Electronic Supplementary Information (ESI)

The solvent-controlled Al_{12}-Oxo molecular ring and Al_{24}-Oxo truncated metallo-cube

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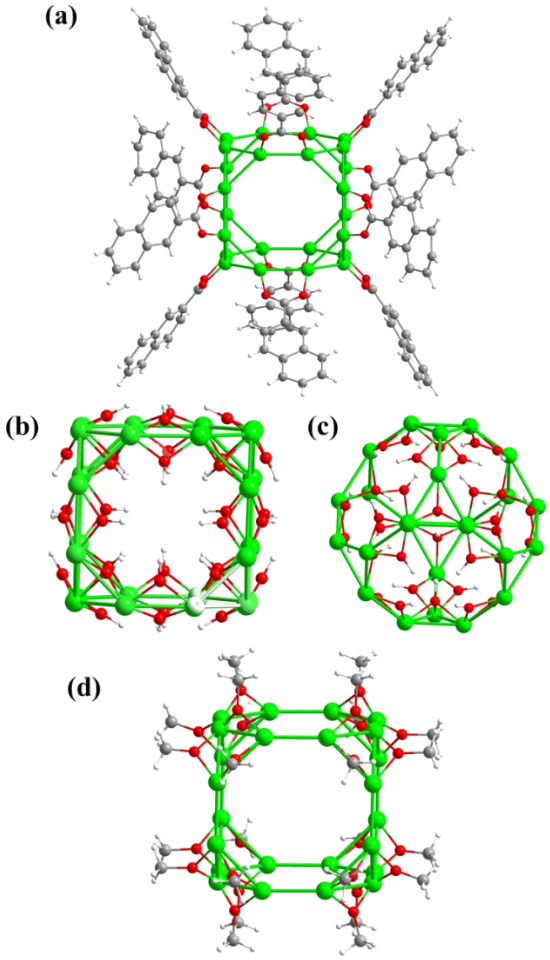

Fig. S1 The coordinated spatial positions of NAP^- ligands, OH^- and CH_3O^- in Al_{24} cluster.

Table S1. The formulas assignment of two sets of species of the negative-ion ESI-MS of Al_{24} in CH_3OH/CH_2Cl_2 solution.

Species	Peak assignment	Exp.*m/z*	Sim.*m/z*
1a	$[Al_{24}(OH)_{34}(CH_3O)_{26}(NAP)_{11}(H_2O)_4Cl_3]^{2-}$	2045.78	2045.70
1b	$[Al_{24}(OH)_{34}(CH_3O)_{23}(NAP)_{11}(H_2O)_4Cl_6]^{2-}$	2052.20	2052.21
1c	$[Al_{24}(OH)_{32}(CH_3O)_{28}(NAP)_{11}(H_2O)_4Cl_3]^{2-}$	2059.79	2059.72
1d	$[Al_{24}(OH)_{32}(CH_3O)_{25}(NAP)_{11}(H_2O)_4Cl_6]^{2-}$	2066.22	2066.27
1e	$[Al_{24}(OH)_{31}(CH_3O)_{30}(NAP)_{11}(H_2O)_1Cl_4H_2]^{2-}$	2073.79	2073.74
1f	$[Al_{24}(OH)_{31}(CH_3O)_{31}(NAP)_{11}Cl_4H_3]^{2-}$	2080.79	2080.75
1g	$[Al_{24}(OH)_{34}(CH_3O)_{23}(NAP)_{11}(H_2O)_6Cl_7H_1]^{2-}$	2088.20	2088.25
2a	$[Al_{22}(OH)_{23}(CH_3O)_{25}(NAP)_{12}(H_2O)_2Cl_7]^{-}$	4097.45	4097.41
2b	$[Al_{22}(OH)_{23}(CH_3O)_{26}(NAP)_{12}(H_2O)_1Cl_7H_1]^{-}$	4111.47	4111.43
2c	$[Al_{22}(OH)_{23}(CH_3O)_{27}(NAP)_{12}Cl_7H_2]^{-}$	4125.48	4125.44

Table S2. The formulas assignment of two sets of species of the positive-ion ESI-MS of Al_{24} in CH_3OH/CH_2Cl_2 solution.

Species	Peak assignment	Exp.m/z	Sim.m/z
1a	$[Al_{24}(OH)_{32}(CH_3O)_{25}(NAP)_{10}Cl_5(H_2O)_5H_2]^{2+}$	1974.24	1974.23
1b	$[Al_{24}(OH)_{32}(CH_3O)_{26}(NAP)_{10}Cl_5(H_2O)_4H_3]^{2+}$	1981.25	1981.25
1c	$[Al_{24}(OH)_{32}(CH_3O)_{26}(NAP)_{10}Cl_5(H_2O)_3(CH_3OH)_1H_3]^{2+}$	1988.26	1988.25
1d	$[Al_{24}(OH)_{32}(CH_3O)_{26}(NAP)_{10}Cl_5(H_2O)_2CH_3OH)_2H_3]^{2+}$	1995.27	1995.26
1e	$[Al_{24}(OH)_{32}(CH_3O)_{26}(NAP)_{10}Cl_5(H_2O)_1(CH_3OH)_3H_3]^{2+}$	2002.28	2002.26
1f	$[Al_{24}(OH)_{32}(CH_3O)_{26}(NAP)_{10}Cl_5(CH_3OH)_4H_3]^{2+}$	2009.28	2009.27
2a	$[Al_{24}(OH)_{32}(CH_3O)_{26}(NAP)_{10}Cl_5(H_2O)_1(CH_3CN)_2(CH_3OH)_3H_3]^{2+}$	2043.29	2043.29
2b	$[Al_{24}(OH)_{32}(CH_3O)_{26}(NAP)_{10}Cl_5(CH_3CN)_2(CH_3OH)_4H_3]^{2+}$	2050.30	2050.30
2c	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_2(H_2O)_3]^{2+}$	2057.31	2057.30
2d	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_2(H_2O)_2(CH_3OH)_1]^{2+}$	2064.32	2064.30
2e	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_2(H_2O)_1(CH_3OH)_2]^{2+}$	2071.33	2071.31
2f	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_2(CH_3OH)_3]^{2+}$	2078.33	2078.32
2g	$[Al_{24}(OH)_{32}(CH_3O)_{25}(NAP)_{12}Cl_1(H_2O)_1(CH_3OH)_3]^{2+}$	2085.34	2085.35
3a	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_2(H_2O)_5(CH_3CN)_1(CH_3OH)_1]^{2+}$	2111.84	2111.83
3b	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_2(H_2O)_3(CH_3CN)_3]^{2+}$	2119.35	2119.34
3c	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_2(H_2O)_2(CH_3CN)_3(CH_3OH)_1]^{2+}$	2126.36	2126.35
3d	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_3(H_2O)_4(CH_3OH)_3H_1]$	2132.87	2132.83

