New Compounds Constructed from Polyoxometalates and Transition Metal Coordination Complexes with Lower Positive Charge

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Supplementary information for paper c1ce05633f:

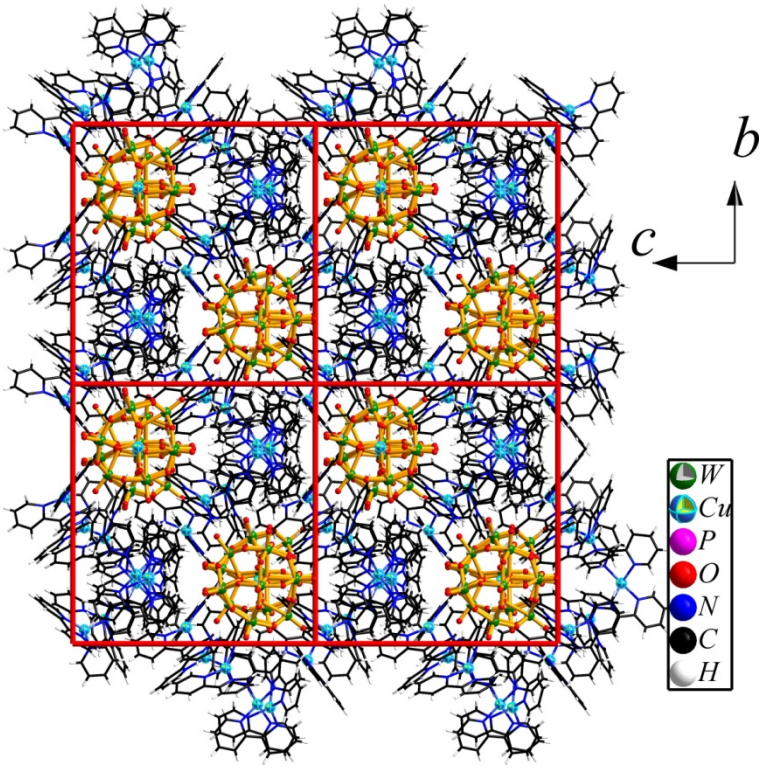

Fig. S1

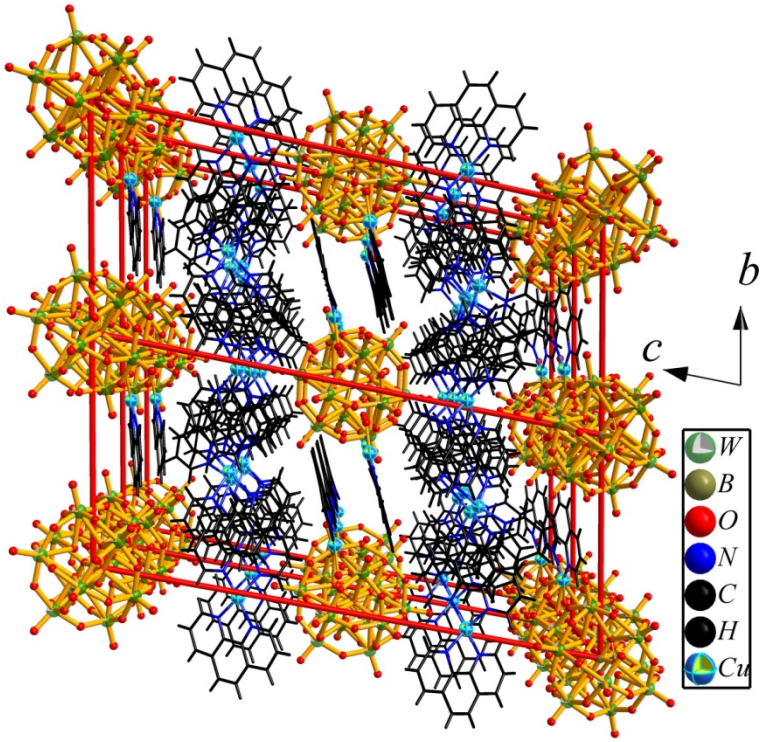

Fig. S2

