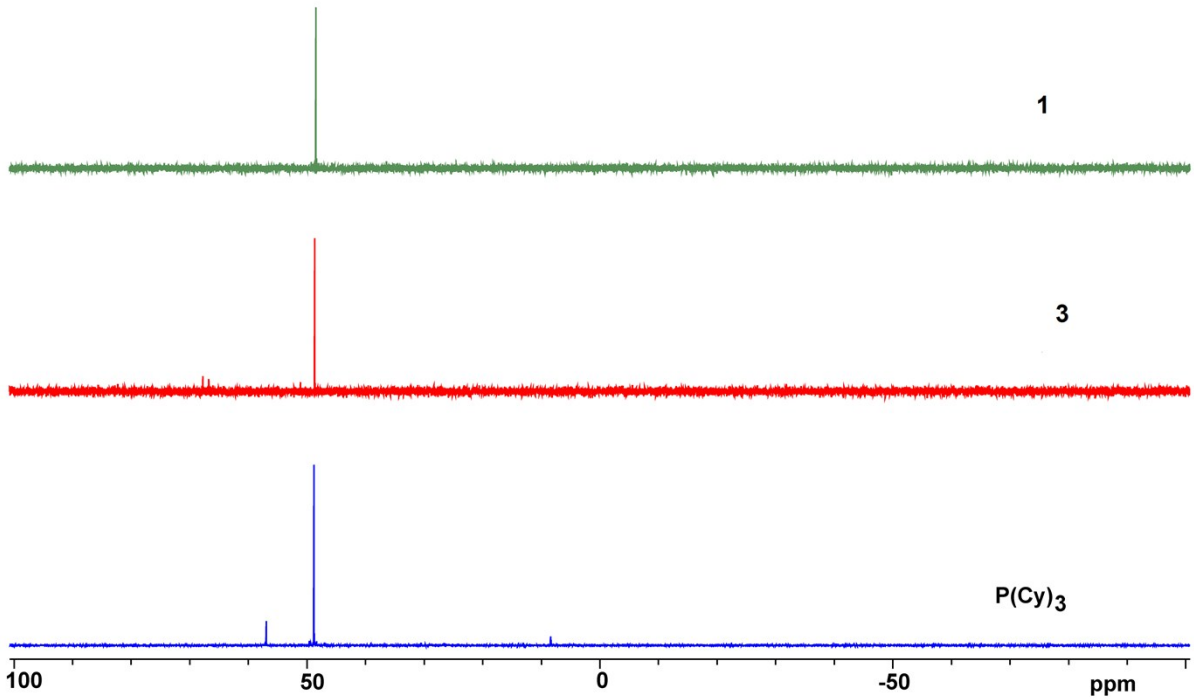


Figure S6. ^{31}P-{^{1}H} NMR spectra of free ligand, **3**, and **1** in dmso–d_6.

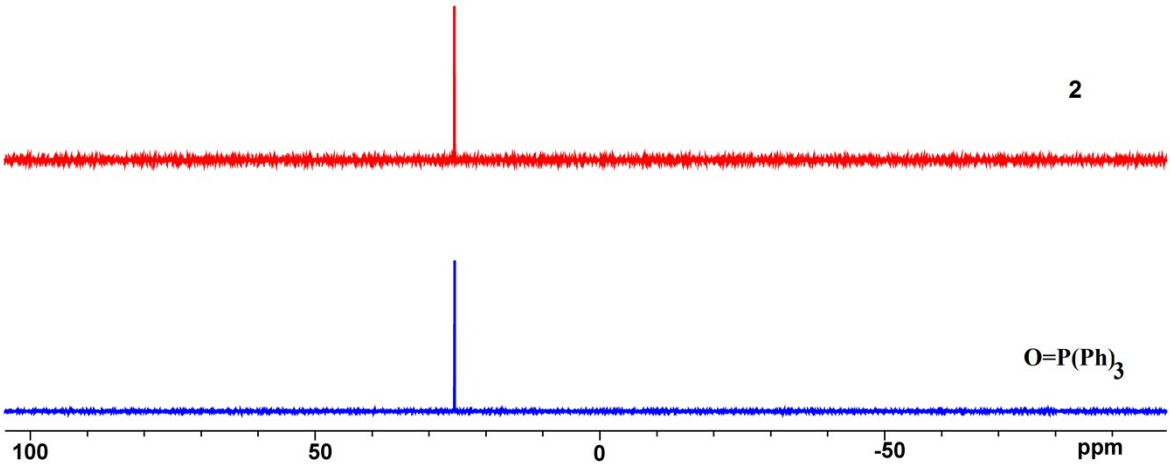


Figure S7. ^{31}P-{^{1}H} NMR spectra of free ligand, and **2** in dmso–d_6.

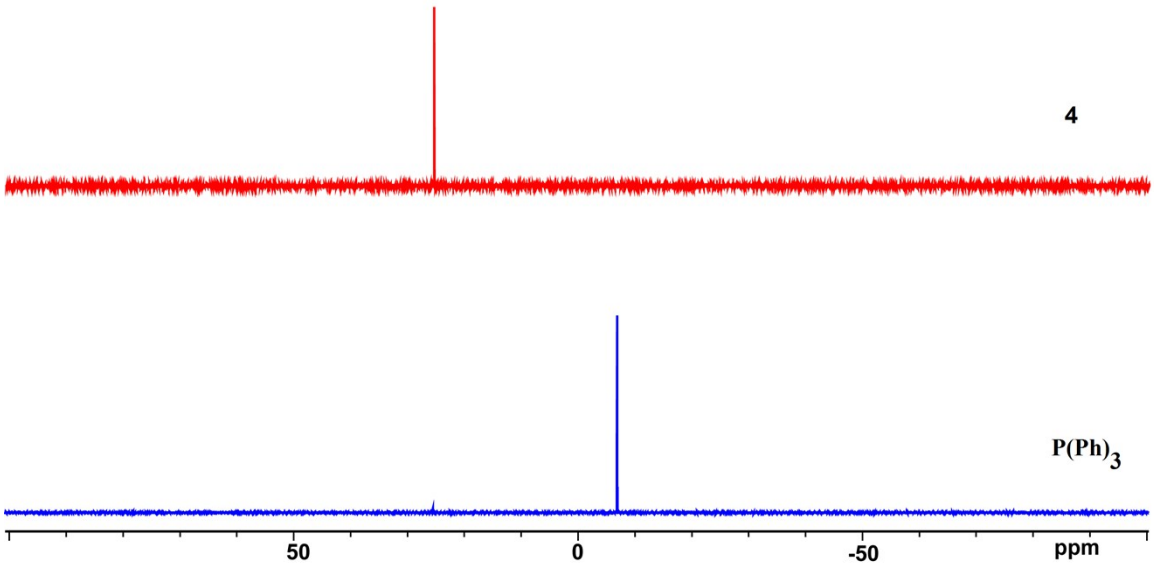


Figure S8. ^{31}P-{^{1}H} NMR spectra of free ligand and **4** in dmso–d_6.

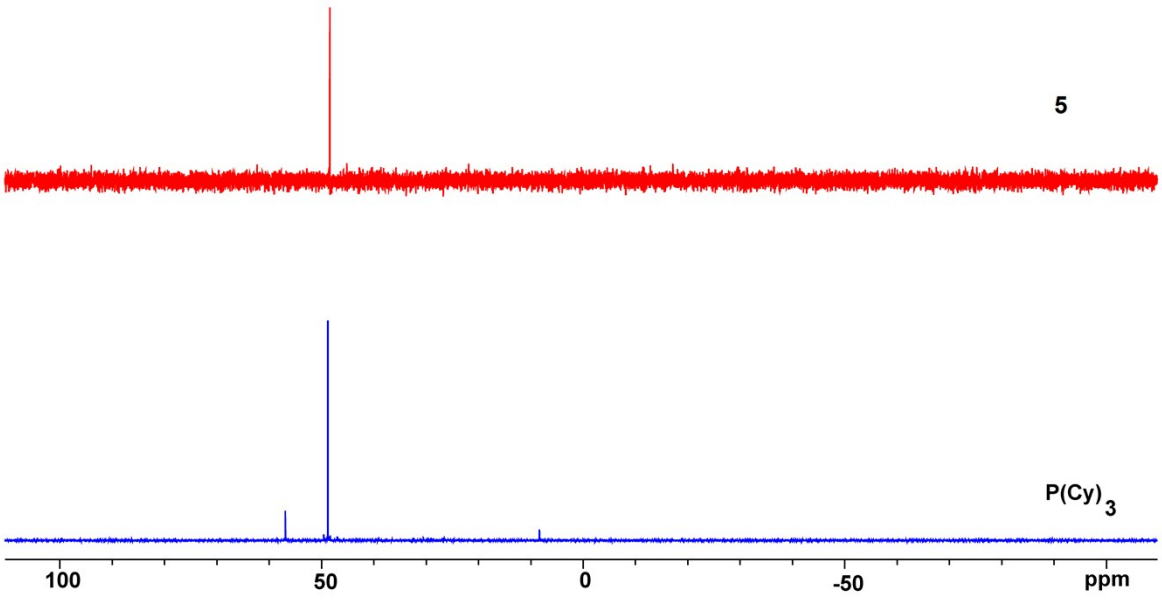


Figure S9. ^{31}P-{^{1}H} NMR spectra of free ligand, and **5** in dmso–d_6.

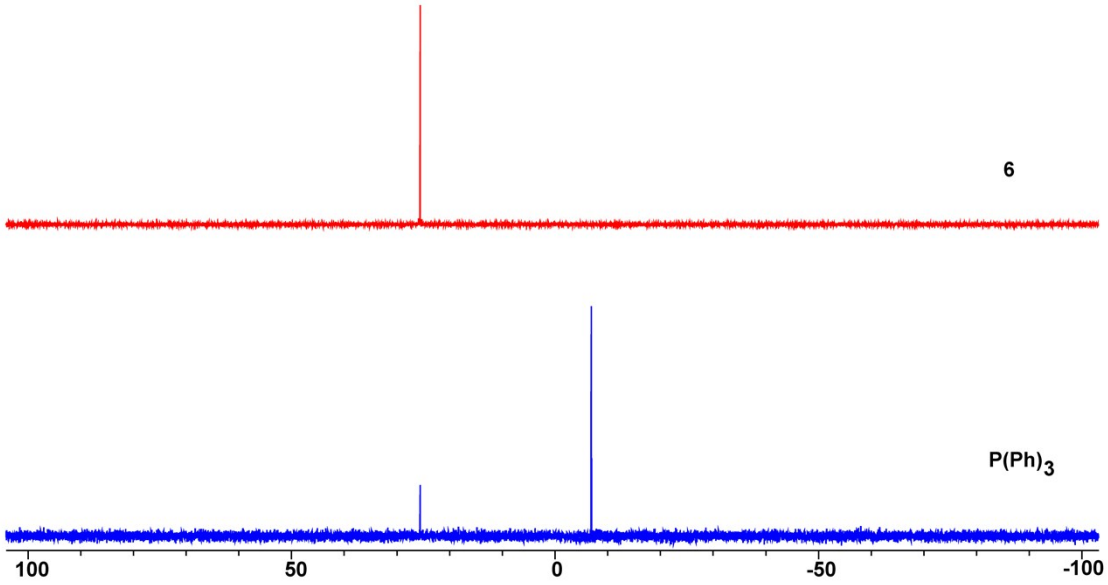
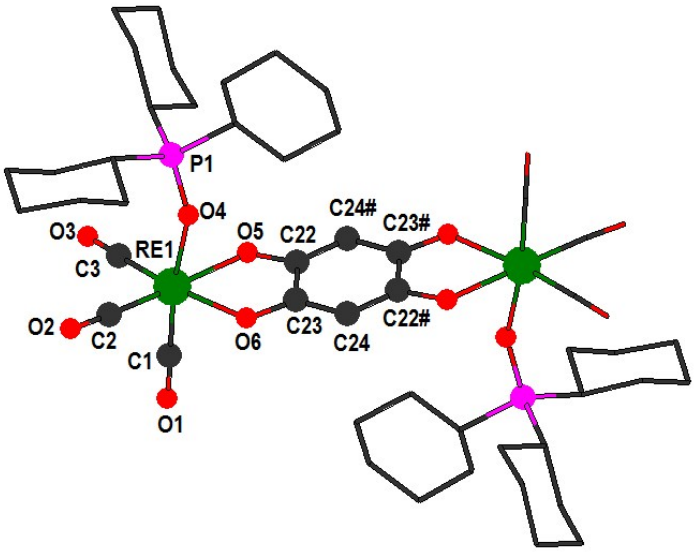


Figure S10. ^{31}P-{^{1}H} NMR spectra of free ligand, and **6** in dmso– d_6.

Table S1a. Crystal data and structure refinement for **1**.

Empirical formula	$C_{48}H_{68}O_{12}P_2Re_2$	
Formula weight	1271.36	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.8509(6) Å	α = 90°.
	b = 15.6904(10) Å	β = 104.812(2)°.
	c = 16.8984(11) Å	γ = 90°.
Volume	2525.1(3) Å^3	
Z	2	
Density (calculated)	1.672 Mg/m^3	
Absorption coefficient	4.911 mm^{-1}	
F(000)	1264	
Crystal size	0.080 x 0.060 x 0.050 mm^3	
Theta range for data collection	2.493 to 27.145°.	
Index ranges	-12<=h<=12, -20<=k<=20, -21<=l<=21	
Reflections collected	73754	
Independent reflections	5586 [R(int) = 0.0608]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.791 and 0.695	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5586 / 0 / 288	
Goodness-of-fit on F^2	1.027	
Final R indices [I>2sigma(I)]	$R1$ = 0.0309, $wR2$ = 0.0735	
R indices (all data)	$R1$ = 0.0388, $wR2$ = 0.0779	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.122 and -1.570 e.Å^{-3}	

Table S1b. Selected bond lengths [Å] and angles [°] for **1**.



Re(1)-C(1)	1.878(5)	O(6)-C(23)	1.270(5)	P(1)-O(4)	1.508(3)
Re(1)-C(3)	1.889(5)	O(5)-C(22)	1.264(5)		
Re(1)-C(2)	1.916(5)	C(23)-C(24)	1.392(6)		
Re(1)-O(5)	2.131(3)	C(24)-C(22)#1	1.381(6)		
Re(1)-O(6)	2.144(3)	C(23)-C(22)	1.515(5)		
Re(1)-O(4)	2.136(3)				

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z+1

C(1)-Re(1)-C(3)	87.9(2)	O(5)-Re(1)-O(4)	80.80(12)	P(1)-O(4)-Re(1)	151.6(2)
C(1)-Re(1)-C(2)	89.1(2)	C(1)-Re(1)-O(6)	91.93(19)		
C(3)-Re(1)-C(2)	88.2(2)	C(3)-Re(1)-O(6)	169.92(17)		
C(1)-Re(1)-O(5)	95.8(2)	C(2)-Re(1)-O(6)	101.90(17)		
C(3)-Re(1)-O(5)	95.23(17)	O(5)-Re(1)-O(6)	74.76(10)		
C(2)-Re(1)-O(5)	174.12(17)	O(4)-Re(1)-O(6)	80.11(12)		
C(1)-Re(1)-O(4)	171.9(2)				
C(3)-Re(1)-O(4)	99.72(19)				
C(2)-Re(1)-O(4)	93.92(18)				

Table S1c. Intermolecular hydrogen bonds for **1** [Å and °].