	$^{2+}$		
3e	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_4(H_2O)_1(CH_3OH)_4H_2]^{2+}$	2140.38	2140.32
3f	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_4(CH_3OH)_5H_2]^{2+}$	2147.38	2147.32
3g	$[Al_{24}(OH)_{32}(CH_3O)_{25}(NAP)_{11}Cl_4(H_2O)_3(CH_3CN)_4(CH_3OH)_3H_2]^{2+}$	2154.39	2154.35
4a	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_2(H_2O)_3(CH_3CN)_4(CH_3OH)_3]^{2+}$	2187.90	2187.89
4b	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_2(H_2O)_2(CH_3CN)_4(CH_3OH)_4]^{2+}$	2194.91	2194.90
4c	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_2(H_2O)_1(CH_3CN)_4(CH_3OH)_5]^{2+}$	2201.91	2201.91
4d	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{12}Cl_2(CH_3CN)_4(CH_3OH)_6]^{2+}$	2208.92	2208.91
4e	$[Al_{24}(OH)_{32}(CH_3O)_{24}(NAP)_{13}Cl_1(H_2O)_6(CH_3OH)_4]^{2+}$	2216.43	2216.40

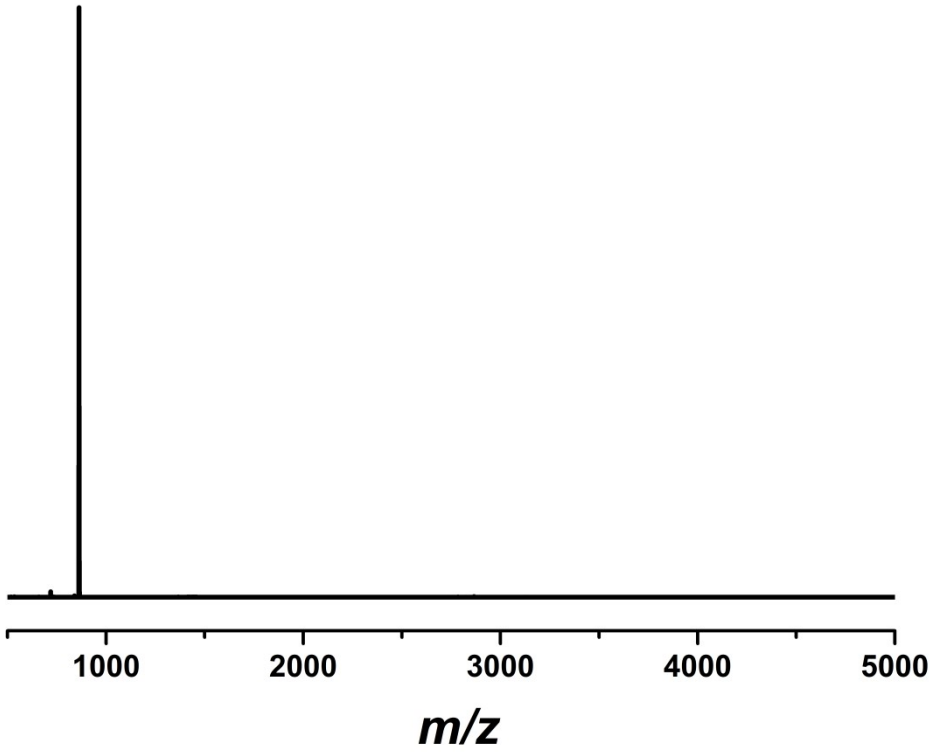

Fig. S2 The negative-ion ESI-MS of Al_{12} in CH_3OH/CH_2Cl_2

Table S3. The formulas assignment of two sets of species of Al_{12} in CH_3OH/CH_2Cl_2 solution.

Species	Peak assignment	Exp.m/z	Sim.m/z
1a	$[Al_{12}(CH_3O)_{17}(NAP)_{17}(H_2O)_8]^{2+}$	1953.40	1953.48
1b	$[Al_{12}(CH_3O)_{16}(NAP)_{18}(H_2O)_1]^{2+}$	1960.40	1960.45
1c	$[Al_{12}(CH_3O)_{17}(NAP)_{18}H_1]^{2+}$	1967.40	1967.46
1d	$[Al_{12}(CH_3O)_{20}(NAP)_{17}(H_2O)_5H_3]^{2+}$	1974.42	1974.50
1e	$[Al_{12}(CH_3O)_{21}(NAP)_{17}(H_2O)_4H_4]^{2+}$	1981.43	1981.51
1f	$[Al_{11}(CH_3O)_{12}(NAP)_{19}(H_2O)_3]^{2+}$	1988.42	1988.46
1g	$[Al_{11}(CH_3O)_{13}(NAP)_{19}(H_2O)_2H_1]^{2+}$	1995.43	1995.47
1h	$[Al_{11}(CH_3O)_{14}(NAP)_{19}(H_2O)_1H_2]^{2+}$	2002.44	2002.47
1i	$[Al_{11}(CH_3O)_{15}(NAP)_{19}H_3]^{2+}$	2009.44	2009.48
1j	$[Al_{10}(CH_3O)_8(NAP)_{20}(H_2O)_5]^{2+}$	2016.46	2016.50
2a	$[Al_{13}(CH_3O)_{20}(NAP)_{19}(H_2O)_1H_2]^{2+}$	2122.54	2122.51
2b	$[Al_{13}(CH_3O)_{21}(NAP)_{19}H_3]^{2+}$	2129.55	2129.52
2c	$[Al_{12}(CH_3O)_{14}(NAP)_{20}(H_2O)_5]^{2+}$	2136.56	2136.50
2d	$[Al_{12}(CH_3O)_{15}(NAP)_{20}(H_2O)_4H_1]^{2+}$	2143.56	2143.51
2e	$[Al_{12}(CH_3O)_{16}(NAP)_{20}(H_2O)_3H_2]^{2+}$	2150.57	2150.52
2f	$[Al_{12}(CH_3O)_{17}(NAP)_{20}(H_2O)_2H_3]^{2+}$	2157.58	2157.52
3a	$[Al_{14}(CH_3O)_{20}(NAP)_{20}(H_2O)_9]^{2+}$	2292.59	2292.56
3b	$[Al_{14}(CH_3O)_{21}(NAP)_{20}(H_2O)_8H_1]^{2+}$	2299.58	2299.57
3c	$[Al_{14}(CH_3O)_{22}(NAP)_{20}(H_2O)_7H_2]^{2+}$	2306.60	2306.57
3d	$[Al_{14}(CH_3O)_{23}(NAP)_{20}(H_2O)_6H_3]^{2+}$	2313.60	2313.58
3e	$[Al_{14}(CH_3O)_{24}(NAP)_{20}(H_2O)_5H_4]^{2+}$	2320.61	2320.59
3f	$[Al_{14}(CH_3O)_{25}(NAP)_{20}(H_2O)_4H_5]^{2+}$	2327.62	2327.60

Table S4. The hydrogen bond interactions of cluster Al_{24}.