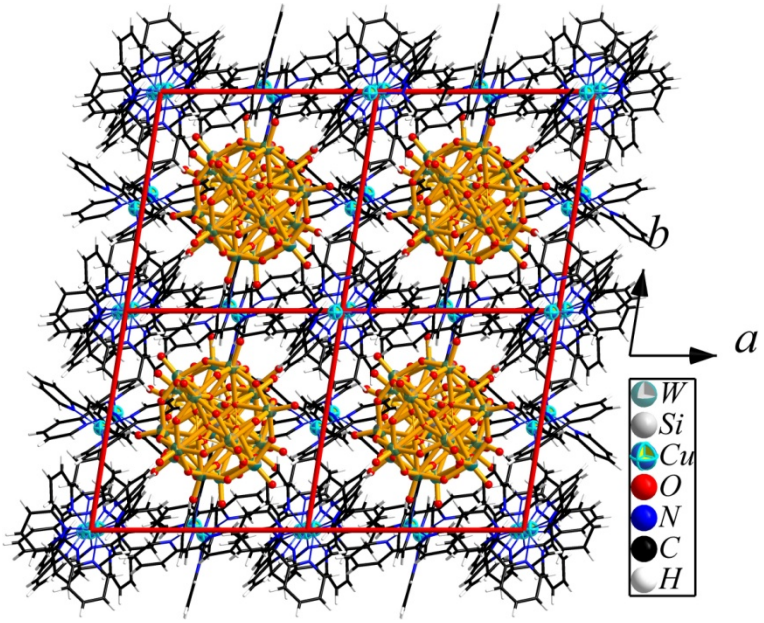

Fig. S3

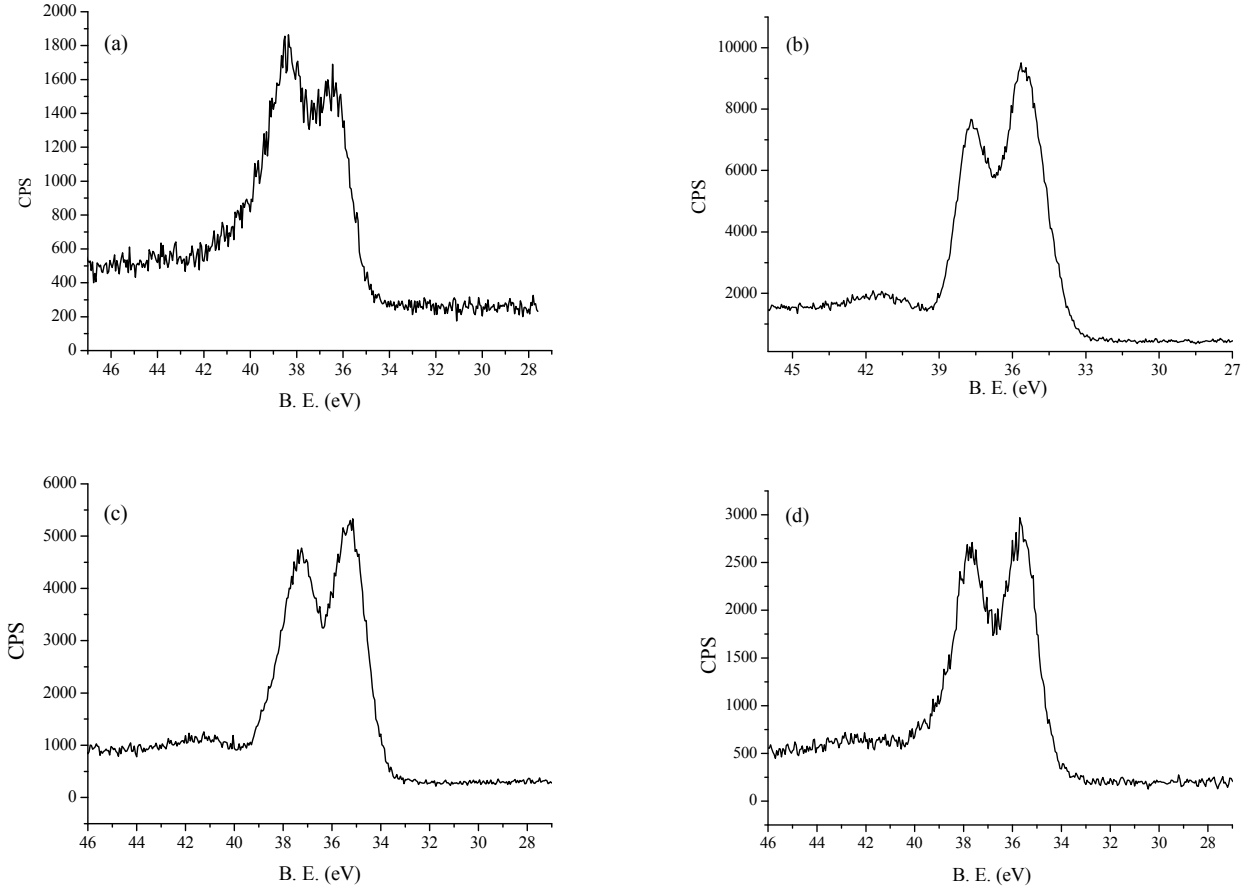

Fig. s4. The XPS spectra for tungsten in compound **1** (a), **2** (b), **3** (c) and **4**(d).

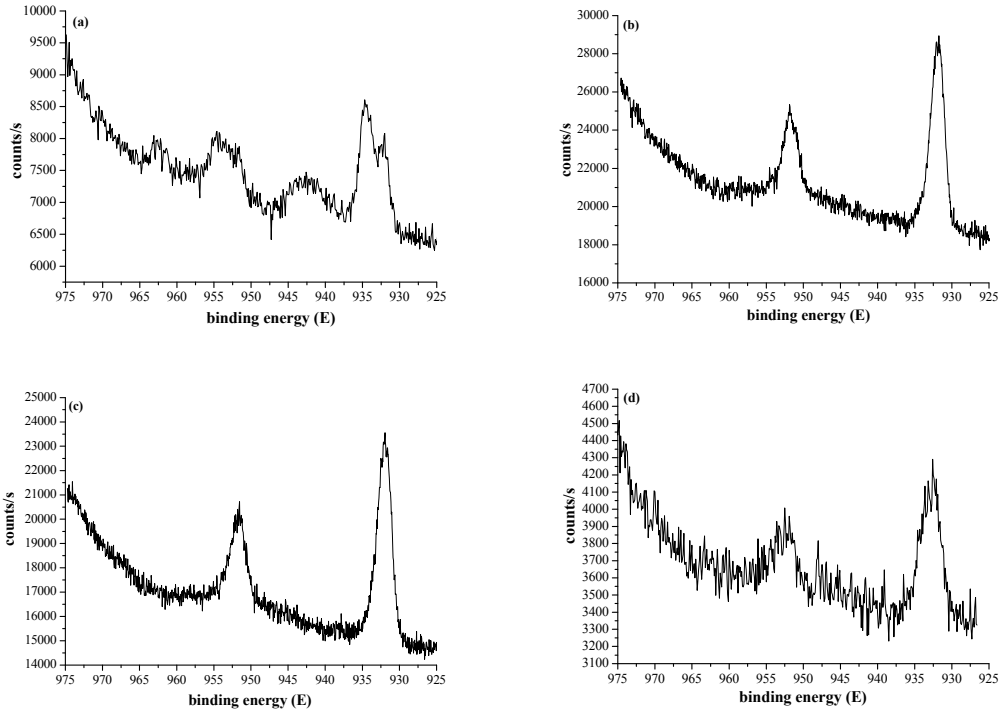

Fig. s5. The XPS spectra for copper in compound **1** (a), **2** (b), **3** (c) and **4**(d).

