Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Magnesium cations as templates for the self-assembly of supramolecular luminescent {Mg@[$B_{18}\varphi_{34–35}$]}-clusters

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1. Reagents

H_3BO_3 (NevaReaktiv, Russia, 99.8 %), $Mg(NO_3)_2 \cdot 6H_2O$ (Lenreactiv, Russia, 99.0 %) and N,N-dimethylformamide (Lenreactiv, Russia, 99.0 %), were used as received. Phase identification of the prepared samples was carried out using Rigaku SmartLab SE diffractometer (3 kW sealed X-ray tube, D/teX Ultra 250 silicon strip detector, vertical type θ-θ geometry, HyPix-400 (2D HPAD) detector).

2. Synthesis

A mixture of H_3BO_3 (618.0 mg, 10.0 mmol) and $Mg(NO_3)_2 \cdot 6H_2O$ was added to 3.0 mL N,N-dimethylformamide (DMF) and stirred for about 1 h. Synthesis was performed with different amounts $Mg(NO_3)_2 \cdot 6H_2O$. It was used 0.3 mmol (76.9 mg), 0.4 mmol (102.6 mg), 0.5 mmol (128.2 mg), 0.6 mmol (153.8 mg), 0.8 mmol (205.1 mg), 1.0 mmol (256.4 mg) $Mg(NO_3)_2 \cdot 6H_2O$ for the samples "Mg0.3", "Mg0.4", "Mg0.5", "Mg0.6", "Mg0.8", "Mg1.0", respectively. The final solution was put into a 30 mL Teflon liner. The liner was sealed and placed into an autoclave and heated in an oven. The oven was heated at 220 ℃ for 7 days and then cooled to room temperature. X-ray phase analysis showed the presence of several compounds in the resulted samples (Figure S1). All samples contained the impurity of $[(CH_3)_2NH_2]_2[B_5O_6(OH)_4]_2[HCON(CH_3)_2]$.[1] The "Mg1.0" sample consisted of 97 % of the $MgB_{17}O_{28}[NH(CH_3)_3][NH_2CH_3]_2[NHCH_3]_6$ (**2**) phase and this sample was characterized thoroughly. The yield of **1**, **3**, **4**, **5** and **6** was 16% ("Mg0.8" sample), 4 % ("Mg1.0"), 13 % ("Mg1.0"), 21 % ("Mg0.6"), and 37 % ("Mg0.8"), respectively.

3. Thermal behavior study

The sample of **2** was heat-treated at 300 °C for 2 h. As a result, the mass decreased by 27.69 %, and the sample became amorphous (Figure S2). Then the sample was heat-treated at 800 °C for 86 h. As the result the formation of $Mg_2B_2O_5$ [2] was observed.

4. X-ray Powder Diffraction

A Rietveld refinement of **2** was performed on the powder diffraction patterns, to check the consistency between the single crystal and powder sample used for study of properties. The final structure model of **2** obtained from single-crystal data (see below) were used in the refinement utilizing RietveldToTensor software.[3] Final Rietveld refinement results are presented in Table S1. Pseudo-Voigt functions were used for fitting the reflection profiles. The background was described by a Chebyshev polynomial function (17th order) and the preferred orientation (direction [001]) was modeled by the March-Dollase approach. The atomic coordinates were not refined. The final Rietveld refinement plot is given in Figure S3. They show good agreement with the single-crystal data. The lattice parameters obtained from the powder diffraction data are in good agreement with those derived from the single-crystal data.

5. Structure determination

Single crystals of $\{Mg@[B_{17}O_{26}(OH)_4\}[N(CH_3)_3][NH(CH_3)_3]_3$ (**1**), $\{Mg@[B_{17}O_{27}(OH)_3]\}[NH(CH_3)_3]_{0.5}[NH(CH_3)_2)][NH_2(CH_3)_2]_{2.5}[CH_3NH_3]_{0.5}(H_2O)_{1.5}$ (**4**) and $\{Mg@[B_{17}O_{26.5}(OH)_4\}[NH(CH_3)_3]_{1.25}[N(CH_3)_3][NH_2(CH_3)_2]_{2.25}[CH_3NH_3]_{0.5}(H_2O)_{1.5}$ (**5**) were selected from «Mg0.6» sample. Single crystal of $\{Mg@[B_{17}O_{28}]\}[NH(CH_3)_3]_2[N(CH_3)_3]_4[NH_2(CH_3)_2][NH(CH_3)_2]_2(H_2O)_2$ (**3**) was selected from «Mg1.0» sample. Single crystal of $\{Mg@[B_{17}O_{26.5}(OH)_4]\}[HDMF][NH(CH_3)_3]_2[NH_2(CH_3)_2](NH_3)_{0.5}$ (**6**) was selected from «Mg0.4» sample. Single crystal of $MgB_{17}O_{28}[NH(CH_3)_3][NH_2(CH_3)_2]_2[NH(CH_3)_2]_6$ (**2**) was selected from «Mg0.2» sample.

