Supplementary Information

Polynuclear cage-like Au(I) phosphane complexes based on S^{2-} template; observation of multiple luminescence in coordinated polyaromatic systems.

Julia R. Shakirova,[a] Elena V. Grachova,[a] Vladimir V. Sizov,[a] Galina L. Starova,[a] Igor O. Koshevoy,[b] Alexey S. Melnikov,[c,d] M. Concepción Gimeno,[e] Antonio Laguna,[e] and Sergey P. Tunik[a]*

[a.] *St. Petersburg State University, Institute of Chemistry, Universitetskii pr. 26, 198504 St. Petersburg, Russia. E-mail: stunik@inbox.ru*
[b.] *University of Eastern Finland, 80101 Joensuu, Finland*
[c.] *St. Petersburg State University, Department of Physics, 198504 St. Petersburg, Russia*
[d.] *Institute of Nanobiotechnologies, Peter the Great St. Petersburg Polytechnic University, 195251 St. Petersburg, Russia*
[e.] *Universidad de Zaragoza-CSIC, Departamento de Química Inorgánica, Instituto de Síntesis Química y Catálisis Homogénea (ISQCH), 50009 Zaragoza, Spain*

XRD experimental detailes:

Single crystals of $C_{108}H_{84}P_6S_2Au_6$ (**1**) were growth from dichloromethane. A suitable crystal was selected and mounted in inert oil on a glass fiber and transferred to the cold gas stream of an Xcalibur diffractometer equipped with a low-temperature attachment. The crystal was measured at 100(2) K. Data were collected using monochromated Mo Kα radiation (λ= 0.71073 Å). Scan type: ω. Absorption correction based on multiple scans was applied using spherical harmonics implemented in SCALE3 ABSPACK [1] scaling algorithm. Using Olex2 [1], the structure was solved with the SIR2004 [2] structure solution program using Direct Methods and refined with the ShelXL [3] refinement package using Least Squares minimisation. Supplementary crystallographic data for this paper have been deposited at Cambridge Crystallographic Data Centre (1511913) and can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

1. CrysAlisPro, Agilent Technologies, Version 1.171.35.11. Multi-scans absorption correction with SCALE3 ABSPACK scaling algorithm.
2. Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.
3. Burla, M.C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G.L., De Caro, L., Giacovazzo, C., Polidori, G., Siliqi, D., Spagna, R. (2007). J. Appl. Cryst. 40, 609-613.
4. Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

Crystal structure determination of (1).

Crystal Data for $C_{108}H_{84}P_6S_2Au_6$ (*M* =2813.49 g/mol): monoclinic, space group $P2_1/c$ (no. 14), a = 14.730(3) Å, b = 28.092(6) Å, c = 29.978(6) Å, β = 95.63(3)°, V = 12345(4) Å^3, Z = 4, T = 100(2) K, μ(MoKα) = 7.252 mm^{-1}, *Dcalc* = 1.514 g/cm^3, 92928 reflections measured (8.344° ≤ 2Θ ≤ 51°), 22788 unique (R_{int} = 0.1321, R_{sigma} = 0.1540) which were used in all calculations. The final R_1 was 0.1363 (I > 2σ(I)) and wR_2 was 0.3846 (all data).

Refinement model description

Number of restraints - 5, number of constraints - unknown.
Details:
1. Fixed Uiso
At 1.2 times of:
All C(H) groups
2. Restrained distances
C57-C58
1.39 with sigma of 0.02
C90-C89
1.39 with sigma of 0.02
C89-C91
1.39 with sigma of 0.02
C91-C92
1.39 with sigma of 0.02
3. Restrained planarity
C90, C89, C91, C92

with sigma of 0.1

4.a Aromatic/amide H refined with riding coordinates:
C8(H8), C9(H9), C10(H10), C11(H11), C12(H12), C56(H56), C55(H55), C53(H53), C52(H52), C26(H26), C50(H50), C49(H49), C48(H48), C47(H47), C46(H46), C73(H73), C140(H140), C76(H76), C74(H74), C44(H44), C43(H43), C42(H42), C41(H41), C40(H40), C34(H34), C35(H35), C37(H37), C38(H38), C2(H2), C3(H3), C4(H4), C5(H5), C6(H6), C23(H23), C25(H25), C28(H28), C32(H32), C31(H31), C30(H30), C29(H29), C98(H98), C97(H97), C96(H96), C95(H95), C94(H94), C91(H91), C22(H22), C14(H14), C18(H18), C17(H17), C15(H15), C58(H58), C24(H24), C90(H90), C82(H82), C81(H81), C80(H80), C79(H79), C78(H78), C59(H59), C92(H92), C106(H106), C88(H88), C87(H87), C86(H86), C85(H85), C84(H84), C20(H20), C71(H71), C70(H70), C69(H69), C68(H68), C67(H67), C107(H107), C65(H65), C61(H61), C62(H62), C63(H63), C64(H64), C100(H100), C101(H101), C102(H102), C103(H103), C104(H104)

4.b Fitted hexagon refined as free rotating group:
C7(C8,C9,C10,C11,C12), C51(C56,C55,C54,C53,C52), C45(C50,C49,C48,C47,C46), C73(C72,C140,C76,C75,C74), C39(C44,C43,C42,C41,C40), C33(C34,C35,C36,C37,C38), C1(C2,C3,C4,C5,C6), C28(C27,C32,C31,C30,C29), C93(C98,C97,C96,C95,C94), C14(C13,C18,C17,C16,C15), C77(C82,C81,C80,C79,C78), C83(C88,C87,C86,C85,C84), C66(C71,C70,C69,C68,C67), C65(C60,C61,C62,C63,C64), C99(C100,C101,C102,C103, C104)

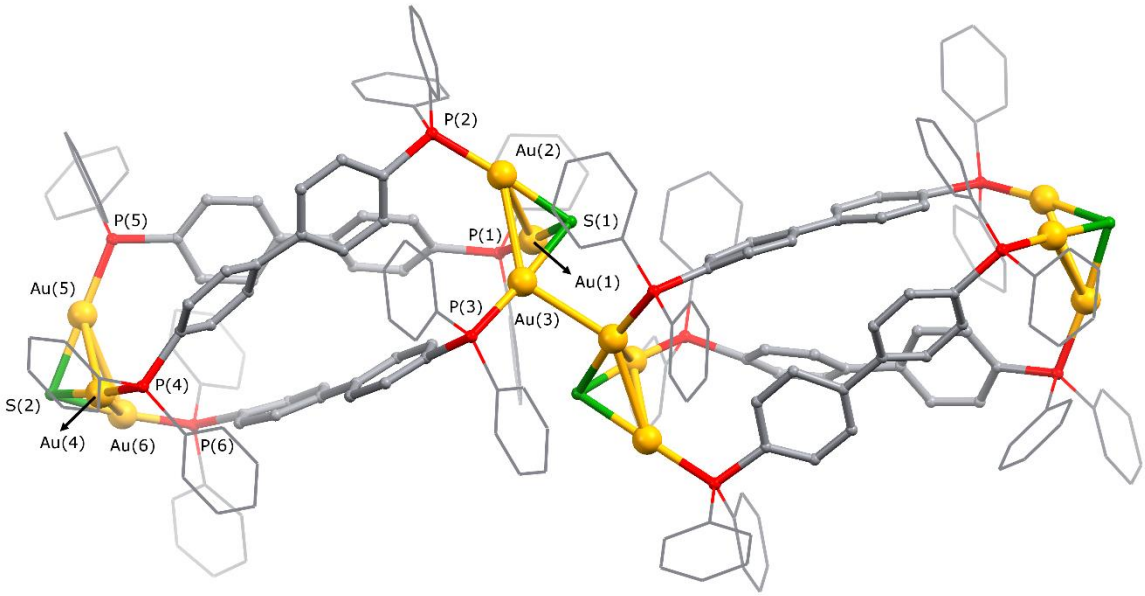

Figure S1. Solid-state structure of dication **1** (hydrogen atoms and counterions are omitted for clarity).

Table S1. Crystal data and structure refinement for **1**.

Identification code	c345
Empirical formula	$C_{108}H_{84}P_6S_2Au_6$
Formula weight	2813.49
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	14.730(3)
b/Å	28.092(6)
c/Å	29.978(6)
α/°	90
β/°	95.63(3)
γ/°	90
Volume/Å^3	12345(4)
Z	4
ρ_{calc}g/cm^3	1.514
μ/mm^{-1}	7.252
F(000)	5312.0
Crystal size/mm^3	0.40 × 0.05 × 0.04
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	8.344 to 51
Index ranges	-17 ≤ h ≤ 17, -34 ≤ k ≤ 33, -36 ≤ l ≤ 36
Reflections collected	92928
Independent reflections	22788 [R_{int} = 0.1321, R_{sigma} = 0.1540]
Data/restraints/parameters	22788/5/379
Goodness-of-fit on F^2	1.132
Final R indexes [I>=2σ (I)]	R_1 = 0.1363, wR_2 = 0.3504
Final R indexes [all data]	R_1 = 0.1980, wR_2 = 0.3846
Largest diff. peak/hole / e Å^{-3}	12.44/-3.32

Table S2. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for **1**. U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
Au6	6328.5(9)	4785.9(3)	7314.3(4)	42.2(3)
Au1	3958.2(8)	5361.2(3)	8087.4(4)	39.6(3)
Au2	5360.8(8)	5347.1(3)	8957.5(3)	35.7(3)
Au5	6043(1)	4816.5(4)	6273.4(4)	51.3(4)
Au4	4416.7(10)	4801.8(4)	6786.4(4)	56.0(4)
Au3	6155.8(8)	5456.7(3)	8060.2(4)	35.7(3)
S1	5214(6)	4870.3(19)	8320(2)	42.0(18)
P6	7064(5)	4202(2)	7723(3)	40.0(18)
P2	5411(6)	5860(2)	9538(2)	36.9(17)
S2	5631(6)	5339(2)	6826(3)	52(2)
P5	6393(6)	4307(2)	5735(3)	43.5(19)
P3	7085(5)	6056(2)	7857(3)	41.6(19)
P4	3194(7)	4306(3)	6674(3)	55(2)
P1	2713(6)	5798(2)	7887(3)	45.7(19)
C7	1722(13)	5511(7)	8079(7)	42(7)
C8	1437(14)	5080(7)	7886(6)	54(8)
C9	720(14)	4832(6)	8048(7)	58(8)