D-H	*d*(D-H)	*d*(H···A)	<D-H-A	*d*(D···A)	A
O1-H1	0.95	2.321	161.53	3.236	Cl2
O8-H8	0.95	2.353	163.88	3.276	Cl1
O9-H9	0.95	2.301	162.68	3.22	Cl1
O10-H10	0.95	2.318	163.89	3.241	Cl2
O11-H11	0.95	2.337	163.44	3.259	Cl2
O12-H12	0.95	2.331	163.05	3.251	Cl2 [-x+1, -y+1, -z+1]
O13-H13	0.95	2.345	165.17	3.272	Cl3
O15-H15	0.95	2.379	164.55	3.304	Cl3
O16-H16	0.95	2.3	165.46	3.228	Cl1 [-x+1, -y+1, -z+1]
O22-H22	0.95	2.296	162.42	3.214	Cl3
O23-H23	0.95	2.325	161.25	3.239	Cl1
O32-H32	0.95	2.26	161.17	3.174	Cl3

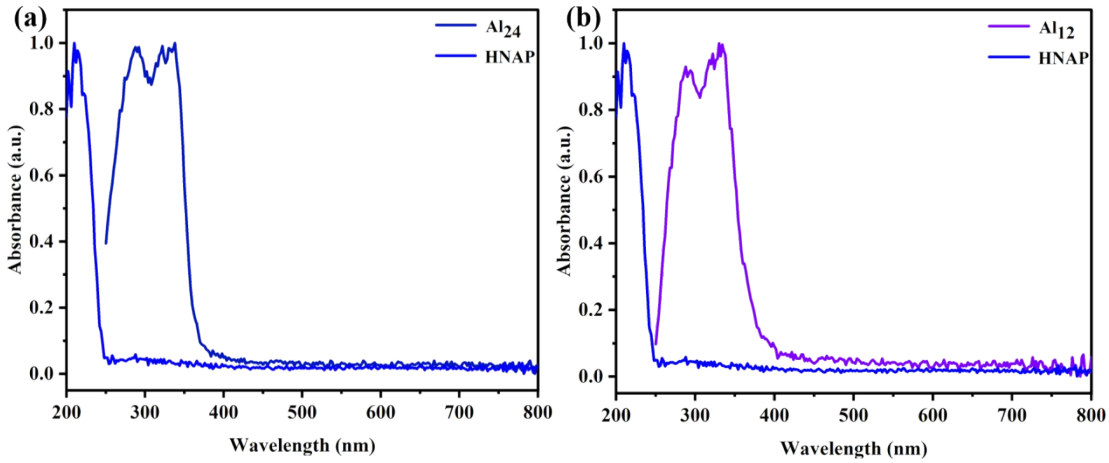

Fig. S3 The solid-state ultraviolet-visible absorption spectra (UV-Vis) of HNAP and Al_{24}, HNAP and Al_{12} under room temperature.

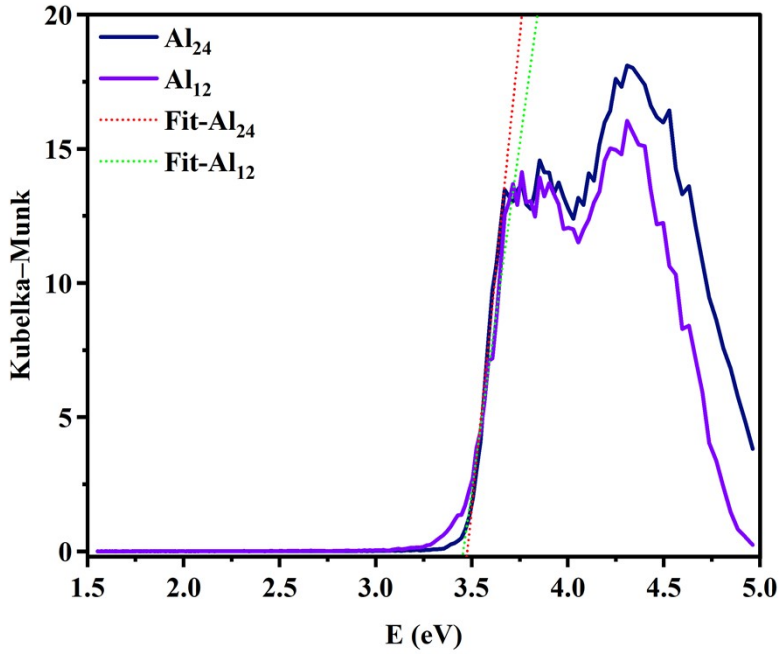

Fig. S4 Absorption spectra of Al_{24} and Al_{12} derived from the diffuse reflectance spectra through Kubelka-Munk function.

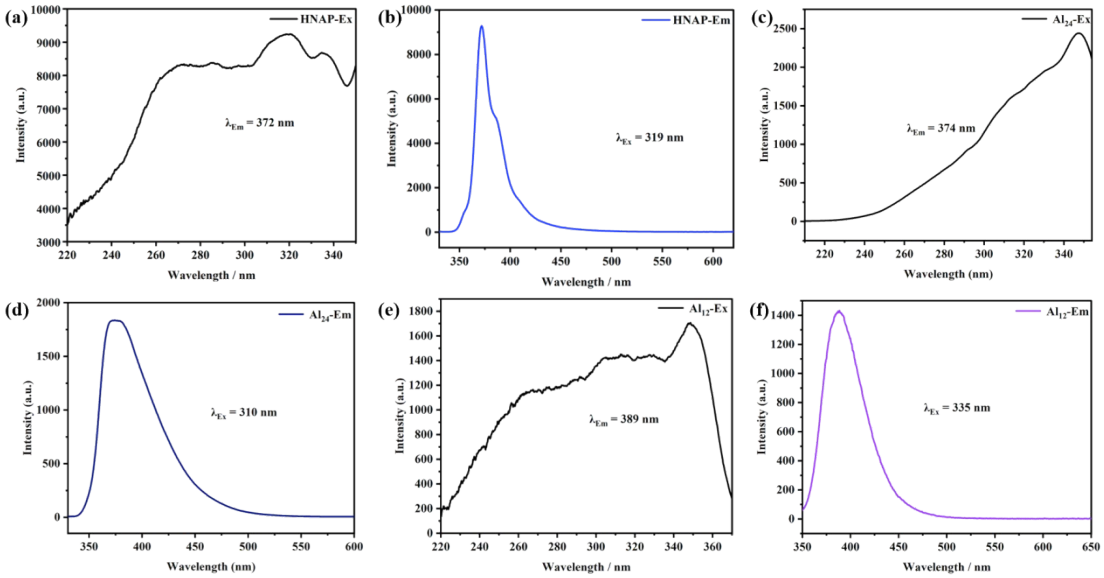

Fig. S5 The emission and excitation spectra of the powder samples of HNAP, Al_{24} and Al_{12} under room temperature.

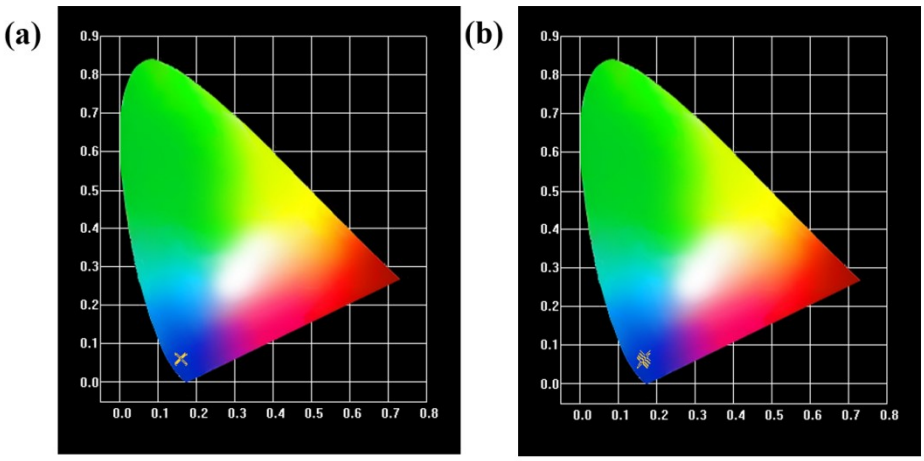

Fig. S6 CIE chromatic coordinates of Al_{24}(a) and Al_{12}(b).

