A novel Cd_4O_4 cubane cluster-based complex and its bifunctional catalytic activity aiming for artificial photosynthesis

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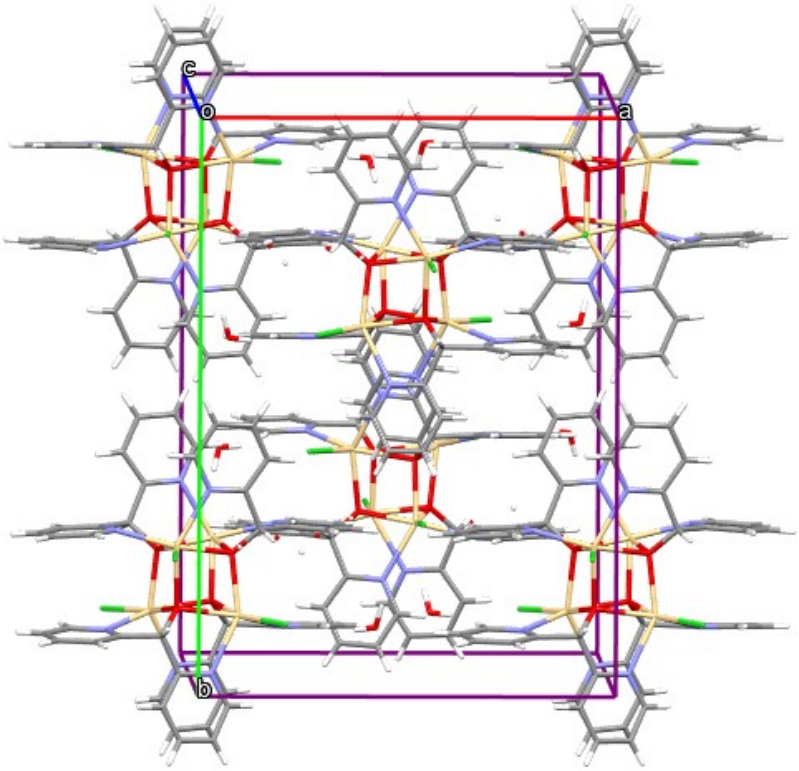

Fig. S1. The crystal packing of complex **1** observed along the c-axis.

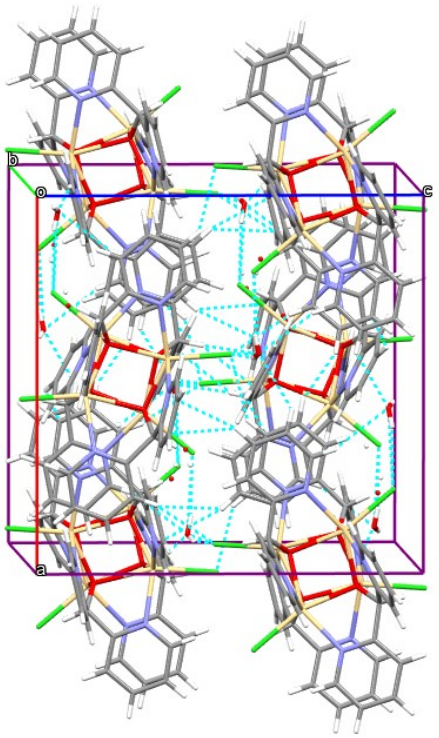

Fig. S2. Relevant hydrogen bonding interactions of complex **1,** in the lattice observed along the b axis, indicated by dashed lines.

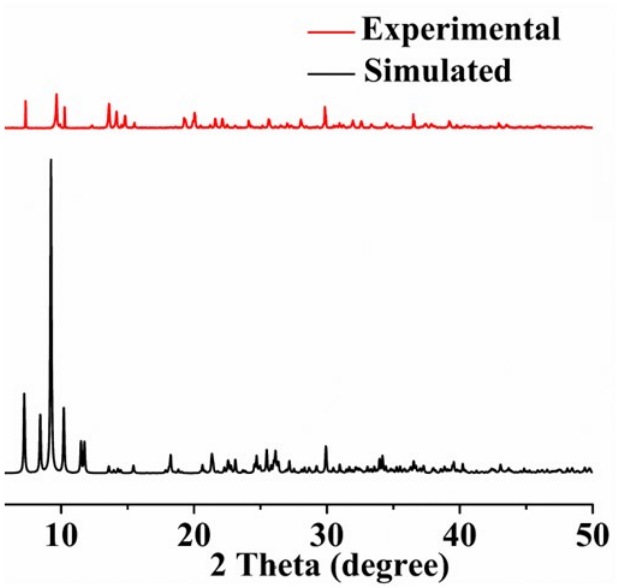

Fig. S3. Overlay of the experimental and simulated PXRD patterns of complex **1**.

