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Synthesis, crystal structure, and optical characteristics of $[Pd_2Hg_4Cl_6\{Te(DMB)\}_6]\cdot 2DMF$, $[HgClTe(DMB)]_4$, and the ring-forming cluster $[Pd_{12}(TePh)_{24}]\cdot 2DMF$

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Table S1. Crystallographic data and refinement parameters for **1, 2** and **3**

	1	**2**	**3**
Empirical formula	$C_{54}H_{68}Cl_6Hg_4N_2O_{14}Pd_2Te_6$	$C_{32}H_{36}Cl_4Hg_4O_8Te_4$	$C_{150}H_{134}N_2O_2Pd_{12}Te_{24}$
Fw	2962.56	2003.17	6335.78
T (K)	293(2)	296(2)	293(2)
Crystal system	triclinic	monoclinic	monoclinic
Space group	$P\bar{1}$	$P2_1/c$	$C2/c$
a/Å	10.5718(4)	13.6219(17)	35.392(3)
b/Å	11.4215(5)	12.3303(14)	19.4685(17)
c/Å	15.7806(7)	14.266(2)	25.583(2)
α/deg	79.158(2)	90	90
β/deg	81.398(2)	114.291(3)	92.237(6)
γ/deg	80.819(2)	90	90
V/Å^3	1833.36(13)	2184.0(5)	17614(3)
Z	1	2	4
ρ_{calcd} (g cm^{-3})	2.683	3.046	2.389
μ (Mo Kα) (mm^{-1})	11.438	16.923	5.134
λ/Å	0.71073	0.71073	0.71073
F (000)	1344	1776	11456
Index ranges	−14<h<14,−15<k<15,−22<l<21	−18<h<18,−17<k<16,−19<l<19	−48<h<49,−27<k<25,−35<l<35
Collected reflns.	36375	22911	175629
Unique reflns.	10372	6133	24752
GOF (F^2)	1.050	1.040	1.026
R_1[a] {[I>2σ(I)]}	0.0404	0.0199	0.0749
wR_2[b] (all data)	0.0971	0.0413	0.2018

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR_2 = \{\sum w(F_o^2 - F_c^2)^2/\sum w(F_o^2)^2\}^{1/2}$.

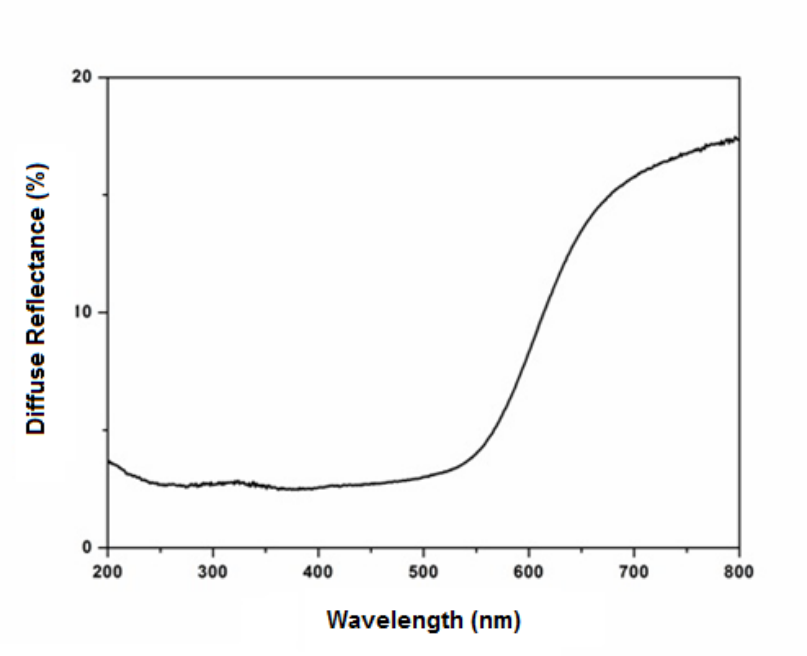

Figure S1. Diffuse reflectance spectrum {r = (R_{Sample}/(R_{Std} – R_{Noise})} of **1**.