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠D–H···A
C21–H21B···O3	0.970	2.541	3.401	147.64

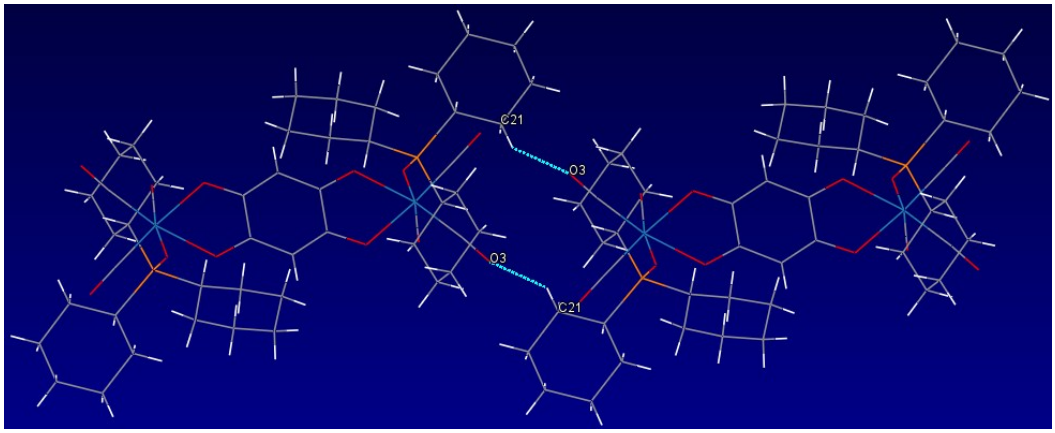
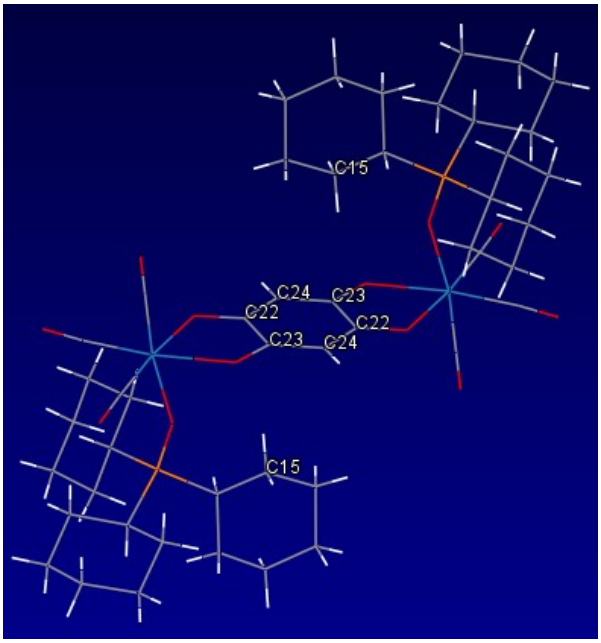


Table S1d. Intramolecular aliphatic C–H···π contacts for **1** [Å and °].

D–H···A(π)	*d*(D···A)	∠D–H···A
C15–H15A···C24	4.104	127
C15–H15A···C23	3.837	137
C15–H15A···C22	3.992	164



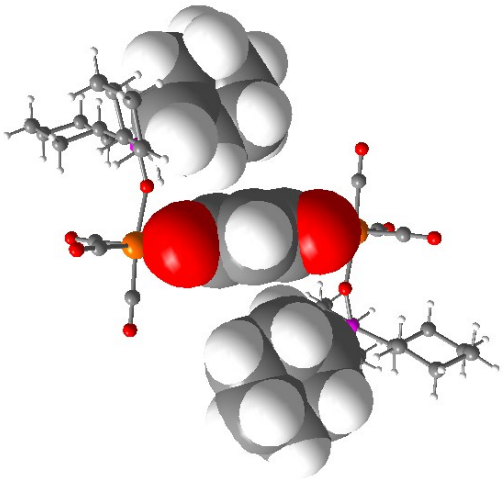
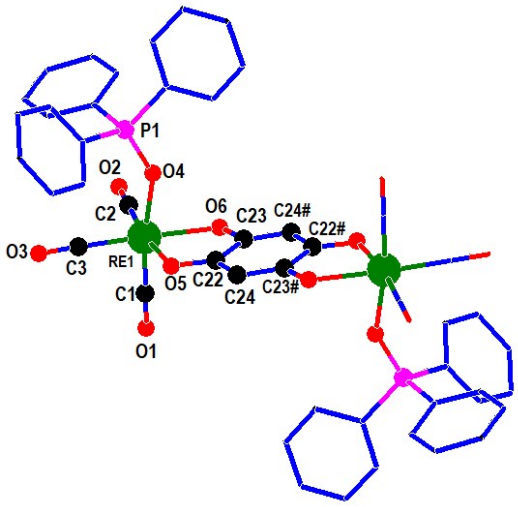


Table S2a. Crystal data and structure refinement for **2**.

Empirical formula	$C_{48}H_{32}O_{12}P_2Re_2$	
Formula weight	1235.07	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 23.052(3) Å	α= 90°.
	b = 9.4296(10) Å	β= 107.377(5)°.
	c = 26.152(3) Å	γ = 90°.
Volume	5425.1(11) $Å^3$	
Z	4	
Density (calculated)	1.512 Mg/m^3	
Absorption coefficient	4.570 mm^{-1}	
F(000)	2384	
Crystal size	0.080 x 0.070 x 0.050 mm^3	
Theta range for data collection	2.350 to 27.212°.	
Index ranges	-29<=h<=29, -12<=k<=12, -33<=l<=33	
Reflections collected	67528	
Independent reflections	6004 [R(int) = 0.1561]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.804 and 0.711	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6004 / 0 / 289	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0507, wR2 = 0.1036	
R indices (all data)	R1 = 0.1153, wR2 = 0.1259	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.075 and -0.924 $e.Å^{-3}$	

Table S2b. Selected bond lengths [Å] and angles [°] for **2**.



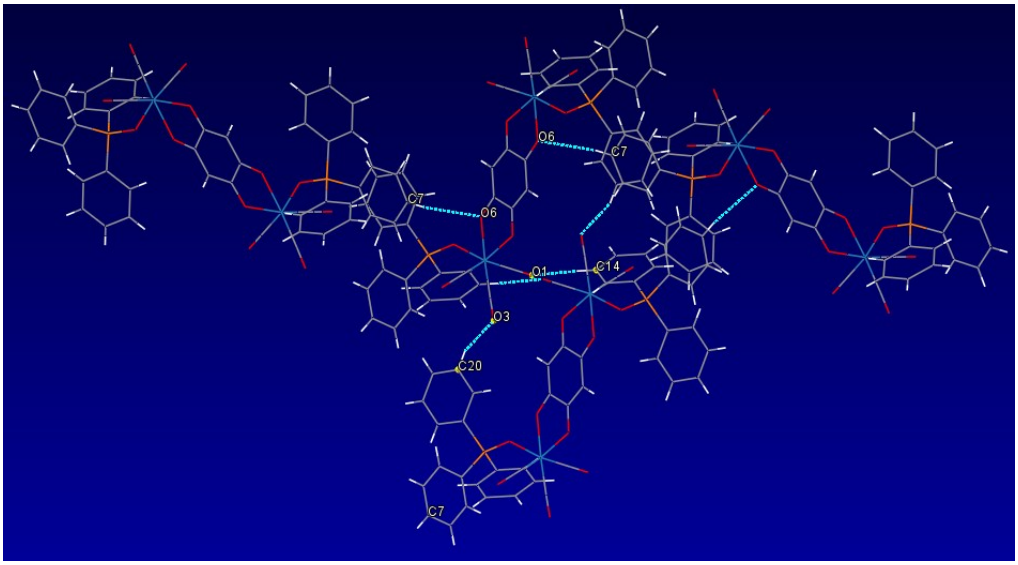
Re(1)-C(1)	1.858(12)	O(5)-C(22)	1.272(9)	P(1)-O(4)	1.502(6)
Re(1)-C(2)	1.892(11)	O(6)-C(23)	1.275(9)		
Re(1)-C(3)	1.902(12)	C(22)-C(24)	1.380(11)		
		C(22)-C(23)	1.513(11)		
Re(1)-O(6)	2.135(6)	C(23)-C(24)#1	1.373(12)		
Re(1)-O(5)	2.146(5)				
Re(1)-O(4)	2.144(6)				

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+3/2,-z+1

C(1)-Re(1)-C(2)	89.2(4)	C(3)-Re(1)-O(4)	98.2(4)
C(1)-Re(1)-C(3)	87.4(5)	O(6)-Re(1)-O(4)	79.7(2)
C(2)-Re(1)-C(3)	87.9(4)	C(1)-Re(1)-O(5)	94.2(3)
C(1)-Re(1)-O(6)	94.3(4)	C(2)-Re(1)-O(5)	172.3(3)
C(2)-Re(1)-O(6)	98.1(3)	C(3)-Re(1)-O(5)	99.1(3)
C(3)-Re(1)-O(6)	173.8(3)	O(6)-Re(1)-O(5)	74.8(2)
C(1)-Re(1)-O(4)	172.3(4)	O(4)-Re(1)-O(5)	79.6(2)
C(2)-Re(1)-O(4)	96.3(3)	P(1)-O(4)-Re(1)	139.6(3)

Table S2c. Intermolecular hydrogen bonds for **2** [Å and °].

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠D–H···A
C7–H···O6	0.929	2.683	3.527	151.60
C14–H···O1	0.931	2.619	3.266	127.08
C20–H···O3	0.929	2.587	3.361	141.03



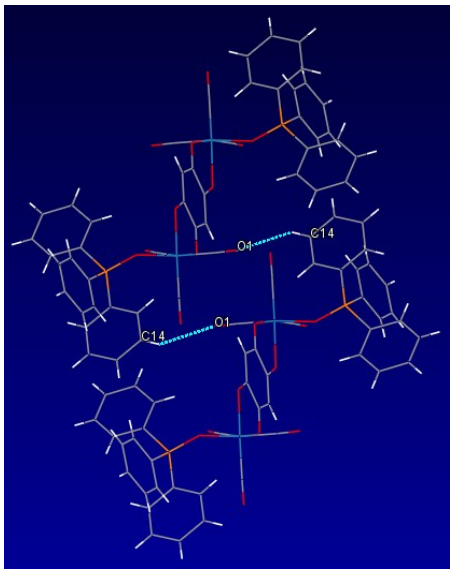
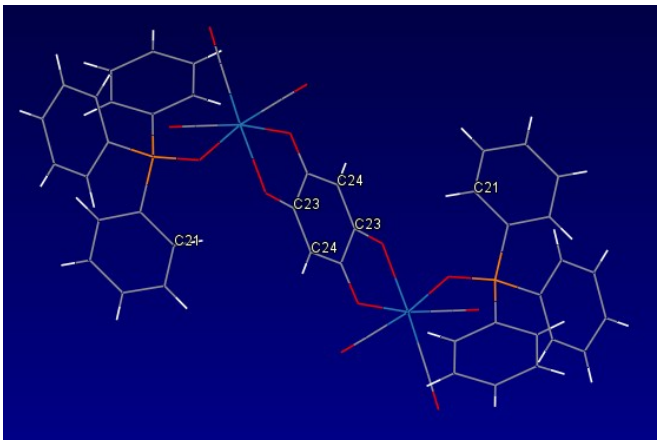


Table S2d. Intramolecular C–H···π contacts for **2** [Å and °].

D–H···A(π)	*d*(D···A)	∠D–H···A
C21–H···C23	4.104	127



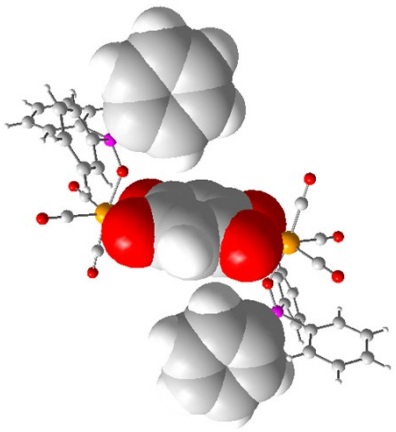
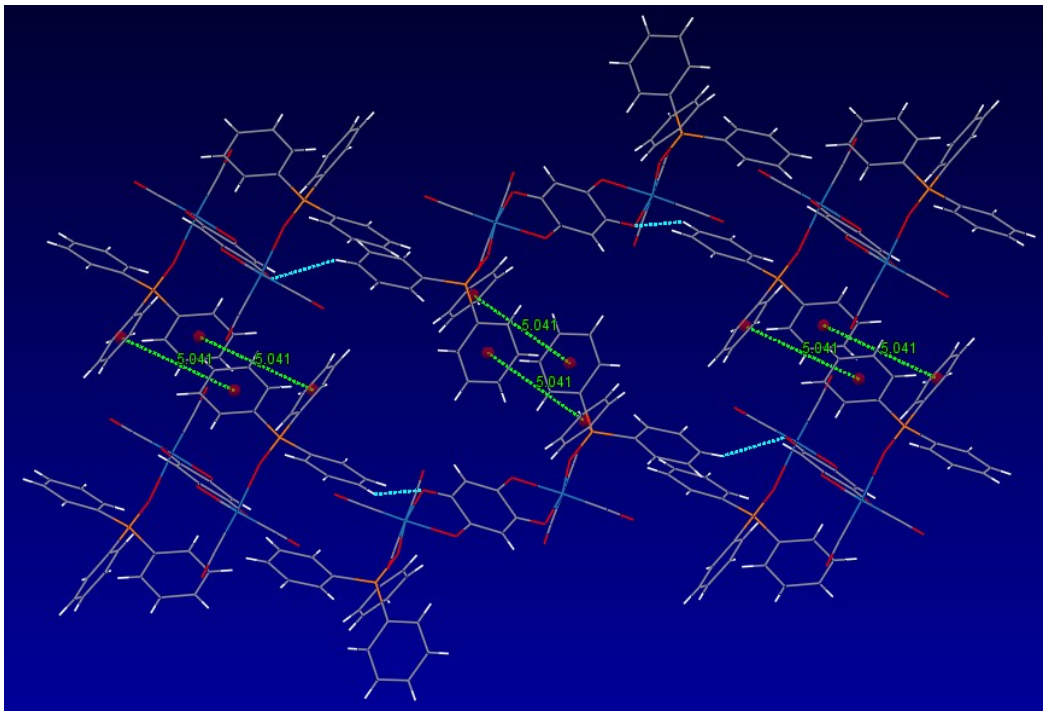


Table S2e. Intermolecular aromatic *edge-to-face* C–H···π contacts for **2** [Å and °].

d(Cg···Cg)	*τ*(arene···arene)
5.041	72



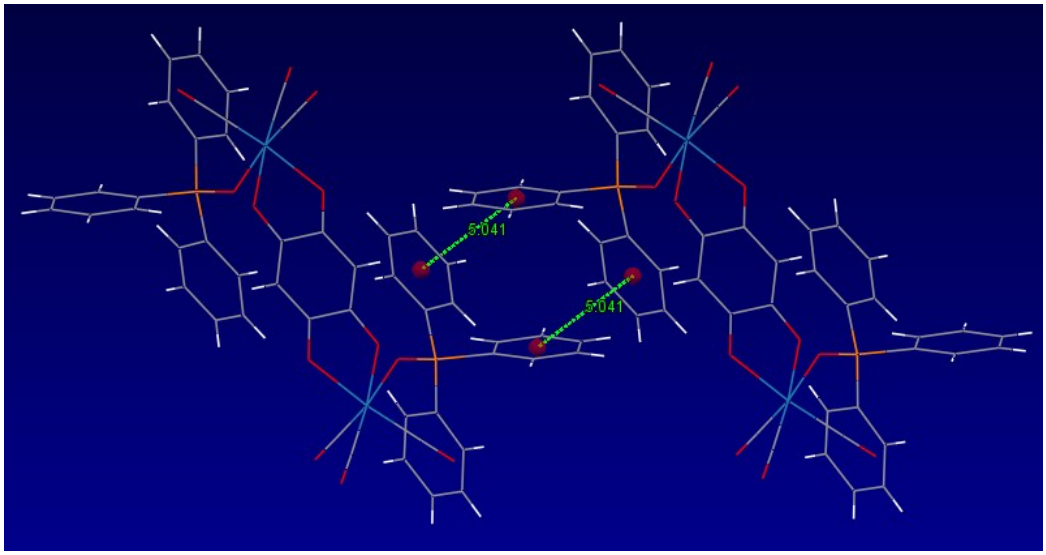
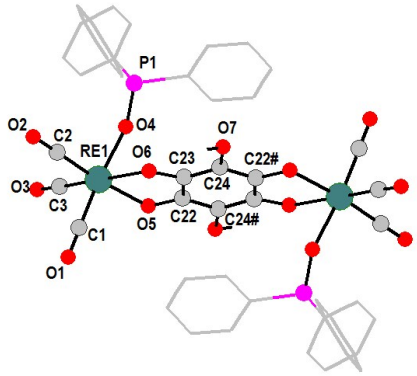


Table S3a. Crystal data and structure refinement for **4**.