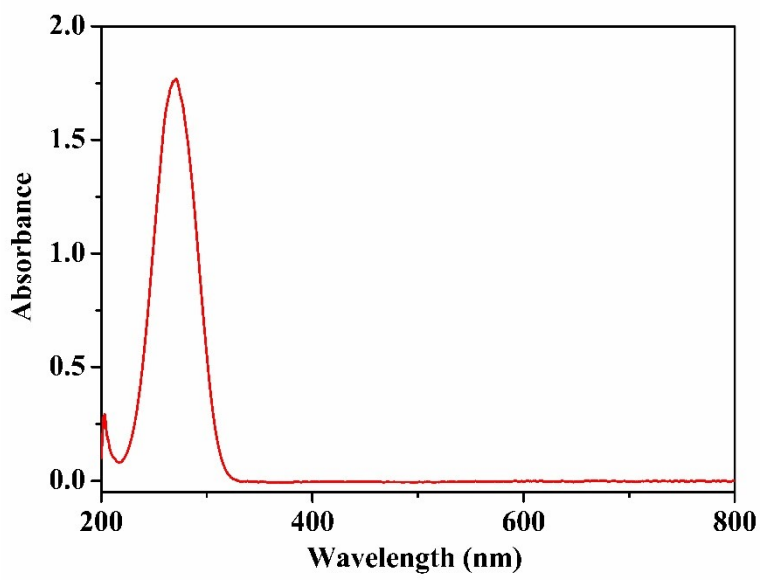

Fig. S4. Solution phase UV-vis spectrum of complex **1** in 10^{-4} M methanol solution.

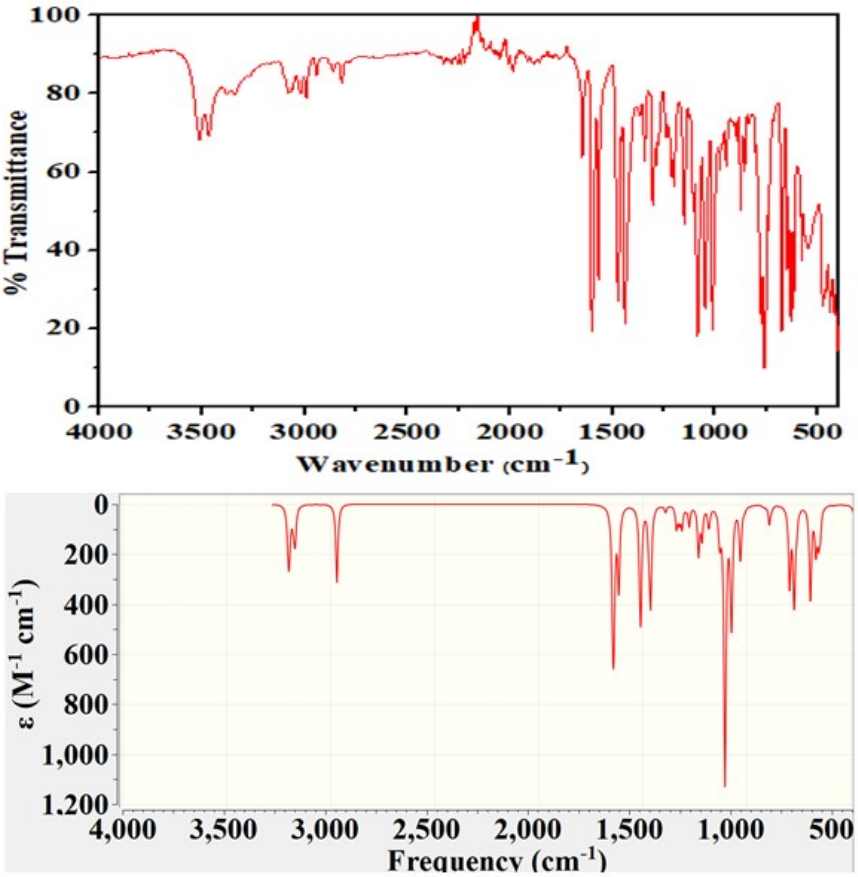

Fig. S5. Experimental (top) and theoretical (bottom) IR spectrum of complex **1**.