C10	290(14)	5016(8)	8403(8)	79(11)
C11	575(17)	5447(9)	8596(7)	93(13)
C12	1292(16)	5695(7)	8434(7)	89(12)
C51	6339(10)	6587(5)	7689(6)	28(5)
C56	5393(11)	6554(4)	7653(6)	41(7)
C55	4864(9)	6960(6)	7567(6)	37(6)
C54	5281(12)	7398(5)	7516(6)	35(6)
C53	6227(12)	7430(5)	7552(7)	79(11)
C52	6756(9)	7025(6)	7639(7)	62(9)
C21	6117(18)	5670(8)	10068(8)	31(6)
C26	5700(20)	5702(10)	10466(9)	47(7)
C45	7685(12)	5932(6)	7386(5)	43(7)
C50	7407(12)	6121(6)	6966(6)	49(7)
C49	7889(14)	6014(7)	6602(5)	75(11)
C48	8649(14)	5719(8)	6659(5)	57(8)
C47	8927(11)	5530(7)	7079(7)	66(9)
C46	8445(13)	5637(6)	7442(5)	37(6)
C73	4217(12)	3533(6)	6466(6)	49(8)
C72	3424(14)	3784(5)	6331(7)	51(8)
C140	2761(12)	3582(7)	6027(7)	77(11)
C76	2891(12)	3129(7)	5858(6)	64(9)
C75	3684(14)	2878(5)	5993(6)	42(7)
C74	4347(11)	3080(6)	6297(7)	56(8)
C39	7952(12)	6243(7)	8303(5)	39(7)
C44	8731(14)	6491(7)	8216(5)	60(9)
C43	9364(12)	6627(8)	8567(8)	72(10)
C42	9217(14)	6515(8)	9006(6)	87(12)
C41	8437(16)	6267(8)	9093(5)	73(10)
C40	7805(12)	6130(7)	8742(6)	47(7)
C33	5853(13)	6430(4)	9376(5)	32(6)
C34	5646(12)	6586(5)	8938(5)	29(6)
C35	5858(12)	7049(5)	8821(4)	34(6)
C36	6277(14)	7356(4)	9141(6)	41(7)
C37	6484(14)	7200(6)	9580(5)	57(8)
C38	6272(14)	6737(6)	9697(4)	52(8)
C1	2461(15)	5895(7)	7302(5)	56(8)
C2	3199(12)	5919(8)	7047(7)	53(8)
C3	3061(14)	6038(8)	6595(7)	91(13)
C4	2185(16)	6132(8)	6398(5)	63(9)
C5	1448(12)	6108(8)	6653(7)	66(9)
C6	1586(13)	5990(8)	7105(7)	61(9)
C23	7610(20)	5475(9)	10444(9)	45(7)
C25	6260(17)	5589(8)	10873(8)	31(6)
C89	6477(17)	3707(8)	5927(7)	38(6)
C28	3598(13)	5694(5)	9557(6)	49(7)
C27	4302(10)	6014(7)	9670(7)	53(8)
C32	4112(11)	6458(6)	9845(6)	50(8)
C31	3219(13)	6581(5)	9905(6)	50(8)
C30	2515(10)	6260(7)	9791(7)	52(8)
C29	2705(11)	5817(6)	9617(6)	54(8)
C93	7296(13)	4306(6)	8320(5)	41(7)
C98	6939(13)	4034(6)	8649(6)	45(7)
C97	7131(16)	4153(7)	9098(6)	79(11)

C96	7679(16)	4544(8)	9219(5)	67(10)
C95	8035(14)	4816(6)	8890(6)	56(8)
C94	7844(14)	4697(6)	8441(6)	48(7)
C91	6411(17)	3299(7)	5655(9)	48(7)
C22	6913(17)	5577(8)	10023(8)	32(6)
C14	2266(12)	6778(6)	7952(5)	49(8)
C13	2753(13)	6392(5)	8142(6)	49(8)
C18	3351(12)	6455(5)	8526(6)	30(6)
C17	3462(12)	6903(6)	8720(5)	48(7)
C16	2974(14)	7289(5)	8530(6)	50(8)
C15	2376(13)	7226(5)	8146(6)	55(8)
C58	3781(15)	7803(9)	7348(8)	33(6)
C24	7090(20)	5491(11)	10845(11)	61(9)
C90	6656(18)	3621(9)	6381(7)	39(6)
C57	4715(15)	7818(9)	7410(9)	38(6)
C77	5594(13)	4291(7)	5254(5)	50(8)
C82	5822(11)	4354(7)	4819(6)	32(6)
C81	5154(15)	4317(7)	4459(5)	86(12)
C80	4258(13)	4217(8)	4535(6)	56(8)
C79	4030(11)	4153(9)	4970(8)	100(14)
C78	4698(15)	4190(8)	5330(6)	73(10)
C59	3282(18)	8207(8)	7255(8)	31(6)
C19	3180(20)	7779(10)	8740(10)	47(7)
C105	6427(18)	3664(9)	7681(8)	35(6)
C92	6552(17)	2846(8)	5835(8)	34(6)
C106	5480(20)	3663(10)	7612(9)	45(7)
C83	7481(12)	4420(7)	5562(7)	46(7)
C88	7959(16)	4042(6)	5398(7)	67(10)
C87	8836(15)	4113(8)	5277(8)	95(13)
C86	9236(13)	4561(9)	5321(8)	71(10)
C85	8758(16)	4938(7)	5485(9)	115(16)
C84	7880(15)	4868(6)	5606(8)	59(9)
C20	3100(30)	8170(12)	8422(12)	67(10)
C66	2352(16)	4637(8)	6357(8)	48(7)
C71	1502(18)	4685(9)	6516(7)	92(13)
C70	826(15)	4954(10)	6278(10)	128(18)
C69	1000(18)	5175(9)	5880(9)	92(13)
C68	1850(20)	5128(9)	5721(7)	82(12)
C67	2527(15)	4859(9)	5959(8)	102(14)
C107	4970(30)	3279(11)	7565(11)	63(9)
C65	3094(16)	4219(7)	7585(8)	83(12)
C60	2781(16)	4039(7)	7166(6)	50(8)
C61	2238(15)	3634(7)	7133(5)	64(9)
C62	2008(15)	3408(6)	7519(7)	51(8)
C63	2320(17)	3588(8)	7938(6)	72(10)
C64	2863(18)	3993(9)	7971(6)	94(13)
C99	8152(14)	4080(8)	7533(7)	43(7)
C100	8340(15)	4246(8)	7116(7)	82(11)
C101	9144(18)	4114(9)	6942(7)	75(11)
C102	9759(15)	3815(10)	7186(10)	101(14)
C103	9571(17)	3648(9)	7603(10)	130(20)
C104	8767(19)	3780(9)	7777(7)	95(13)

Table S3. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **1**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+...+2hka \times b \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Au6	65.0(8)	18.4(5)	46.3(7)	-3.6(4)	21.4(6)	-2.6(5)
Au1	50.3(7)	20.5(5)	48.1(7)	-1.4(4)	6.1(5)	-0.2(4)
Au2	53.3(7)	17.7(5)	37.0(6)	0.1(4)	9.0(5)	-1.0(4)
Au5	88.8(10)	22.5(5)	45.9(7)	5.6(5)	24.2(7)	10.8(6)
Au4	80.6(10)	22.3(6)	68.1(9)	-5.7(5)	21.8(7)	1.9(6)
Au3	47.6(7)	17.2(5)	44.0(7)	-0.2(4)	13.4(5)	2.2(4)
S1	71(5)	9(3)	46(4)	-2(3)	9(4)	5(3)
P6	36(4)	28(3)	57(5)	-12(3)	14(4)	1(3)
P2	63(5)	15(3)	33(4)	5(3)	3(3)	1(3)
S2	82(6)	26(3)	51(5)	4(3)	16(4)	-8(4)
P5	61(5)	27(3)	47(5)	8(3)	22(4)	6(3)
P3	36(4)	16(3)	76(6)	-5(3)	16(4)	2(3)
P4	67(6)	25(4)	74(6)	-8(4)	7(5)	-4(4)
P1	50(5)	26(4)	61(5)	-7(3)	6(4)	-2(3)

Table S4. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **1**.

Atom	*x*	*y*	*z*	U(eq)
H8	1725	4957	7649	65
H9	529	4544	7919	69
H10	−190	4851	8511	95
H11	287	5570	8833	112
H12	1483	5983	8563	107
H56	5114	6261	7686	49
H55	4231	6938	7543	44
H53	6506	7723	7519	94
H52	7389	7046	7663	74
H26	5097	5792	10468	56
H50	6899	6318	6928	59
H49	7703	6140	6321	90
H48	8971	5647	6415	68
H47	9435	5332	7116	79
H46	8631	5511	7723	44
H73	4661	3668	6669	59
H140	2231	3750	5937	92
H76	2448	2994	5654	77
H74	4878	2912	6387	67
H44	8830	6566	7922	72
H43	9885	6793	8509	86
H42	9640	6606	9241	104
H41	8339	6192	9387	87
H40	7283	5964	8800	56
H34	5366	6381	8724	35

H35	5719	7153	8527	41
H37	6764	7405	9794	68
H38	6411	6633	9990	62
H2	3785	5856	7178	64
H3	3554	6054	6424	109
H4	2093	6211	6096	76
H5	862	6171	6522	79
H6	1092	5974	7276	73
H23	8234	5416	10443	54
H25	6018	5589	11149	37
H28	3725	5397	9440	58
H32	4583	6672	9921	60
H31	3092	6878	10021	60
H30	1917	6343	9831	62
H29	2234	5602	9541	65
H98	6573	3772	8568	54
H97	6893	3971	9318	94
H96	7807	4624	9519	81
H95	8402	5078	8971	67
H94	8082	4879	8220	57
H91	6269	3333	5347	58
H22	7108	5566	9737	38
H14	1866	6736	7695	59
H18	3677	6197	8652	35
H17	3862	6945	8977	58
H15	2050	7484	8019	66
H58	3483	7513	7369	40
H24	7422	5417	11115	73
H90	6615	3878	6573	47
H82	6421	4422	4768	38
H81	5306	4360	4168	103
H80	3811	4192	4295	67
H79	3431	4085	5021	121
H78	4546	4147	5621	87
H59	2680	8165	7137	37
H92	6455	2583	5648	41
H106	5180	3956	7599	54
H88	7691	3743	5369	80
H87	9156	3860	5168	114
H86	9823	4608	5240	85
H85	9025	5238	5514	138
H84	7561	5121	5716	71
H20	2913	8131	8120	81
H71	1385	4537	6782	110
H70	257	4986	6384	154
H69	548	5355	5721	110
H68	1968	5276	5455	98

H67	3096	4827	5853	123
H107	4341	3322	7509	75
H65	3457	4490	7608	100
H61	2029	3513	6853	77
H62	1644	3137	7497	62
H63	2166	3437	8196	87
H64	3073	4114	8252	113
H100	7928	4447	6953	98
H101	9270	4226	6663	90
H102	10297	3726	7070	121
H103	9982	3448	7767	162
H104	8641	3669	8057	115

Table S5. Selected bond lengths and angles for **1**.