Empirical formula	$C_{48}H_{32}O_{14}P_2Re_2$	
Formula weight	1267.07	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 25.0720(18) Å	α= 90°.
	b = 12.5382(10) Å	β= 97.093(2)°.
	c = 14.8004(12) Å	γ = 90°.
Volume	4617.0(6) $Å^3$	
Z	4	
Density (calculated)	1.823 Mg/m^3	
Absorption coefficient	5.376 mm^{-1}	
F(000)	2448	
Crystal size	0.080 x 0.070 x 0.070 mm^3	
Theta range for data collection	2.225 to 27.577°.	
Index ranges	-32<=h<=32, -16<=k<=16, -19<=l<=19	
Reflections collected	67057	
Independent reflections	5327 [R(int) = 0.0496]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.705 and 0.673	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5327 / 1 / 280	
Goodness-of-fit on F^2	1.119	
Final R indices [I>2sigma(I)]	R1 = 0.0319, wR2 = 0.0654	
R indices (all data)	R1 = 0.0468, wR2 = 0.0705	
Extinction coefficient	n/a	
Largest diff. peak and hole	1.332 and -0.892 $e.Å^{-3}$	

Table S3b. Selected bond lengths [Å] and angles [°] for **4**.



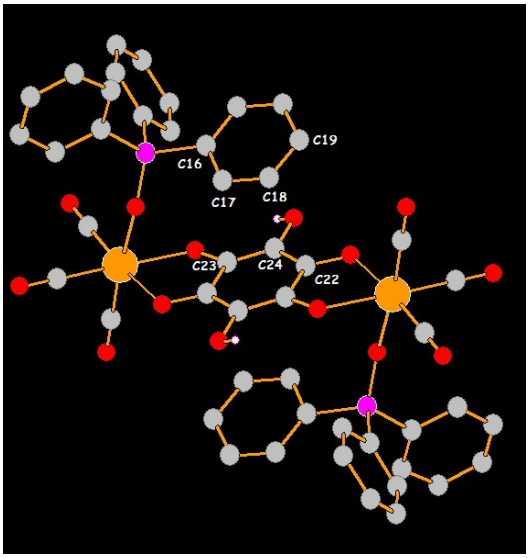
Re(1)-C(3)	1.890(5)	O(6)-C(23)	1.275(5)	P(1)-O(4)	1.491(3)
Re(1)-C(1)	1.897(6)	O(5)-C(22)	1.261(5)		
Re(1)-C(2)	1.913(6)	C(23)-C(24)	1.378(4)		
Re(1)-O(6)	2.145(3)	C(23)-C(22)	1.515(6)		
Re(1)-O(5)	2.147(3)	C(22)-C(24)#1	1.388(4)		
Re(1)-O(4)	2.156(3)				

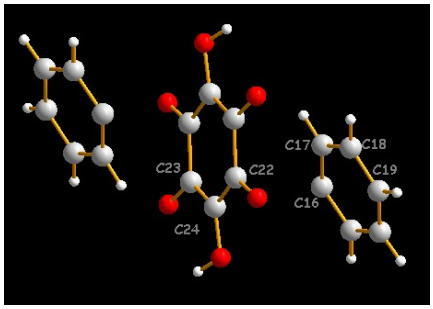
Symmetry transformations used to generate equivalent atoms: #1 -x+3/2,-y+3/2,-z+1

C(3)-Re(1)-C(1)	88.0(2)	O(6)-Re(1)-O(5)	74.97(11)	P(1)-O(4)-Re(1)	147.6(2)
C(3)-Re(1)-C(2)	88.2(2)	C(3)-Re(1)-O(4)	94.77(19)		
C(1)-Re(1)-C(2)	87.0(2)	C(1)-Re(1)-O(4)	173.86(19)		
C(3)-Re(1)-O(6)	170.93(18)	C(2)-Re(1)-O(4)	98.6(2)		
C(1)-Re(1)-O(6)	97.09(17)	O(6)-Re(1)-O(4)	79.49(12)		
C(2)-Re(1)-O(6)	99.51(18)	O(5)-Re(1)-O(4)	78.95(12)		
C(3)-Re(1)-O(5)	97.13(18)				
C(1)-Re(1)-O(5)	95.28(19)				
C(2)-Re(1)-O(5)	174.24(17)				

Table S3c. Intramolecular slipped π···π stacking contacts for **4** [Å and °].

d(Cg···Cg)	*α*(arene···arene)
3.9	21





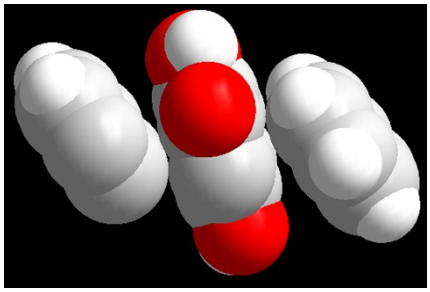


Table S3d. Intermolecular aromatic *edge-to-face* C–H···π contacts for **4** [Å and °].

d(Cg···Cg)	*τ*(arene···arene)
5.30	73
5.24	60

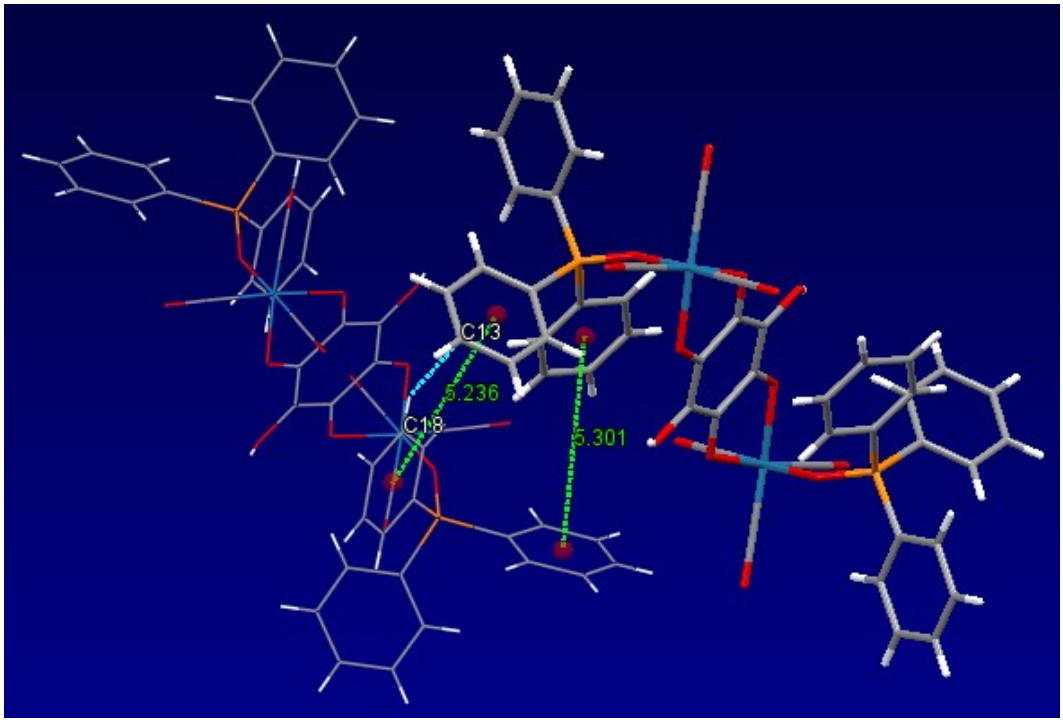
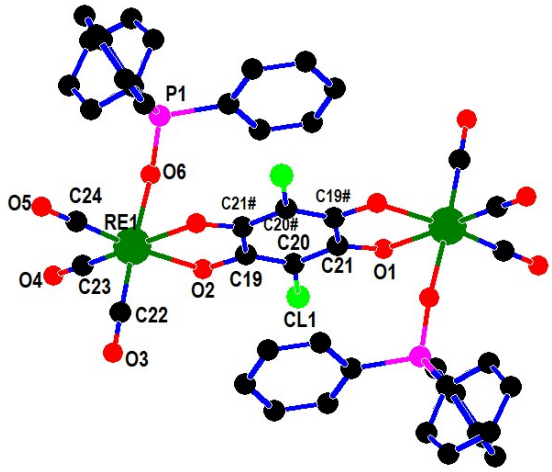


Table S4a. Crystal data and structure refinement for **6**.

Empirical formula	$C_{48}H_{30}Cl_2O_{12}P_2Re_2$	
Formula weight	1303.96	
Temperature	296(2) K	
Wavelength	0.71075 Å	
Crystal system	Monoclinic	
Space group	I2/a	
Unit cell dimensions	a = 25.917(4) Å	α = 90°.
	b = 9.2842(11) Å	β = 111.474(10)°.
	c = 29.980(4) Å	γ = 90°.
Volume	6713.0(16) $Å^3$	
Z	4	
Density (calculated)	1.290 Mg/m^3	
Absorption coefficient	3.774 mm^{-1}	
F(000)	2512	
Crystal size	0.090 x 0.070 x 0.050 mm^3	
Theta range for data collection	2.926 to 25.000°.	
Index ranges	-30<=h<=26, -11<=k<=10, -35<=l<=30	
Reflections collected	15131	
Independent reflections	5822 [R(int) = 0.0409]	
Completeness to theta = 25.000°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.834 and 0.728	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5822 / 0 / 289	
Goodness-of-fit on F^2	1.104	
Final R indices [I>2sigma(I)]	R1 = 0.0516, wR2 = 0.1145	
R indices (all data)	R1 = 0.0556, wR2 = 0.1168	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.834 and -1.402 e.$Å^{-3}$	

Table S4b. Selected bond lengths [Å] and angles [°] for **6**.



Re(1)-C(24)	1.897(9)	O(2)-C(19)	1.269(8)	P(1)-O(6)	1.508(5)
Re(1)-C(22)	1.897(9)	O(1)-C(21)	1.278(8)		
Re(1)-C(23)	1.903(9)	C(21)-C(20)	1.398(7)		
Re(1)-O(2)	2.150(5)	C(21)-C(19)#1	1.495(10)		
Re(1)-O(1)#1	2.160(5)	C(19)-C(20)	1.405(7)		
Re(1)-O(6)	2.140(5)	C(20)-Cl(1)	1.674(3)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1/2,-y+3/2,-z+1/2

C(24)-Re(1)-C(22)	86.8(4)	C(23)-Re(1)-O(2)	98.4(3)
C(24)-Re(1)-C(23)	88.9(4)	O(6)-Re(1)-O(2)	80.4(2)
C(22)-Re(1)-C(23)	88.6(3)	C(24)-Re(1)-O(1)#1	98.4(3)
C(24)-Re(1)-O(6)	97.0(3)	C(22)-Re(1)-O(1)#1	96.9(3)
C(22)-Re(1)-O(6)	176.0(3)	C(23)-Re(1)-O(1)#1	171.1(3)
C(23)-Re(1)-O(6)	92.6(3)	O(6)-Re(1)-O(1)#1	81.56(19)
C(24)-Re(1)-O(2)	172.3(3)	O(2)-Re(1)-O(1)#1	74.15(18)
C(22)-Re(1)-O(2)	95.7(3)	P(1)-O(6)-Re(1)	149.7(4)

Table S4c. Intramolecular slipped π···π contacts for **6** [Å and °].

d(Cg···Cg)	*τ*(arene···arene)
3.736	11

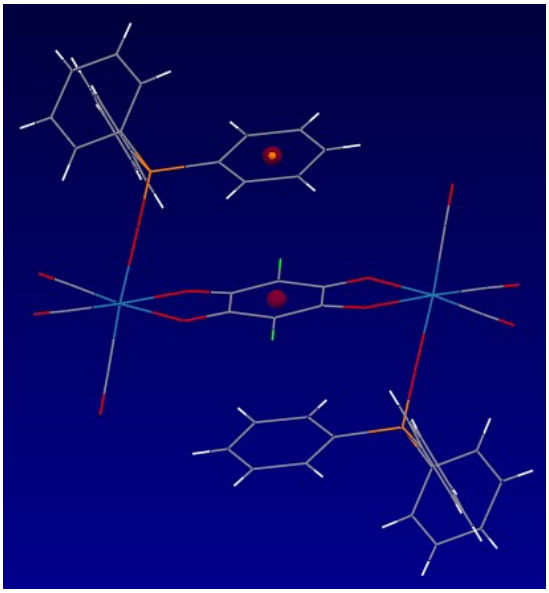
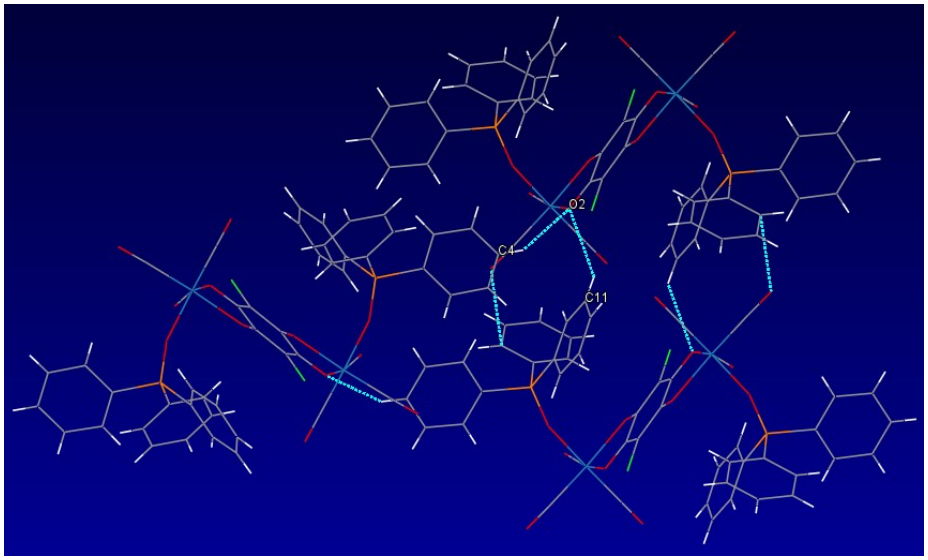


Table S4d. Intermolecular hydrogen bonds for **6** [Å and °].