A single crystals were selected in polarized light using an optical microscope and attached to a glass fiber using epoxy glue. Measurements of the **1**, **2, 3, 6** was performed at 25 °C, while the measurements of **4** and **5** was performed at −173 °C. The experimental data were collected on a Rigaku XtaLAB Synergy-S four-circle diffractometer. MoKα radiation was used for the crystals of **1**, **2**, **4** and **5**. CuKα radiation was used for the crystals of **3** and **6**. A nitrogen blower (Oxford Cryosystems, Oxford, UK) was used for temperature control. Lorentz and polarization corrections were applied. The multi-scan absorption correction was performed.[3] The observed Laue symmetry and systematic absences indicated $P4_2/n$, $P\bar{4}2_1m$, $I\bar{4}2d$, $P2_1/c$, Pc and $P2_1$ space groups for **1**, **2**, **3**, **4**, **5** and **6**, respectively. The structures were solved using a charge-flipping method[4] implemented in JANA2020[5] and refined using OLEX2 software.[6] The crystal structure of **6** was refined starting from positional parameters of $MgB_{17}O_{26.5}(OH)_4[HDMF][NH(CH_3)_3]_2[NH_2(CH_3)_2](NH_3)_{0.5}$ using OLEX2 software.[6] Further checks using PLATON[7] did not indicate possible higher symmetry. Analysis of electron density maps suggested the presence of three TMA molecules in the structure of **1**, one TMA and eight DMA molecules in the structure of **2**, two TMA, one DMA, and one water molecule in the structure of **3** *pfu*. The structure of **4** contained four TMA, twenty DMA, four MA, and twelve water molecules per unit cell. The structure of **5** is assumed to contain ten TMA, eighteen DMA, four MA, and twelve water molecules. As location of hydrogen atoms

faces essential difficulties, only the CNO backbone of the organic species could be identified and the true nature of these may occur to differ from our suggestions. For compensation of the negative charges of ($\{Mg@[B_{17}O_{30}]\}^{7-}$ in **1** and **4**, $\{Mg@[B_{17}O_{28}]\}^{3-}$ in **2** and **3**, and $\{Mg@[B_{17}O_{30.5}]\}^{8-}$ in **5** and **6**, at least some of their oxygen atoms, as well as the nitrogen atoms of the organic species, are actually protonated. The choice of these atoms was made based on the maxima on the difference Fourier maps. Attempts to refine the organic species faced several problems mostly concerning thermal parameters and bond distances and angles. In addition, the data/parameter ratio was low. Therefore, solvent masking was applied to the structures (Table S7). The void volume was estimated to be 798, 1729, 3230, 3436, 4446, 2008 Å^3 with 267, 516, 1244, 1107, 1405, 581 electrons removed during masking for **1**, **2**, **3**, **4**, **5**, **6**, respectively. The number of electrons was correlated to the suggested filling of the structures **1** (286 $\bar{e}$), **2** (490 $\bar{e}$), and **6** (572 $\bar{e}$), b ut exceed that for **3** (428 $\bar{e}$), **4** (900 $\bar{e}$), and **5** (1064 $\bar{e}$). The structure **3** contains large cavities wherein not all organic species could be localized from the electron density maps. The **4** and **5** are the most complex and low-symmetrical with cell volumes exceeding 7000 and 8000 Å^3, therefore, the corresponding numbers of independent atoms are very large; the problems with the identification of the organic species, which may be partially disordered, are not surprising. Our suggestion is that the structures of **3**, **4**, and **5** contain the TMA, DMA, and water species which leads to the proposed formulae. $\{Mg@[B_{17}O_{26}(OH)_4\}[N(CH_3)_3][NH(CH_3)_3]_3$ (**1**), $\{Mg@[B_{17}O_{28}]\}[NH(CH_3)_3][NH_2(CH_3)_2]_2[NH(CH_3)_2]_6$ (**2**), $\{Mg@[B_{17}O_{28}]\}[NH(CH_3)_3]_2[N(CH_3)_3]_4[NH_2(CH_3)_2][NH(CH_3)_2]_2(H_2O)_2$ (**3**), $\{Mg@[B_{17}O_{27}(OH)_3]\}[NH(CH_3)_3]_{0.5}[NH(CH_3)_2)][NH_2(CH_3)_2]_{2.5}[CH_3NH_3]_{0.5}(H_2O)_{1.5}$ (**4**), $\{Mg@[B_{17}O_{26.5}(OH)_4\}[NH(CH_3)_3]_{1.25}[N(CH_3)_3][NH_2(CH_3)_2]_{2.25}[CH_3NH_3]_{0.5}(H_2O)_{1.5}$ (**5**), and $\{Mg@[B_{17}O_{26.5}(OH)_4]\}[HDMF][NH(CH_3)_3]_2[NH_2(CH_3)_2](NH_3)_{0.5}$ (**6**). Data visualization was performed with the Vesta[8] and ATOMS[9] software. The main features of the X-ray diffraction experiment and structure refinement are summarized in Table S8. Final atomic positional and displacement parameters, selected bond lengths and angles are given in Tables S9−S23.