Bond Lengths		
Atom1	Atom2	Length, Å
Au6	Au5	3.1086(18)
Au6	Au4	3.092(2)
Au6	Au3	2.954(15)
Au5	Au4	2.971(2)
Au2	Au3	3.0530(16)
Au1	Au2	3.1650(19)
Au1	Au3	3.25773(17)
Au2	S1	2.325(7)
Au3	S1	2.340(6)
Au1	S1	2.358(7)
Au6	S2	2.306(8)
Au4	S2	2.335(8)
Au5	S2	2.337(8)
Au1	P1	2.239(8)
Au2	P2	2.256(7)
Au3	P3	2.289(7)
Au5	P5	2.253(7)
Au4	P4	2.276(9)
Au6	P6	2.260(8)

Angles			
Atom1	Atom2	Atom3	Angle, °
S2	Au6	P6	173.4(3)
S1	Au1	P1	176.6(3)
S1	Au2	P2	174.4(2)
S2	Au5	P5	178.2(3)
S2	Au4	P4	174.0(3)
S1	Au3	P3	175.8(3)
Au1	S1	Au2	85.0(2)
Au1	S1	Au3	87.9(2)
Au2	S1	Au3	81.8(2)

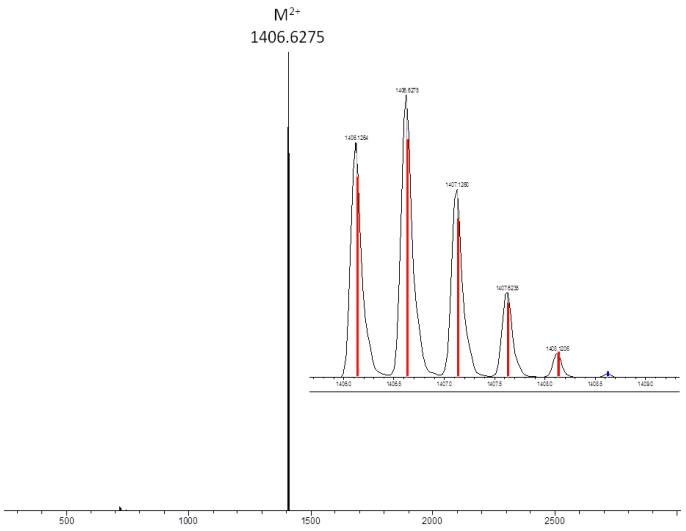

Figure S2. ESI$^+$ mass spectrum of **1**: experimental (black) and calculated (red).

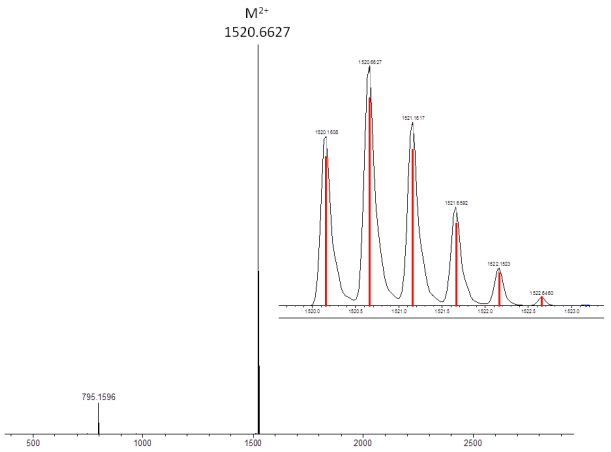

Figure S3. ESI$^+$ mass spectrum of **2**: experimental (black) and calculated (red).

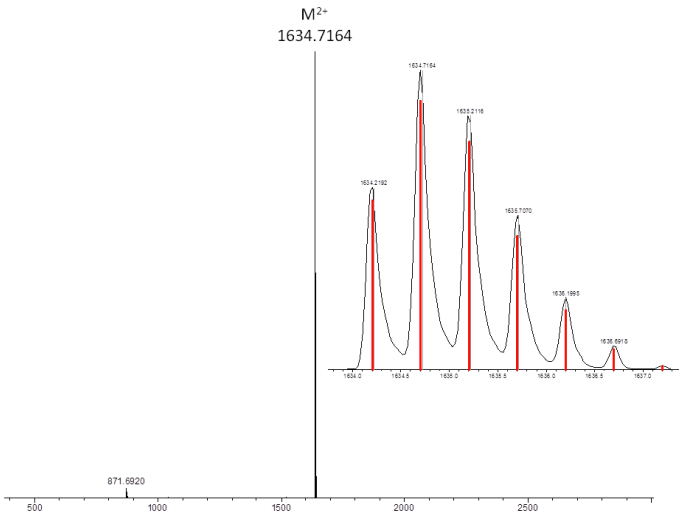

Figure S4. ESI$^+$ mass spectrum of **3**: experimental (black) and calculated (red).

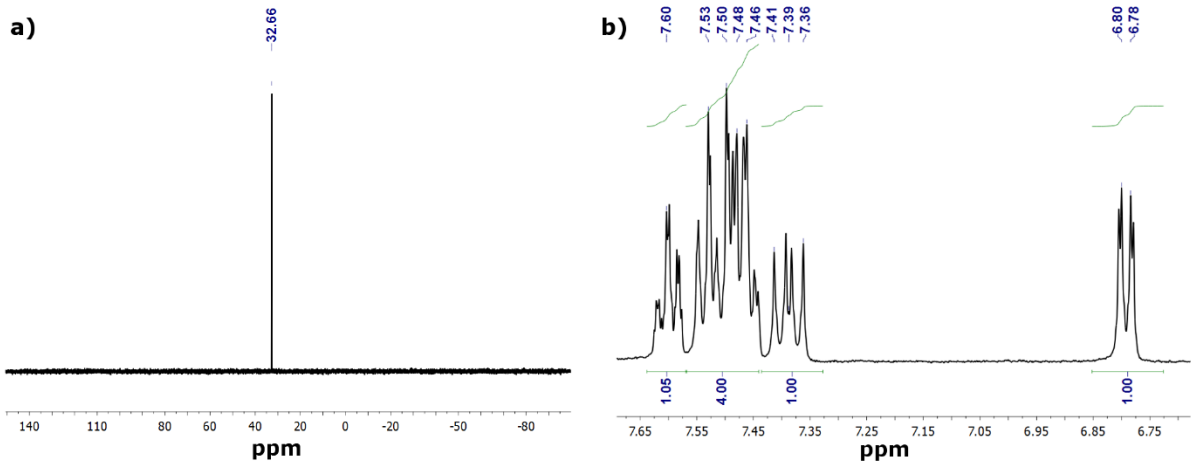

Figure S5. ^{31}P NMR spectrum (a) and fragment of ^{1}H NMR spectrum (b) of **1**.

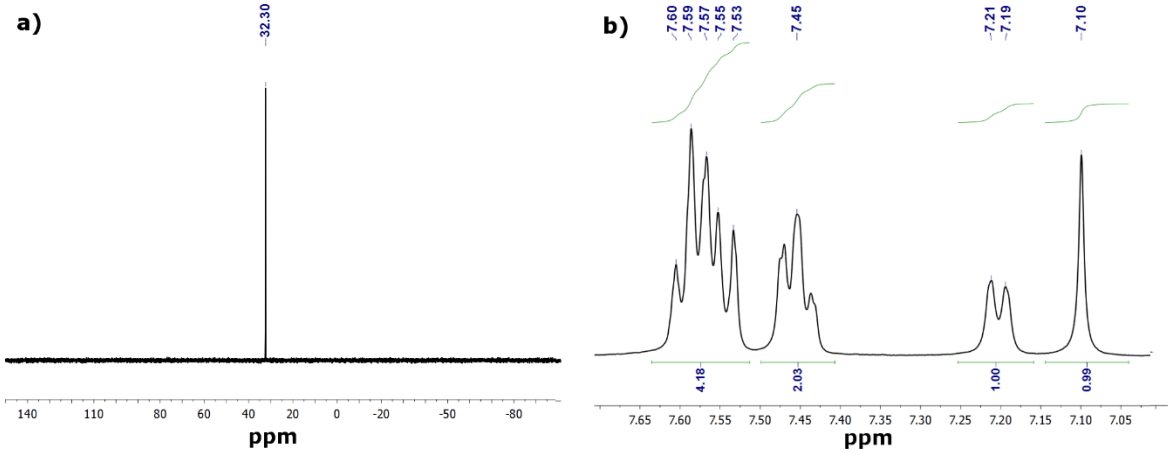

Figure S6. ^{31}P NMR spectrum (a) and fragment of ^{1}H NMR spectrum (b) of **2**.