D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠D–H···A
C4–H···O2	0.930	2.600	3.409	146
C11–H···O2	0.930	2.599	3.373	141
C16–H···O5				
C23–O4···π(C18)		3.151		120



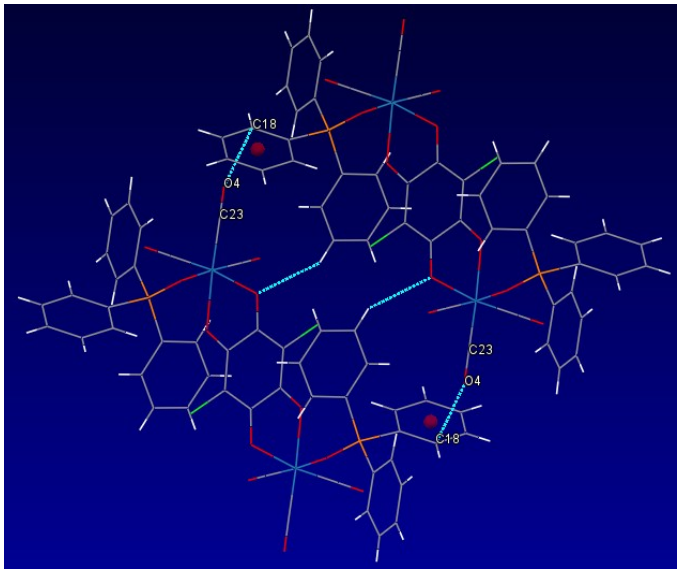
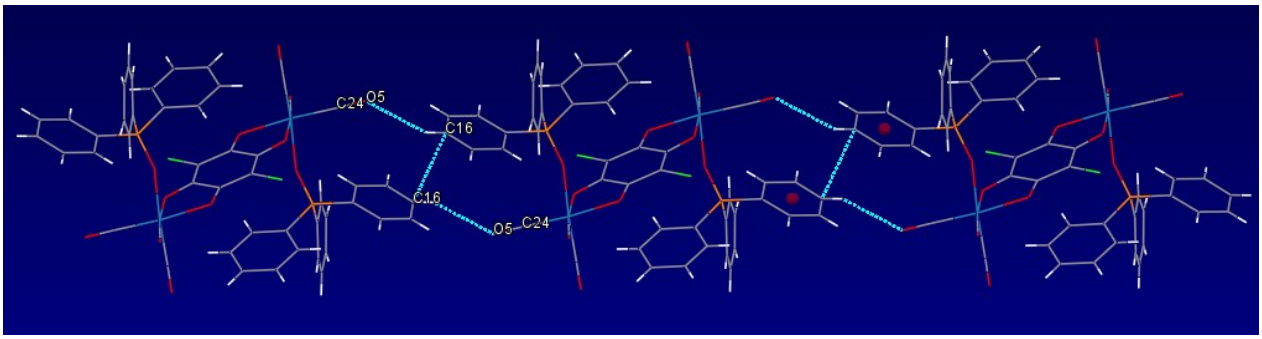


Table S4e. Intermolecular slipped π···π contacts for **6** [Å and °].

d(Cg···Cg)	*d*(D···A)	*τ*(arene···arene)
4.603		0
C16···C16	3.349	



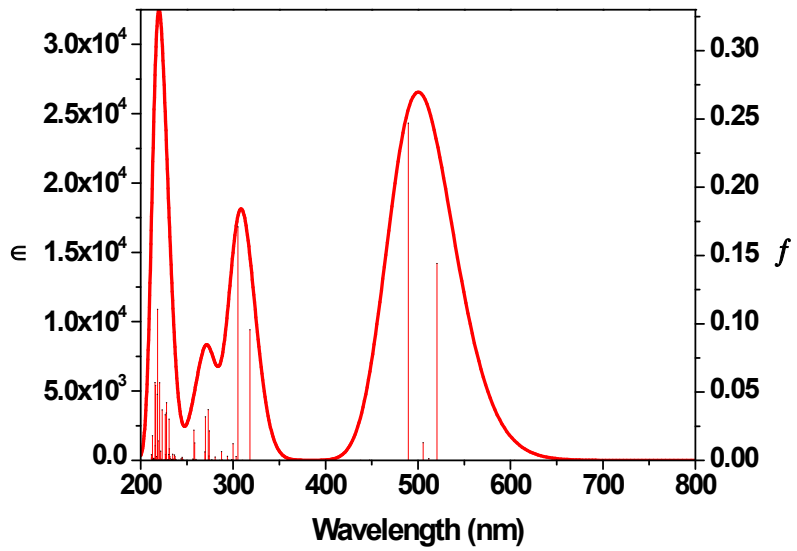


Figure S11. Simulated absorption spectrum of **1** with oscillator strength (f) values (shown as vertical bars, same color code).

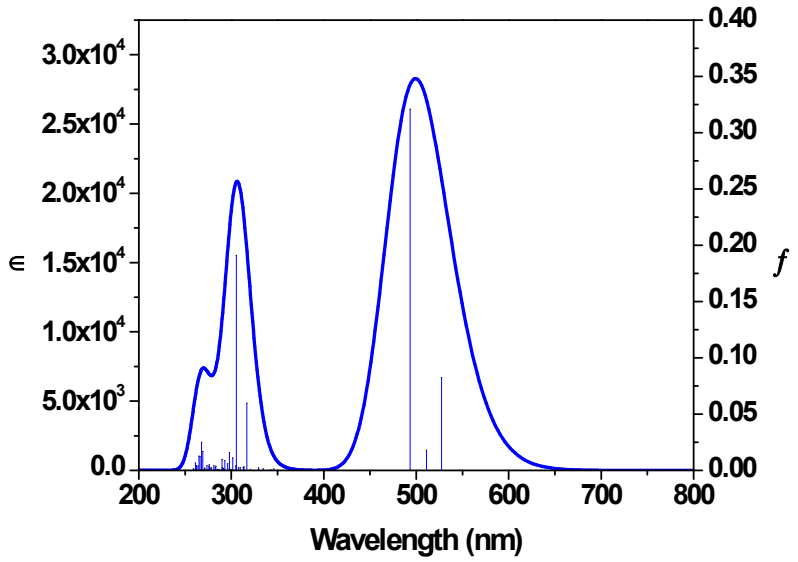


Figure S12. Simulated absorption spectrum of **2** with oscillator strength (f) values (shown as vertical bars, same color code).

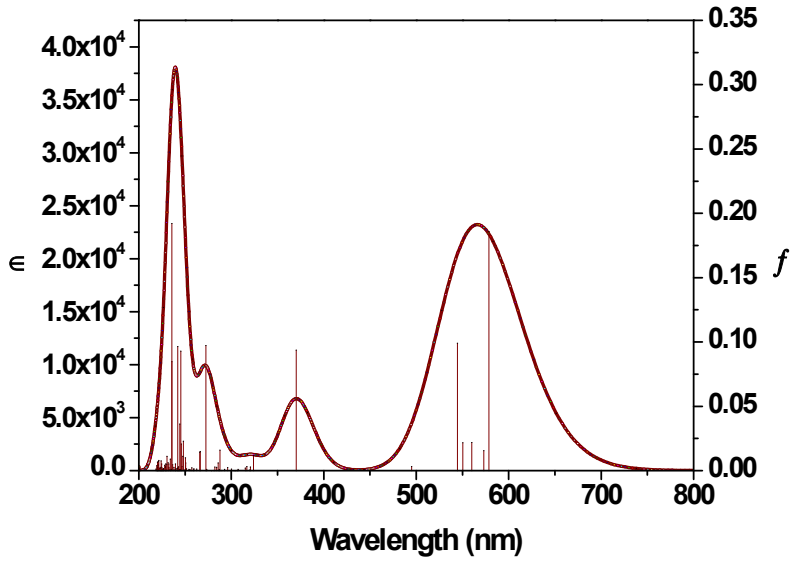


Figure S13. Simulated absorption spectrum of **3** with oscillator strength (f) values (shown as vertical bars, same color code).

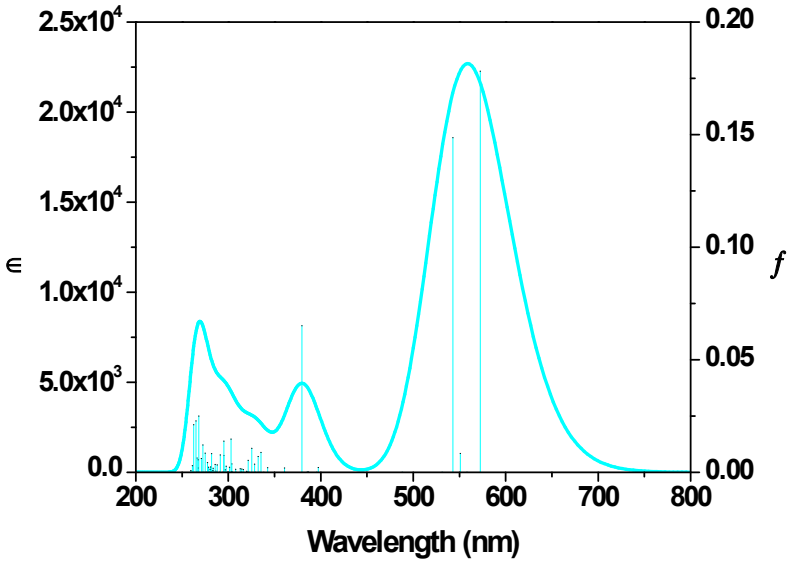


Figure S14. Simulated absorption spectrum of **4** with oscillator strength (f) values (shown as vertical bars, same color code).

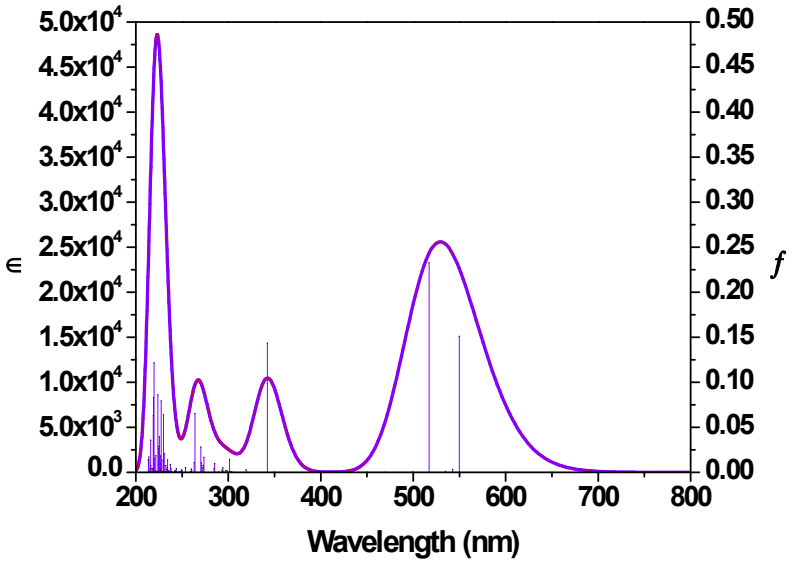


Figure S15. Simulated absorption spectrum of **5** with oscillator strength (f) values (shown as vertical bars, same color code).

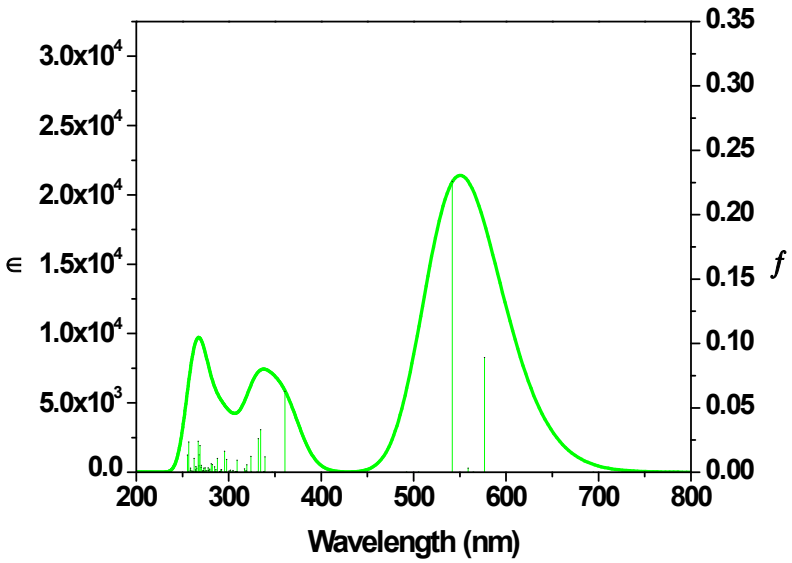


Figure S16. Simulated absorption spectrum of **6** with oscillator strength (f) values (shown as vertical bars, same color code).

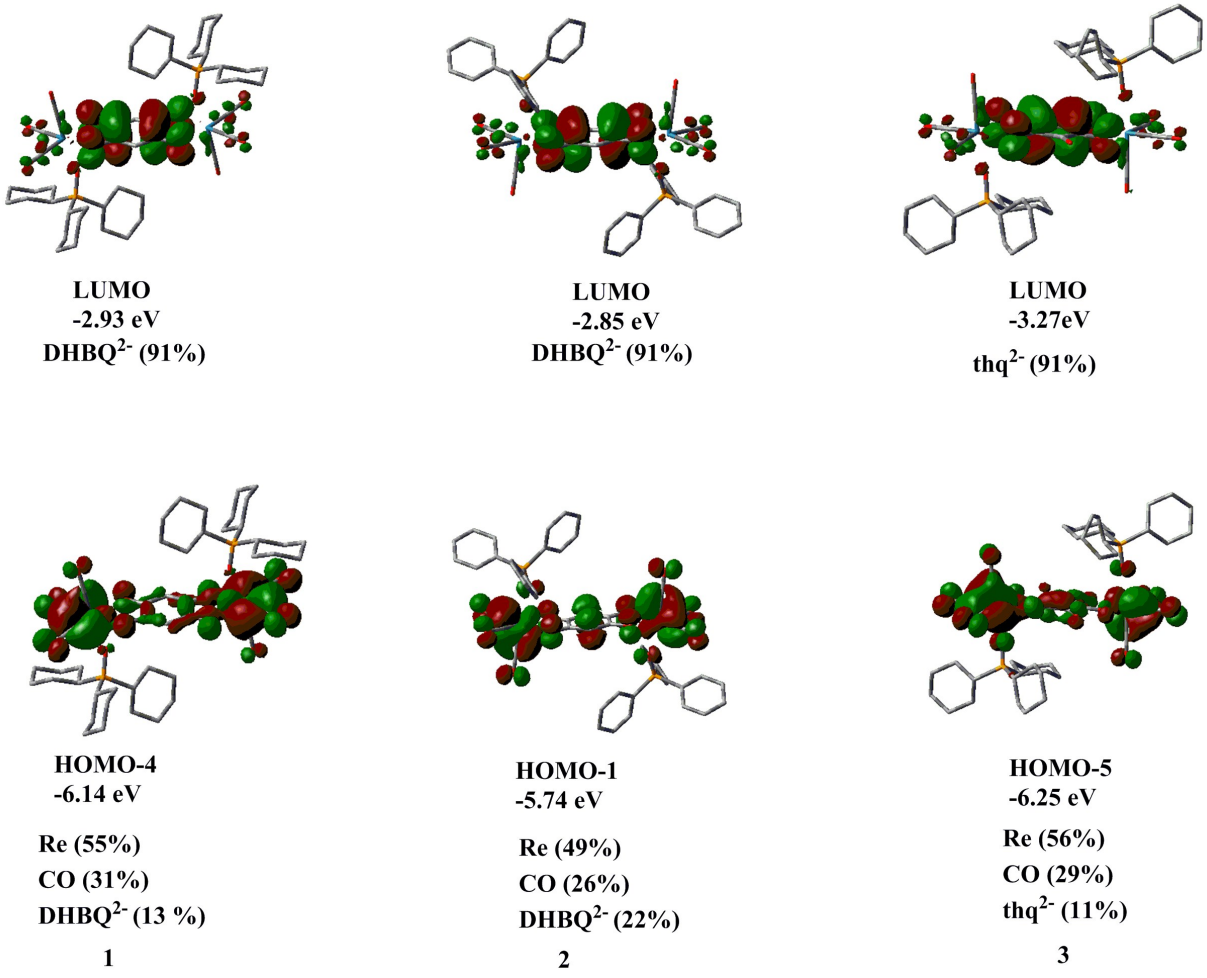


Figure S17a. Frontier molecular orbitals involved in TDDFT transition of **1**-**3**.

