Supporting Information

Table S1. Elemental analysis results (%).

Results	1	2	3	4	5	6	7	8	9	10	11	12
C calculate	19.09	19.01	19.72	20.44	18.71	18.16	18.59	17.60	19.39	19.32	17.74	16.75
found	18.99	18.87	19.71	20.27	18.79	18.01	18.79	17.84	19.27	19.23	18.00	17.05
H calculate	4.65	4.63	5.04	4.82	5.24	5.37	5.20	5.48	5.04	5.02	5.46	5.76
found	4.45	4.53	5.01	4.62	5.04	5.27	5.01	5.28	4.94	4.89	5.16	5.46
N calculate	14.84	14.78	15.33	15.90	14.56	14.13	14.45	13.68	15.08	15.03	13.79	13.03
found	14.98	14.87	15.57	15.99	14.82	14.20	14.55	13.74	15.23	15.17	13.99	13.32

Table S2. Crystal data and structure refinement details for compounds in the second and third isomorphous groups.

Compound	1	2	3	4	5	6	7	8	9	10	11	12
Empirical formula	$C_{42}H_{122}N_{28}O_{54}Cu_2La_2Cl_{10}$	$C_{42}H_{122}N_{28}O_{54}Cu_2Nd_2Cl_{10}$	$C_{42}H_{128}N_{28}O_{57}CoLa_2Cl_8$	$C_{42}H_{118}N_{28}O_{52}CoCe_2Cl_8$	$C_{42}H_{140}N_{28}O_{63}CuEu_2Cl_8$	$C_{42}H_{148}N_{28}O_{67}CuGd_2Cl_8$	$C_{42}H_{140}N_{28}O_6{}_3CoDy_2Cl_8$	$C_{42}H_{156}N_{28}O_7{}_1CoEr_2Cl_8$	$C_{42}H_{130}N_{28}O_5{}_8CoEu_2Cl_8$	$C_{42}H_{130}N_{28}O_5{}_8CoGd_2Cl_8$	$C_{42}H_{154}N_{28}O_7{}_0CuDy_2Cl_8$	$C_{42}H_{172}N_{28}O_7{}_9CuHo_2Cl_8$
Formula weight	2643.08	2653.74	2558.07	2470.41	2696.88	2779.52	2713.35	2867.00	2602.19	2612.77	2844.07	3006.47
Crystal system	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	triclinic	monoclinic	monoclinic	monoclinic	monoclinic
Spacegroup	P-1	P-1	P-1	P-1	P-1	P-1	P-1	P-1	P21/c	P21/c	P21/c	P21/c
a, Å	17.267(6)	17.2440(6)	17.1376(9)	17.0773(11)	17.0566(17)	17.045(4)	16.979(3)	17.085(4)	17.0739(11)	17.0997(11)	17.084(2)	17.1162(13)
b, Å	17.380(6)	17.3617(6)	17.4128(8)	17.3435(11)	17.1421(17)	17.080(4)	17.140(3)	17.228(4)	27.7218(18)	27.7353(19)	27.493(4)	27.675(2)
c, Å	18.306(10)	18.1955(11)	18.4104(9)	18.243(2)	20.041(3)	19.983(7)	20.168(3)	20.219(6)	20.6280(14)	20.6163(13)	20.428(3)	20.4248(16)
α, deg	102.659(5)	102.902(2)	103.314(2)	103.410(3)	97.415(5)	112.825(11)	97.223(7)	97.325(10)	90.00	90.00	90.00	90.00
β, deg	103.677(5)	103.810(2)	103.349(2)	103.249(3)	112.647(5)	96.852(11)	113.441(6)	113.561(7)	97.558(2)	97.468(2)	99.261(4)	97.399(2)
γ, deg	110.207(3)	110.4590(10)	110.196(2)	110.144(2)	111.089(4)	111.574(8)	111.556(6)	111.615(7)	90.00	90.00	90.00	90.00
V, $Å^3$	4729(3)	4666.2(4)	4718.9(4)	4643.2(7)	4795.8(10)	4748(2)	4747.3(14)	4801(2)	9678.8(11)	9694.7(11)	9470(2)	9594.4(13)
Z	2	2	2	2	2	2	2	2	4	4	4	4
Dcalcd, g cm^{-3}	1.856	1.889	1.800	1.767	1.868	1.944	1.898	1.983	1.787	1.790	1.995	2.081
T, K	223	223	223	223	223	223	223	223	223	223	223	223
μ, mm^{-1}	1.726	1.946	1.407	1.483	1.859	1.959	2.081	2.261	1.787	1.858	2.146	2.174
Unique reflns	16672	16427	16635	16543	16826	16910	16666	16592	17146	17169	18333	18676
Obsd reflns	9307	13482	11474	12136	13122	12439	12014	10343	12777	12787	10670	10691
Params	991	991	964	964	932	911	962	857	949	955	955	952
Rint	0.0540	0.0422	0.0782	0.0624	0.0747	0.0801	0.0906	0.0950	0.0676	0.0597	0.1255	0.1098
R[I> 2σ(I)] [a]	0.0749	0.0529	0.0567	0.0499	0.0822	0.1009	0.0886	0.1200	0.0433	0.0404	0.1016	0.0890
wR[I> 2σ(I)] [b]	0.2014	0.1654	0.1605	0.1438	0.2319	0.2818	0.2353	0.3102	0.1185	0.1155	0.2586	0.2336
R(all data)	0.1162	0.0615	0.0778	0.0659	0.0938	0.1167	0.1058	0.1497	0.0566	0.0538	0.1373	0.1281
wR(all data)	0.2528	0.1756	0.1782	0.1568	0.2455	0.3035	0.2524	0.3393	0.1243	0.1217	0.2797	0.2583
GOF on F2	1.004	1.110	0.923	1.027	1.125	1.155	1.022	1.114	1.016	0.951	1.023	1.030

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; [b] $wR_2 = |\Sigma w(|F_o|^2 - |F_c|^2)|/\Sigma|w(F_o)^2|^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$; $P = (F_o^2 + 2F_c^2)/3$.

Crystal structures details of compounds in the first group are shown in Figures S1–S4:

Figure S1. X-ray crystal structure of compound **1**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of La^{3+} cations and Q[7] molecules surrounded by the $[CuCl_4]^{2-}$ anions; (**c**) coordination of the La^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four La^{3+} cations coordinated to a Q[7] molecule.