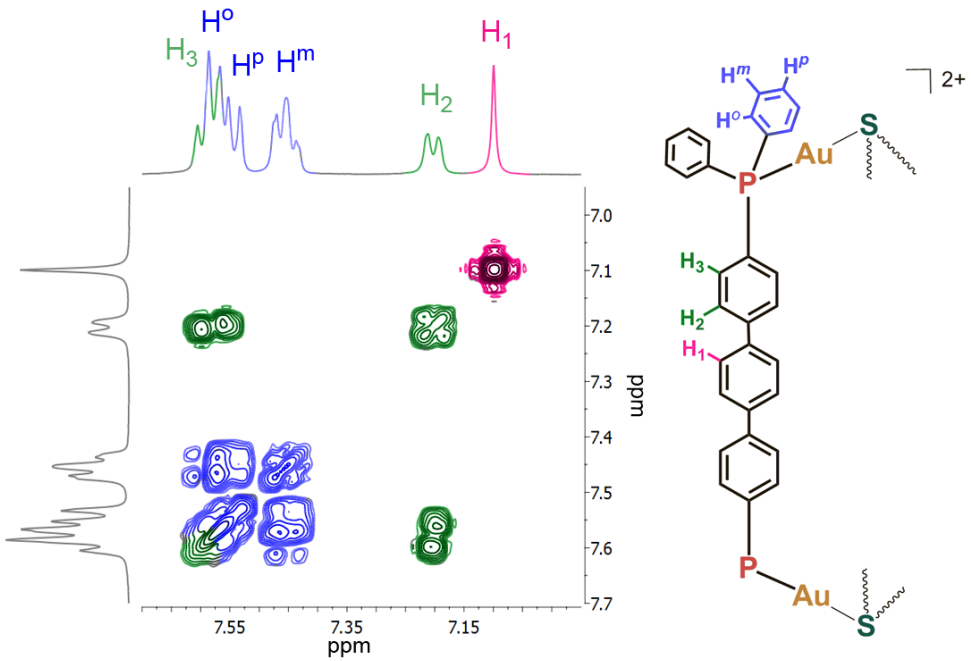

Figure S7. Fragment of ^{1}H - ^{1}H COSY NMR spectrum of **2** with assignment.

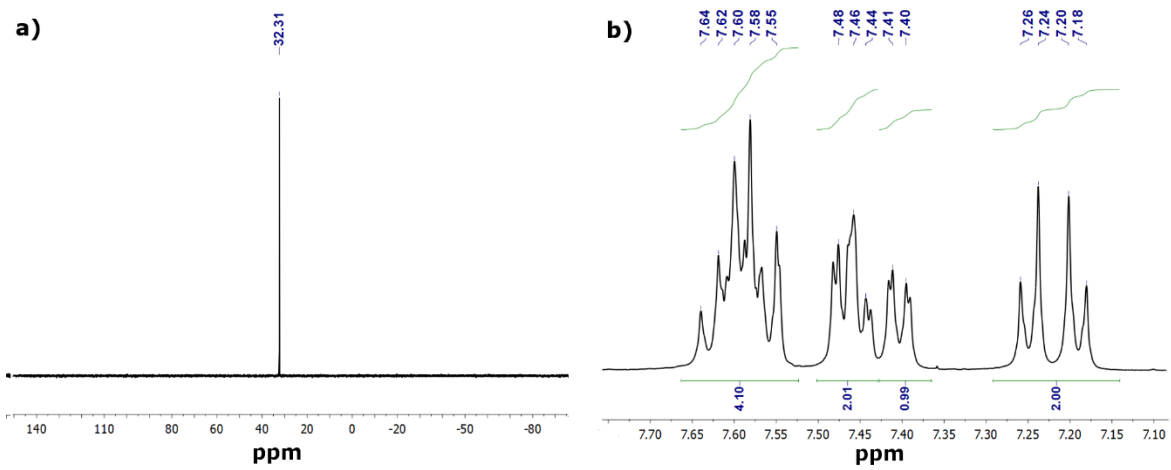

Figure S8. ^{31}P NMR spectrum (a) and fragment of ^{1}H NMR spectrum (b) of **3**.

Optimized cartesian coordinates of the studied systems in atomic units:

Table S6. 1

S	7.552239	0.076796	0.095524
Au	6.277607	2.040758	0.522871
Au	6.299091	-1.362953	1.518759
Au	6.377180	-0.516759	-1.888154
P	-5.083938	-3.599549	-1.969885
P	5.164425	-2.822875	2.942400
P	5.270070	-1.112466	-3.851957
C	-3.316776	-3.188117	-2.249799
C	-2.283428	-4.092760	-1.968653
C	-2.988667	-1.926964	-2.775869
C	-5.752044	-4.075106	-3.610304
C	-7.140655	-4.011154	-3.815564
C	-7.687433	-4.393044	-5.040817
C	-6.854046	-4.832283	-6.073186
C	-5.472490	-4.892019	-5.877392
C	-4.919913	-4.516246	-4.650907
C	-5.099668	-5.118275	-0.942060
C	-5.108935	-6.400129	-1.513744
C	-5.102952	-7.531573	-0.695061
C	-5.085644	-7.393425	0.694599
C	-5.077424	-6.119666	1.269599
C	-5.089467	-4.985966	0.456766
C	-1.338200	-0.321035	2.710709
C	-1.530260	-1.740989	4.648434
C	5.919451	-2.902675	4.611079
C	6.551446	-1.757139	5.123580
C	7.116267	-1.777334	6.399275
C	7.063663	-2.941672	7.169838
C	6.443209	-4.086145	6.663321
C	5.871818	-4.070223	5.389488
C	5.126870	-4.541130	2.300464
C	4.053755	-5.407096	2.565229
C	4.075028	-6.716838	2.081281
C	5.162429	-7.171139	1.331307
C	6.232201	-6.313267	1.062358
C	6.214766	-5.002573	1.540632
C	-1.662496	-1.588165	-3.026550
C	-0.955542	-3.745695	-2.213797

C	5.314057	0.198231	-5.134394
C	5.303558	1.543898	-4.729902
C	5.350180	-0.109245	-6.503629
C	5.318542	2.564239	-5.681237
C	5.352667	2.251570	-7.042829
C	5.369419	0.916175	-7.451483
C	5.967394	-2.619548	-4.629906
C	7.353295	-2.837913	-4.553181
C	7.921876	-3.957700	-5.160760
C	7.112828	-4.872261	-5.840546
C	5.733748	-4.663768	-5.914864
C	5.159643	-3.541755	-5.313278
H	-2.508577	-5.075007	-1.566439
H	-3.771442	-1.203070	-2.986636
H	-7.791825	-3.659481	-3.019661
H	-8.761809	-4.339955	-5.190554
H	-7.280421	-5.123152	-7.028897
H	-4.821495	-5.230402	-6.678239
H	-3.844700	-4.564883	-4.509702
H	-5.126013	-6.519114	-2.592522
H	-5.114578	-8.519837	-1.145377
H	-5.084691	-8.275655	1.328234
H	-5.071797	-6.007909	2.349973
H	-5.097840	-3.996919	0.907324
H	-0.751039	0.113733	1.907739
H	-1.109228	-2.462235	5.341996
H	6.607811	-0.853398	4.522561
H	7.605151	-0.887718	6.785554
H	7.510642	-2.958975	8.159592
H	6.405340	-4.994852	7.256922
H	5.397167	-4.967445	5.004446
H	3.201598	-5.063328	3.143357
H	3.240678	-7.380079	2.290443
H	5.174497	-8.189593	0.954038
H	7.077060	-6.660248	0.474643
H	7.044512	-4.336250	1.319873
H	-1.432980	-0.600726	-3.415507
H	-0.175094	-4.472721	-2.010894
H	5.370374	-1.143305	-6.832951
H	5.291928	1.793480	-3.672132
H	5.314561	3.601298	-5.358320
H	5.372839	3.046506	-7.782719
H	5.401480	0.669006	-8.508569
H	7.985168	-2.135297	-4.015953
H	8.994010	-4.118686	-5.096341
H	7.555804	-5.747184	-6.307443
H	5.101581	-5.373922	-6.439924
H	4.086413	-3.390081	-5.375066
S	-7.559797	-0.090196	-0.027212
Au	-6.273648	-1.843824	-0.997087
Au	-6.330735	0.000218	2.009774
Au	-6.363135	1.676431	-1.082685
P	5.099846	4.009459	0.941229
P	-5.251729	3.441737	-2.124636
P	-5.198025	0.086723	4.047556
C	-3.452280	-0.462959	3.898794
C	-2.672932	0.046664	2.846076
C	-2.865021	-1.364680	4.796591
C	-5.968352	-0.968358	5.334506

C	-6.646569	-2.134313	4.941361
C	-7.222575	-2.969716	5.899131
C	-7.134710	-2.644816	7.255090
C	-6.468410	-1.483051	7.652357
C	-5.886428	-0.645810	6.698684
C	-5.121259	1.780493	4.748776
C	-4.014162	2.227094	5.487576
C	-4.008156	3.513707	6.031369
C	-5.102701	4.360677	5.843888
C	-6.207571	3.921590	5.108593
C	-6.217418	2.638853	4.559718
C	-1.812546	3.443602	0.111735
C	-1.120286	3.734182	-2.180424
C	5.778858	5.445743	0.024255
C	7.168920	5.525033	-0.166241
C	7.725315	6.616359	-0.833700
C	6.900244	7.632140	-1.324287
C	5.110673	4.473590	2.715734
C	5.155184	5.812323	3.134003
C	4.955299	6.468745	-0.470687
C	5.517440	7.556317	-1.143119
C	5.085202	5.099892	5.447498
C	5.143381	6.120680	4.496245
C	5.042226	3.764656	5.036889
C	5.059957	3.450742	3.677906
C	-3.478142	3.505492	-1.654679
C	-2.451854	3.680611	-2.592988
C	-5.294022	4.488701	-4.760291
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C	-5.374829	1.958142	-5.950921
C	-5.362013	3.106196	-6.747310
C	-5.322938	4.368924	-6.151077
C	-5.943649	5.079584	-1.675658
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C	-7.082266	7.560760	-1.042840
C	-5.701908	7.451069	-1.225610
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H	-7.747399	-3.867056	5.584572
H	-7.590012	-3.291417	7.999622
H	-6.403563	-1.223667	8.705033
H	-5.376872	0.257742	7.018650
H	-3.157428	1.577789	5.638356
H	-3.147363	3.851278	6.601587
H	-5.093789	5.361478	6.266061
H	-7.059043	4.578422	4.956171
H	-7.075811	2.305472	3.982095
H	-1.574849	3.326594	1.164778
H	-0.343823	3.895803	-2.922080
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H	7.333893	8.478156	-1.849661
H	4.872917	8.342647	-1.525147
H	3.879175	6.419065	-0.336751