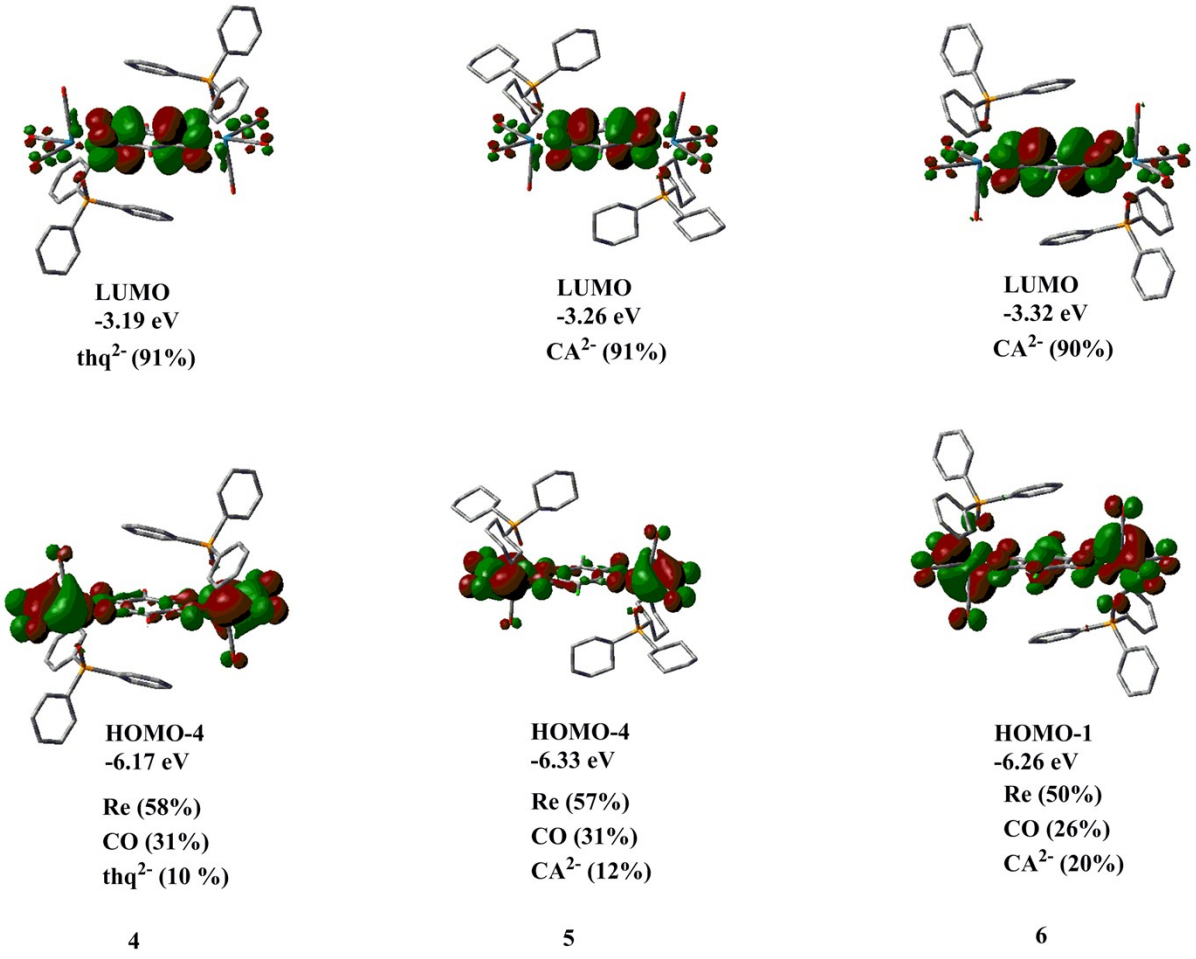


Figure S17b. Frontier molecular orbitals involved in TDDFT transition of **4**-**6**.

Table S5. Selected singlet excited state transitions for **1** as obtained from TDDFT calculations in the gas phase.

Trans band	Wavelength (nm)	Oscillator strength (f)	Major contribution [%]	Character
2	521	0.1442	H–4 → LUMO (42%) H–1→ LUMO (53%)	Re (48%) CO (26 %) → $DHBQ^{2-}$ (91 %) $DHBQ^{2-}$ (23 %)
5	490	0.247	H–4 → LUMO (55%) H–1 → LUMO (40%)	Re (55%) CO (31%) → $DHBQ^{2-}$ (91%) $DHBQ^{2-}$ (13 %)
8	318	0.0956	H–12 →LUMO (21%) H–10 →LUMO (21%) H–7 →LUMO (39%)	Re (13%) CO (4 %) → $DHBQ^{2-}$ (91 %) $DHBQ^{2-}$ 67%) $Cy_3P=O$ (15%)
10	305	0.171	H–12 →LUMO (17%) H–10 →LUMO (12%) H–7 →LUMO (49%)	Re (13%) CO (4 %) → $DHBQ^{2-}$ (91 %) $DHBQ^{2-}$ (67%) $Cy_3P=O$ (15%)

Table S6. Selected singlet excited state transitions for **2** as obtained from TDDFT calculations in the gas phase.

Trans band	Wavelength (nm)	Oscillator strength (f)	Major contribution [%]	Character
2	527	0.0824	H–4 → LUMO (53%) H–1 → LUMO (37%)	Re (56%) CO (31 %) → $DHBQ^{2-}$ (91%) $DHBQ^{2-}$ (12%)
5	493	0.321	H–4→ LUMO (43%) H–1→ LUMO (54%)	Re (49%) CO (26 %) → $DHBQ^{2-}$ (91%) $DHBQ^{2-}$ (22 %)
18	317	0.0597	H–20 → LUMO (49%) H–18→ LUMO (10%) H–7 → LUMO (26%)	Re (13%) CO (5%) → $DHBQ^{2-}$ (91 %) $DHBQ^{2-}$ (65 %) Ph_3P=O tppo (17%)
28	306	0.1909	H-20 → LUMO (20%) H-7 → LUMO (53%)	Re (14%)CO (5%) $DHBQ^{2-}$ (66%) → $DHBQ^{2-}$ (91 %) Ph_3P=O (15%)

Table S7. Selected singlet excited state transitions for **3** as obtained from TDDFT calculations in the gas phase.

Trans band	Wavelength (nm)	Oscillator strength (f)	Major contribution [%]	Character
2	579	0.186	H–5→ LUMO (14%) H–1 → LUMO (63%)	Re (43%) CO (24 %) → thq^{2-} (91 %) thq^{2-} (29%)
6	545	0.099	H–5→ LUMO (76%) H–1→ LUMO (19%)	Re (56%) CO (29 %) → thq^{2-} (91 %) thq^{2-} (11 %)
8	370	0.0936	H–7 → LUMO (89%)	Re (17%) CO (6%) → thq^{2-} (91 %) thq^{2-} (65 %) $Cy_3P=O$ (12%)

Table S8. Selected singlet excited state transitions for **4** as obtained from TDDFT calculations in the gas phase.

Trans band	Wavelength (nm)	Oscillator strength (f)	Major contribution [%]	Character	
2	572	0.1782	H-4→LUMO (31%) H-1→LUMO (62%)	Re (42%) CO (23%) thq^{2-} (32%)	→ thq^{2-} (91%)
5	543	0.1486	H-4→LUMO (66%) H-1→LUMO (31%)	Re (58%) CO (31%) thq^{2-} (10%)	→ thq^{2-} (91%)
12	380	0.0651	H-7→LUMO (88%)	Re (20%) CO (7%) thq^{2-} (58%) $Ph_3P=O$ (16%)	→ thq^{2-} (91%)

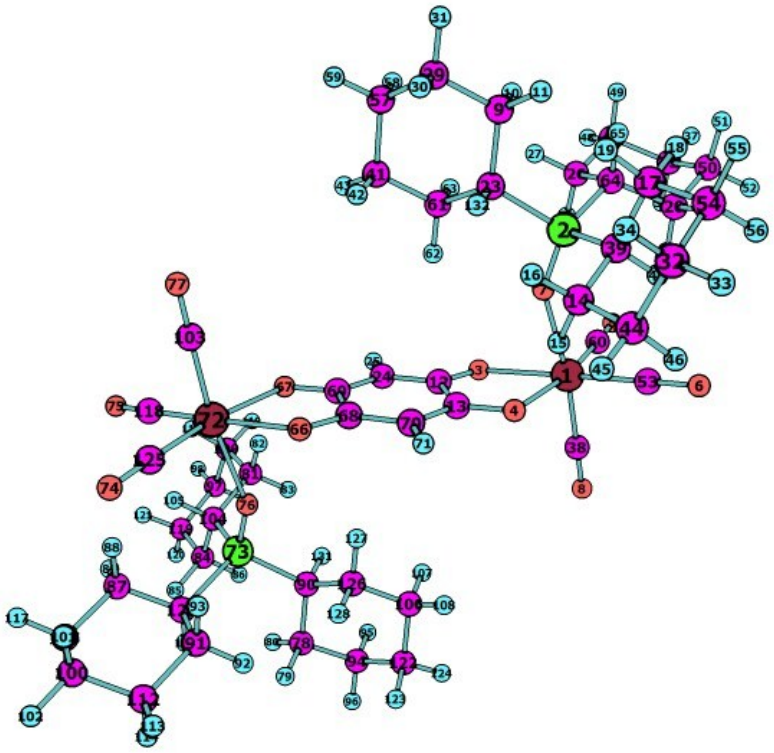
Table S9. Selected singlet excited state transitions for **5** as obtained from TDDFT calculations in the gas phase.

Trans band	Wavelength (nm)	Oscillator strength (f)	Major contribution [%]	Character
2	550	0.151	H–4 → LUMO (37%) H–1 → LUMO (57%)	Re (48%) CO (25 %) → CA^{2-} (91 %) CA^{2-} (23%)
5	517	0.2327	H–4→ LUMO (56%) H–1→ LUMO (40%)	Re (57%) CO (31 %) → CA^{2-} (91 %) CA^{2-} (12 %)
8	342	0.1435	H–7 → LUMO (90%)	Re (14%) CO (5 %) → CA^{2-} (91 %) CA^{2-} (71%) $Cy_3P{=}O$ (10%)

Table S10. Selected singlet excited state transitions for **6** as obtained from TDDFT calculations in the gas phase.

Trans band	Wavelength (nm)	Oscillator strength (f)	Major contribution [%]	Character	
2	577	0.0891	H-4→LUMO (48%) H-1→LUMO (47%)	Re (58%) CO (31%) CA^{2-} (11%)	→ CA^{2-} (90%)
5	542	0.2257	H-4→LUMO (48%) H-1→LUMO (50%)	Re (50%) CO (26%) CA^{2-} (20%)	→ CA^{2-} (90%)
8	361	0.0629	H-7→LUMO (85%)	Re (9%) CO (3%) CA^{2-} (55%) $Cy_3P{=}O$ (32%)	→ CA^{2-} (90%)
12	334	0.0331	H-11→LUMO (62%) HOMO→ L+1 (21%)	Re (2%) CO (1%) CA^{2-} (13%) $Cy_3P{=}O$ (83%)	→ CA^{2-} (90 %)

Cartesian coordinates of the DFT/B3LYP/SDD optimized structure of **1.**



Atom	X	Y	Z
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8	-2.042492000	1.248009000	1.285319000
8	-5.323378000	3.245368000	-2.294800000
8	-5.596126000	2.861355000	2.128394000
8	-4.101000000	0.089034000	-0.293529000
8	-2.290612000	5.015488000	0.294124000
6	-5.304082000	-3.811763000	-0.642824000
1	-5.849859000	-3.595161000	-1.568050000
1	-6.055592000	-3.906688000	0.145750000
6	-0.966429000	0.804744000	-0.777140000

6	-1.063797000	0.650325000	0.737105000
6	-4.267699000	-1.050670000	2.736321000
1	-3.538511000	-0.300524000	2.425919000
1	-3.783465000	-2.029010000	2.625398000
6	-6.574481000	-2.026343000	2.301467000
1	-7.478991000	-1.976807000	1.687184000
1	-6.167743000	-3.036958000	2.181101000
6	-7.522282000	0.354140000	-0.432062000
1	-6.936131000	1.274970000	-0.507621000
1	-7.785781000	0.237940000	0.622605000
6	-4.314137000	-2.664073000	-0.345381000
6	0.082458000	0.206378000	-1.479241000
1	0.148164000	0.317145000	-2.554998000
6	-6.378918000	-0.720204000	-2.435332000
1	-5.832091000	-1.597099000	-2.792053000
1	-5.725490000	0.140331000	-2.606781000
6	-4.556945000	-5.145310000	-0.805390000
1	-4.101812000	-5.422965000	0.154026000
1	-5.272957000	-5.937787000	-1.046926000
6	-5.700609000	-1.847377000	4.681998000
1	-5.985256000	-1.642365000	5.719080000
1	-5.274539000	-2.859424000	4.674479000
6	-8.506846000	0.629841000	-2.758941000
1	-7.959142000	1.561401000	-2.944395000
1	-9.439729000	0.697959000	-3.327951000
6	-2.753531000	3.965247000	0.168373000
6	-5.527959000	-0.988327000	1.844474000
1	-5.963653000	0.010676000	1.971061000