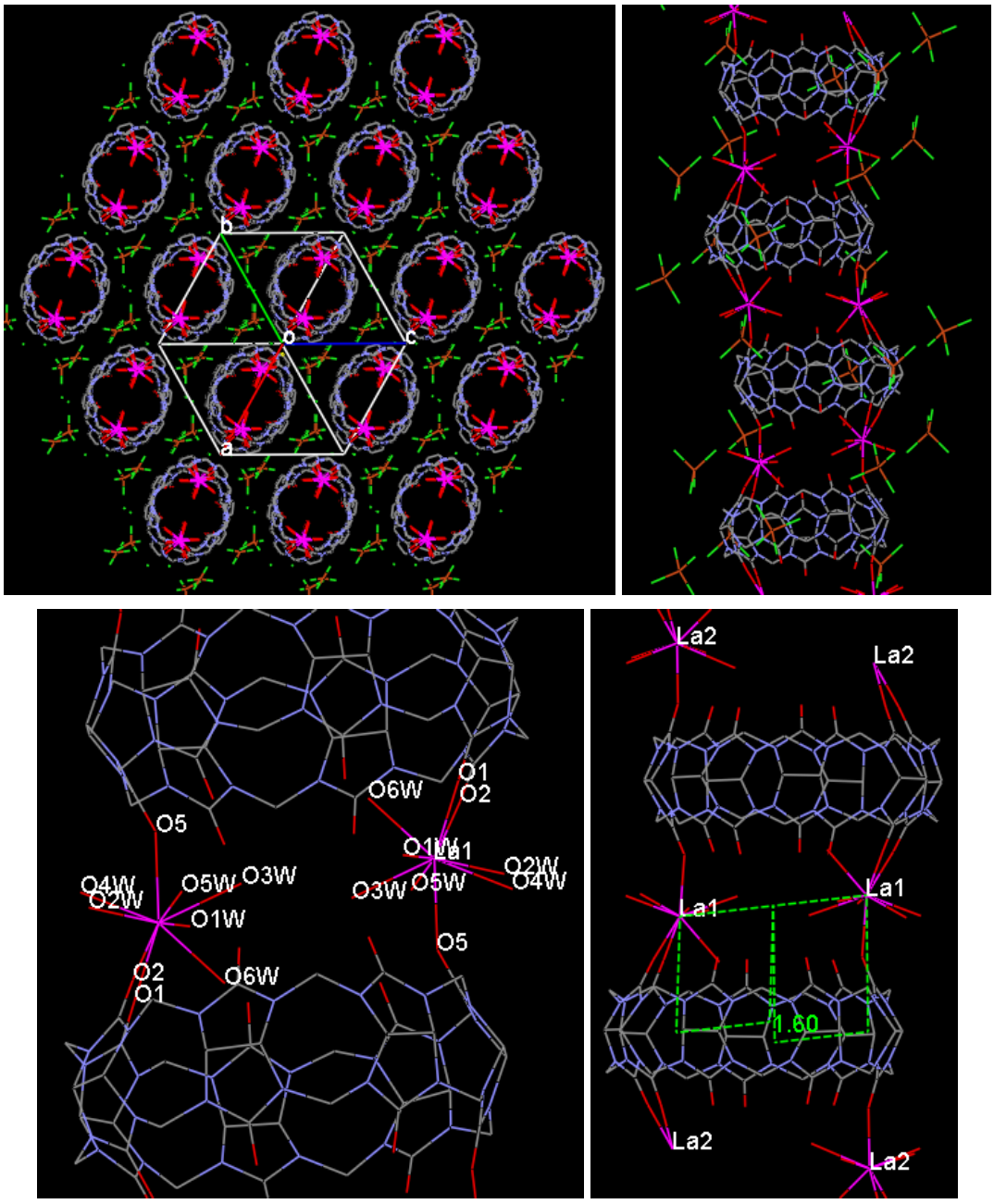


Figure S2. X-ray crystal structure of compound **2**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of Nd^{3+} cations and Q[7] molecules surrounded by the $[CuCl_4]^{2-}$ anions; (**c**) coordination of the Nd^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four Nd^{3+} cations coordinated to a Q[7] molecule.