H	5.204133	6.613335	2.403256
H	5.182153	7.159207	4.811670
H	5.079726	5.343344	6.506015
H	5.005040	2.967266	5.773451
H	5.041225	2.410739	3.362467
H	-2.685484	3.787007	-3.647328
H	-3.919337	3.222392	0.446280
H	-5.270848	5.475267	-4.307949
H	-5.378158	1.177412	-3.944096
H	-5.414854	0.974616	-6.410100
H	-5.389426	3.017236	-7.829511
H	-5.319133	5.263562	-6.766884
H	-7.966468	4.317671	-1.572461
H	-8.968965	6.511454	-1.026002
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H	-5.066163	8.325570	-1.121772
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C	2.307833	4.458271	1.225350
C	2.998661	3.219122	-0.731573
C	3.333512	3.889729	0.456901
C	0.795226	-2.134353	-3.019810
C	1.145908	-1.362573	-4.139885
C	1.824912	-2.567478	-2.164153
C	2.476781	-1.040490	-4.405402
C	3.153166	-2.241777	-2.420787
C	3.496834	-1.479789	-3.550134
C	0.685982	-1.614634	3.463017
C	1.288722	-1.700377	2.193567
C	1.476682	-1.901993	4.587974
C	2.627727	-2.051772	2.058761
C	2.815627	-2.270076	4.456667
C	3.407499	-2.350099	3.189128
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C	-0.619817	-2.491316	-2.749536
C	-0.738774	-1.223537	3.609585
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H	2.539489	4.984214	2.145985
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H	0.376100	-1.032996	-4.831185
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H	2.715855	-0.454417	-5.287003
H	3.926666	-2.577494	-1.735296
H	0.703261	-1.506602	1.299960
H	1.051984	-1.817130	5.583306
H	3.066093	-2.100766	1.065783
H	3.396295	-2.485300	5.347633

Table S7. 2

S	9.725441	0.073406	0.080764
Au	8.413082	0.918946	-1.723587
Au	8.378441	1.203899	1.685181
Au	8.530239	-1.985967	0.148489
P	-7.073910	-1.241483	3.797664

P	7.113327	2.356828	3.268845
P	7.378638	-4.013731	0.182449
C	-5.310733	-1.561516	3.403515
C	-4.281919	-1.305353	4.322900
C	-4.977080	-2.101281	2.150442
C	-7.709241	-2.773166	4.584087
C	-9.093514	-3.014296	4.563395
C	-9.618553	-4.151413	5.177852
C	-8.767391	-5.061986	5.809762
C	-7.389852	-4.832258	5.827349
C	-6.859414	-3.692997	5.217966
C	-7.072581	0.047961	5.103032
C	-7.104396	-0.273440	6.468397
C	-7.084035	0.741931	7.427728
C	-7.030806	2.080324	7.033475
C	-7.001041	2.406681	5.674646
C	-7.026860	1.397195	4.712533
C	-3.530009	2.516506	-0.391919
C	-3.545806	4.764347	0.477976
C	7.806092	4.010709	3.655829
C	8.426452	4.739159	2.626610
C	8.944362	6.009635	2.878656
C	8.856320	6.559906	4.160339
C	8.247593	5.838034	5.189261
C	7.722719	4.567628	4.941322
C	6.999056	1.457880	4.863487
C	5.850391	1.512887	5.668083
C	5.816035	0.831253	6.886784
C	6.923538	0.093199	7.310407
C	8.069572	0.033552	6.512605
C	8.107587	0.708340	5.292226
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C	7.394693	-4.868166	-1.440513
C	7.643654	-4.124295	-2.605347
C	7.153437	-6.248250	-1.542456
C	7.642213	-4.749902	-3.853550
C	7.398847	-6.121774	-3.947846
C	7.155538	-6.869118	-2.792030
C	8.050411	-5.208209	1.400435
C	9.436424	-5.225018	1.629830
C	9.990225	-6.150441	2.515012
C	9.166505	-7.059438	3.184345
C	7.786998	-7.042774	2.966077
C	7.227633	-6.121895	2.077749
H	-4.509335	-0.886370	5.298262
H	-5.754557	-2.288798	1.414659
H	-9.758533	-2.315451	4.062795
H	-10.689853	-4.328658	5.155942
H	-9.176263	-5.950185	6.282743
H	-6.724408	-5.539459	6.313917
H	-5.786799	-3.526982	5.235145
H	-7.150640	-1.310185	6.786337
H	-7.112426	0.484010	8.482385
H	-7.018668	2.867377	7.781937
H	-6.967402	3.446628	5.362977
H	-7.018299	1.656795	3.656993
H	-3.009055	1.592428	-0.622993
H	-3.051344	5.590553	0.979645

H	8.511448	4.309019	1.631998
H	9.424784	6.563965	2.077662
H	9.266863	7.545979	4.357607
H	8.182426	6.260001	6.187928
H	7.256033	4.012881	5.749171
H	4.983134	2.081566	5.346751
H	4.922818	0.877967	7.503052
H	6.892740	-0.437668	8.257531
H	8.930943	-0.543964	6.835316
H	8.996675	0.650122	4.669603
H	-3.419068	-2.775882	0.845302
H	-2.183293	-1.409773	4.738278
H	6.971621	-6.840556	-0.650892
H	7.846605	-3.058894	-2.535383
H	7.840231	-4.166495	-4.748061
H	7.404452	-6.609539	-4.918341
H	6.971934	-7.937332	-2.861291
H	10.080475	-4.513460	1.119583
H	11.062661	-6.155606	2.686498
H	9.598294	-7.775301	3.877772
H	7.142975	-7.745167	3.487183
H	6.153596	-6.114033	1.919915
S	-9.706350	-0.004593	0.083878
Au	-8.335437	-0.616461	1.936967
Au	-8.486295	1.971013	-0.445236
Au	-8.473337	-1.410849	-1.393131
P	7.168506	1.743069	-3.515572
P	-7.258769	-2.804765	-2.815611
P	-7.336909	3.933648	-0.962533
C	-5.568951	3.832951	-0.485960
C	-4.872276	2.638387	-0.735810
C	-4.887614	4.896800	0.122080
C	-8.024150	5.399960	-0.102322
C	-8.541920	5.236636	1.193851
C	-9.057882	6.331079	1.887901
C	-9.070866	7.595060	1.291774
C	-8.564049	7.762735	0.001242
C	-8.040923	6.671368	-0.696076
C	-7.360194	4.321083	-2.754740
C	-6.270660	4.933526	-3.393215
C	-6.335817	5.232165	-4.756062
C	-7.484506	4.924091	-5.488526
C	-8.571810	4.312694	-4.858212
C	-8.510421	4.007545	-3.498221
C	-3.873902	-0.532687	-3.269183
C	-3.120501	-2.731905	-2.631438
C	7.769067	1.120491	-5.133677
C	9.152877	0.963602	-5.322083
C	9.648673	0.517416	-6.547229
C	8.769224	0.214799	-7.590597
C	7.192506	3.573587	-3.627130
C	7.137215	4.241392	-4.860346
C	6.890842	0.814029	-6.184515
C	7.392611	0.362268	-7.407370
C	7.190827	6.374857	-3.715972
C	7.137480	5.637393	-4.900922
C	7.247466	5.715385	-2.485138
C	7.253588	4.321148	-2.439014
C	-5.495417	-2.300062	-2.883823

C	-4.442638	-3.177090	-2.589870
C	-7.100669	-5.606617	-3.209057
C	-5.194040	-0.967579	-3.215787
C	-7.279502	-4.561472	-2.288355
C	-7.468976	-4.864698	-0.929778
C	-7.467845	-6.192084	-0.498396
C	-7.286889	-7.226778	-1.419254
C	-7.105006	-6.932563	-2.773030
C	-7.856692	-2.776852	-4.548523
C	-9.235738	-2.645090	-4.782725
C	-9.730515	-2.654747	-6.087198
C	-8.854150	-2.787631	-7.167598
C	-7.481606	-2.913773	-6.941401
C	-6.981090	-2.909543	-5.637692
H	-5.379595	1.799232	-1.204605
H	-5.403367	5.827715	0.335187
H	-8.548002	4.252718	1.655611
H	-9.457977	6.194204	2.888320
H	-9.480367	8.445327	1.829485
H	-8.577022	8.742370	-0.467528
H	-7.654023	6.812294	-1.700343
H	-5.372582	5.174030	-2.832550
H	-5.488014	5.704887	-5.243451
H	-7.531030	5.155465	-6.548755
H	-9.464517	4.065858	-5.425444
H	-9.353886	3.521328	-3.014935
H	-3.667022	0.504531	-3.514988
H	-2.319686	-3.435563	-2.424492
H	9.840742	1.185983	-4.510363
H	10.719718	0.399232	-6.683339
H	9.156162	-0.139029	-8.541870
H	6.705630	0.125368	-8.214636
H	5.818863	0.922986	-6.051744
H	7.099443	3.677246	-5.786919
H	7.098563	6.146488	-5.859528
H	7.194394	7.460459	-3.751517
H	7.297171	6.285144	-1.561803
H	7.313683	3.811445	-1.480883
H	-4.646446	-4.213298	-2.340489
H	-5.993771	-0.263587	-3.430810
H	-6.966062	-5.390298	-4.264235
H	-7.626291	-4.064149	-0.211795
H	-7.619100	-6.416157	0.553567
H	-7.294201	-8.260035	-1.084330
H	-6.970558	-7.734815	-3.492699
H	-9.920497	-2.530938	-3.946391
H	-10.797967	-2.551149	-6.258573
H	-9.239688	-2.788610	-8.183043
H	-6.797263	-3.014415	-7.778832
H	-5.912030	-3.003816	-5.473666
C	-1.402942	-0.937920	-3.032942
C	-0.980977	-0.036996	-4.026270
C	-0.448289	-1.383854	-2.102368
C	0.340528	0.393788	-4.090901
C	0.872416	-0.949011	-2.164888
C	-1.203138	-2.439821	2.405855
C	-0.866437	-3.548353	1.608511
C	-0.154098	-1.623835	2.864585
C	0.457925	-3.821889	1.276307