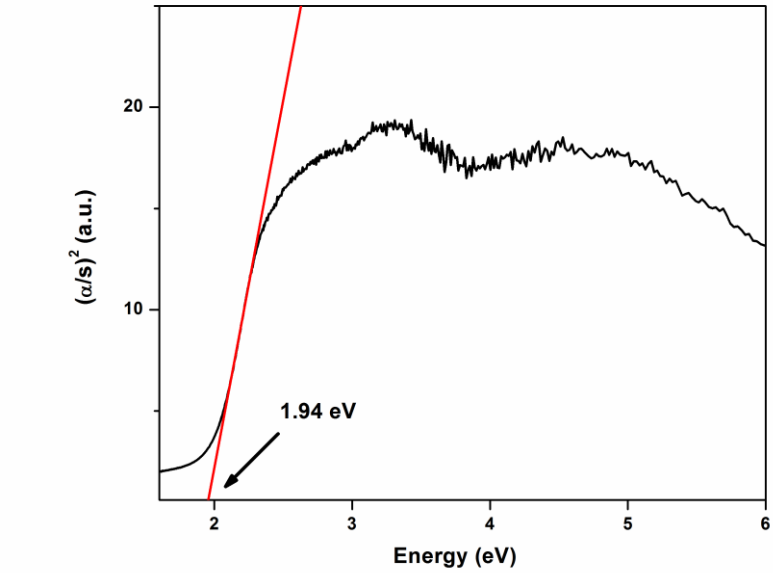

Figure S2. Graphical determination of the E_g value of **1** (1.94 eV).[20]

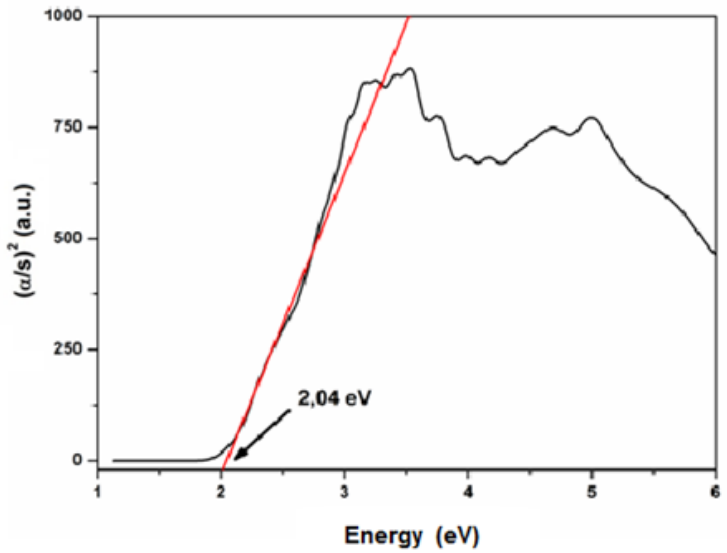

Figure S3. Graphical determination of the E_g value of **2** (2.04 eV).[20]

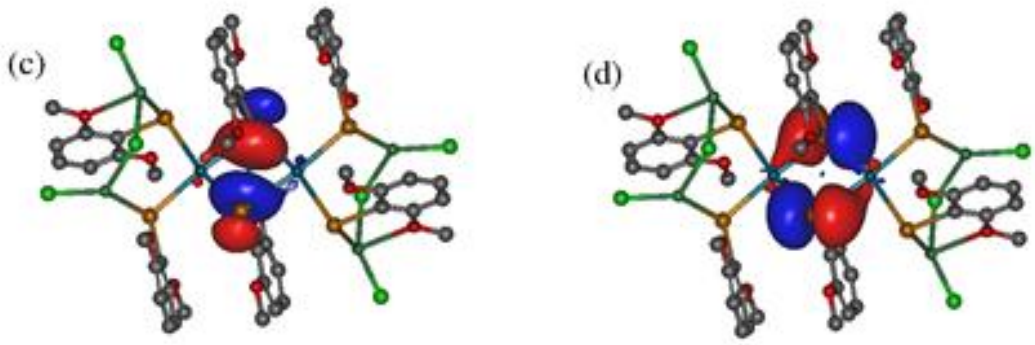

Figure S4. The two anti-bonding 'bridging' Te1–Te1' orbitals of **1**,