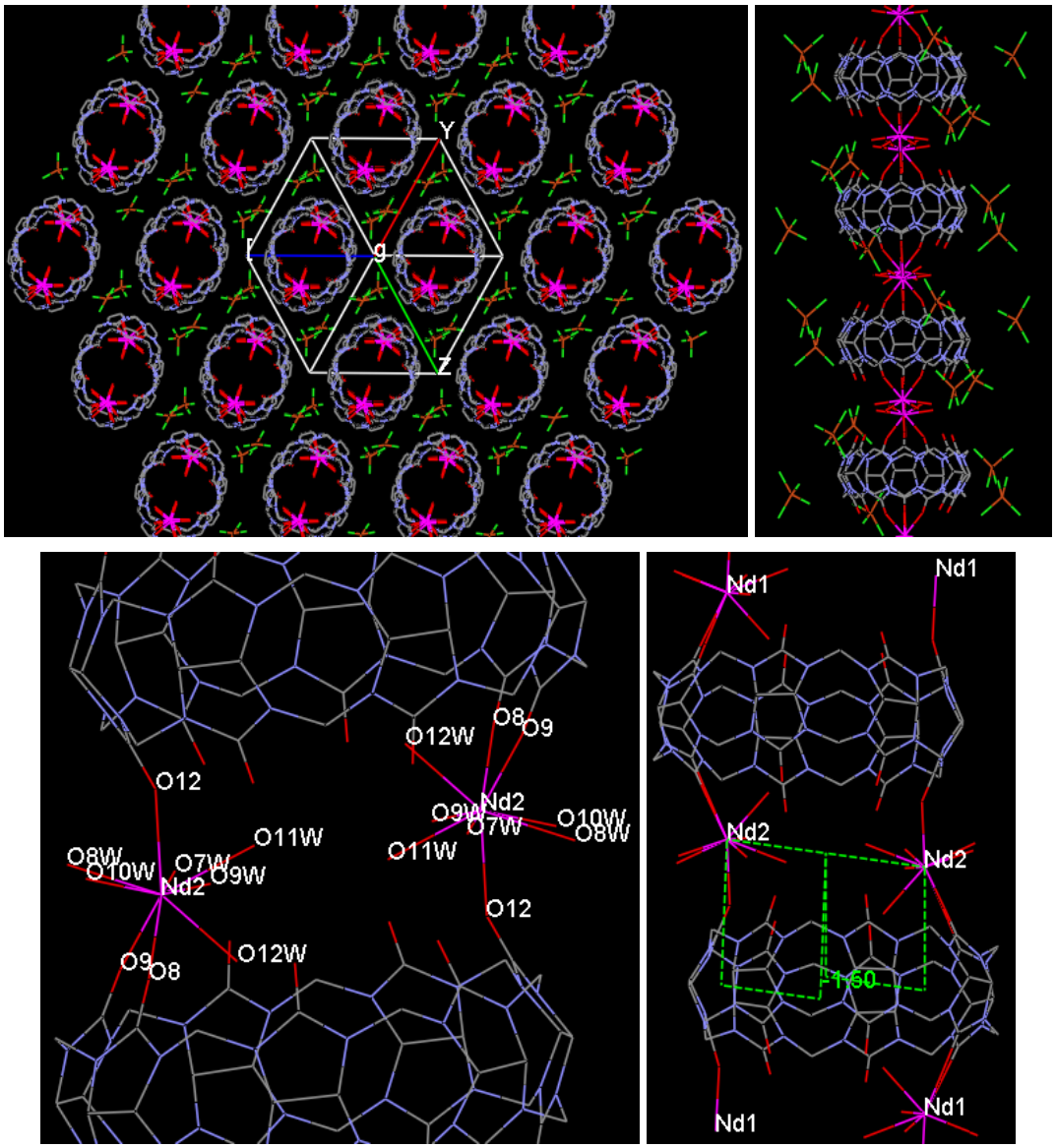


Figure S3. X-ray crystal structure of compound **3**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of La^{3+} cations and Q[7] molecules surrounded by the $[CoCl_4]^{2-}$ anions; (**c**) coordination of the La^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four La^{3+} cations coordinated to a Q[7] molecule.

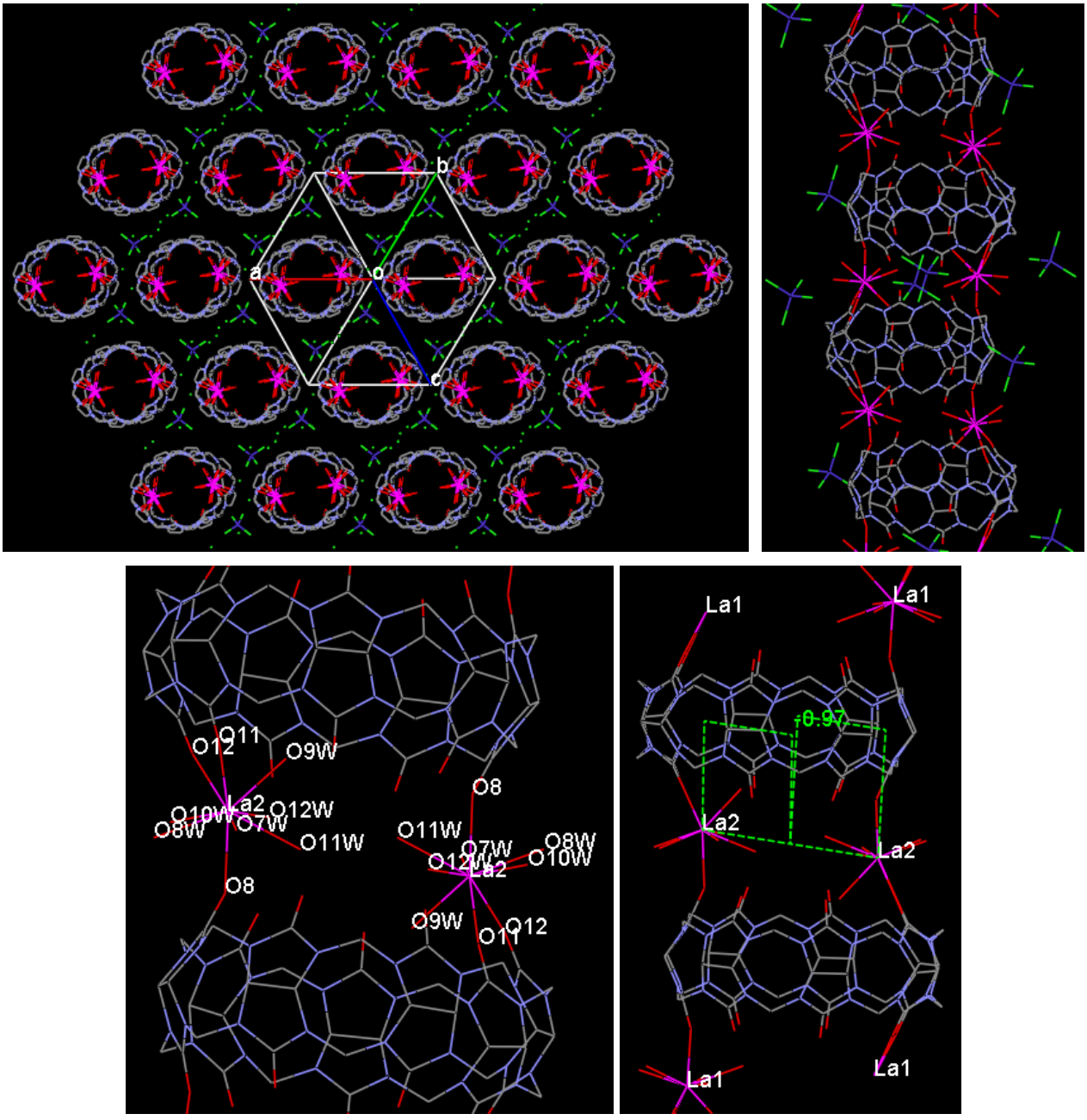
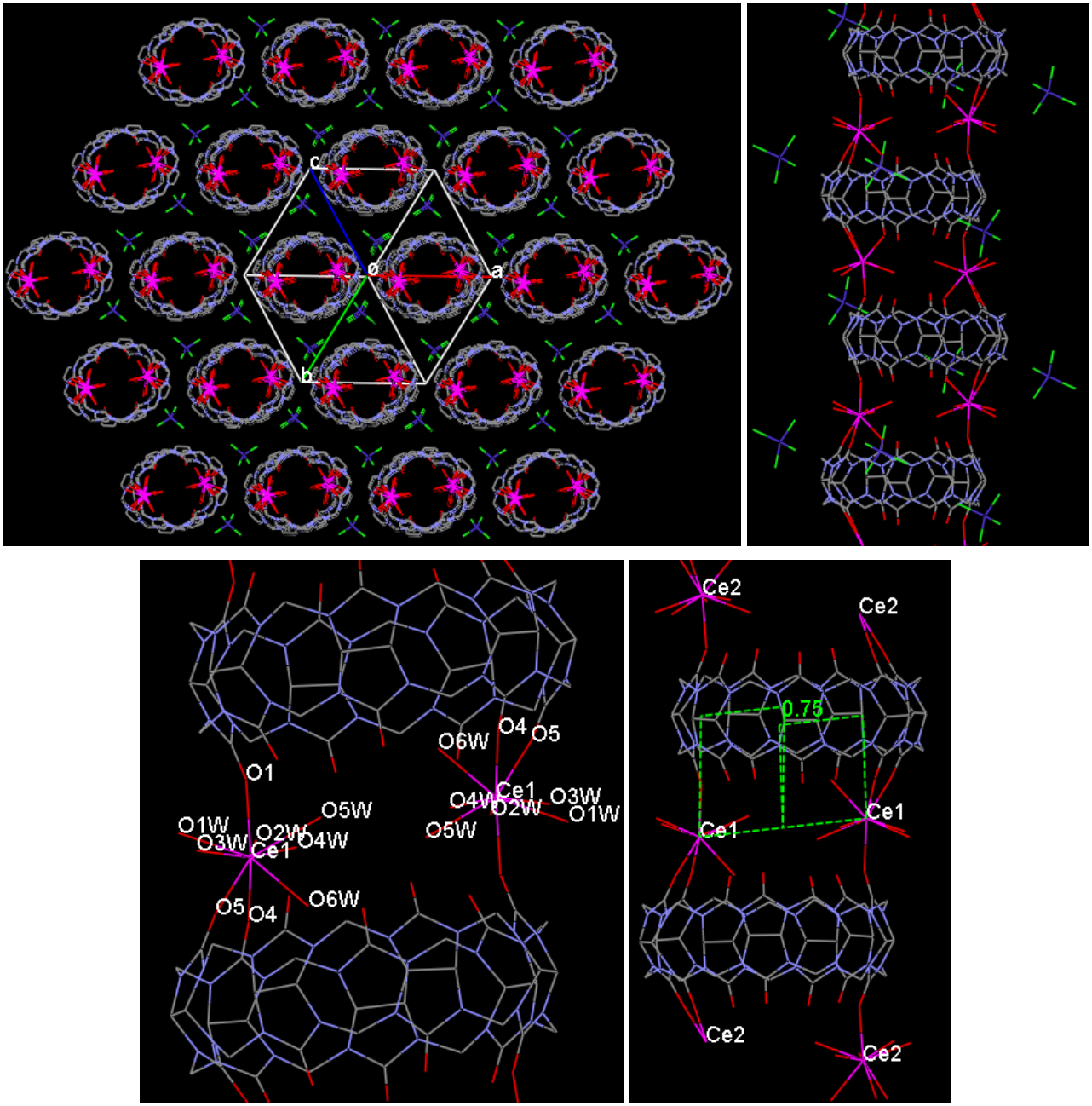