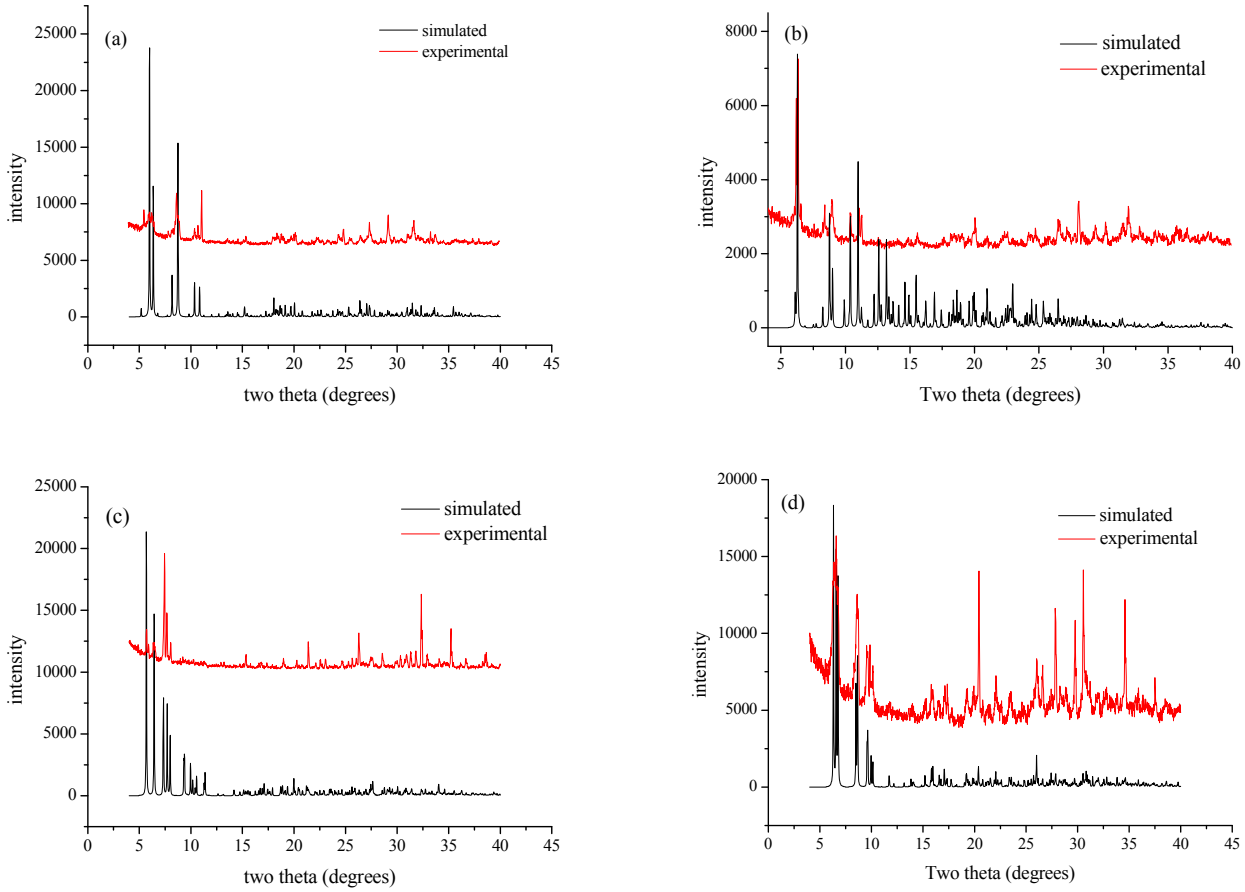

Fig. s6. (a) The experimental and simulated XRD pattern for compound **1**. (b) The experimental and simulated XRD pattern for compound **2**. (c) The experimental and simulated XRD pattern for compound **3**. (d) The experimental and simulated XRD pattern for compound **4**.