6	-2.504237000	-3.897640000	-1.615148000
1	-1.925566000	-4.103130000	-0.705595000
1	-1.774116000	-3.814378000	-2.425985000
6	-4.638736000	-0.845361000	4.213130000
1	-3.737574000	-0.929506000	4.828734000
1	-5.010702000	0.177310000	4.350475000
6	-7.671010000	-0.556520000	-3.250233000
1	-7.416945000	-0.432933000	-4.307849000
1	-8.265382000	-1.477470000	-3.180476000
6	-8.806845000	0.507226000	-1.261285000
1	-9.457889000	-0.360126000	-1.087476000
1	-9.360308000	1.383444000	-0.908967000
6	-4.824418000	2.636803000	1.293650000
6	-6.940450000	-1.814668000	3.779889000
1	-7.660006000	-2.578956000	4.091714000
1	-7.448247000	-0.848206000	3.889893000
6	-3.468145000	-5.060820000	-1.881892000
1	-3.940610000	-4.923859000	-2.863587000
1	-2.917089000	-6.005012000	-1.935513000
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1	-2.542406000	-1.759829000	-1.225898000
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8	1.821612000	-1.428100000	1.260160000
8	2.012774000	-1.138527000	-1.335636000
6	0.926050000	-0.709421000	0.724326000

6	1.031763000	-0.543733000	-0.788393000
6	-0.114370000	-0.099124000	1.428189000
1	-0.180314000	-0.210724000	2.503847000
75	3.434114000	-2.164399000	-0.018942000
15	5.151315000	1.003985000	-0.009118000
8	5.177944000	-3.322690000	2.241290000
8	5.528857000	-2.850006000	-2.169897000
8	4.098273000	-0.071775000	0.282322000
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1	6.228201000	3.846604000	-0.050826000
6	4.469773000	1.032399000	-2.749133000
1	3.699243000	0.308847000	-2.477283000
1	4.010985000	2.026227000	-2.673023000
6	6.775331000	1.941295000	-2.185013000
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1	6.391795000	2.964078000	-2.095260000
6	7.486889000	-0.460374000	0.596305000
1	6.854686000	-1.353123000	0.623426000
1	7.822884000	-0.347620000	-0.438067000
6	4.408334000	2.675675000	0.319954000
6	6.273463000	0.659890000	2.534701000
1	5.748976000	1.561960000	2.861408000
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6	6.041141000	1.768095000	-4.611717000
1	6.380320000	1.544251000	-5.628262000
1	5.646730000	2.792637000	-4.637727000
6	8.307603000	-0.794555000	2.978285000
1	7.702360000	-1.697483000	3.122052000
1	9.198125000	-0.912842000	3.604108000
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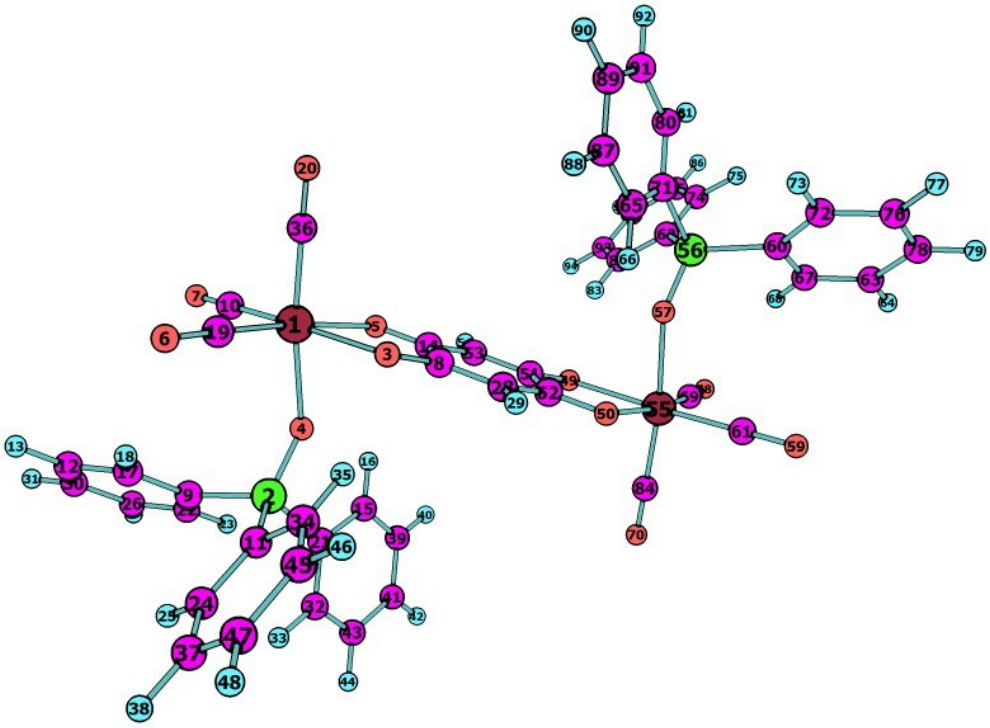
6	5.673668000	0.937756000	-1.784790000
1	6.085177000	-0.074372000	-1.882940000
6	2.566053000	3.985555000	1.462372000
1	2.059663000	4.211506000	0.515208000
1	1.779680000	3.933217000	2.221486000
6	4.922680000	0.802928000	-4.199569000
1	4.063201000	0.908425000	-4.869099000
1	5.270761000	-0.231657000	-4.306146000
6	7.504788000	0.431603000	3.424299000
1	7.181866000	0.319519000	4.464286000
1	8.148101000	1.321376000	3.394487000
6	8.707189000	-0.680516000	1.503590000
1	9.409847000	0.154385000	1.378046000
1	9.238041000	-1.581391000	1.179862000
6	4.754367000	-2.614306000	-1.340742000
6	7.223492000	1.707176000	-3.636657000
1	7.982621000	2.447591000	-3.909818000
1	7.708060000	0.725420000	-3.709258000
6	3.555934000	5.109430000	1.794371000
1	3.954037000	4.956190000	2.806166000
1	3.041629000	6.075496000	1.810229000

6	4.541259000	-2.902089000	1.371647000
6	3.260677000	2.620720000	1.351642000
1	2.543200000	1.848483000	1.073197000
1	3.654819000	2.331050000	2.331913000
6	6.660309000	0.767814000	1.041211000
1	7.275449000	1.666557000	0.904364000
1	3.957269000	2.943197000	-0.644874000
1	-3.784461000	-2.913643000	0.583570000

Cartesian coordinates of the DFT/B3LYP/SDD optimized structure of **2.**



Atom	X	Y	Z
75	3.511987000	2.121546000	0.126786000
15	5.116872000	-1.085161000	0.012776000
8	2.045034000	1.235019000	-1.246728000

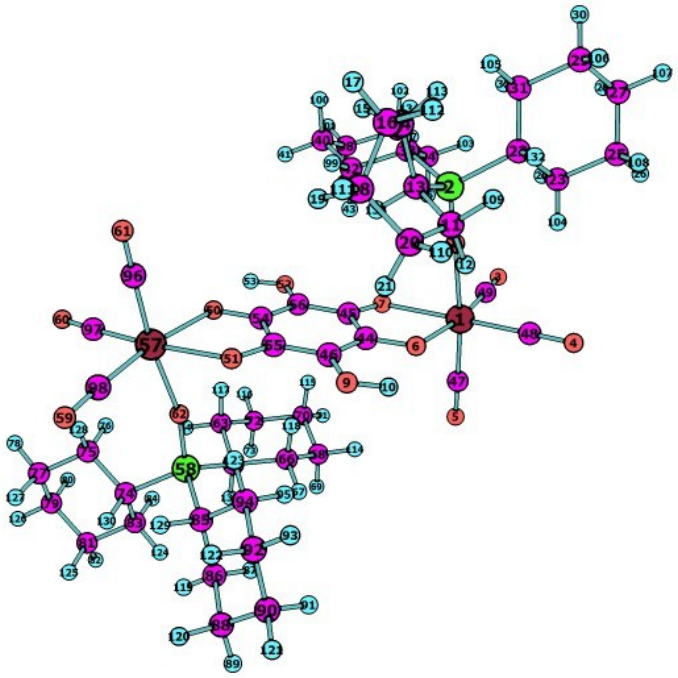
8	4.061326000	-0.017398000	0.275082000
8	1.877292000	1.355065000	1.364871000
8	5.654794000	2.861411000	-1.958056000
8	5.327023000	3.019965000	2.450006000
6	1.054045000	0.627189000	-0.730969000
6	6.706719000	-0.745554000	0.830944000
6	4.666497000	2.696440000	1.559864000
6	5.455614000	-1.270829000	-1.764539000
6	8.704710000	0.610600000	0.993515000
1	9.336445000	1.399516000	0.599831000
6	0.960237000	0.696739000	0.789450000
6	3.372371000	-2.620577000	1.516937000
1	2.932211000	-1.665595000	1.777995000
6	7.533981000	0.268783000	0.325168000
1	7.266241000	0.794270000	-0.585025000
6	4.857329000	2.600282000	-1.159725000
8	2.345568000	4.960512000	-0.068699000
6	4.472410000	-2.661574000	0.652560000
6	7.065945000	-1.404160000	2.013072000
1	6.431175000	-2.184675000	2.416693000
6	6.644802000	-1.838935000	-2.240616000
1	7.428305000	-2.133865000	-1.550617000
6	8.241211000	-1.058643000	2.675695000
1	8.513850000	-1.573397000	3.590899000
6	0.088432000	-0.062201000	-1.460389000
1	0.150573000	-0.115585000	-2.540909000
6	9.059535000	-0.052965000	2.167480000
1	9.972466000	0.217949000	2.687615000
6	5.031506000	-3.894142000	0.293358000

1	5.870025000	-3.940223000	-0.393351000
6	4.468049000	-0.859769000	-2.669159000
1	3.558770000	-0.392420000	-2.307835000
6	2.790100000	3.897299000	0.007620000
6	6.837370000	-2.005330000	-3.609081000
1	7.761379000	-2.441250000	-3.974281000
6	2.842106000	-3.806175000	2.021204000
1	1.982775000	-3.770563000	2.682022000
6	3.404111000	-5.030321000	1.666901000
1	2.983780000	-5.952222000	2.055082000
6	4.498433000	-5.073686000	0.803282000
1	4.929876000	-6.027361000	0.517997000
6	4.671932000	-1.025436000	-4.036708000
1	3.909353000	-0.696498000	-4.734405000
6	5.850740000	-1.600206000	-4.506650000
1	6.005558000	-1.725001000	-5.573419000
8	-2.044853000	-1.234815000	1.246466000
8	-1.877246000	-1.354658000	-1.365148000
6	-1.053893000	-0.626933000	0.730703000
6	-0.960134000	-0.696414000	-0.789719000
6	-0.088311000	0.062495000	1.460122000
1	-0.150463000	0.115895000	2.540640000
75	-3.511757000	-2.121450000	-0.127004000
15	-5.117053000	1.085097000	-0.012649000
8	-4.061464000	0.017429000	-0.275118000
8	-5.654057000	-2.861847000	1.958165000
8	-5.327080000	-3.019852000	-2.450013000
6	-6.707019000	0.745375000	-0.830542000
6	-4.666427000	-2.696345000	-1.559961000

6	-5.455556000	1.270694000	1.764725000
6	-8.704949000	-0.610920000	-0.992712000
1	-9.336548000	-1.399883000	-0.598904000
6	-3.372627000	2.620715000	-1.516681000
1	-2.932214000	1.665793000	-1.777530000
6	-7.534109000	-0.269026000	-0.324605000
1	-7.266150000	-0.794499000	0.585532000
6	-4.856803000	-2.600517000	1.159690000
8	-2.345012000	-4.960314000	0.067959000
6	-4.472851000	2.661574000	-0.652538000
6	-7.066535000	1.403957000	-2.012594000
1	-6.431900000	2.184510000	-2.416353000
6	-6.644690000	1.838770000	2.240972000
1	-7.428295000	2.133683000	1.551081000
6	-8.241916000	1.058365000	-2.674977000
1	-8.514774000	1.573105000	-3.590123000
6	-9.060066000	0.052629000	-2.166599000
1	-9.973088000	-0.218343000	-2.686545000
6	-5.032333000	3.894060000	-0.293648000
1	-5.871014000	3.940045000	0.392869000
6	-4.467878000	0.859603000	2.669203000
1	-3.558640000	0.392273000	2.307749000
6	-2.789643000	-3.897127000	-0.008157000
6	-6.837083000	2.005128000	3.609464000
1	-7.761047000	2.441033000	3.974795000
6	-2.842545000	3.806366000	-2.021018000
1	-1.983074000	3.770864000	-2.681659000
6	-3.404930000	5.030426000	-1.667027000
1	-2.984756000	5.952371000	-2.055273000

6	-4.499447000	5.073655000	-0.803646000
1	-4.931194000	6.027268000	-0.518612000
6	-4.671587000	1.025230000	4.036785000
1	-3.908918000	0.696269000	4.734373000
6	-5.850333000	1.599987000	4.506895000
1	-6.005013000	1.724756000	5.573688000

Cartesian coordinates of the DFT/B3LYP/SDD optimized structure of **3.**



Atom	X	Y	Z
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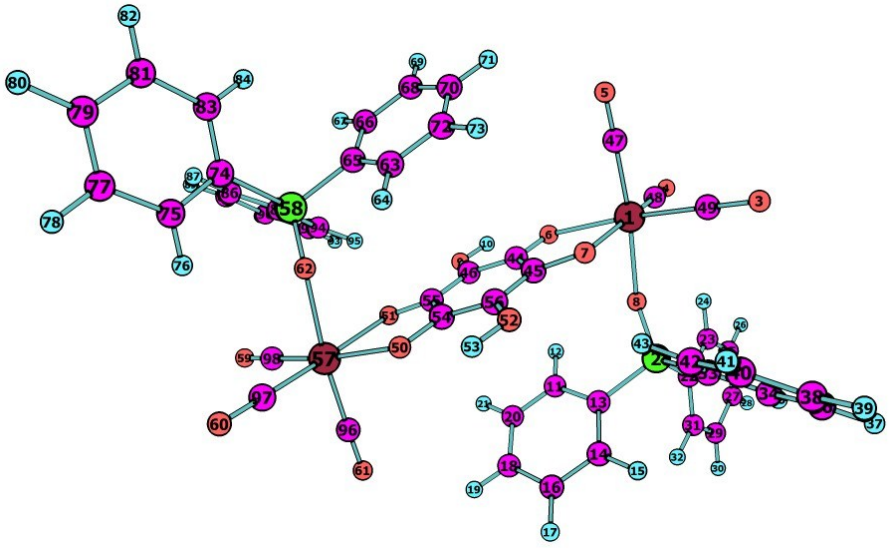
15	4.849647000	1.059632000	0.013883000
8	5.215700000	-3.390390000	-2.108640000
8	5.092104000	-3.408123000	2.321777000
8	1.725261000	-4.959094000	0.011467000
8	1.831136000	-1.321709000	1.355171000
8	1.892914000	-1.299533000	-1.276682000
8	4.230646000	-0.330775000	0.078314000
8	-0.057835000	0.003129000	2.865416000
1	0.654417000	-0.599974000	3.125246000
6	3.897340000	1.595800000	2.607889000
1	3.718886000	0.519144000	2.593112000
6	3.927649000	2.164012000	1.174278000
6	4.360371000	3.652608000	1.185114000