Figure S4. X-ray crystal structure of compound **4**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of Ce^{3+} cations and Q[7] molecules surrounded by the $[CoCl_4]^{2-}$ anions; (**c**) coordination of the Ce^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four Ce^{3+} cations coordinated to a Q[7] molecule.



Crystal structures details of compounds in the second group are shown in Figures S5–S8:

Figure S5. X-ray crystal structure of compound **5**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of Eu^{3+} cations and Q[7] molecules surrounded by the $[CuCl_4]^{2-}$ anions; (**c**) coordination of the Eu^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four Eu^{3+} cations coordinated to a Q[7] molecule.

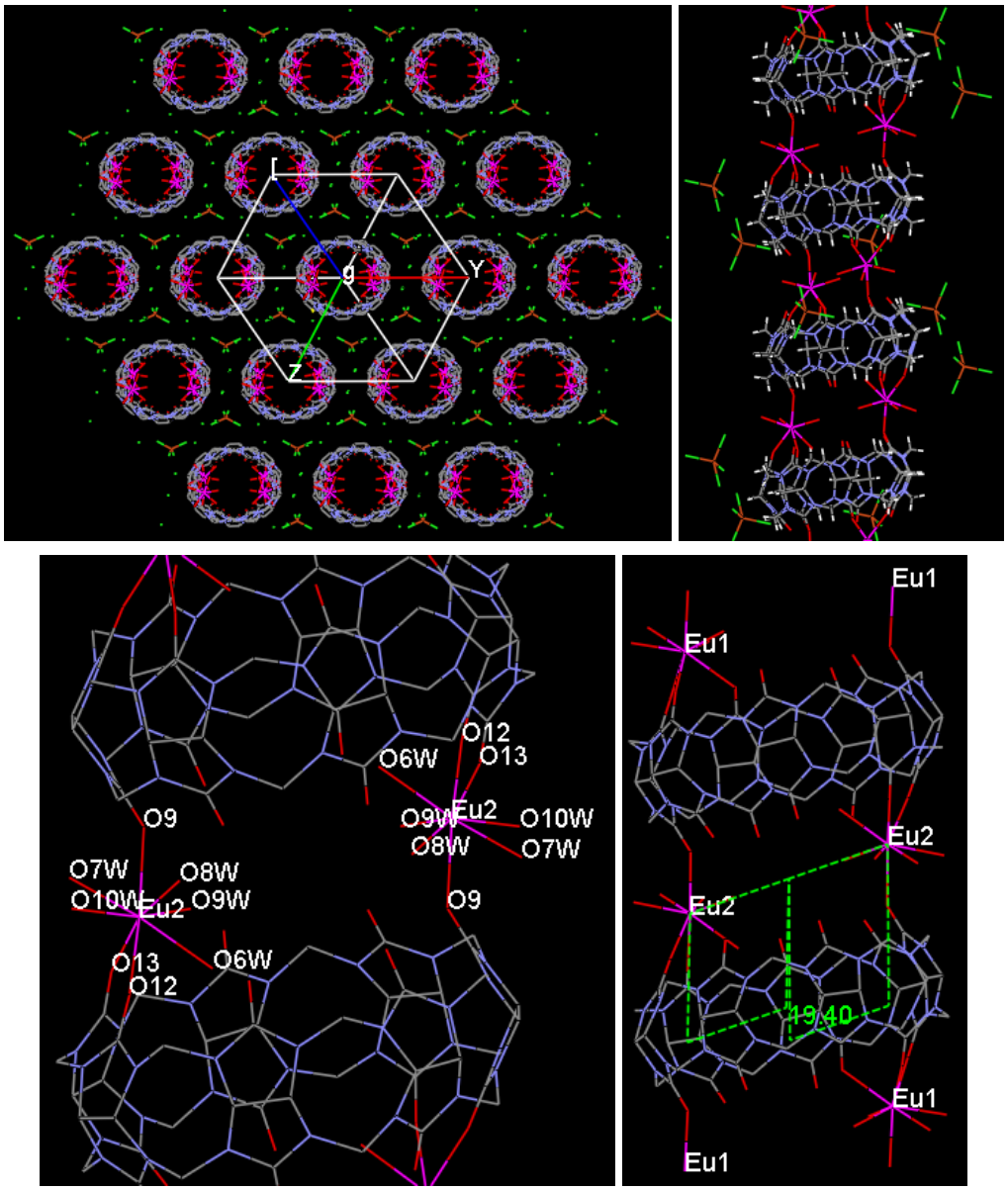


Figure S6. X-ray crystal structure of compound **6**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of Gd^{3+} cations and Q[7] molecules surrounded by the $[CuCl_4]^{2-}$ anions; (**c**) coordination of the Gd^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four Gd^{3+} cations coordinated to a Q[7] molecule.

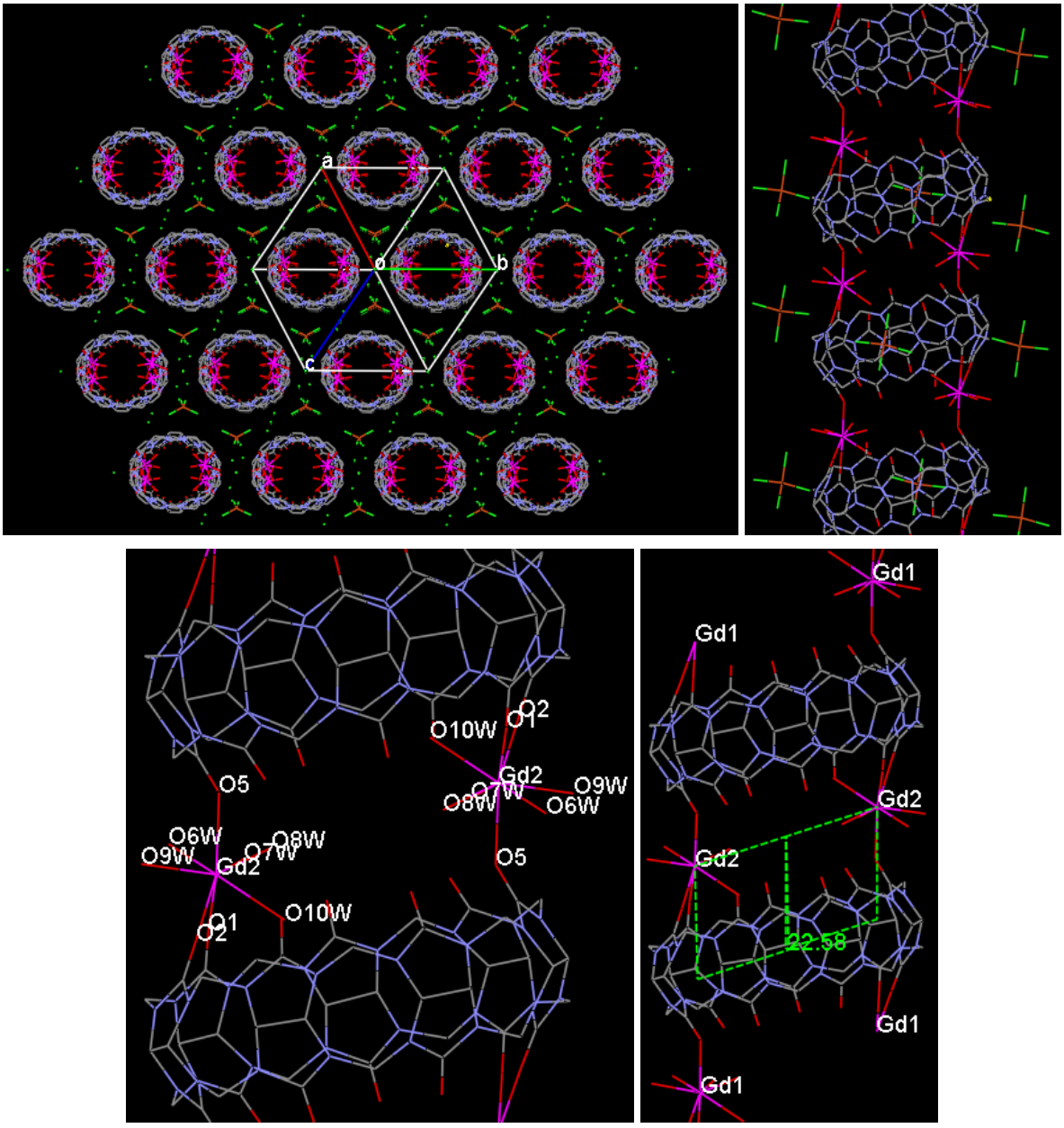


Figure S7. X-ray crystal structure of compound **7**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of Dy^{3+} cations and Q[7] molecules surrounded by the $[CoCl_4]^{2-}$ anions; (**c**) coordination of the Dy^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four Dy^{3+} cations coordinated to a Q[7] molecule.