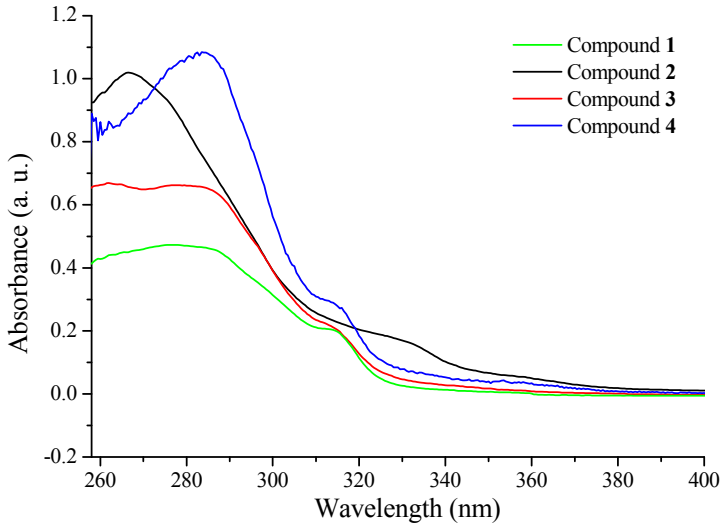

Fig. s7. The UV-Vis spectra for compound **1**, **2, 3** and **4**.

Table s1.

The π···π interactions in compound 1

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I) Res(I)	Cg(J) [ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(33) [3]	-> Cg(37) [3545.04]	3.7853	-0.1601-0.3061 0.9384	14.5163	24.15	29.19	5.85	3.766	3.305
Cg(36) [4]	-> Cg(45) [1555.05]	3.8018	-0.5551 0.8007-0.2253	1.3912	3.59	20.89	17.38	3.628	3.552
Cg(37) [4]	-> Cg(33) [3554.03]	3.7853	0.4963-0.0680 0.8655	4.6601	24.15	5.85	29.19	3.305	3.766
Cg(45) [5]	-> Cg(36) [1555.04]	3.8018	-0.5225 0.8329-0.1825	6.0570	3.59	17.38	20.89	3.552	3.628