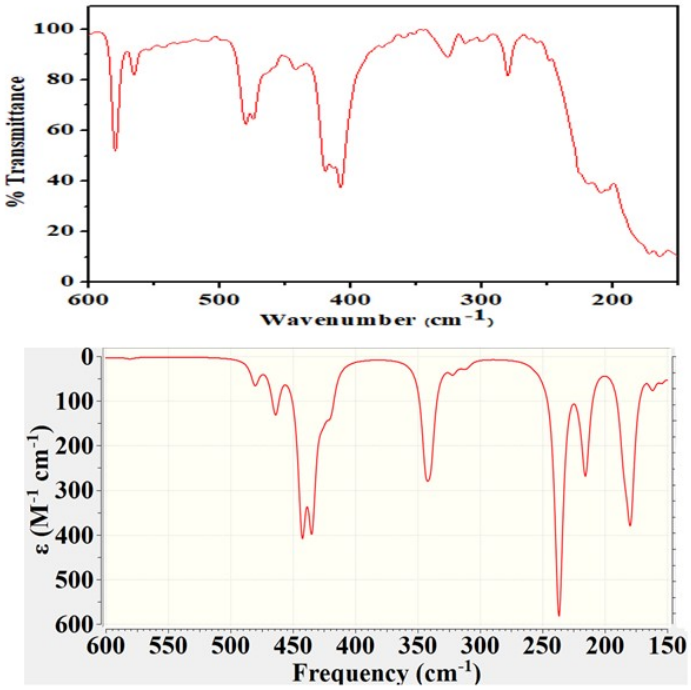

Fig. S6. Experimental (top) and theoretical (bottom) Far IR spectrum of complex **1**.

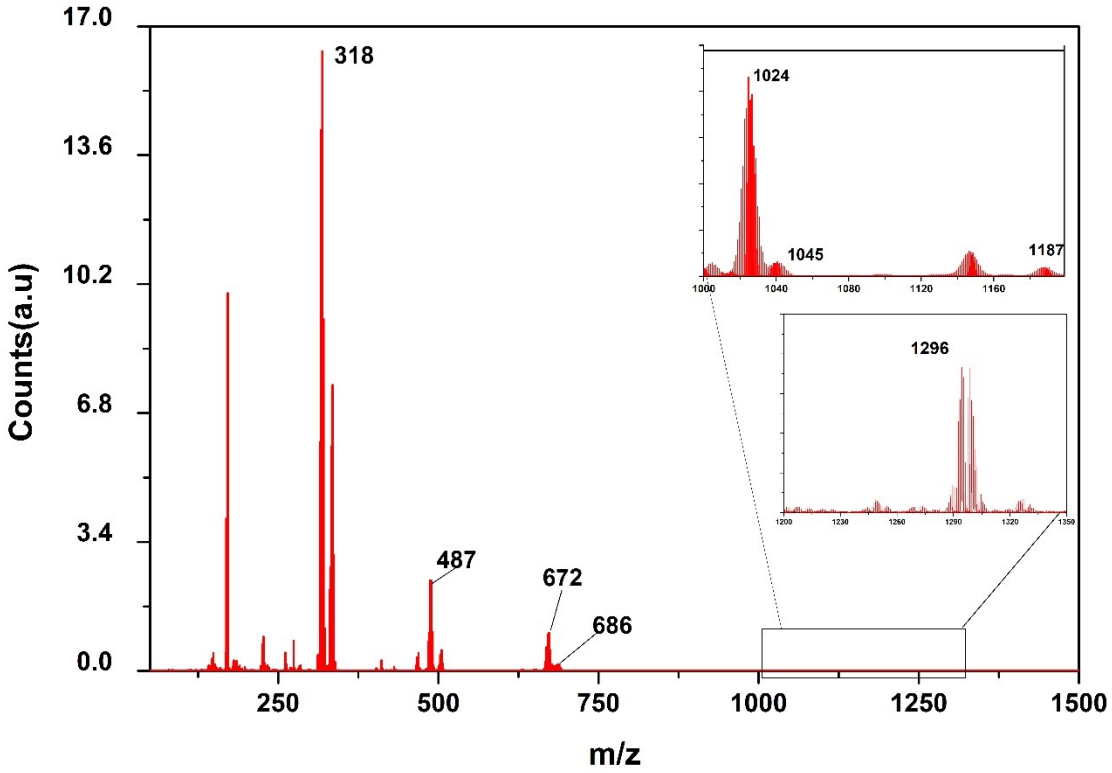

Fig. S7. ESI-MS spectrum of complex **1** in methanol, showing relevant peaks.