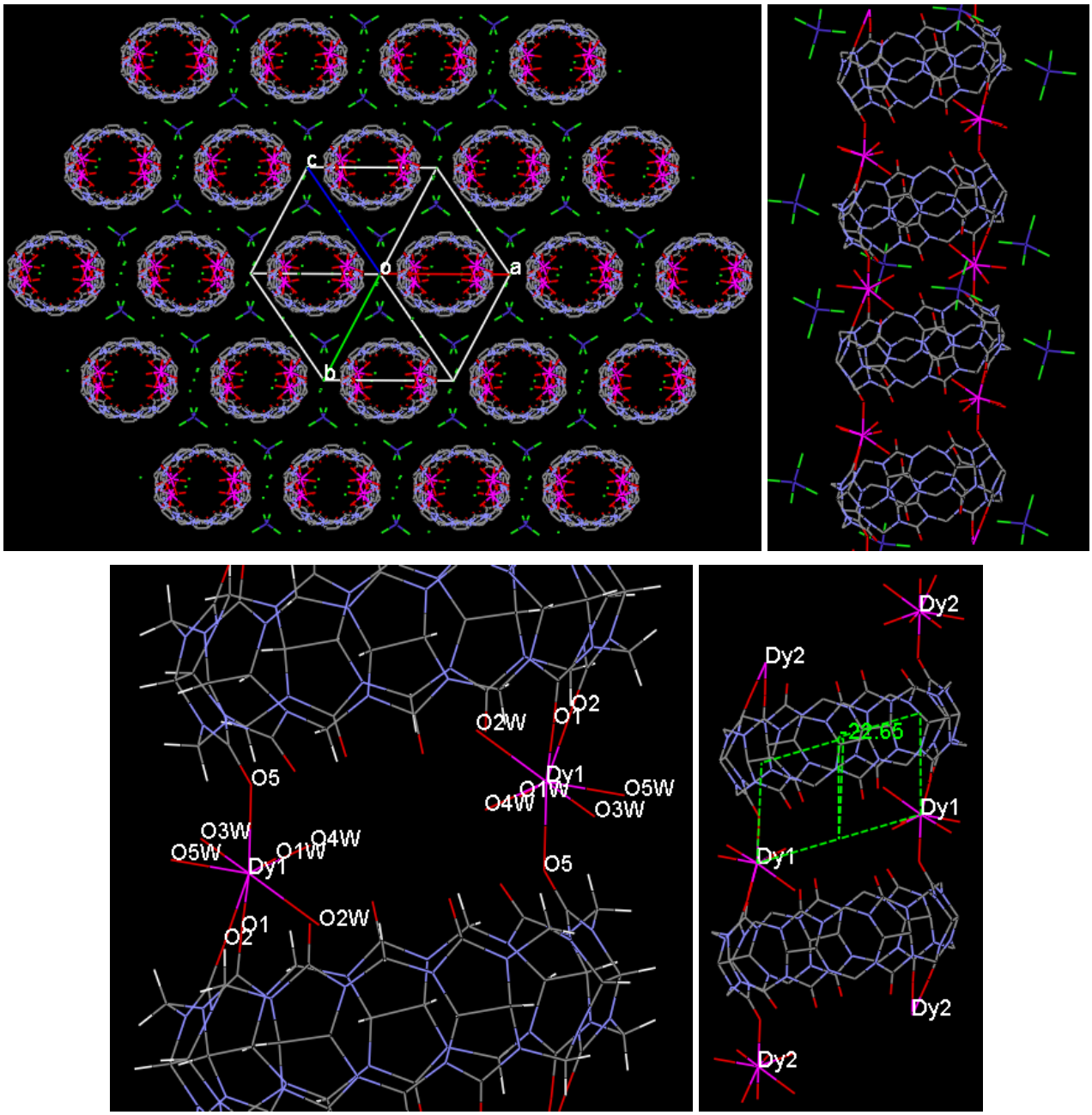
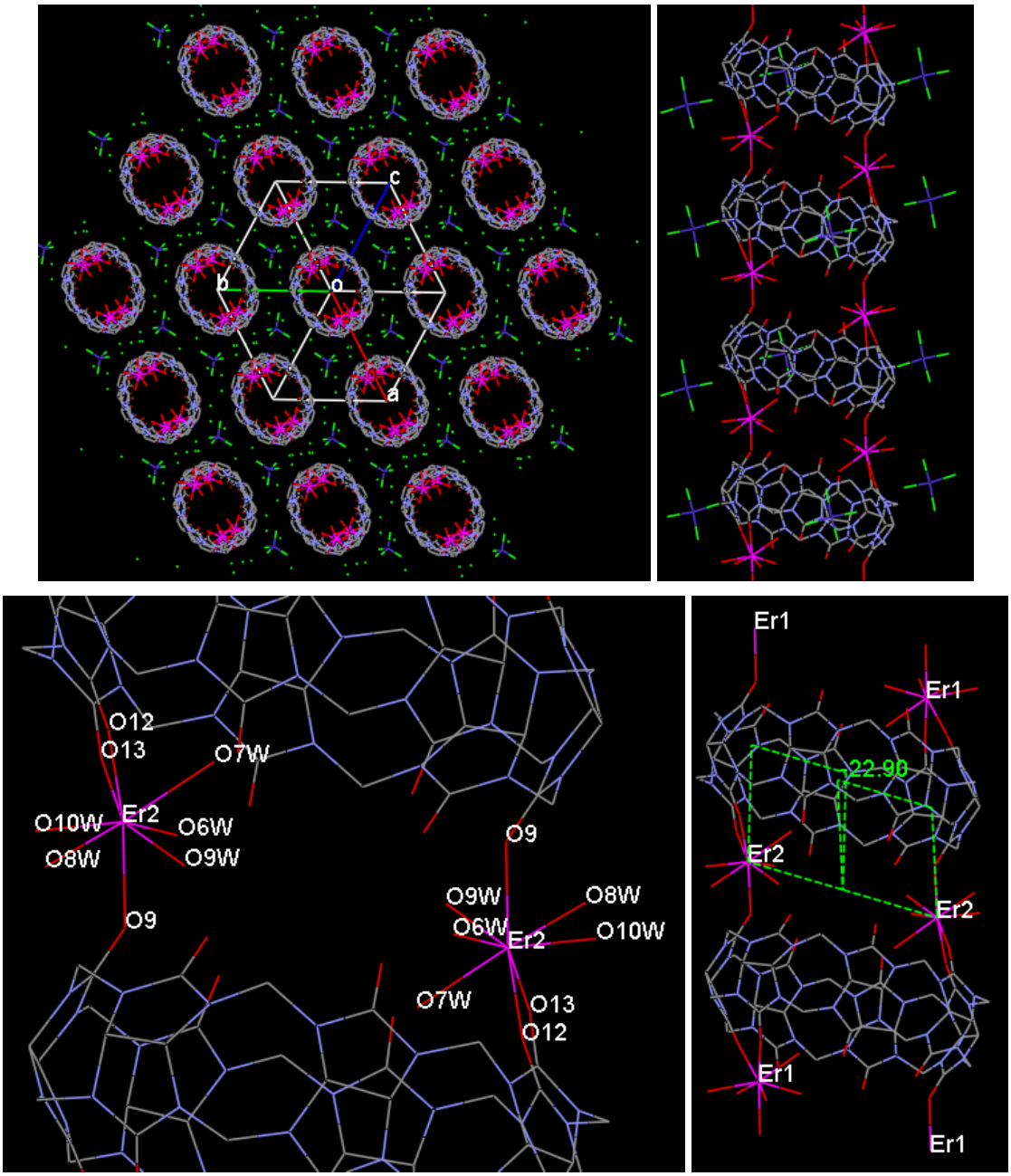


Figure S8. X-ray crystal structure of compound **8**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of Er^{3+} cations and Q[7] molecules surrounded by the $[CoCl_4]^{2-}$ anions; (**c**) coordination of the Er^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four Er^{3+} cations coordinated to a Q[7] molecule.