C	1.169425	-1.895114	2.529032
C	-1.419219	3.426077	0.631167
C	-0.916949	2.185087	1.060564
C	-0.531262	4.516275	0.603662
C	0.411608	2.041580	1.445754
C	0.797283	4.373737	0.994805
C	-2.809408	-1.405817	-2.975103
C	-2.615111	-2.140691	2.750350
C	-2.840215	3.574098	0.231354
C	2.707564	0.399320	-3.240129
C	3.764469	-0.461480	-2.889700
C	3.031836	1.697995	-3.669139
C	5.088397	-0.040387	-2.964177
C	4.357320	2.121685	-3.755173
C	5.403588	1.255512	-3.406361
C	2.917092	-3.273589	1.352321
C	3.976526	-2.944176	2.220207
C	3.241591	-3.862089	0.118275
C	5.300154	-3.179174	1.862559
C	4.566279	-4.115236	-0.238922
C	5.613259	-3.775223	0.628103
C	2.707600	2.971507	1.857614
C	3.412813	1.782957	1.589729
C	3.377650	3.991773	2.554161
C	4.730178	1.619895	2.006812
C	4.696535	3.831927	2.978090
C	5.387851	2.640322	2.714526
C	1.296895	-0.053556	-3.162484
C	1.297440	3.132750	1.426207
C	1.506535	-2.997408	1.722927
H	-1.685400	0.302355	-4.779972
H	-0.746327	-2.053446	-1.300623
H	0.639570	1.059453	-4.895039
H	1.574540	-1.287600	-1.408891
H	-1.644995	-4.227059	1.272848
H	-0.376786	-0.746662	3.464777
H	0.680137	-4.708431	0.690067
H	1.947637	-1.221656	2.875397
H	-1.578909	1.326966	1.128587
H	-0.873756	5.482132	0.244348
H	0.753917	1.073663	1.797949
H	1.460886	5.231433	0.934319
H	3.551022	-1.477029	-2.570207
H	2.239368	2.397040	-3.918212
H	5.881501	-0.728704	-2.684303
H	4.569708	3.133268	-4.086050
H	3.764101	-2.516799	3.195251
H	2.453289	-4.111143	-0.585350
H	6.091232	-2.908692	2.556973
H	4.776456	-4.572121	-1.200277
H	2.936136	0.989398	1.022573
H	2.855302	4.913297	2.792871
H	5.252061	0.696322	1.770999
H	5.180011	4.636964	3.522472

Table S8. 3

S	-11.915895	0.046156	-0.110213

Au	-10.710550	0.305027	1.927351
Au	-10.614054	1.663987	-1.274776
Au	-10.724102	-1.902501	-0.782746
P	9.470939	-0.922986	-3.809015
P	-9.456352	3.322512	-2.437523
P	-9.633993	-3.845910	-1.475906
C	7.675842	-1.140019	-3.498606
C	6.702372	-0.556716	-4.322110
C	7.259428	-1.929432	-2.412665
C	10.021513	-2.446498	-4.669850
C	11.376768	-2.810936	-4.601835
C	11.834007	-3.945082	-5.273771
C	10.942557	-4.729097	-6.010860
C	9.592673	-4.375915	-6.077140
C	9.130504	-3.239071	-5.410746
C	9.612018	0.440963	-5.028940
C	9.701230	0.197620	-6.407933
C	9.794143	1.265884	-7.303297
C	9.794697	2.580121	-6.831814
C	9.705044	2.828962	-5.459268
C	9.619616	1.766059	-4.560216
C	5.763763	2.665014	0.935051
C	5.847362	4.851510	-0.071322
C	-10.155029	4.990791	-2.129927
C	-10.664433	5.284556	-0.853811
C	-11.182069	6.550088	-0.577428
C	-11.205323	7.529776	-1.573809
C	-10.707841	7.241832	-2.846592
C	-10.183152	5.978179	-3.126996
C	-9.504248	3.072155	-4.255136
C	-8.428851	3.435536	-5.080544
C	-8.513774	3.252759	-6.462612
C	-9.668645	2.709326	-7.029685
C	-10.742397	2.344841	-6.212754
C	-10.661108	2.520605	-4.831131
C	5.905043	-2.143054	-2.171400
C	5.347780	-0.767981	-4.071397
C	-9.891317	-5.263059	-0.339280
C	-9.983681	-5.014265	1.040583
C	-9.978991	-6.582525	-0.809734
C	-10.150300	-6.071423	1.935401
C	-10.234577	-7.383376	1.461348
C	-10.150226	-7.636670	0.090446
C	-10.205304	-4.402769	-3.128309
C	-11.569827	-4.278443	-3.441194
C	-12.049232	-4.711263	-4.677396
C	-11.171306	-5.261893	-5.615447
C	-9.813332	-5.381589	-5.313086
C	-9.328620	-4.955429	-4.074051
H	6.995662	0.055038	-5.168991
H	7.995608	-2.375716	-1.748846
H	12.071877	-2.210564	-4.020698
H	12.883378	-4.218915	-5.214996
H	11.298202	-5.615230	-6.528655
H	8.896349	-4.984733	-6.646518
H	8.079085	-2.974577	-5.467197
H	9.702291	-0.819735	-6.785690
H	9.866965	1.067824	-8.368722
H	9.869319	3.408380	-7.530587

H	9.710529	3.849442	-5.087247
H	9.563127	1.965636	-3.493069
H	5.209326	1.789594	1.258590
H	5.367906	5.678696	-0.585187
H	-10.662614	4.520776	-0.080548
H	-11.575564	6.766736	0.411448
H	-11.615782	8.512495	-1.360319
H	-10.729195	7.998662	-3.625314
H	-9.803654	5.763858	-4.121098
H	-7.526089	3.856627	-4.649040
H	-7.676008	3.534733	-7.093839
H	-9.730491	2.565951	-8.104595
H	-11.640257	1.916560	-6.648698
H	-11.495069	2.225303	-4.199714
H	5.607114	-2.739436	-1.313997
H	4.613107	-0.328396	-4.739148
H	-9.919640	-6.789217	-1.873726
H	-9.932736	-3.994833	1.413936
H	-10.223488	-5.868973	2.999992
H	-10.371617	-8.205283	2.158160
H	-10.220193	-8.654455	-0.282237
H	-12.255110	-3.839729	-2.720480
H	-13.105450	-4.611215	-4.909796
H	-11.544610	-5.592166	-6.580533
H	-9.127143	-5.805816	-6.040351
H	-8.270801	-5.051633	-3.850482
S	11.994654	-0.060740	0.081375
Au	10.689587	-0.496885	-1.866895
Au	10.772882	1.905630	0.637594
Au	10.705907	-1.581281	1.382242
P	-9.560227	0.528720	3.945055
P	9.470256	-3.123016	2.618743
P	9.675728	3.894033	1.168186
C	7.879640	3.851971	0.800399
C	7.134718	2.718142	1.167869
C	7.217903	4.917152	0.173378
C	10.356211	5.321327	0.237617
C	10.817324	5.114887	-1.073545
C	11.324441	6.181163	-1.816649
C	11.383715	7.459870	-1.255907
C	10.931997	7.670672	0.048707
C	10.418975	6.607638	0.795341
C	9.817436	4.322355	2.946503
C	8.787611	4.983597	3.633613
C	8.944521	5.313709	4.981648
C	10.126325	4.989095	5.651449
C	11.154763	4.329561	4.972858
C	11.001437	3.992687	3.627758
C	5.967547	-1.038595	3.096207
C	5.347810	-3.212482	2.260498
C	-10.045921	-0.757791	5.161710
C	-11.400870	-1.123533	5.242184
C	-11.816729	-2.081400	6.166795
C	-10.884352	-2.690588	7.011467
C	-9.842405	2.143826	4.769643
C	-9.990764	2.255034	6.160433
C	-9.114665	-1.373755	6.011225
C	-9.535864	-2.337395	6.931001
C	-10.230345	4.655964	5.950787

C	-10.184752	3.508879	6.745447
C	-10.084892	4.550811	4.564404
C	-9.896938	3.301235	3.974502
C	7.686701	-2.694469	2.642107
C	6.689637	-3.592471	2.238915
C	9.432177	-5.956373	2.742980
C	7.308802	-1.407031	3.062495
C	9.588946	-4.820097	1.933214
C	9.830600	-4.981398	0.558647
C	9.903347	-6.259160	0.002216
C	9.744520	-7.385486	0.813316
C	9.510682	-7.232404	2.182212
C	9.981844	-3.233304	4.375643
C	11.335736	-3.043023	4.698703
C	11.764668	-3.159082	6.021319
C	10.846574	-3.457182	7.031740
C	9.497810	-3.640526	6.717779
C	9.063542	-3.529992	5.395297
H	7.624321	1.875638	1.649444
H	7.768848	5.800117	-0.133846
H	10.785922	4.119658	-1.509369
H	11.681721	6.010809	-2.828120
H	11.786069	8.288027	-1.832142
H	10.980628	8.661933	0.489954
H	10.075764	6.782113	1.810251
H	7.864155	5.237951	3.122718
H	8.141698	5.823533	5.506387
H	10.244209	5.244891	6.700494
H	12.073094	4.069661	5.491305
H	11.800150	3.469614	3.108030
H	5.701866	-0.036214	3.418833
H	4.590874	-3.934795	1.970387
H	-12.128926	-0.661963	4.580098
H	-12.865970	-2.356607	6.221473
H	-11.208072	-3.441190	7.726751
H	-8.807634	-2.810651	7.583272
H	-8.063985	-1.107702	5.957494
H	-9.960207	1.369418	6.787199
H	-10.301531	3.585697	7.822560
H	-10.384125	5.628771	6.408863
H	-10.126624	5.439746	3.941660
H	-9.797827	3.222727	2.894931
H	6.951678	-4.595819	1.919541
H	8.065481	-0.686042	3.361596
H	9.257028	-5.849906	3.808980
H	9.971044	-4.107847	-0.072709
H	10.094370	-6.373274	-1.060923
H	9.809220	-8.379954	0.381237
H	9.392730	-8.105802	2.816925
H	12.051330	-2.799792	3.917649
H	12.813091	-3.009219	6.262045
H	11.180780	-3.541112	8.061815
H	8.780911	-3.868395	7.501235
H	8.012241	-3.669114	5.162453
C	3.525608	-1.552488	2.733451
C	3.014280	-0.753227	3.770905
C	2.628103	-2.003592	1.749536
C	1.658084	-0.445442	3.839608
C	1.273996	-1.692214	1.816876