1	3.963062000	4.151783000	0.296296000
6	3.868371000	4.382396000	2.460914000
1	3.734031000	5.445686000	2.242877000
6	2.574069000	3.766194000	3.000288000
1	1.800036000	3.812361000	2.225797000
6	2.799462000	2.302319000	3.439911000
1	1.861179000	1.747408000	3.359483000
6	6.634107000	1.002374000	0.555423000
6	7.239416000	-0.407988000	0.377069000
1	7.278914000	-0.663468000	-0.687663000
6	8.653817000	-0.477059000	0.970723000
1	9.070980000	-1.474313000	0.799480000
6	9.576583000	0.597589000	0.384036000
1	9.744822000	0.391071000	-0.681005000
6	8.969705000	1.996911000	0.538008000
1	9.610611000	2.746753000	0.062708000
6	7.557474000	2.074417000	-0.064725000
1	7.626047000	1.920301000	-1.147053000
6	4.734593000	1.770041000	-1.689866000
6	5.332221000	0.800375000	-2.735388000
1	4.774851000	-0.140552000	-2.703511000
6	5.256434000	1.387803000	-4.152807000
1	5.655868000	0.659784000	-4.866197000
6	3.822192000	1.774411000	-4.530235000
1	3.204996000	0.870216000	-4.592475000
6	3.214839000	2.724933000	-3.493304000
1	2.170729000	2.940005000	-3.740550000
6	3.283827000	2.138238000	-2.075081000
1	2.658843000	1.242089000	-2.032954000
6	0.932553000	-0.624543000	0.770947000
6	0.973244000	-0.609919000	-0.741055000
6	-0.040699000	0.059132000	1.495593000
6	2.333759000	-3.975810000	0.030008000
6	4.436798000	-3.022839000	1.450775000
6	4.508652000	-3.010289000	-1.277833000
8	-1.827599000	1.543903000	-1.300236000
8	-1.941017000	1.458124000	1.326697000
8	0.037082000	0.189784000	-2.809474000
1	-0.689085000	0.776134000	-3.068973000
6	-0.940162000	0.834316000	-0.715759000
6	-0.998989000	0.796571000	0.795463000
6	0.025648000	0.140787000	-1.440221000
75	-3.413154000	2.372344000	-0.026189000
15	-4.870377000	-1.016439000	0.096913000
8	-5.515586000	3.125880000	2.093842000
8	-5.160078000	3.410576000	-2.339960000
8	-2.129495000	5.156267000	0.202681000
8	-4.085273000	0.269412000	-0.163430000
6	-3.845398000	-1.953308000	-2.310777000
1	-4.788928000	-1.648456000	-2.772500000
6	-4.066607000	-2.395800000	-0.843487000
6	-2.739106000	-2.882526000	-0.221879000

1	-2.905564000	-3.260832000	0.789040000
6	-2.089914000	-3.986432000	-1.072299000
1	-2.728108000	-4.880172000	-1.048890000
6	-1.881984000	-3.546819000	-2.525019000
1	-1.462809000	-4.370806000	-3.110964000
6	-3.198427000	-3.068295000	-3.145490000
1	-3.894055000	-3.914094000	-3.229230000
6	-6.656189000	-0.878615000	-0.458814000
6	-6.880111000	0.317047000	-1.408161000
1	-6.319034000	0.167241000	-2.337073000
6	-8.370458000	0.494846000	-1.733326000
1	-8.489842000	1.324956000	-2.436322000
6	-8.992172000	-0.785712000	-2.302013000
1	-8.547980000	-1.002192000	-3.282366000
6	-8.759386000	-1.977380000	-1.366099000
1	-9.158091000	-2.896158000	-1.808697000
6	-7.267565000	-2.168635000	-1.049689000
1	-6.742872000	-2.436384000	-1.972994000
6	-4.997856000	-1.350953000	1.918896000
6	-5.640949000	-2.708878000	2.274355000
1	-4.990120000	-3.524833000	1.938366000
6	-5.862720000	-2.833364000	3.791007000
1	-6.274204000	-3.822285000	4.018685000
6	-4.572584000	-2.592011000	4.583372000
1	-3.859943000	-3.400202000	4.372316000
6	-3.937611000	-1.245525000	4.215574000
1	-2.989487000	-1.108575000	4.743827000
6	-3.690049000	-1.122602000	2.705115000
1	-2.937280000	-1.859498000	2.410250000
6	-2.620338000	4.114600000	0.113469000
6	-4.531895000	3.029107000	-1.447807000
6	-4.733491000	2.870492000	1.281425000
1	2.862261000	2.857574000	-1.367540000
1	3.745660000	3.686198000	-3.517928000
1	3.803061000	2.234424000	-5.523718000
1	5.904919000	2.271987000	-4.217137000
1	6.370373000	0.555254000	-2.494879000
1	6.598021000	-1.154444000	0.846149000
1	7.153813000	3.080297000	0.078788000
1	8.923203000	2.260689000	1.602532000
1	10.560020000	0.558084000	0.863379000
1	8.594230000	-0.352429000	2.059772000
1	4.875737000	1.747508000	3.077375000
1	3.086775000	2.270790000	4.495959000
1	2.189554000	4.355737000	3.836994000
1	4.639744000	4.327789000	3.237642000
1	5.448367000	3.745300000	1.127547000
1	-1.137033000	-4.279060000	-0.621684000
1	-1.144836000	-2.735826000	-2.563478000
1	-3.030929000	-2.704292000	-4.164368000
1	-3.202133000	-1.068456000	-2.316228000
1	-2.047717000	-2.038243000	-0.133064000

1	-6.597833000	-2.840292000	1.760853000
1	-6.621877000	-2.104076000	4.101754000
1	-4.778501000	-2.637328000	5.657736000
1	-4.593220000	-0.428561000	4.543747000
1	-3.269028000	-0.144390000	2.475219000
1	-7.144065000	-3.014685000	-0.367828000
1	-9.311819000	-1.821039000	-0.430475000
1	-10.063933000	-0.644550000	-2.474871000
1	-8.906853000	0.785495000	-0.820616000
1	-6.487043000	1.229283000	-0.959692000
1	-5.697526000	-0.560425000	2.230470000
1	-7.194943000	-0.656875000	0.472714000
1	-4.778501000	-3.230490000	-0.828363000
1	6.578078000	1.195793000	1.635082000
1	2.903699000	2.101593000	0.787402000
1	5.334635000	2.689938000	-1.674090000

Cartesian coordinates of the DFT/B3LYP/SDD optimized structure of **4.**

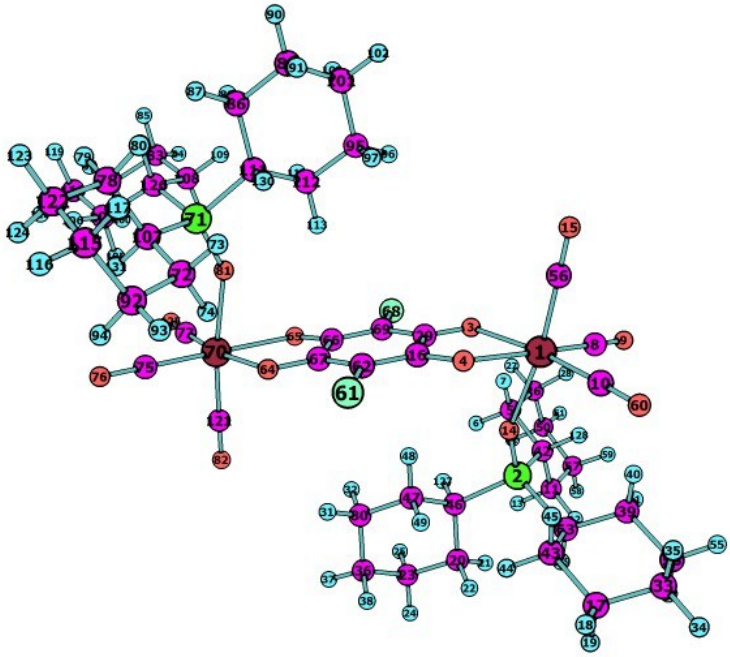


Atom	X	Y	Z
75	-3.948577000	0.752337000	0.781874000
15	-2.795214000	-0.760258000	3.854228000
8	-6.454854000	-1.010927000	1.108046000
8	-5.437604000	3.213269000	1.886458000
8	-4.823895000	1.442432000	-2.081353000
8	-1.979689000	1.707829000	0.557240000
8	-2.562366000	-0.825980000	0.160849000
8	-3.087118000	0.265807000	2.764701000
8	0.574353000	2.749184000	0.417475000
1	-0.279546000	3.183773000	0.558254000
6	-0.136926000	-0.012908000	3.690041000
1	-0.536320000	0.953208000	3.402499000
6	-1.008210000	-1.077646000	3.958880000

6	-0.486877000	-2.329109000	4.308846000
1	-1.150658000	-3.164949000	4.500030000
6	0.892338000	-2.511546000	4.384646000
1	1.292635000	-3.486194000	4.643246000
6	1.755514000	-1.452809000	4.109261000
1	2.829117000	-1.601682000	4.142991000
6	1.239140000	-0.203945000	3.764026000
1	1.909406000	0.617921000	3.537026000
6	-3.330882000	-0.080464000	5.456602000
6	-4.317293000	0.912707000	5.460517000
1	-4.722036000	1.273572000	4.522294000
6	-4.761066000	1.447226000	6.667639000
1	-5.522137000	2.220231000	6.664607000
6	-4.223740000	0.996493000	7.871471000
1	-4.568455000	1.417182000	8.810491000
6	-3.235454000	0.012795000	7.871005000
1	-2.807091000	-0.329975000	8.807019000
6	-2.786534000	-0.524237000	6.667934000
1	-2.004116000	-1.275678000	6.675285000
6	-3.630674000	-2.358194000	3.611428000
6	-4.570115000	-2.841014000	4.531061000
1	-4.798018000	-2.276371000	5.427516000
6	-5.220765000	-4.049684000	4.294947000
1	-5.949705000	-4.416269000	5.009998000
6	-4.941554000	-4.778578000	3.141800000
1	-5.453681000	-5.717267000	2.956731000
6	-4.011261000	-4.299229000	2.220379000
1	-3.798791000	-4.857802000	1.315295000
6	-3.354416000	-3.094652000	2.448210000
1	-2.651457000	-2.726891000	1.709798000
6	-0.997903000	0.936264000	0.293059000
6	-1.330255000	-0.520982000	0.071899000
6	0.306766000	1.421092000	0.212678000
6	-4.506463000	1.188627000	-0.997930000
6	-4.906572000	2.279228000	1.461256000
6	-5.526093000	-0.334848000	0.992092000
8	1.979689000	-1.707829000	-0.557240000
8	2.562366000	0.825980000	-0.160849000
8	-0.574353000	-2.749184000	-0.417475000
1	0.279546000	-3.183773000	-0.558254000
6	0.997903000	-0.936264000	-0.293059000
6	1.330255000	0.520982000	-0.071899000
6	-0.306766000	-1.421092000	-0.212678000
75	3.948577000	-0.752337000	-0.781874000
15	2.795214000	0.760258000	-3.854228000
8	6.454854000	1.010927000	-1.108046000
8	5.437604000	-3.213269000	-1.886458000
8	4.823895000	-1.442432000	2.081353000
8	3.087118000	-0.265807000	-2.764701000
6	0.136926000	0.012908000	-3.690041000
1	0.536320000	-0.953208000	-3.402499000
6	1.008210000	1.077646000	-3.958880000

6	0.486877000	2.329109000	-4.308846000
1	1.150658000	3.164949000	-4.500030000
6	-0.892338000	2.511546000	-4.384646000
1	-1.292635000	3.486194000	-4.643246000
6	-1.755514000	1.452809000	-4.109261000
1	-2.829117000	1.601682000	-4.142991000
6	-1.239140000	0.203945000	-3.764026000
1	-1.909406000	-0.617921000	-3.537026000
6	3.330882000	0.080464000	-5.456602000
6	4.317293000	-0.912707000	-5.460517000
1	4.722036000	-1.273572000	-4.522294000
6	4.761066000	-1.447226000	-6.667639000
1	5.522137000	-2.220231000	-6.664607000
6	4.223740000	-0.996493000	-7.871471000
1	4.568455000	-1.417182000	-8.810491000
6	3.235454000	-0.012795000	-7.871005000
1	2.807091000	0.329975000	-8.807019000
6	2.786534000	0.524237000	-6.667934000
1	2.004116000	1.275678000	-6.675285000
6	3.630674000	2.358194000	-3.611428000
6	4.570115000	2.841014000	-4.531061000
1	4.798018000	2.276371000	-5.427516000
6	5.220765000	4.049684000	-4.294947000
1	5.949705000	4.416269000	-5.009998000
6	4.941554000	4.778578000	-3.141800000
1	5.453681000	5.717267000	-2.956731000
6	4.011261000	4.299229000	-2.220379000
1	3.798791000	4.857802000	-1.315295000
6	3.354416000	3.094652000	-2.448210000
1	2.651457000	2.726891000	-1.709798000
6	4.506463000	-1.188627000	0.997930000
6	4.906572000	-2.279228000	-1.461256000
6	5.526093000	0.334848000	-0.992092000

Cartesian coordinates of the DFT/B3LYP/SDD optimized structure of **5.**

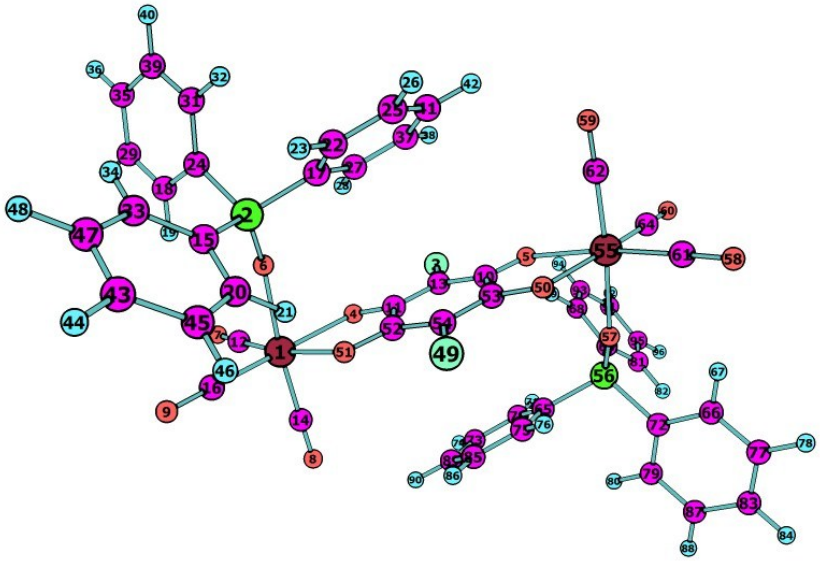


Atom	X	Y	Z
75	3.607094000	2.248471000	-0.079664000
15	5.001464000	-1.073832000	0.038502000
8	2.100395000	1.321060000	-1.383370000
8	1.916892000	1.675162000	1.192351000
6	4.607408000	-0.970144000	-2.749517000
1	4.023530000	-1.898769000	-2.747183000
1	3.904266000	-0.164342000	-2.533319000
6	4.979103000	2.561412000	-1.387905000
8	5.786151000	2.720829000	-2.202418000
6	4.770778000	2.898641000	1.306622000
6	6.712261000	-2.172822000	-1.988025000
1	7.507972000	-2.221814000	-1.238228000
1	6.196953000	-3.139903000	-1.962294000
8	4.043614000	0.109113000	0.241913000
8	2.566480000	5.111065000	-0.527015000
6	1.010808000	0.965604000	0.681772000
6	6.997646000	-0.813355000	3.719993000
1	6.576665000	-0.647771000	4.716773000
1	7.495044000	-1.792027000	3.753173000
6	4.885075000	-3.872242000	0.717957000
1	5.773656000	-4.014934000	0.097014000
1	5.242121000	-3.694666000	1.738527000
6	4.035527000	-5.153807000	0.704873000
1	4.635802000	-5.992265000	1.073271000
1	3.767454000	-5.398107000	-0.331071000
6	5.224953000	-0.776340000	-4.142528000
1	4.428088000	-0.763175000	-4.892287000
1	5.707026000	0.207618000	-4.187598000
6	1.118860000	0.753286000	-0.828274000