Table S5. The corresponding chromaticity coordinates of Al_{24} and Al_{12}.

	Al_{24}		Al_{12}	
	x	y	x	y
300K	0.1571	0.0614	0.1623	0.053
270K	0.1575	0.0588	0.1631	0.0525
240K	0.158	0.0565	0.1637	0.0549
210K	0.159	0.0555	0.1644	0.0572
180K	0.1598	0.0548	0.1658	0.061
150K	0.1609	0.0562	0.1672	0.0646
120K	0.1618	0.0577	0.169	0.0695
90K	0.1625	0.0591	0.17	0.0726

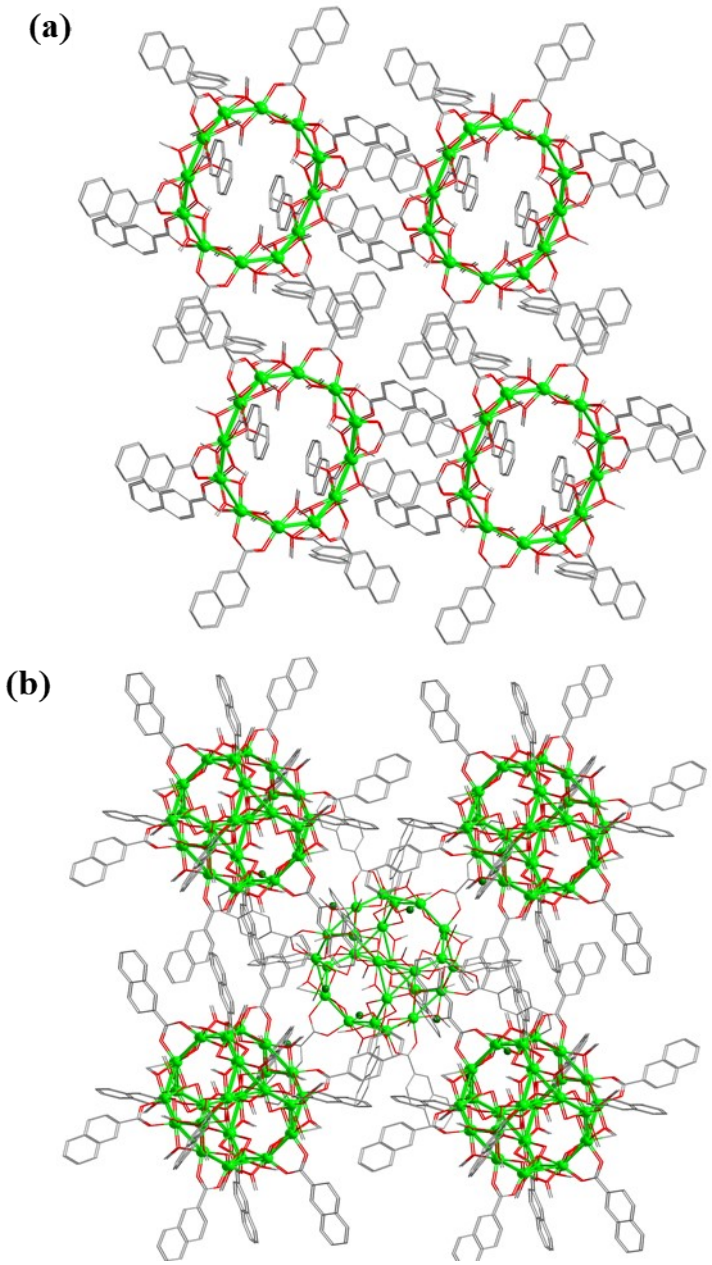

Fig. S7 The packing structures of Al_{12}(a) and Al_{24}(b).