C	3.476254	-1.802338	-2.759129
C	3.001292	-3.054966	-2.331756
C	2.531092	-0.785979	-2.983458
C	1.638462	-3.287922	-2.159819
C	1.170390	-1.018151	-2.807796
C	3.625072	3.681323	0.069082
C	2.961873	2.465322	-0.175853
C	2.849938	4.855069	0.082082
C	1.587684	2.425102	-0.396714
C	1.478367	4.815849	-0.147350
C	4.958362	-1.933435	2.692202
C	4.921426	-1.567449	-2.997384
C	5.088298	3.731686	0.311243
C	-0.698920	-0.650817	2.975204
C	-1.635744	-1.630370	2.600030
C	-1.192878	0.569202	3.470594
C	-3.002245	-1.406208	2.726303
C	-2.561563	0.795234	3.593875
C	-0.765006	-2.526613	-2.261761
C	-1.689043	-1.895650	-3.114210
C	-1.274287	-3.398687	-1.282903
C	-3.056369	-2.116388	-2.986874
C	-2.643274	-3.618667	-1.153893
C	-0.645285	3.566241	-0.643376
C	-1.453468	2.538698	-0.126227
C	-1.268990	4.566402	-1.410012
C	-2.824833	2.512764	-0.365730
C	-2.638493	4.537643	-1.653661
C	0.755605	-0.920359	2.871865
C	0.815948	3.600283	-0.392175
C	0.690671	-2.277535	-2.403772
H	3.675879	-0.406397	4.559497
H	2.994754	-2.582136	0.906486
H	1.289478	0.134525	4.680699
H	0.612650	-2.032748	1.025910
H	3.700822	-3.871852	-2.178239
H	2.864841	0.205659	-3.274730
H	1.305278	-4.281655	-1.875000
H	0.471497	-0.202539	-2.967754
H	3.527700	1.539920	-0.227698
H	3.317457	5.808954	0.306756
H	1.115291	1.470450	-0.609885
H	0.907214	5.738688	-0.103425
H	-1.289301	-2.594473	2.240128
H	-0.499447	1.360462	3.740354
H	-3.692857	-2.203072	2.467567
H	-2.905906	1.760241	3.953910
H	-1.331904	-1.247980	-3.909217
H	-0.594856	-3.892958	-0.594424
H	-3.733921	-1.636664	-3.686785
H	-2.999461	-4.273004	-0.363554
H	-1.011303	1.770615	0.501716
H	-0.669085	5.358238	-1.849337
H	-3.421586	1.724226	0.083298
H	-3.077795	5.306287	-2.282599
C	-4.955817	0.026019	3.388994
C	-5.875482	-0.558955	2.499092
C	-5.465745	0.807742	4.441410
C	-7.246506	-0.385686	2.665108

H	-5.516681	-1.135874	1.652177
C	-6.836928	0.987893	4.609472
H	-4.784574	1.259945	5.155542
C	-7.746915	0.382224	3.728772
H	-7.932465	-0.840624	1.955594
H	-7.193868	1.594567	5.436211
C	-5.026368	-3.203547	-1.863963
C	-5.539275	-4.445289	-1.448582
C	-5.945128	-2.174570	-2.145191
C	-6.911159	-4.654448	-1.318078
H	-4.860343	-5.267985	-1.246402
C	-7.315651	-2.377813	-2.015577
H	-5.584651	-1.195555	-2.445832
C	-7.818413	-3.622827	-1.603497
H	-7.271068	-5.627746	-0.999453
H	-7.999235	-1.559670	-2.226375
C	-4.905601	3.477779	-1.412364
C	-5.645356	4.665413	-1.549610
C	-5.592243	2.257091	-1.554802
C	-7.008376	4.640752	-1.840429
H	-5.155350	5.624134	-1.411123
C	-6.955623	2.226022	-1.832028
H	-5.048847	1.320989	-1.468662
C	-7.679920	3.419103	-1.993887
H	-7.545788	5.578301	-1.941012
H	-7.457308	1.267546	-1.936523
C	-3.447884	3.509652	-1.137747
C	-3.566170	-2.979621	-2.000865
C	-3.496964	-0.190118	3.230337

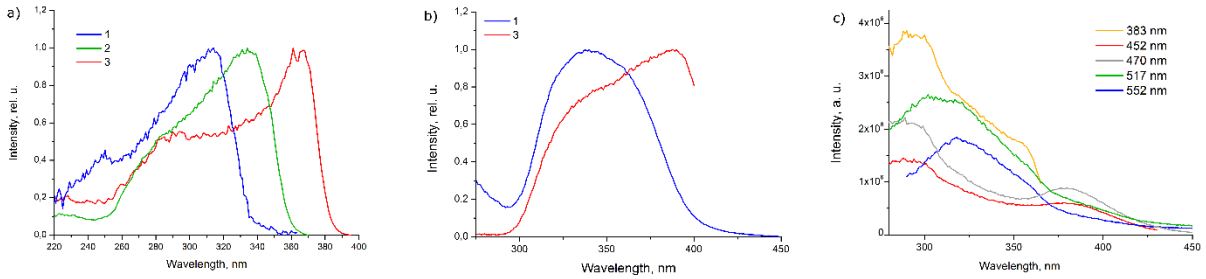


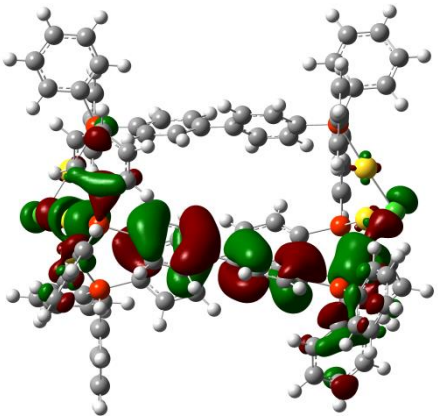
Figure S9. Excitation spectra of **1** – **3** in dichloromethane solution (a), excitation spectra of **1**, **3** in solid state (b) and excitation spectra of **2** in solid state (c).

Table S9. Calculated energies of HOMO/LUMO orbitals of 1 – 3.

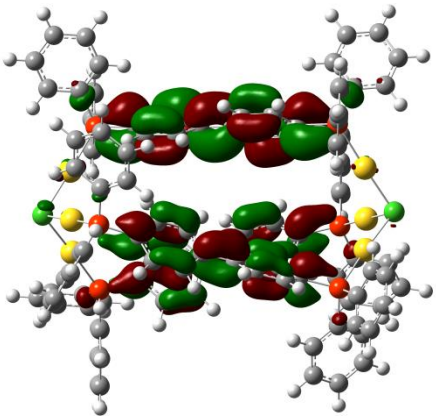
Complex	Orbital	E, eV
1	HOMO	-6.807
	LUMO	-2.166
2	HOMO	-6.479
	LUMO	-2.182
3	HOMO	-6.220
	LUMO	-2.106

Figure S10. Highest occupied and lowest vacant molecular orbitals for complex **1**

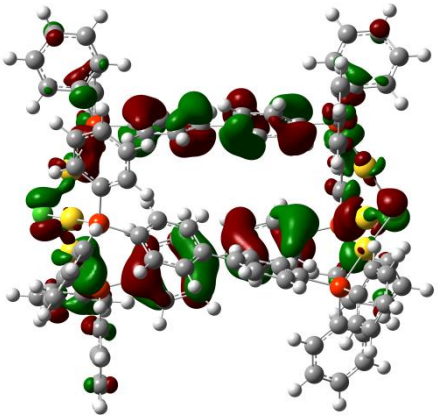
HOMO



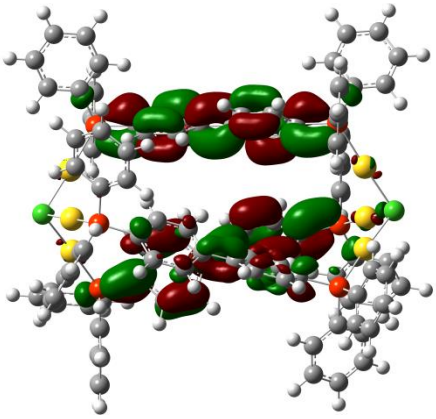
LUMO+2



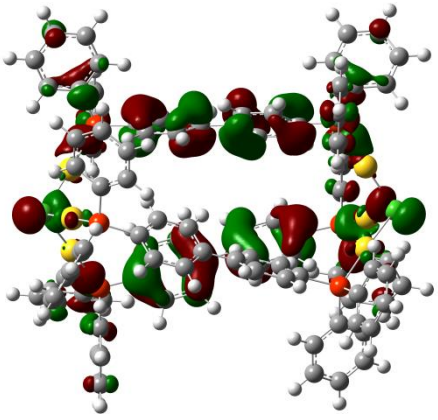
HOMO–1



LUMO+1



HOMO–2



LUMO

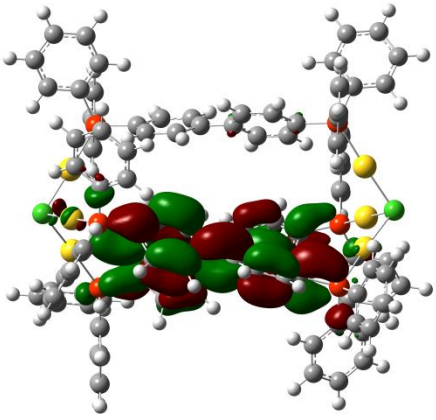
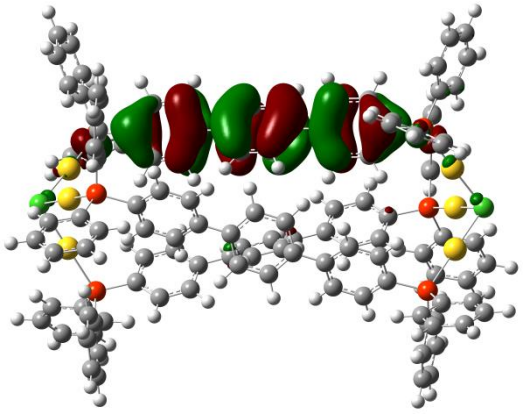
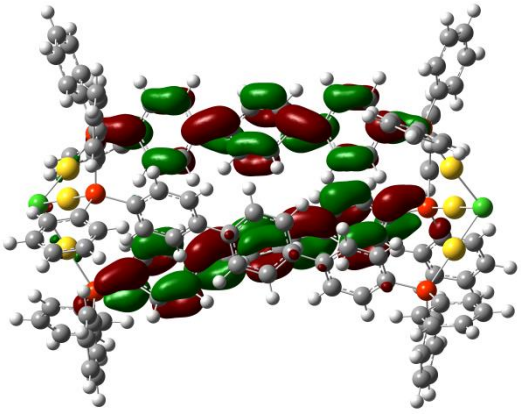