Crystal structures details of compounds in the third group are shown in Figures S9–S12:

Figure S9. X-ray crystal structure of compound **9**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of Eu^{3+} cations and Q[7] molecules surrounded by the $[CoCl_4]^{2-}$ anions; (**c**) coordination of the Eu^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four Eu^{3+} cations coordinated to a Q[7] molecule.

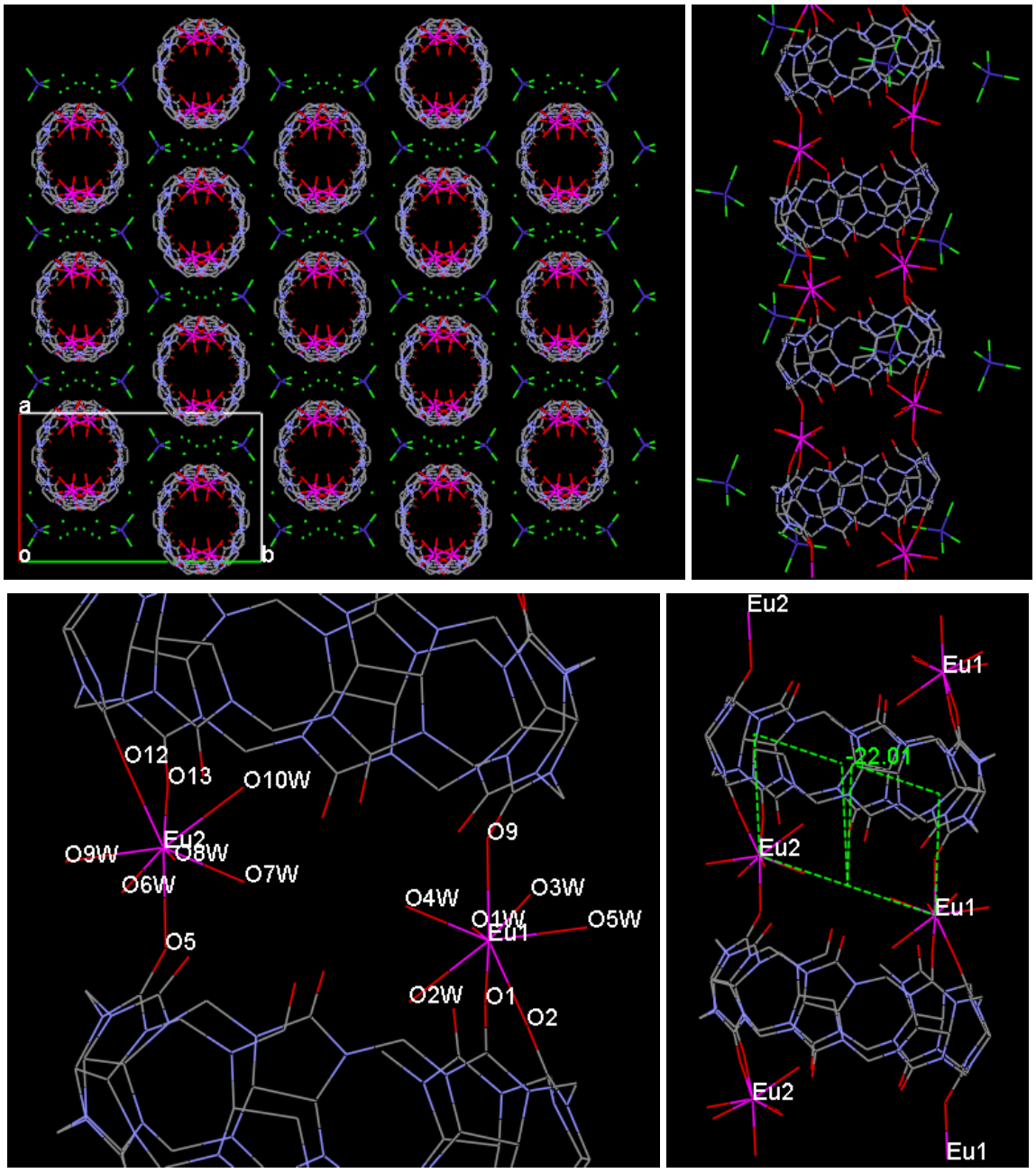


Figure S10. X-ray crystal structure of compound **10**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of Gd^{3+} cations and Q[7] molecules surrounded by the $[CoCl_4]^{2-}$ anions; (**c**) coordination of the Gd^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four Gd^{3+} cations coordinated to a Q[7] molecule.