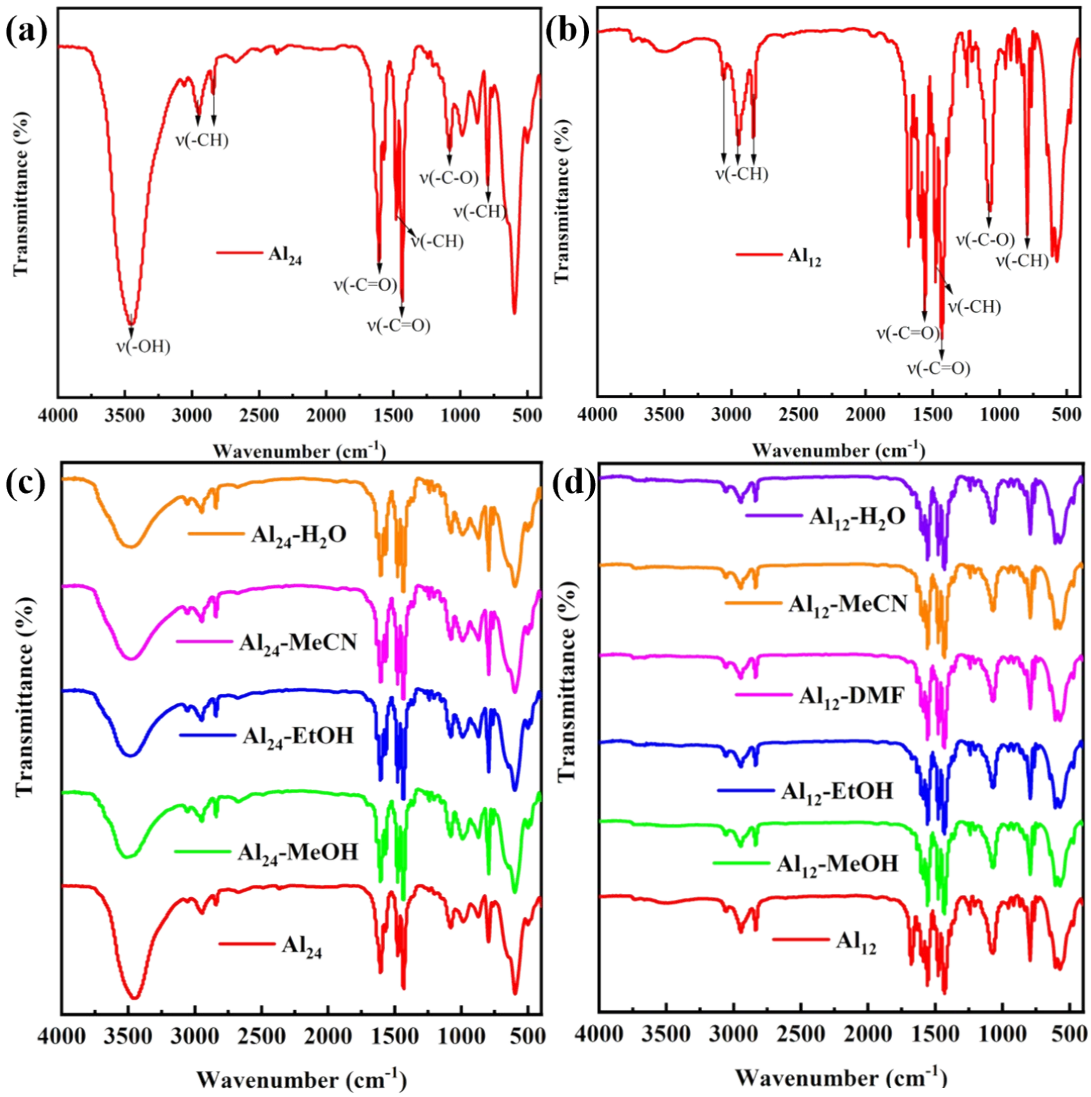

Fig. S8 The IR spectra of Al_{24} (a), Al_{12} (b), and IR of the crystal after soaking in different solvents (c, d).

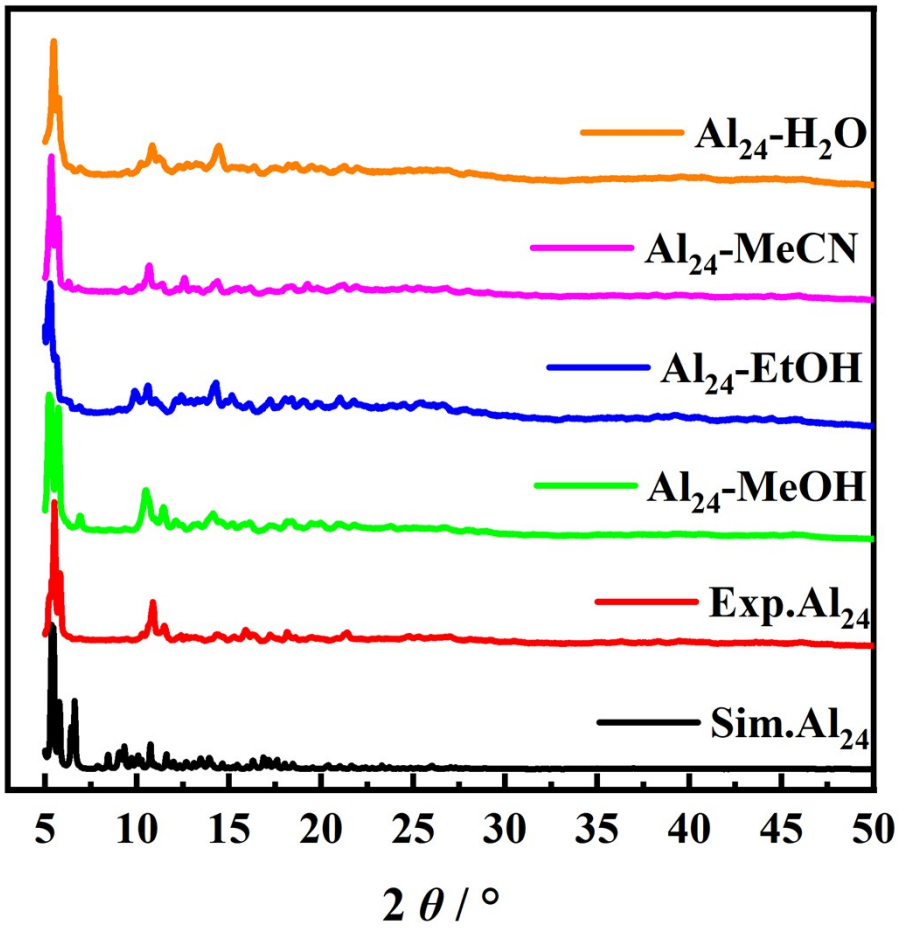

Fig. S9 The simulated and experimental PXRD of Al_{24} and the crystal after soaking in different solvents for 24h.

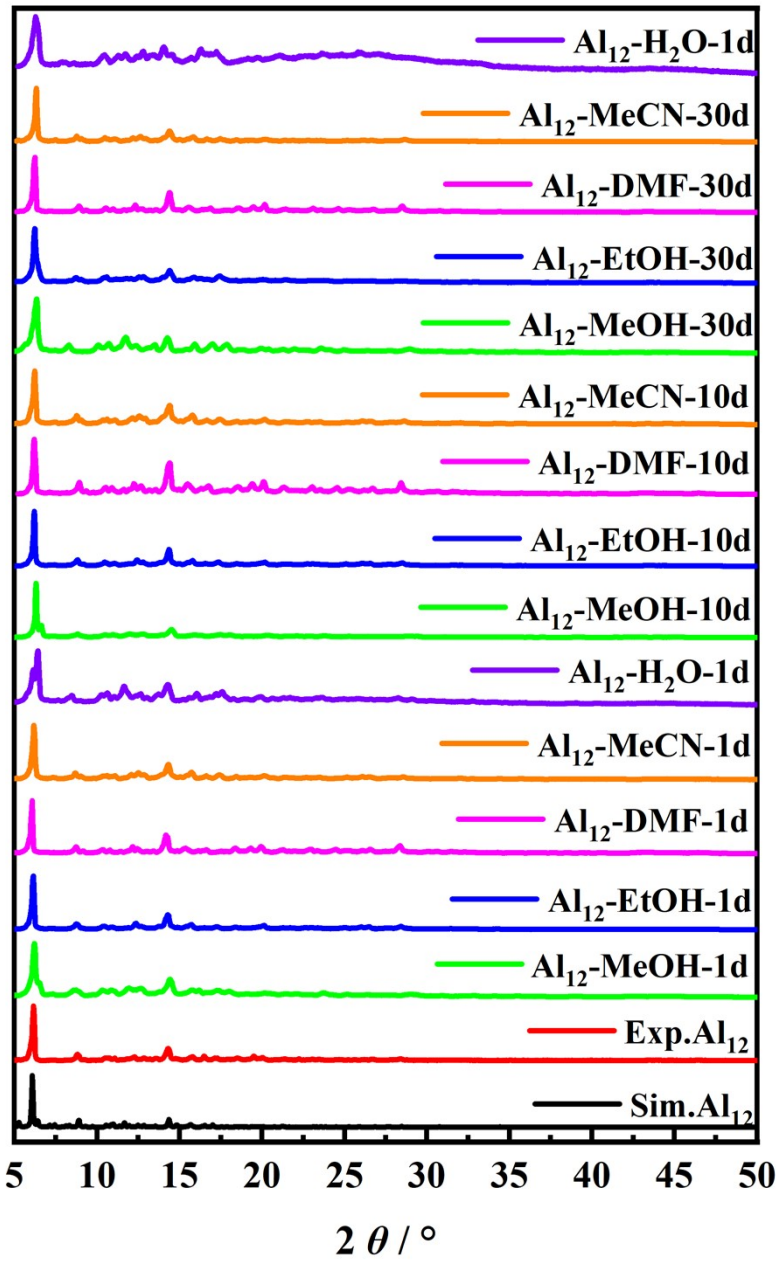

Fig. S10 The simulated and experimental PXRD of Al_{12} and the crystal after soaking in different solvents from 1d to 30d.