Figure S11. Highest occupied and lowest vacant molecular orbitals for complex **2**

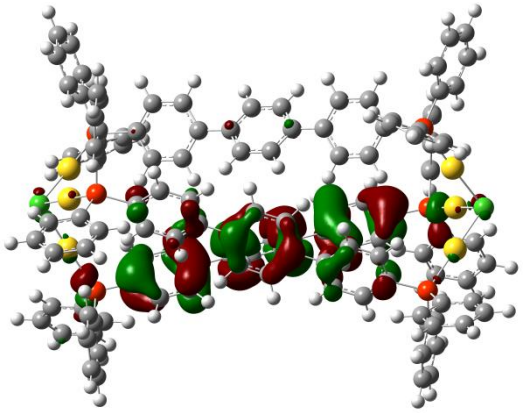
HOMO



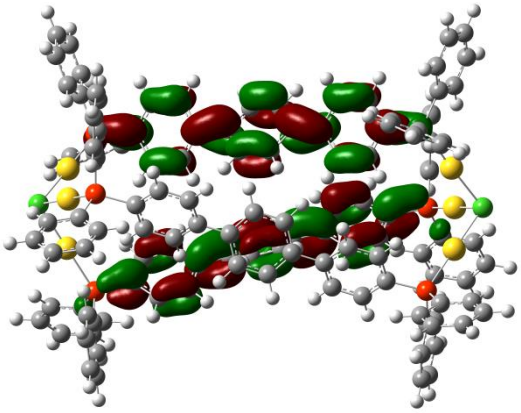
LUMO+2



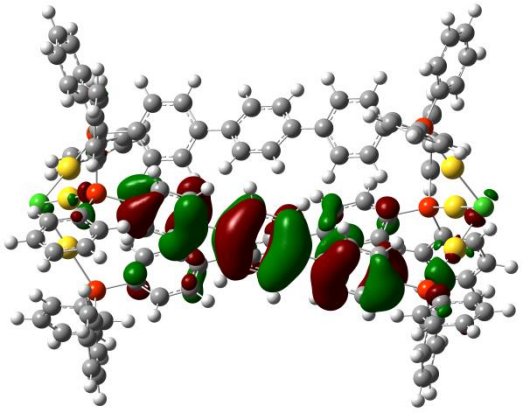
HOMO–1



LUMO+1



HOMO–2



LUMO

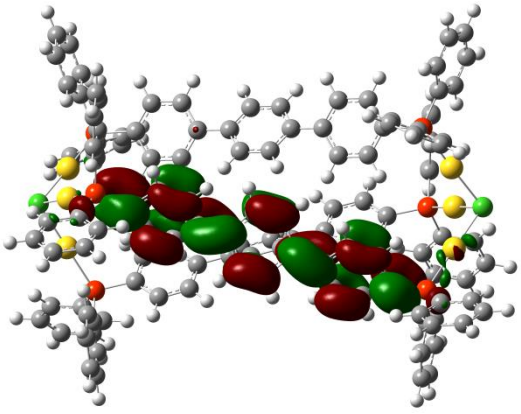
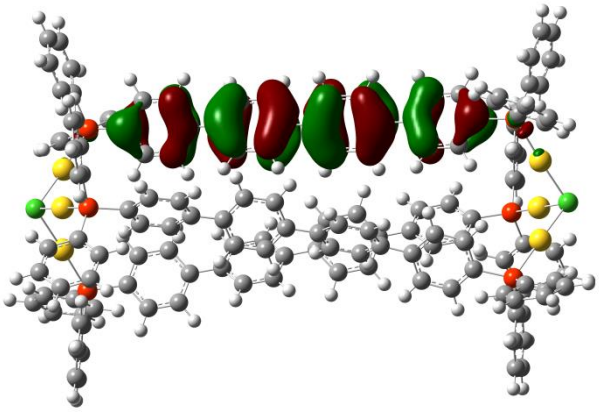
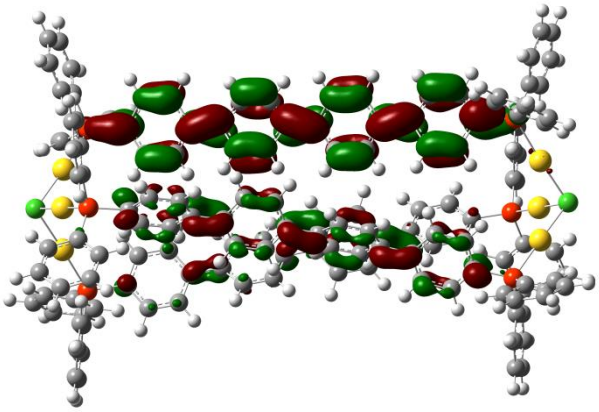


Figure S12. Highest occupied and lowest vacant molecular orbitals for complex **3**

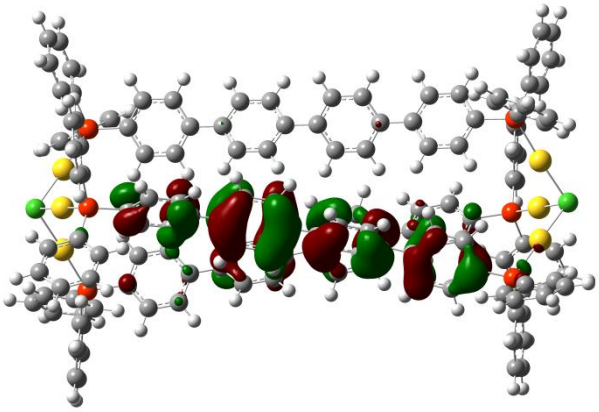
HOMO



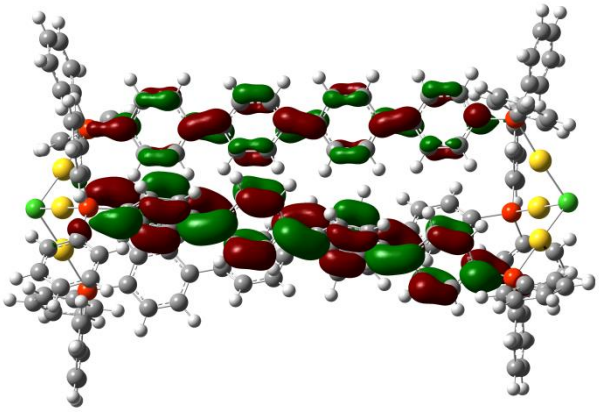
LUMO+2



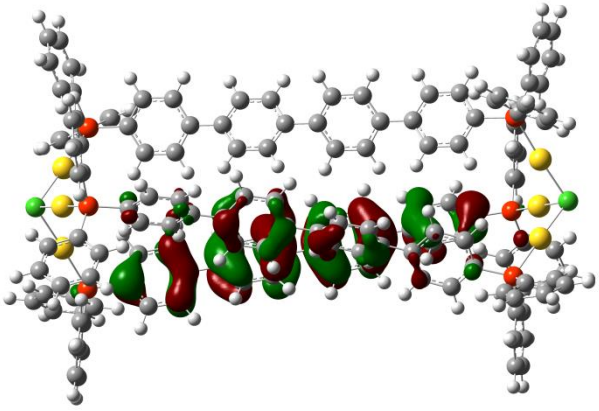
HOMO–1



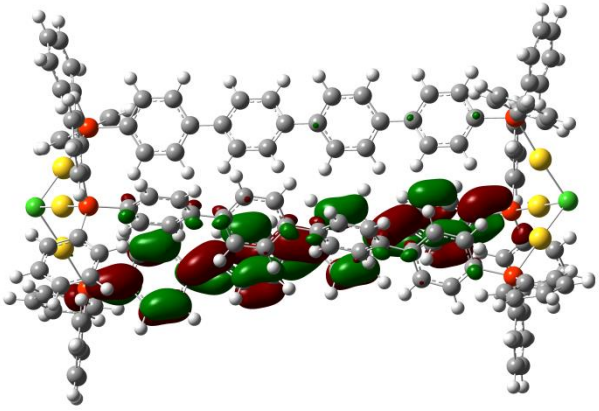
LUMO+1

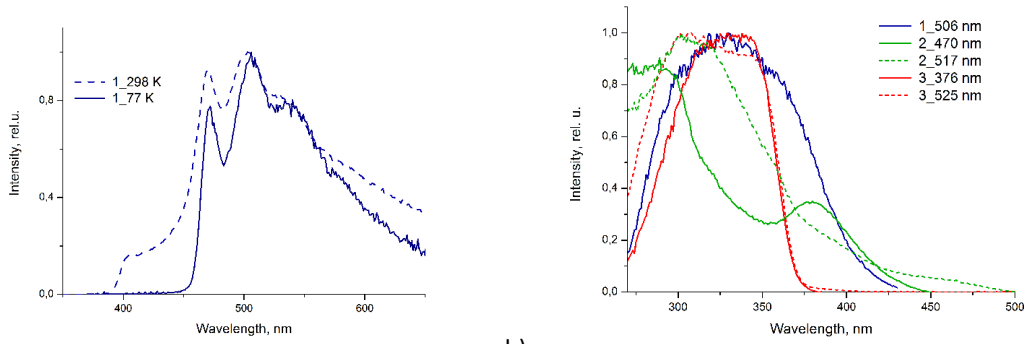


HOMO–2



LUMO





a) b)

Figure S13. Emission spectra of **1**, λ_{ex} = 340 nm in solid state at room temperature and 77K (**a**), excitation spectra of 1 – 3 at 77K (b).