The π···π interactions in compound 3

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I) Res(I)	Cg(J) [ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg2 [2]	-> Cg3 [1555.02]	3.2773	-0.1348 0.8267 0.5463	10.8861	33.11	17.37	15.78	3.154	3.128
Cg3 [2]	-> Cg2 [1555.02]	3.2773	0.1268 0.9897 0.0670	4.2760	33.11	15.78	17.37	3.128	3.154
Cg12 [3]	-> Cg31 [1555.05]	3.7142	0.8388 0.0876 0.5373	10.1421	2.32	18.77	19.70	3.497	3.517
Cg12 [3]	-> Cg33 [1555.05]	3.7174	0.8372 0.0576 0.5438	10.0295	1.99	22.17	20.35	3.485	3.443
Cg13 [3]	-> Cg22 [1455.04]	3.5998	0.8638 0.0293 0.5029	2.5041	2.78	18.69	18.90	3.406	3.410
Cg14 [3]	-> Cg32 [1545.05]	3.6803	0.8428 0.0529-0.5357	0.5879	3.35	24.86	25.19	3.330	3.339
Cg15 [3]	-> Cg20 [1445.04]	3.6822	0.8000 0.1646-0.5770	-6.8824	3.63	22.35	20.08	3.458	3.406
Cg15 [3]	-> Cg24 [1445.04]	3.6301	0.8207 0.1658-0.5467	-6.6609	4.64	17.65	16.82	3.475	3.459
Cg16 [3]	-> Cg25 [1455.04]	3.5907	0.8909 0.0245 0.4536	2.0709	7.11	5.62	5.71	3.573	3.573
Cg16 [3]	-> Cg31 [1555.05]	3.7386	0.8388 0.0876 0.5373	10.1421	1.52	18.55	18.28	3.550	3.544
Cg17 [3]	-> Cg20 [1445.04]	3.6735	0.8000 0.1646-0.5770	-6.8824	3.60	22.08	21.72	3.413	3.404
Cg17 [3]	-> Cg29 [1545.05]	3.6862	0.8520 0.0535-0.5208	0.7396	5.24	22.17	23.06	3.392	3.414
Cg17 [3]	-> Cg32 [1545.05]	3.5818	0.8428 0.0529-0.5357	0.5879	4.45	21.97	18.64	3.394	3.322
Cg18 [4]	-> Cg28 [1555.05]	3.6875	0.8546 0.0225-0.5187	1.6525	9.61	14.30	4.69	3.675	3.573
Cg19 [4]	-> Cg30 [1555.05]	3.7332	0.8308 0.0375 0.5553	9.9508	6.83	23.60	24.67	3.392	3.421
Cg20 [4]	-> Cg15 [1665.03]	3.6822	0.7983 0.1034-0.5934	8.3533	3.63	20.08	22.35	3.406	3.458
Cg20 [4]	-> Cg17 [1665.03]	3.6735	0.8060 0.1023-0.5830	8.5337	3.60	21.72	22.08	3.404	3.413
Cg21 [4]	-> Cg32 [1555.05]	3.4673	0.8428 0.0529-0.5357	1.7689	3.65	12.28	8.65	3.428	3.388
Cg22 [4]	-> Cg13 [1655.03]	3.5998	0.8404 0.0124 0.5419	16.6978	2.78	18.90	18.69	3.410	3.406
Cg22 [4]	-> Cg30 [1555.05]	3.6145	0.8308 0.0375 0.5553	9.9508	3.58	17.50	14.20	3.504	3.447
Cg22 [4]	-> Cg33 [1555.05]	3.8298	0.8372 0.0576 0.5438	10.0295	3.23	22.83	23.26	3.519	3.530
Cg24 [4]	-> Cg15 [1665.03]	3.6301	0.7983 0.1034-0.5934	8.3533	4.64	16.82	17.65	3.459	3.475