6. EDX.

Energy-dispersive X-ray spectroscopy (EDX) was performed on a Zeiss EVO-25 scanning electron microscope (SEM) equipped with an Oxford Instruments Ultum-Max 100 Energy Dispersive Spectrometer. The electron-beam accelerating voltage was 20 kV and the current 2 nA; defocused beam (up to 4 μm spot size) was used and the X-ray acquisition time was 100 s. The chemical composition was measured on different spots on several crystals and eventually averaged. The final composition was normalized to 100 %. The Cu signal is due to the conductive copper coating. Energy dispersive X-ray analysis yielded Mg:O:N:C:B molar ratios of approximately 1.0:32.8:7.4:20.1:12.7 for **2**, which is close to the expected 1:28:9:19:17 (Figure S5).

7. Variable-temperature X-ray powder diffraction. Thermal expansion of **2** was studied by high-temperature X-ray powder diffraction using a Rigaku Ultima IV diffractometer (Co Kα radiation, 40 kV/30 mA, Bragg-Brentano geometry, PSD D-Tex Ultra) with 5 °C temperature increments in the range 25–100 °C (Rigaku R-300 high-temperature attachment). The unit cell parameters were refined at different temperatures by the Rietveld method using RietveldToTensor software.[10] The structure models of **2** obtained from a single crystal were used as starting models for further refinement. Pseudo-Voigt functions were used for fitting the reflection profiles. The background was described by a Chebyshev polynomial function (26th order). Temperature dependences of unit-cell parameters and volume of 2 in the 25–100 °C temperature range (Figure S6) can be described by the following equations:

$a = 16.0335(35) + 0.000117(52)t$

$c = 10.0118(18) + 0.000125(26)t$

$V = 559.053(56) + 0.070(21)t$

8. Thermal analysis.

2 was studied by thermal analysis on a NETZSCH STA 429 thermal analyzer. The polycrystalline sample (4.668 mg) was placed in a corundum crucible. The samples were studied at 40–800 °C (10 °C / min) (Figure S9).

9. Spectroscopy

Infrared spectrum (IR) for **2** in the 800−4000 cm^{-1} range was collected with a Thermo Scientific Nicolet 8700 spectrometer (spectral resolution 2 cm^{-1}) (Figure S8a). KBr was used as the reference pellet and the samples were mixed thoroughly with it. The Raman spectrum for **2** was measured using a FTIR Raman spectrometer based on Bruker IFS 125 HR with YAG:Nd laser @ 1064 nm, pair of RazorEdge Semrock long-pass edge filters @ 1064 nm and liquid-nitrogen cooled Ge-detector Bruker Senterra (Figure S8b). The UV–Vis–NIR absorbance spectrum for **2** was collected with the Perkin Elmer Lambda 1050

spectrophotometer equipped with a 150 mm integrating sphere. Absorbance spectra were measured at room temperature in the spectral range of 200−2500 nm with 1 nm resolution. $BaSO_4$ disk was used as a reference sample.

Photoluminescence emission (PL) and excitation (PLE, Figure S10) spectra for **2** in visible region were recorded on an Agilent Cary Eclipse fluorescence spectrometer with a 75 kW xenon light source (pulse length τ = 2 μs, pulse frequency ν = 80 Hz, and wavelength resolution 0.15 nm; PMT Hamamatsu R928). The measured spectra were corrected for the sensitivity of the spectrometer.