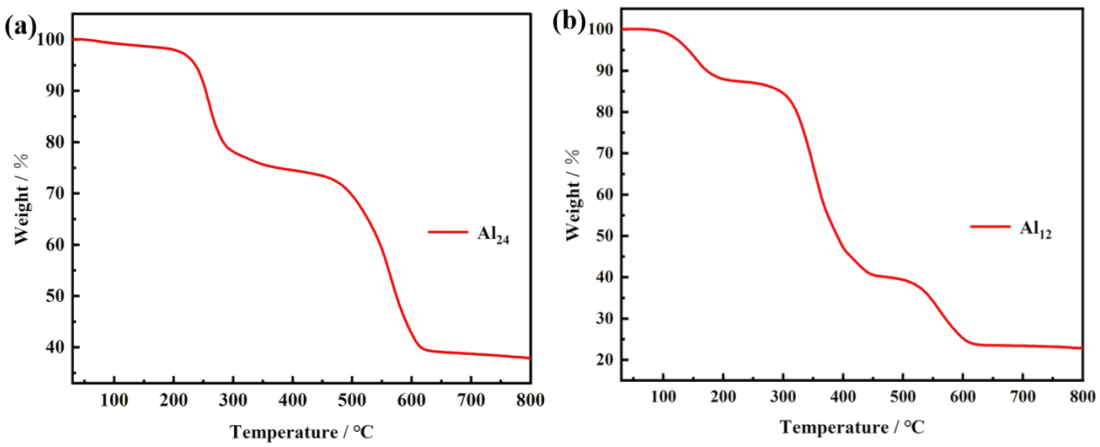

Fig. S11 The TGA of Al_{24} and Al_{12}.

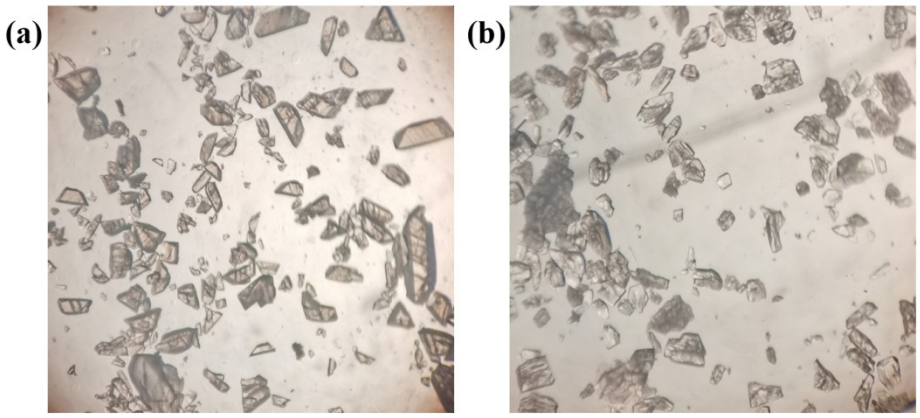

Fig. S12 Microscope photographs of crystals of Al_{24}(a) and Al_{12}(b).

Table S6. Crystal data for Al_{24} and Al_{12}.

Identification code	**Al_{24}**	**Al_{12}**
Empirical formula	$C_{158}H_{202}Al_{24}Cl_6O_{84}$	$C_{170}H_{196}Al_{12}N_4O_{56}$
Formula weight	4305.51	3515.14
Temperature/K	120.00(10)	293(2)
Crystal system	monoclinic	triclinic
Space group	$P2_1/n$	P-1
a/Å	22.4243(8)	14.9026(6)
b/Å	20.9573(4)	17.4708(5)
c/Å	26.8950(5)	18.5727(3)
α/°	90	100.822(2)
β/°	97.007(2)	92.904(2)
γ/°	90	101.735(3)
Volume/Å^3	12545.0(6)	4630.4(2)
Z	2	1
ρ_{calc}g/cm^3	1.113	1.121
μ/mm^{-1}	2.06	1.196
F(000)	4356	1634.0
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.362 to 154.214	4.864 to 154.856
Index ranges	-23 ≤ h ≤ 28, -25 ≤ k ≤ 26, -33 ≤ l ≤ 32	-18 ≤ h ≤ 18, -21 ≤ k ≤ 22, -15 ≤ l ≤ 23
Reflections collected	83142	58907
Independent reflections	23912 [R_{int} = 0.0376, R_{sigma} = 0.0366]	18569 [R_{int} = 0.0480, R_{sigma} = 0.0354]
Data/restraints/parameters	23912/584/1162	18569/108/959
Goodness-of-fit on F^2	0.993	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.1026, wR_2 = 0.2768	R_1 = 0.0875, wR_2 = 0.2687
Final R indexes [all data]	R_1 = 0.1667, wR_2 = 0.3528	R_1 = 0.1091, wR_2 = 0.2983
Largest diff. peak/hole / e Å^{-3}	0.45/-0.23	1.05/-0.55

Table S7. Selected bond distances (Å) and angles (°) for Al_{24} and Al_{12}.

Al_{24}			
Al1—O6	1.987 (4)	Al6—O34	1.839 (5)
Al1—O12	1.881 (5)	Al6—O36	1.859 (5)
Al1—O20	1.855 (4)	Al7—O15	1.883 (6)
Al1—O22	1.874 (4)	Al7—O16	1.867 (4)
Al1—O25	1.889 (6)	Al7—O35	1.861 (4)
Al1—O30	1.927 (4)	Al7—O37^{i}	1.867 (7)
Al2—O4	1.972 (3)	Al7—O38	1.908 (5)
Al2—O14	1.849 (4)	Al8—O10	1.850 (4)
Al2—O15	1.869 (4)	Al8—O13	1.860 (4)
Al2—O16	1.881 (5)	Al8—O18	1.860 (5)
Al2—O18	1.875 (6)	Al8—O19	1.874 (4)
Al2—O40	1.926 (4)	Al8—O26	1.957 (7)
Al3—O1^{i}	1.868 (5)	Al9—O3^{i}	1.958 (5)
Al3—O5^{i}	1.915 (4)	Al9—O11	1.890 (5)
Al3—O6	1.971 (4)	Al9—O21	1.854 (4)
Al3—O9	1.887 (4)	Al9—O23	1.866 (4)
Al3—O17	1.860 (5)	Al9—O24	1.919 (6)
Al3—O20	1.849 (4)	Al9—O37	1.852 (5)
Al4—O4	1.973 (3)	Al10—O17	1.865 (4)
Al4—O7	1.914 (4)	Al10—O25	1.855 (5)
Al4—O9^{i}	1.851 (5)	Al10—O27	1.942 (6)
Al4—O14	1.885 (4)	Al10—O32	1.856 (4)
Al4—O19	1.893 (5)	Al11—O11	1.823 (5)
Al5—O12	1.856 (4)	Al11—O23	1.872 (4)
Al5—O21^{i}	1.898 (5)	Al11—O28	1.918 (5)
Al5—O22	1.867 (6)	Al11—O29	1.859 (5)
Al5—O31	1.908 (4)	Al11—O34	1.866 (5)
Al5—O35	1.856 (4)	Al12—O13	1.886 (5)
Al6—O8	1.835 (4)	Al12—O29	1.881 (5)
Al6—O32	1.853 (5)	Al12—O36	1.869 (5)
Al6—O33	1.939 (5)	Al12—O39	1.952 (5)
O12—Al1—O6	99.72 (18)	O15—Al7—O3	97.01 (18)
O12—Al1—O25	169.90 (18)	O15—Al7—O38	93.6 (2)
O12—Al1—O30	93.0 (2)	O16—Al7—O3	98.48 (16)
O20—Al1—O6	78.24 (15)	O16—Al7—O15	76.80 (19)
O20—Al1—O12	95.4 (2)	O16—Al7—O37^{i}	94.5 (2)
O20—Al1—O22	170.4 (2)	O16—Al7—O38	93.65 (18)
O20—Al1—O25	93.9 (2)	O35—Al7—O3	77.84 (16)