Cg25 [4]	-> Cg16 [1655.03]	3.5907	0.8305 0.0678 0.5528	16.9656	7.11	5.71	5.62	3.573	3.573
Cg25 [4]	-> Cg30 [1555.05]	3.6899	0.8308 0.0375 0.5553	9.9508	6.81	20.68	26.96	3.289	3.452
Cg28 [5]	-> Cg18 [1555.04]	3.6875	0.7936 0.1632-0.5861	5.6962	9.61	4.69	14.30	3.573	3.675
Cg29 [5]	-> Cg17 [1565.03]	3.6862	0.8060 0.1023-0.5830	-1.5466	5.24	23.06	22.17	3.414	3.392
Cg30 [5]	-> Cg19 [1555.04]	3.7332	0.8904 0.0134 0.4551	13.1159	6.83	24.67	23.60	3.421	3.392
Cg30 [5]	-> Cg22 [1555.04]	3.6145	0.8638 0.0293 0.5029	13.3073	3.58	14.20	17.50	3.447	3.504
Cg30 [5]	-> Cg25 [1555.04]	3.6899	0.8909 0.0245 0.4536	13.2122	6.81	26.96	20.68	3.452	3.289
Cg31 [5]	-> Cg12 [1555.03]	3.7142	0.8189 0.0727 0.5692	6.7200	2.32	19.70	18.77	3.517	3.497
Cg31 [5]	-> Cg16 [1555.03]	3.7386	0.8305 0.0678 0.5528	6.5789	1.52	18.28	18.55	3.544	3.550
Cg32 [5]	-> Cg14 [1565.03]	3.6803	0.8109 0.0721-0.5808	-1.8966	3.35	25.19	24.86	3.339	3.330
Cg32 [5]	-> Cg17 [1565.03]	3.5818	0.8060 0.1023-0.5830	-1.5466	4.45	18.64	21.97	3.322	3.394
Cg32 [5]	-> Cg21 [1555.04]	3.4673	0.8193 0.1051-0.5637	5.4390	3.65	8.65	12.28	3.388	3.428
Cg33 [5]	-> Cg12 [1555.03]	3.7174	0.8189 0.0727 0.5692	6.7200	1.99	20.35	22.17	3.443	3.485
Cg33 [5]	-> Cg22 [1555.04]	3.8298	0.8638 0.0293 0.5029	13.3073	3.23	23.26	22.83	3.530	3.519
Cg34 [6]	-> Cg37 [2665.06]	3.3688	-0.2498 0.0461-0.9672	0.4050	4.13	3.28	3.92	3.361	3.363
Cg35 [6]	-> Cg36 [2665.06]	3.4172	-0.2109 0.0495-0.9763	0.6408	0.82	5.13	5.35	3.402	3.404
Cg36 [6]	-> Cg35 [2665.06]	3.4172	-0.1971 0.0467-0.9793	0.8092	0.82	5.35	5.13	3.404	3.402
Cg37 [6]	-> Cg34 [2665.06]	3.3688	-0.2272 0.1146-0.9671	1.0571	4.13	3.92	3.28	3.363	3.361
Cg38 [7]	-> Cg38 [2566.07]	3.8142	0.0112 0.2266-0.9739	-14.4836	0.00	28.80	28.80	3.342	3.342
Cg38 [7]	-> Cg39 [2566.07]	3.6027	-0.0030 0.2310-0.9730	-14.4616	0.86	22.72	21.88	3.343	3.323
Cg38 [7]	-> Cg41 [2566.07]	3.5070	0.0050 0.2314-0.9728	-14.4423	0.45	16.59	17.04	3.353	3.361
Cg39 [7]	-> Cg38 [2566.07]	3.6027	0.0112 0.2266-0.9739	-14.4836	0.86	21.88	22.72	3.323	3.343
Cg39 [7]	-> Cg40 [2566.07]	3.4564	-0.0074 0.2644-0.9644	-13.9585	1.99	15.61	16.80	3.309	3.329
Cg40 [7]	-> Cg39 [2566.07]	3.4564	-0.0030 0.2310-0.9730	-14.4616	1.99	16.80	15.61	3.329	3.309