6	1.947246000	-3.774680000	1.103998000
1	1.076294000	-3.645635000	1.753172000
1	1.552905000	-3.938616000	0.093132000
6	8.026366000	0.272807000	3.387072000
1	8.848126000	0.251932000	4.110154000
1	7.555651000	1.258962000	3.477996000
6	2.758421000	-4.999859000	1.540763000
1	2.147130000	-5.904424000	1.465980000
1	3.029478000	-4.897545000	2.599796000
6	7.441648000	0.067028000	0.920367000
1	6.952407000	1.045414000	0.890731000
1	7.872608000	-0.096575000	-0.071107000
6	5.710944000	-1.042533000	-1.670394000
6	5.859302000	-0.852318000	2.690314000
1	5.166394000	-1.660087000	2.941059000
1	5.281524000	0.074948000	2.747335000
6	4.051897000	-2.661495000	0.242354000
6	2.791561000	-2.492766000	1.118398000
1	2.202086000	-1.645379000	0.769006000
1	3.081229000	-2.257888000	2.148403000
6	6.249290000	-1.870149000	-4.470023000
1	6.714239000	-1.676685000	-5.442062000
1	5.733314000	-2.835051000	-4.562601000
6	8.568860000	0.099317000	1.964333000
1	9.146122000	-0.833030000	1.903427000
1	9.263810000	0.908570000	1.718796000
6	2.963342000	4.041471000	-0.356866000
6	7.326731000	-1.975910000	-3.383708000
1	8.010059000	-2.803033000	-3.602668000
1	7.935979000	-1.063242000	-3.382260000
8	5.442467000	3.268043000	2.172042000
17	-0.168332000	0.638050000	3.118132000
6	-0.050785000	0.394107000	1.394475000
6	6.399575000	-1.025402000	1.251873000
8	-1.948212000	-1.003308000	1.297600000
8	-1.766938000	-1.356910000	-1.277614000
6	-0.881714000	-0.615592000	-0.773508000
6	-0.988770000	-0.403434000	0.735463000
17	0.276641000	-0.259886000	-3.215934000
6	0.160908000	-0.017950000	-1.491859000
75	-3.350736000	-2.123862000	0.030290000
15	-5.178815000	0.976040000	-0.011063000
6	-4.510484000	1.041884000	2.733761000
1	-4.089345000	2.051936000	2.657663000
1	-3.708587000	0.349804000	2.472173000
6	-4.637741000	-2.605363000	1.372700000
8	-5.394074000	-2.863328000	2.210596000
6	-4.441149000	-2.942052000	-1.327758000
6	-6.845167000	1.861251000	2.153590000
1	-7.702459000	1.754652000	1.481768000
1	-6.500499000	2.897597000	2.062002000
8	-4.097995000	-0.074428000	-0.301020000

8	-1.916010000	-4.809767000	0.478751000
6	-7.505347000	0.337705000	-3.450814000
1	-7.178007000	0.237335000	-4.490525000
1	-8.174439000	1.208129000	-3.419849000
6	-5.511023000	3.747388000	-0.708782000
1	-6.318732000	3.793431000	0.026885000
1	-5.977466000	3.499750000	-1.668716000
6	-4.838613000	5.125192000	-0.823129000
1	-5.584663000	5.871812000	-1.114515000
1	-4.468177000	5.428622000	0.164453000
6	-4.961845000	0.800360000	4.182586000
1	-4.109352000	0.941442000	4.853885000
1	-5.270133000	-0.246508000	4.292217000
6	-2.660251000	4.012331000	-1.485562000
1	-1.872373000	3.975520000	-2.243914000
1	-2.161596000	4.253311000	-0.537894000
6	-8.272668000	-0.912381000	-3.008269000
1	-9.159156000	-1.054785000	-3.634692000
1	-7.641892000	-1.797415000	-3.154459000
6	-3.675868000	5.111163000	-1.822650000
1	-3.184420000	6.088952000	-1.842184000
1	-4.069341000	4.944505000	-2.834047000
6	-7.464018000	-0.558533000	-0.624581000
1	-6.803649000	-1.430806000	-0.653487000
1	-7.803978000	-0.458957000	0.409829000
6	-5.704364000	0.898104000	1.762914000
6	-6.282493000	0.600251000	-2.559226000
1	-5.783600000	1.516974000	-2.884798000
1	-5.555894000	-0.207560000	-2.688400000
6	-4.473612000	2.663168000	-0.341579000
6	-3.323639000	2.632379000	-1.371918000
1	-2.588820000	1.877587000	-1.090245000
1	-3.707968000	2.330559000	-2.352117000
6	-6.118140000	1.723689000	4.585171000
1	-6.454525000	1.490568000	5.600534000
1	-5.762775000	2.762396000	4.609803000
6	-8.676182000	-0.814086000	-1.533486000
1	-9.403432000	-0.000928000	-1.406272000
1	-9.179723000	-1.731244000	-1.211982000
6	-2.462293000	-3.807513000	0.307348000
6	-7.291798000	1.614911000	3.603820000
1	-8.080401000	2.326534000	3.869881000
1	-7.738862000	0.615490000	3.676919000
8	-5.070229000	-3.410946000	-2.176538000
6	-6.675490000	0.695698000	-1.066580000
1	3.706964000	-2.878118000	-0.777300000
1	6.255745000	-0.090296000	-1.696816000
1	6.893706000	-2.002824000	1.180674000
1	-4.031015000	2.941828000	0.623887000
1	-6.079884000	-0.127799000	1.862922000
1	-7.317690000	1.575299000	-0.929955000

Cartesian coordinates of the DFT/B3LYP/SDD optimized structure of **6.**



Atom	X	Y	Z
75	-3.431703000	-2.279924000	-0.177910000
15	-4.803375000	1.076263000	-0.084628000
17	0.387702000	-0.345197000	-3.165081000
8	-1.769642000	-1.474982000	-1.373686000
8	2.107411000	1.185714000	-1.195080000
8	-4.240260000	-0.259944000	-0.552383000
8	-5.063028000	-3.482490000	-2.496824000
8	-2.032028000	-4.974238000	0.295624000
8	-5.617270000	-3.086104000	1.838310000
6	1.095782000	0.600633000	-0.708439000
6	-0.901853000	-0.767517000	-0.799560000
6	-4.462042000	-3.050592000	-1.611236000
6	0.184031000	-0.157178000	-1.441616000
6	-2.568540000	-3.965896000	0.111801000
6	-5.467989000	1.024910000	1.607890000
6	-4.808717000	-2.792150000	1.068582000
6	-3.526911000	2.368613000	-0.150671000

6	-6.858650000	0.577727000	-1.880236000
1	-6.584857000	-0.462543000	-1.748537000
6	-4.645415000	0.533785000	2.633833000
1	-3.637456000	0.195964000	2.420188000
6	-3.380722000	3.335887000	0.850490000
1	-4.029583000	3.326716000	1.719005000
6	-6.146103000	1.576396000	-1.205866000
6	-2.380948000	4.300960000	0.744148000
1	-2.260611000	5.039254000	1.529730000
6	-2.667279000	2.379063000	-1.259109000
1	-2.766121000	1.624227000	-2.031816000
6	-7.902348000	0.924898000	-2.733975000
1	-8.447301000	0.147895000	-3.259349000
6	-6.480332000	2.921982000	-1.401045000
1	-5.917621000	3.704246000	-0.902736000
6	-6.775964000	1.429705000	1.901451000
1	-7.425161000	1.797704000	1.115373000
6	-8.238714000	2.264657000	-2.918449000
1	-9.050473000	2.532675000	-3.586840000
6	-1.671996000	3.345574000	-1.357460000
1	-1.001928000	3.342364000	-2.210322000
6	-7.527191000	3.262167000	-2.253527000
1	-7.780320000	4.306137000	-2.405729000
6	-1.525830000	4.305870000	-0.355567000
1	-0.734335000	5.043667000	-0.426032000
6	-6.431957000	0.869547000	4.223950000
1	-6.807365000	0.805887000	5.240058000
6	-5.131092000	0.459335000	3.935153000
1	-4.491666000	0.073221000	4.721548000

6	-7.252833000	1.352824000	3.208015000
1	-8.268304000	1.664681000	3.428420000
17	-0.385473000	0.356259000	3.160390000
8	1.773864000	1.482633000	1.369845000
8	-2.105207000	-1.174439000	1.190497000
6	-1.093039000	-0.590362000	0.703860000
6	0.905275000	0.776597000	0.795228000
6	-0.181297000	0.167373000	1.437027000
75	3.437346000	2.285096000	0.175110000
15	4.798545000	-1.078243000	0.082382000
8	4.238750000	0.261580000	0.543090000
8	5.073266000	3.477690000	2.496017000
8	2.043343000	4.983671000	-0.290409000
8	5.624491000	3.089907000	-1.839906000
6	4.470524000	3.049380000	1.609934000
6	2.578245000	3.973950000	-0.109751000
6	5.465469000	-1.034939000	-1.609426000
6	4.815346000	2.796493000	-1.070553000
6	3.520440000	-2.368642000	0.151428000
6	6.875404000	-0.579217000	1.853413000
1	6.626517000	0.463501000	1.694177000
6	4.652896000	-0.526246000	-2.634724000
1	3.651504000	-0.169330000	-2.420771000
6	3.373246000	-3.336762000	-0.848747000
1	4.020201000	-3.327269000	-1.718699000
6	6.137116000	-1.578976000	1.208453000
6	2.375676000	-4.303700000	-0.739008000
1	2.254827000	-5.043037000	-1.523531000
6	2.663351000	-2.379387000	1.261844000

1	2.763025000	-1.623920000	2.033859000
6	7.912820000	-0.927281000	2.714180000
1	8.477485000	-0.149276000	3.216766000
6	6.440082000	-2.926118000	1.440053000
1	5.857457000	-3.708137000	0.964820000
6	6.764436000	-1.467395000	-1.903513000
1	7.405762000	-1.849985000	-1.117867000
6	8.217119000	-2.269227000	2.935895000
1	9.023311000	-2.537857000	3.610756000
6	1.670327000	-3.347865000	1.363655000
1	1.002552000	-3.345422000	2.218345000
6	7.480436000	-3.267414000	2.300267000
1	7.708241000	-4.312532000	2.481554000
6	1.523739000	-4.309608000	0.363175000
1	0.734350000	-5.049297000	0.436688000
6	6.431996000	-0.897559000	-4.225373000
1	6.808533000	-0.840780000	-5.241506000
6	5.139987000	-0.460512000	-3.936032000
1	4.508599000	-0.060373000	-4.721891000
6	7.242598000	-1.399397000	-3.210130000
1	8.251111000	-1.732849000	-3.431323000

UOH -SCHOOL OF CHEMISTRY -HRMS

Analysis Info

Analysis Name	D:\Data\2018\PROF MS\aug\RA5-25R.d	Acquisition Date	8/28/2018 2:35:46 PM
Method	tune_wide_PosR.m	Operator	UOH-Chemistry
Sample Name	RA5-25-ACN	Instrument	maXis 10138
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	4200 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	2500.0 Vpp	Set Divert Valve	Source

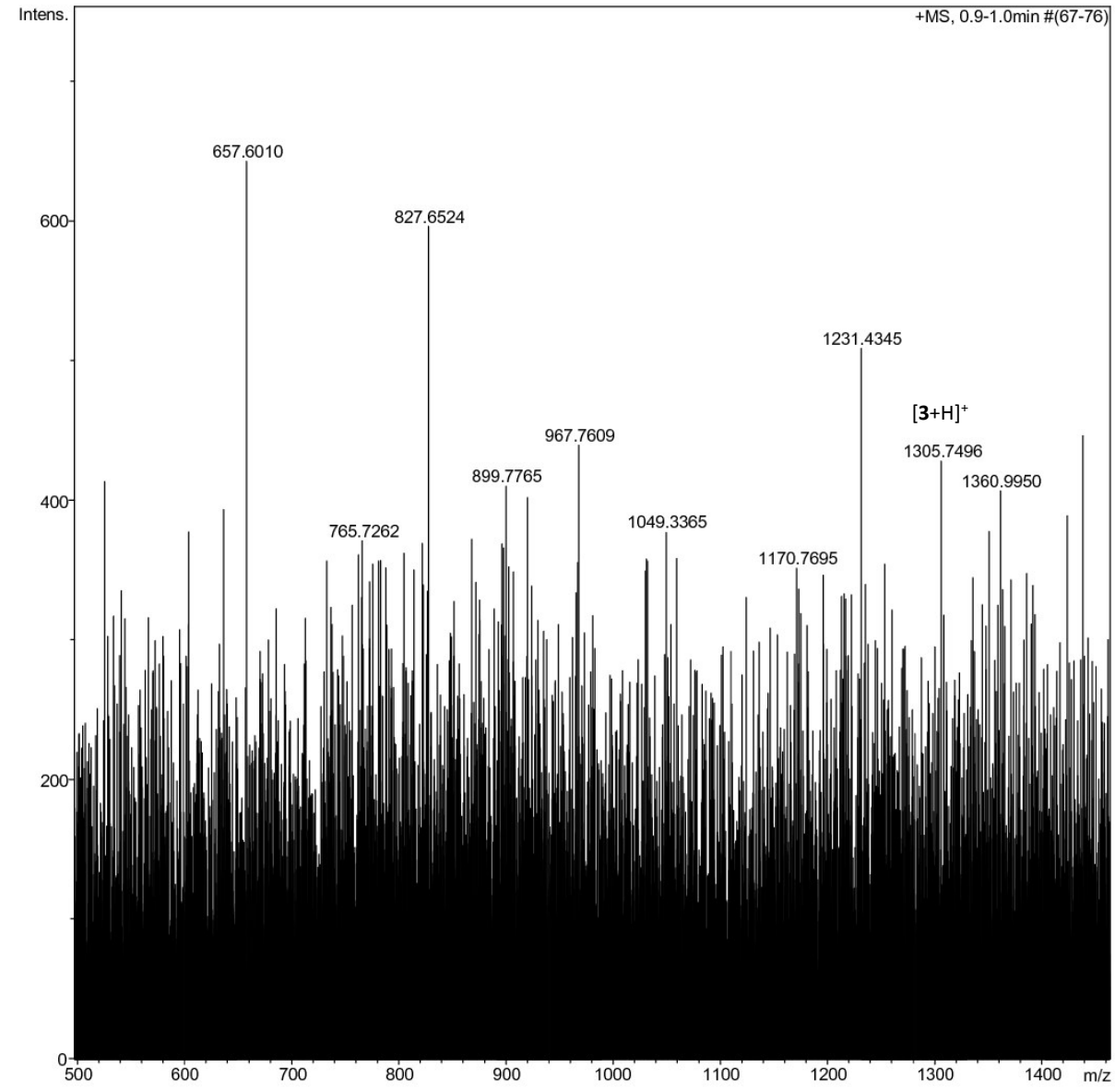


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Figure S18: ESI-TOF Mass spectra of **3** in positive ion mode.