O20—Al1—O30	90.70 (18)	O35—Al7—O15	94.0 (2)
O22—Al1—O6	99.36 (16)	O35—Al7—O16	169.7 (2)
O22—Al1—O12	75.7 (2)	O35—Al7—O37^{i}	94.2 (2)
O22—Al1—O25	94.8 (2)	O35—Al7—O38	91.50 (19)
O22—Al1—O30	93.43 (18)	O37^{i}—Al7—O3	78.4 (2)
O25—Al1—O6	78.43 (18)	O37^{i}—Al7—O15	169.6 (2)
O25—Al1—O30	90.7 (2)	O37^{i}—Al7—O38	92.7 (2)
O30—Al1—O6	163.8 (2)	O38—Al7—O3	165.4 (2)
O14—Al2—O4	78.49 (15)	O10—Al8—O4	99.45 (19)
O14—Al2—O15	169.9 (3)	O10—Al8—O13	75.96 (17)
O14—Al2—O16	93.8 (2)	O10—Al8—O18	170.26 (18)
O14—Al2—O18	94.5 (2)	O10—Al8—O19	94.08 (18)
O14—Al2—O40	92.27 (18)	O10—Al8—O26	91.9 (2)
O15—Al2—O4	99.26 (16)	O13—Al8—O4	99.42 (18)
O15—Al2—O16	76.8 (2)	O13—Al8—O19	169.67 (19)
O15—Al2—O18	94.7 (2)	O13—Al8—O26	91.5 (2)
O15—Al2—O40	91.94 (18)	O18—Al8—O4	78.8 (2)
O16—Al2—O4	99.74 (17)	O18—Al8—O13	94.78 (18)
O16—Al2—O40	93.3 (2)	O18—Al8—O19	95.00 (19)
O18—Al2—O4	78.48 (18)	O18—Al8—O26	91.4 (2)
O18—Al2—O16	171.00 (19)	O19—Al8—O4	79.26 (18)
O18—Al2—O40	90.0 (2)	O19—Al8—O26	91.6 (2)
O40—Al2—O4	164.5 (2)	O26—Al8—O4	165.8 (2)
O1^{i}—Al3—O5^{i}	94.1 (2)	O11—Al9—O3^{i}	99.81 (18)
O1^{i}—Al3—O6	99.65 (17)	O11—Al9—O24	93.1 (2)
O1^{i}—Al3—O9	75.80 (19)	O21—Al9—O3^{i}	80.55 (19)
O5^{i}—Al3—O6	163.6 (2)	O21—Al9—O11	94.8 (2)
O9—Al3—O5^{i}	92.51 (18)	O21—Al9—O23	169.5 (2)
O9—Al3—O6	99.38 (15)	O21—Al9—O24	89.5 (2)
O17—Al3—O1^{i}	168.82 (17)	O23—Al9—O3^{i}	98.46 (17)
O17—Al3—O5^{i}	89.9 (2)	O23—Al9—O11	74.97 (18)
O17—Al3—O6	78.21 (18)	O23—Al9—O24	93.5 (2)
O17—Al3—O9	93.6 (2)	O24—Al9—O3^{i}	164.3 (2)
O20—Al3—O1^{i}	96.1 (2)	O37—Al9—O3^{i}	79.3 (2)
O20—Al3—O5^{i}	91.05 (17)	O37—Al9—O11	169.6 (2)
O20—Al3—O6	78.80 (16)	O37—Al9—O21	95.2 (2)
O20—Al3—O9	171.3 (2)	O37—Al9—O23	94.90 (19)
O20—Al3—O17	94.3 (2)	O37—Al9—O24	89.6 (2)
O1—Al4—O4	98.52 (15)	O8—Al10—O6	99.35 (18)
O1—Al4—O7	93.96 (17)	O8—Al10—O27	92.7 (2)
O1—Al4—O14	170.9 (2)	O17—Al10—O6	78.1 (2)

O1—Al4—O19	94.3 (2)	O17—Al10—O8	94.04 (18)
O7—Al4—O4	164.5 (2)	O17—Al10—O27	90.8 (2)
O9^{i}—Al4—O1	76.92 (19)	O25—Al10—O6	79.7 (2)
O9^{i}—Al4—O4	99.25 (16)	O25—Al10—O8	170.75 (19)
O9^{i}—Al4—O7	92.5 (2)	O25—Al10—O17	94.77 (19)
O9^{i}—Al4—O14	95.4 (2)	O25—Al10—O27	90.0 (2)
O9^{i}—Al4—O19	170.65 (19)	O25—Al10—O32	95.87 (19)
O14—Al4—O4	77.62 (15)	O27—Al10—O6	164.15 (19)
O14—Al4—O7	91.29 (17)	O32—Al10—O6	99.71 (19)
O14—Al4—O19	93.1 (2)	O32—Al10—O8	75.16 (17)
O19—Al4—O4	78.78 (17)	O32—Al10—O17	168.58 (19)
O19—Al4—O7	91.20 (19)	O32—Al10—O27	93.3 (2)
O12—Al5—O3	98.75 (16)	O11—Al11—O2	98.9 (2)
O12—Al5—O21^{i}	94.0 (2)	O11—Al11—O23	76.42 (19)
O12—Al5—O22	76.4 (2)	O11—Al11—O28	93.3 (2)
O12—Al5—O31	93.15 (17)	O11—Al11—O29	93.4 (2)
O12—Al5—O35	170.3 (2)	O11—Al11—O34	170.7 (2)
O21^{i}—Al5—O3	79.26 (18)	O23—Al11—O2	99.16 (18)
O21^{i}—Al5—O31	90.0 (2)	O23—Al11—O28	93.7 (2)
O22—Al5—O3	98.16 (17)	O28—Al11—O2	164.0 (3)
O22—Al5—O21^{i}	169.7 (2)	O29—Al11—O2	78.75 (18)
O22—Al5—O31	94.3 (2)	O29—Al11—O23	169.3 (2)
O31—Al5—O3	164.4 (2)	O29—Al11—O28	90.4 (2)
O35—Al5—O3	78.25 (17)	O29—Al11—O34	94.4 (2)
O35—Al5—O21^{i}	94.5 (2)	O34—Al11—O2	77.7 (2)
O35—Al5—O22	94.8 (2)	O34—Al11—O23	95.4 (2)
O35—Al5—O31	91.56 (18)	O34—Al11—O28	91.7 (2)
O8—Al6—O2	98.95 (19)	O10—Al12—O2	99.9 (2)
O8—Al6—O32	76.09 (17)	O10—Al12—O13	75.26 (18)
O8—Al6—O33	92.9 (2)	O10—Al12—O29	96.10 (19)
O8—Al6—O34	94.9 (2)	O10—Al12—O36	169.4 (2)
O8—Al6—O36	171.2 (2)	O10—Al12—O39	92.7 (2)
O32—Al6—O2	97.91 (19)	O13—Al12—O2	97.70 (18)
O32—Al6—O33	93.0 (2)	O13—Al12—O39	94.6 (2)
O32—Al6—O36	96.0 (2)	O29—Al12—O2	78.92 (18)
O33—Al6—O2	165.5 (2)	O29—Al12—O13	170.2 (2)
O34—Al6—O2	79.2 (2)	O29—Al12—O39	90.4 (2)
O34—Al6—O32	170.1 (2)	O36—Al12—O2	77.81 (19)
O34—Al6—O33	91.5 (2)	O36—Al12—O13	94.7 (2)
O34—Al6—O36	92.7 (2)	O36—Al12—O29	93.6 (2)
O36—Al6—O2	78.25 (19)	O36—Al12—O39	91.4 (2)
O36—Al6—O33	91.1 (2)	O39—Al12—O2	164.2 (2)