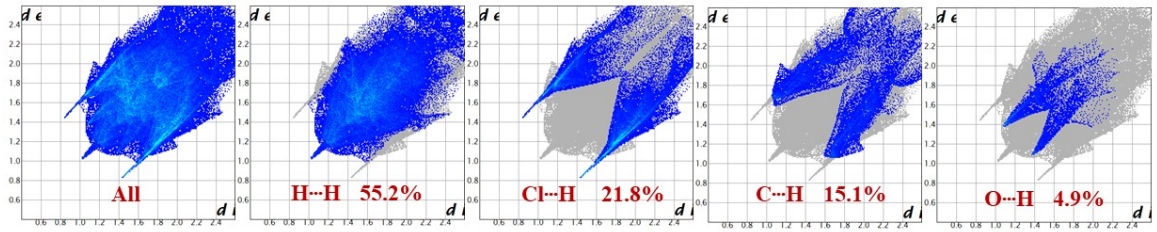

Fig. S8. 2D fingerprint plots of complex **1**.

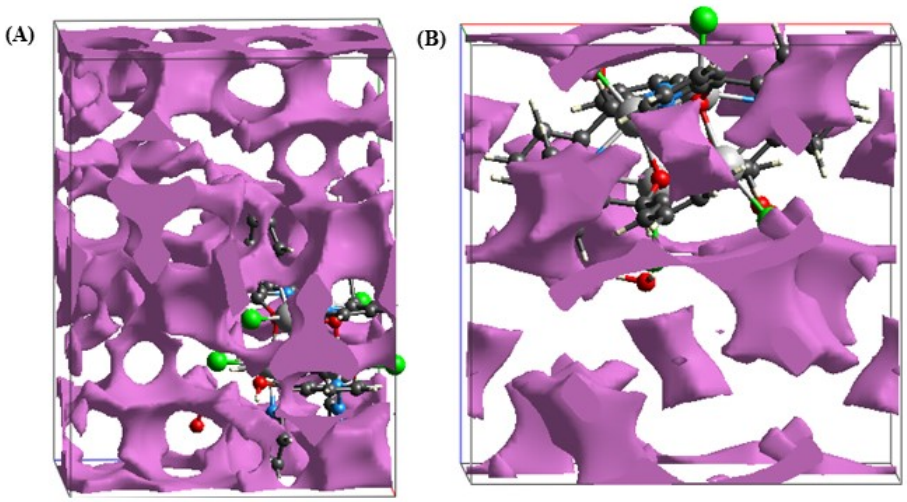

Fig. S9. Void surfaces of complex **1** arising from different isovalues (0.002 au (a) and 0.0008 au (b)) for a unit cell.

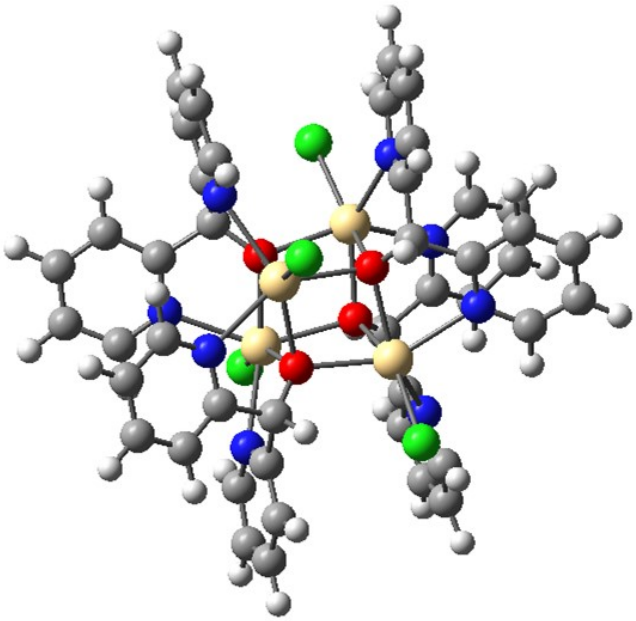

Fig. S10. DFT optimized structure of complex **1**.