Cg41 [7] -> Cg38 [2566.07] 3.5070 0.0112 0.2266-0.9739 -14.4836 0.45 17.04 16.59 3.361 3.353
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Min or Max 3.277 0.00 2.61 89.72 0.027 2.842

[1455] = -1+X,Y,Z
[1555] = X,Y,Z
[1655] = 1+X,Y,Z
[1545] = X,-1+Y,Z
[1555] = X,Y,Z
[1445] = -1+X,-1+Y,Z

The π···π interactions in compound 4

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Angstrom and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang).
- P,Q,R,S = J-Plane Parameters for Carth. Coord. (Xo, Yo, Zo)

Cg(I)	Res(I)	Cg(J)	[ARU(J)]	Cg-Cg	Transformed J-Plane P, Q, R, S				Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg(9)	[3] ->	Cg(17)	[1655.05]	3.8393	-0.3836	0.8652	0.3229	3.0083	15.06	33.47	26.05	3.449	3.203	
Cg(9)	[3] ->	Cg(20)	[1655.05]	3.7050	-0.4679	0.8731	0.1370	0.7794	12.34	21.08	22.09	3.433	3.457	
Cg(17)	[5] ->	Cg(9)	[1455.03]	3.8393	-0.6086	0.7539	0.2474	9.6334	15.06	26.05	33.47	3.203	3.449	
Cg(20)	[5] ->	Cg(9)	[1455.03]	3.7050	-0.6086	0.7539	0.2474	9.6334	12.34	22.09	21.08	3.457	3.433	
Cg(26)	[6] ->	Cg(26)	[2756.06]	3.7283	0.4152	-0.7852	0.4595	13.7454	0.00	11.11	11.11	3.658	3.658	0.718
Min or Max				3.705					0.00	3.12	88.07	0.185	2.481	