Symmetry code: (i) −x+1, −y+1, −z+1.			
Al_{12}			
Al1—O1	1.946 (3)	Al4—O10	1.936 (3)
Al1—O3	1.861 (2)	Al4—O11	1.878 (3)
Al1—O4	1.871 (3)	Al4—O12	1.874 (3)
Al1—O22^{i}	1.933 (3)	Al4—O13	1.927 (3)
Al1—O23^{i}	1.876 (3)	Al4—O15	1.861 (2)
Al1—O24^{i}	1.865 (2)	Al4—O16	1.882 (3)
Al2—O2	1.923 (3)	Al5—O14	1.924 (3)
Al2—O3	1.872 (3)	Al5—O15	1.873 (3)
Al2—O4	1.886 (2)	Al5—O16	1.868 (3)
Al2—O5	1.927 (2)	Al5—O17	1.874 (2)
Al2—O7	1.863 (3)	Al5—O18	1.932 (3)
Al2—O8	1.875 (3)	Al5—O20	1.875 (2)
Al3—O6	1.924 (2)	Al6—O17	1.868 (2)
Al3—O7	1.877 (3)	Al6—O19	1.935 (3)
Al3—O8	1.862 (3)	Al6—O20	1.879 (3)
Al3—O9	1.924 (3)	Al6—O21	1.937 (3)
Al3—O11	1.876 (3)	Al6—O23	1.850 (2)
Al3—O12	1.867 (2)	Al6—O24	1.886 (3)
O3—Al1—O1	92.59 (12)	O11—Al4—O10	91.85 (12)
O3—Al1—O4	77.94 (11)	O11—Al4—O13	92.08 (12)
O3—Al1—O22^{i}	91.70 (11)	O11—Al4—O16	99.69 (12)
O3—Al1—O23^{i}	98.37 (12)	O12—Al4—O10	89.83 (12)
O3—Al1—O24^{i}	174.72 (13)	O12—Al4—O11	77.58 (11)
O4—Al1—O1	89.67 (12)	O12—Al4—O13	168.76 (11)
O4—Al1—O22^{i}	168.05 (11)	O12—Al4—O16	96.64 (12)
O4—Al1—O23^{i}	97.74 (12)	O13—Al4—O10	86.06 (13)
O22^{i}—Al1—O1	84.82 (12)	O15—Al4—O10	91.16 (12)
O23^{i}—Al1—O1	167.83 (12)	O15—Al4—O11	174.80 (12)
O23^{i}—Al1—O22^{i}	89.57 (12)	O15—Al4—O12	98.18 (11)
O24^{i}—Al1—O1	91.55 (11)	O15—Al4—O13	92.36 (12)
O24^{i}—Al1—O4	98.82 (11)	O15—Al4—O16	77.66 (11)
O24^{i}—Al1—O22^{i}	91.94 (12)	O16—Al4—O10	167.75 (13)
O24^{i}—Al1—O23^{i}	77.83 (10)	O16—Al4—O13	89.38 (13)
O2—Al2—O5	84.96 (12)	O14—Al5—O18	84.83 (13)
O3—Al2—O2	93.01 (13)	O15—Al5—O14	89.93 (12)
O3—Al2—O4	77.30 (10)	O15—Al5—O17	99.27 (11)
O3—Al2—O5	91.07 (11)	O15—Al5—O18	167.14 (12)
O3—Al2—O8	98.64 (12)	O15—Al5—O20	97.65 (12)
O4—Al2—O2	89.14 (11)	O16—Al5—O14	91.64 (12)

O4—Al2—O5	166.68 (13)	O16—Al5—O15	77.69 (11)
O7—Al2—O2	91.27 (12)	O16—Al5—O17	175.27 (12)
O7—Al2—O3	174.75 (13)	O16—Al5—O18	90.69 (12)
O7—Al2—O4	99.73 (11)	O16—Al5—O20	99.70 (12)
O7—Al2—O5	92.34 (12)	O17—Al5—O14	91.97 (12)
O7—Al2—O8	77.39 (12)	O17—Al5—O18	92.66 (12)
O8—Al2—O2	167.26 (13)	O17—Al5—O20	77.01 (11)
O8—Al2—O4	98.39 (12)	O20—Al5—O14	167.46 (12)
O8—Al2—O5	89.68 (12)	O20—Al5—O18	89.67 (12)
O7—Al3—O6	89.86 (12)	O17—Al6—O19	92.89 (12)
O7—Al3—O9	167.23 (14)	O17—Al6—O20	77.05 (11)
O8—Al3—O6	92.30 (12)	O17—Al6—O21	92.77 (11)
O8—Al3—O7	77.38 (12)	O17—Al6—O24	99.16 (11)
O8—Al3—O9	91.15 (13)	O19—Al6—O21	84.68 (12)
O8—Al3—O11	174.68 (11)	O20—Al6—O19	89.12 (12)
O8—Al3—O12	98.14 (11)	O20—Al6—O21	167.82 (12)
O9—Al3—O6	84.95 (12)	O20—Al6—O24	98.74 (12)
O11—Al3—O6	92.09 (11)	O23—Al6—O17	174.59 (12)
O11—Al3—O7	99.63 (12)	O23—Al6—O19	90.46 (12)
O11—Al3—O9	92.23 (13)	O23—Al6—O20	98.77 (12)
O12—Al3—O6	168.10 (13)	O23—Al6—O21	91.76 (11)
O12—Al3—O7	97.96 (11)	O23—Al6—O24	77.94 (11)
O12—Al3—O9	89.12 (12)	O24—Al6—O19	166.81 (11)
O12—Al3—O11	77.82 (11)	O24—Al6—O21	89.38 (12)
Symmetry code: (i) −x+1, −y+1, −z+2.			