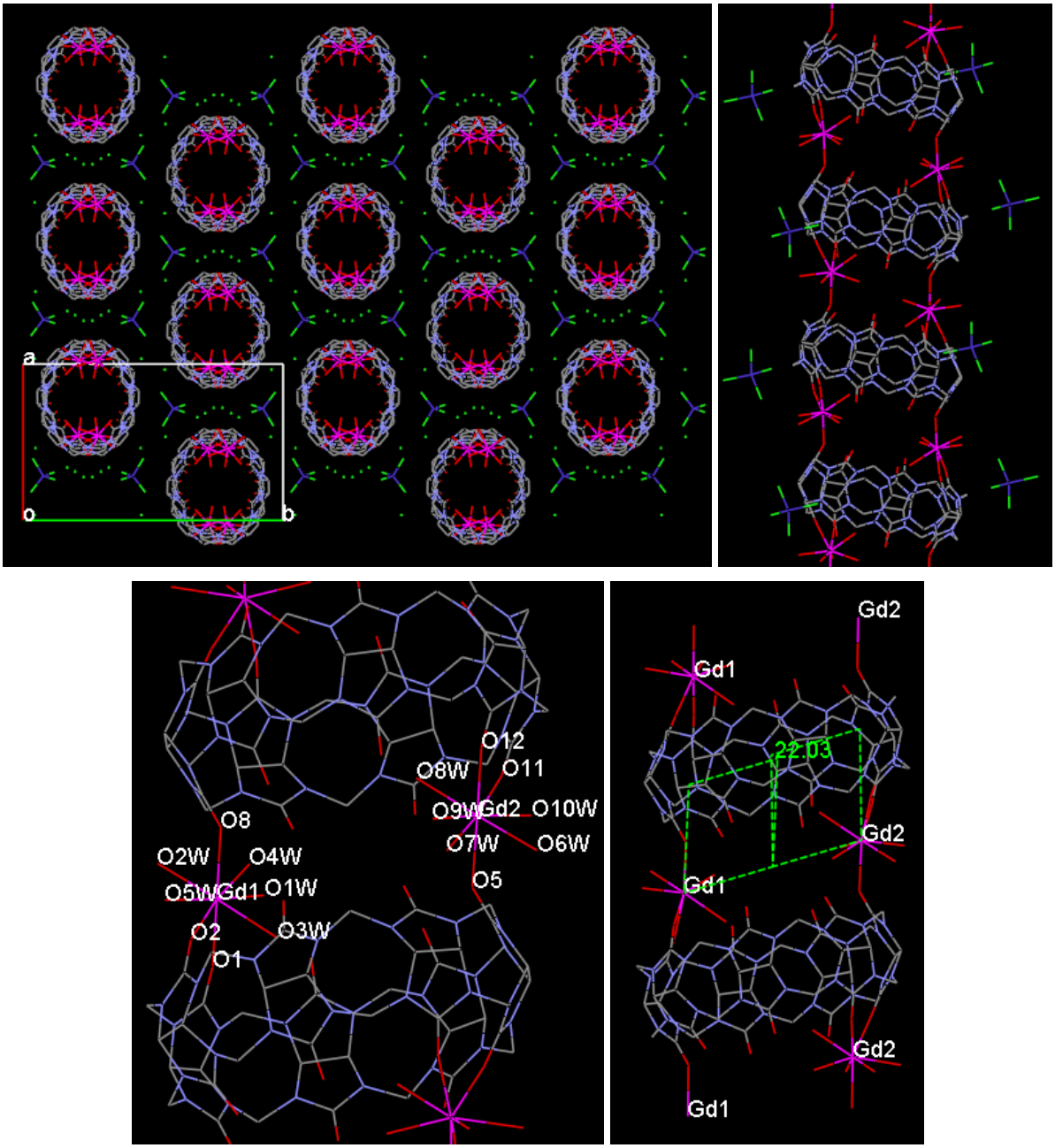


Figure S11. X-ray crystal structure of compound **11**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of Dy^{3+} cations and Q[7] molecules surrounded by the $[CuCl_4]^{2-}$ anions; (**c**) coordination of the Dy^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four Dy^{3+} cations coordinated to a Q[7] molecule.

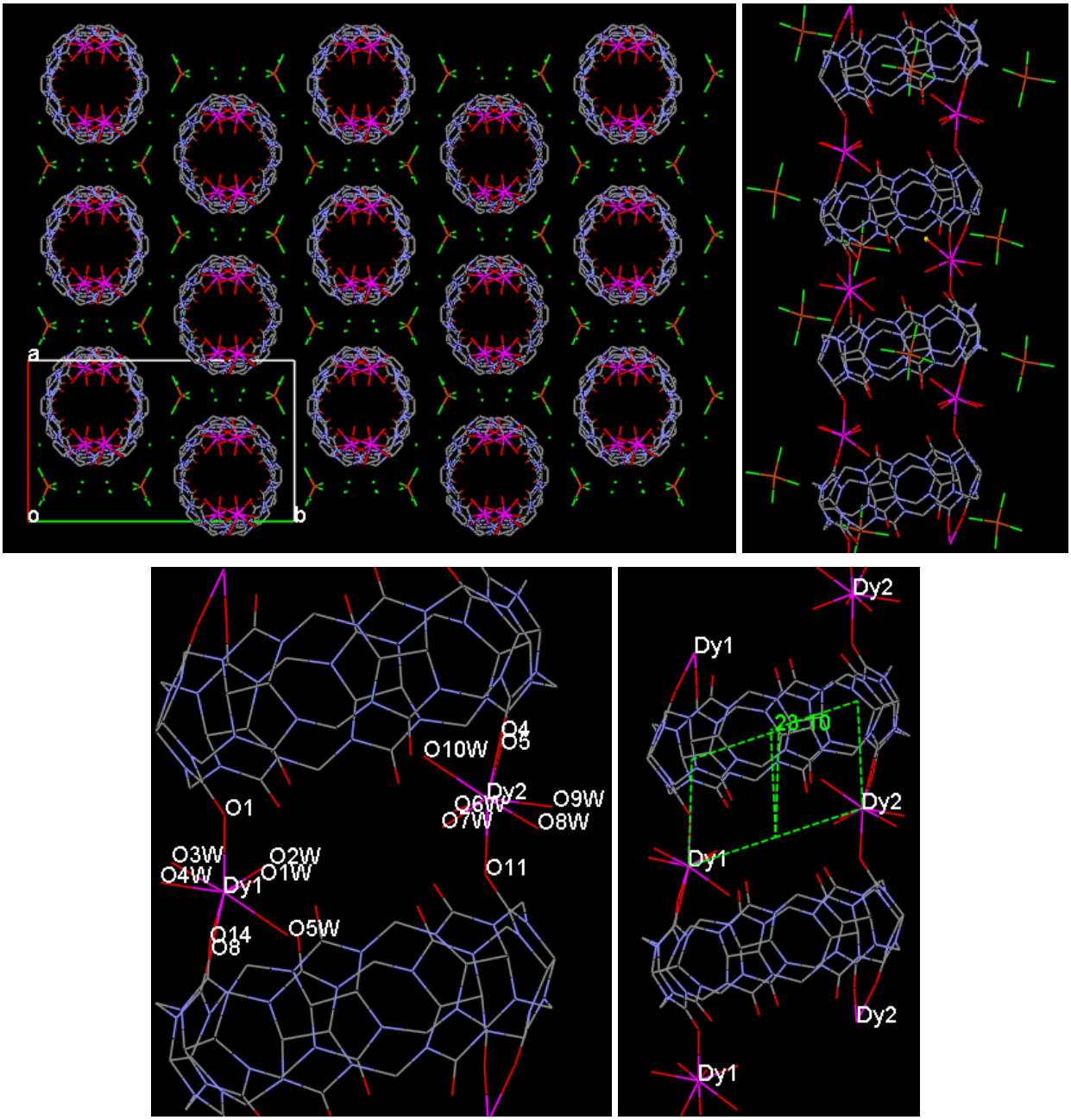


Figure S12. X-ray crystal structure of compound **12**: (**a**) an overall view of the coordination features and supramolecular assembly; (**b**) a 1D coordination polymer of Ho^{3+} cations and Q[7] molecules surrounded by the $[CoCl_4]^{2-}$ anions; (**c**) coordination of the Ho^{3+} cations by the portal carbonyl oxygens of the Q[7] molecules and water molecules; (**e**) torsion of the four Ho^{3+} cations coordinated to a Q[7] molecule.