[1545] = X,-1+Y,Z
[1555] = X,Y,Z
[1555] = X,Y,Z
[1555] = X,Y,Z
[1655] = 1+X,Y,Z
[2775] = 2-X,2-Y,-Z
[1665] = 1+X,1+Y,Z
[1565] = X,1+Y,Z
[1655] = 1+X,Y,Z
[1565] = X,1+Y,Z
[1455] = -1+X,Y,Z
[1465] = -1+X,1+Y,Z
[1445] = -1+X,-1+Y,Z
[1455] = -1+X,Y,Z
[1445] = -1+X,-1+Y,Z
[1455] = -1+X,Y,Z
[1545] = X,-1+Y,Z
[1645] = 1+X,-1+Y,Z
[2756] = 2-X,-Y,1-Z

Table s2. The C-H···O hydrogen bonds in compound **1** and **4**.

D-H···A	H···A[Å]	D···A[Å]	D-H···A[°]	symop-for-A
Compound 1				
C79-H79···O33A	2.55	3.26(3)	134	x, y, -1+z
C32-H32···O38A	2.56	3.09(3)	116	x, y, -1+z
C31-H31···O38A	2.40	3.01(3)	123	x, y, -1+z
C90-H90···O38A	2.40	3.21(4)	146	x, y, -1+z
C23-H23···O26A	2.42	3.17(3)	137	0.5+x,-0.5-y, -1+z
C84-H84···O18A	2.41	3.25(4)	149	0.5+x, -0.5-y, -1+z
C58-H58···O17A	2.63	3.18 (4)	119	-1-x, -y, 0.5+z
C57-H57···O17A	2.49	3.10 (5)	123	-1-x, -y, -0.5+z
C29-H29···O30A	2.58	3.09(4)	115	-1-x, -y, -0.5+z
C28-H28···O30A	2.47	3.04(5)	120	-1-x, -y, -0.5+z
C82-H82···O22A	2.41	3.17(7)	138	-0.5-x,0.5+y,-0.5+z
C47-H47···O24A	2.24	3.16(3)	173	0.5+x, -0.5-y, z
C94-H94···O8	2.64	3.17(4)	117	
C8-H8···O29A	2.54	3.25(3)	134	0.5+x, -0.5-y, z
C98-H98···O29	2.54	3.23(3)	132	
C103-H103···O13A	2.29	3.19(3)	162	-0.5-x,-0.5+y,-0.5+z
C103-H103···O1A	2.72	3.19(3)	112	-0.5-x,-0.5+y, 0.5+z
C103-H103···O15A	2.69	3.20(3)	115	-0.5-x,-0.5+y,-0.5+z
C103-H103···O23A	2.53	3.14(3)	124	-0.5-x,-0.5+y,-0.5+z
C104-H104···O23A	2.64	3.19(3)	119	-0.5-x,-0.5+y,-0.5+z
C2-H2···O26A	2.41	3.22(3)	145	0.5+x,-0.5-y, -1+z
C53-H53···O11A	2.64	3.21(5)	123	-1-x, -y, -0.5+z
C74-H74···O5A	2.41	3.17(3)	138	-1-x,-1-y,-0.5+z
C18-H18···O17A	2.47	3.25(3)	142	-0.5-x,-0.5+y,-0.5+z
Compound 4				
C58-H58···O14A	2.60	3.20(3)	122	-1+x, y, z
C54-H54···O10A	2.59	3.25(2)	128	-x, 1-y, -z
C63-H63···O11A	2.32	3.23(3)	166	1+x, y, z
C11-H11···O15A	2.71	3.21(2)	115	1-x, 2-y, -z
C52-H52···O9	2.39	3.14(2)	121	
C37-H37···O22	2.56	3.21(2)	128	
C70-H70···O40A	2.51	3.16(2)	127	1+x, -2+y, z
C18-H18···O29A	2.58	3.25(2)	129	x, -1+y, z
C23-H23···O43	2.36	3.16(3)	144	
C43-H43···O41A	2.84	3.02(3)	92	x, -1+y, z
C49-H49···O27A	2.95	3.21(3)	98	-1+x, -1+y, z