The CIE 1931 chromaticity coordinates (x, y) have been used for detailed determination of emission color from the sample. The calculations were made using the formula according[11]:

$$x = \frac{X}{X+Y+Z}, y = \frac{Y}{X+Y+Z},$$

while $X = \int I(\lambda)\bar{x}(\lambda)d\lambda$,

$Y = \int I(\lambda)\bar{y}(\lambda)d\lambda$,

$Z = \int I(\lambda)\bar{z}(\lambda)d\lambda$

where $I(\lambda)$ is the intensity at wavelength λ, $\bar{x}$, $\bar{y}$, $\bar{z}$ are the curves of the CIE standard observer for wavelength λ, and provides converting spectral radiance $I(\lambda)$ to a trichromatic color space X, Y, Z.

The calculated CIE coordinates are (0.1939, 0.2108) corresponding to blue area on the CIE color space (Figure S13).

10. Quantum yield measurements. The of study the quantum yield was carry out of the Fluorolog-3 (HORIBA, Irvine, CA, USA)) spectrofluorimeter. Quantum yield was measured in 150 mm integrating sphere. The excitation of the sample was performed at 365 nm, and the emission spectrum was measured in the range of 370–675 nm. A 400 W Xe lamp was used as an excitation source. The measured quantum yield of the synthesized sample of about 9.5%, which shows reliable value in relation to the previously studied amine-functionalized organic/inorganic phosphors.[12]

11. Latent fingerprints collection. Black paper was used to collect fingerprints (Figure S14). A fingerprint was made by pressing a finger against the surface of the glass slide and the aluminum foil. The powder of **2** was brushed on the surface of the paper using a soft feather brush. The as-treated fingerprints were irradiated with a portable UV lamp and the images were captured by a digital single-lens reflex camera.

12. Topological and complexity analysis.

To analyze the topology of nets we used the extended Topological Types Database (TTD)[13] comprising 806 220 topological types up to date. Topological types of nets were classified using RCSR (Reticular Chemistry Structure Resource)[14] and, for those types that are lacking in RCSR, TopCryst.[15] The *p*,*r*-transitivity of a net is established as the number *p* of inequivalent vertices and the number *r* of inequivalent edges for the most symmetric embedding of the net into Euclidean space. In difficult cases, a barycentric placement[16] of the net can be used to find *p* and *r*. The topological density (TD_{10}) of nets was calculated as the sum of all vertices in the first 10 coordination spheres of the initial vertex of the net.

According to Krivovichev,[17] the Shannon-like combinatorial complexity of a crystal structure should be calculated as

$$H_{comb} = -\sum_{i=1}^{v''} \frac{v_i}{v} \log_2 \frac{v_i}{v},$$

where v'' is the number of crystallographic orbits occupied by primary building units (b.u.) under consideration (atoms, molecular centers of gravity, etc.), v_i is the multiplicity of the i-th orbit, and v is the total number of b.u.'s in the reduced cell: $v = v_1 + v_2 + ... + v_{v''}$. Infimal value of H_{comb} corresponds to the most symmetric embedding of a given net. The lower H_{comb}, the higher the configurational entropy of a crystal.[18]

At the second level of consideration, different sources of information originated from secondary b.u.'s of different kind, for example, inequivalent molecules[19] or layers[20] in the same crystal structure can be treated separately with the aid of the strong additivity rule discussed by Hornfeck:[21]

$$H_{comb} = \sum_{j=1}^{b.u.''} \frac{v_j}{\sum_j v_j} H_{comb}^{b.u.j} + H(v_1, v_2, ..., v_{b.u.''}),$$

$$H\left(v_1,v_2,\ldots,v_{b.u.''}\right) = -\sum_{j=1}^{b.u.''}\frac{v_j}{\sum_j v_j}\log_2\frac{v_j}{\sum_j v_j} \equiv wH_{comb}^{mix}$$

$$\frac{v_j}{\sum_j v_j}H_{comb}^{b.u.,j} \equiv wH_{comb}^{b.u.,j}$$

,

,

where b.u.″ is the number of inequivalent secondary b.u.'s, $H_{comb}^{b.u.,j}$ is H_{comb} of the *j*-th secondary b.u., and v_j is the total number of primary b.u.'s included in the *j*-th secondary b.u. (per reduced cell). Such additivity approach has much in common with a so-called ladder of information,[22,23] which reflects a decrease of H_{comb} upon excluding atoms of some sort from consideration, as well as upon finding the idealized symmetry of a secondary b.u.