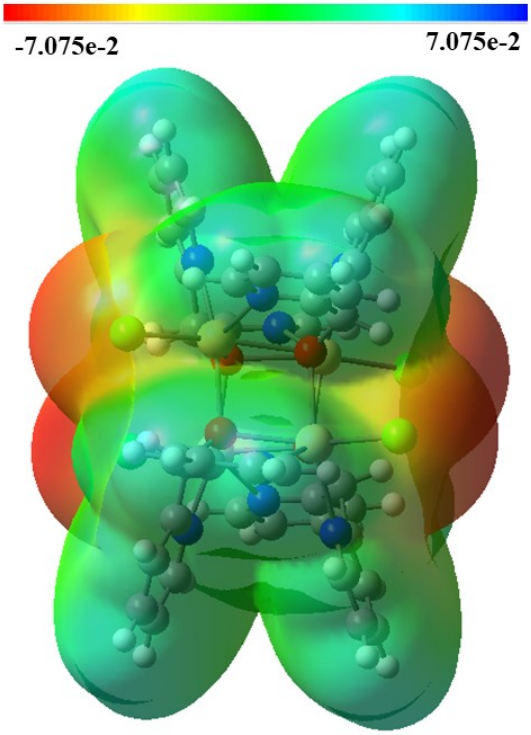

Fig. S11. Molecular electrostatic potential surface of complex **1**.

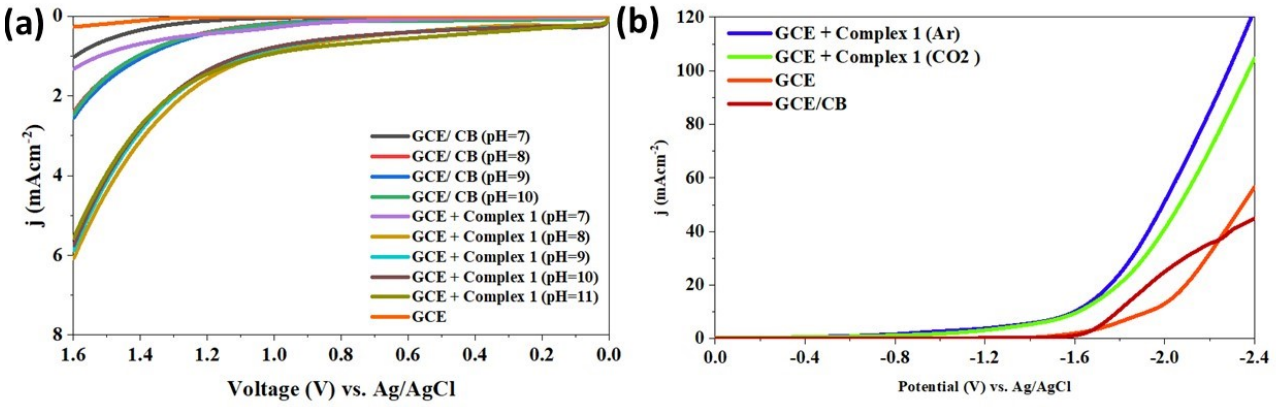

Fig. S12. LSV control experiment for (a) water oxidation and (b) CO_2 reduction activity of complex **1**.

Table S1. Interaction parameters of complex **1**.

C–H···π interactions			
C–H···Cg	H···Cg(Å)	C···Cg(Å)	C–H···Cg(°)
C(6')–H(6')···Cg(3)[a]	2.97	3.934(17)	162
C(6')–H(6')···Cg(4)[b]	2.97	3.934(17)	162
Equivalent position codes: (a) = x, y, z, (b) = 1-x, y, 1/2-z.			
Hydrogen bonding interactions			
D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
O(3)–H(3A)···Cl(2)[a]	0.73(3)	2.54(3)	3.2598(17)	166(3)
O(3)–H(3B)···Cl(1)[b]	0.83(4)	2.45(4)	3.2540(17)	166(3)
C(2)–H(2)···O(3)[c]	0.95	2.58	3.333(3)	136
C(10)–H(10)···Cl(1)[a]	0.95	2.73	3.5357(19)	143
C(11)–H(11)···O(1')[a]	0.95	2.60	3.264(14)	127
C(13)–H(13)···O(3)[d]	0.95	2.59	3.348(2)	137
A = acceptor, D = donor; Equivalent position codes: (a) = 1/2-x, 1/2-y, 1/2+z, (b) = 1-x, y, 1/2-z, (c) = x, -y, -1/2+z, (d) = -1/2+x, 1/2-y, 1-z.				

Table S2. Hirshfeld surface properties of cadmium cubane cluster.

Compound	Volume (Å^3)	Area (Å^2)	Globularity (G)	Asphericity (Ω)
Complex **1**	1174.60	687.03	0.784	0.030