The number of symmetrically inequivalent edges e'' binding secondary b.u.'s into a net[24] is another kind of complexity which, unlike Shannon-like complexity, accounts for rather difficulty-to-create than difficulty-to-describe[11] a crystal structure. As it was previously shown, the infimal value of e'' is strongly dependent on the cardinality of the minimal generating set of a space group.[25,26]

The weighted values wH_{comb} for different sources of structural complexity show that the information originated from Mg^{2+} sublattice makes a very small contribution to the complexity of the whole structure (Figure S15).

13. Computational details.

The band structure calculation was performed within the framework of the density-functional theory (DFT) as implemented in the CASTEP package. The exchange-correlation potential within the Generalized Gradient Approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) parametrization and ultrasoft pseudopotentials technique was used. The energy cutoff value of 571.4 eV and tolerance of 10^{-6} eV/atom were set for the self-consistent field convergence of the total electronic energy. The integration of the Brillouin zone was performed by a 2 × 1 × 4 *k*-point grid sampling for density of states, and the Fermi level (E_f = 0 eV) was selected as the reference.

The result band structure (Figure S17) shows the substance under consideration to be a dielectric. The direct band gap value was found of 4.793 eV which is much closer to experimental value of 4.95 eV. The total and partial density of states (DOS and PDOS respectively) are presented in Figure S18. The VB ranging between −23 and −18 eV is composed of B-2s2p and O-2s2p; between –22 and –21 eV – O-2s2p. The Fermi level in **2** is near the valence band ceiling. It is determined by the acceptor nature of interactions.

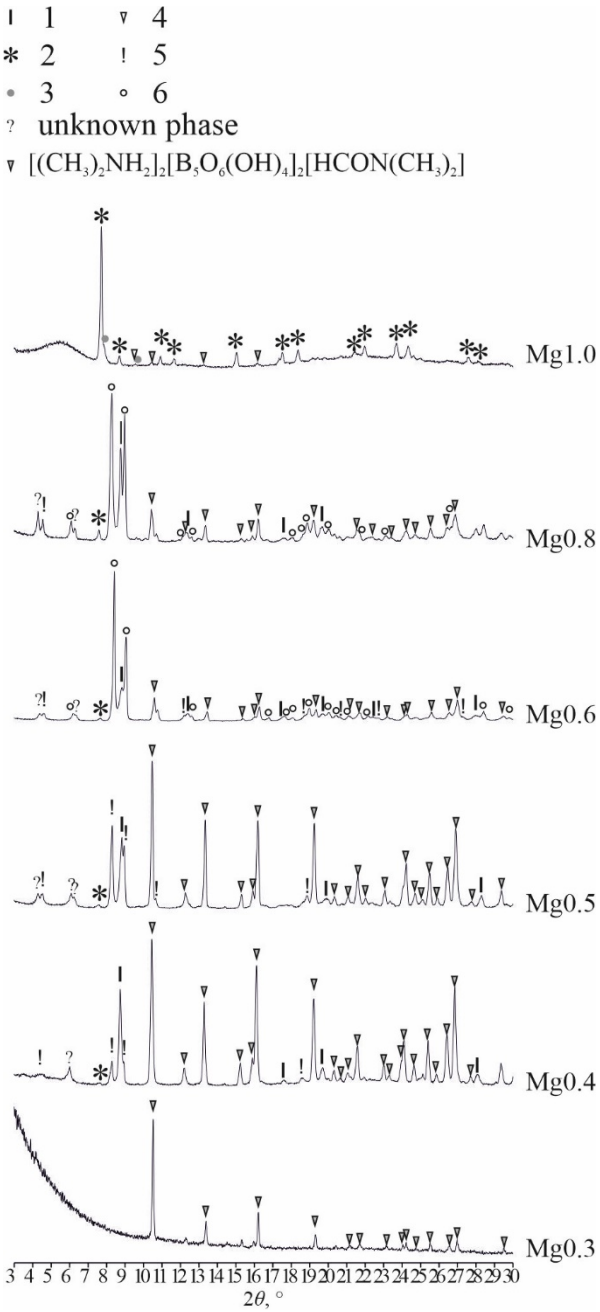


Figure S1. X-ray diffraction patterns of samples “Mg0.3”, “Mg0.4”, “Mg0.5”, “Mg0.6”, “Mg0.8”, “Mg1.0”.

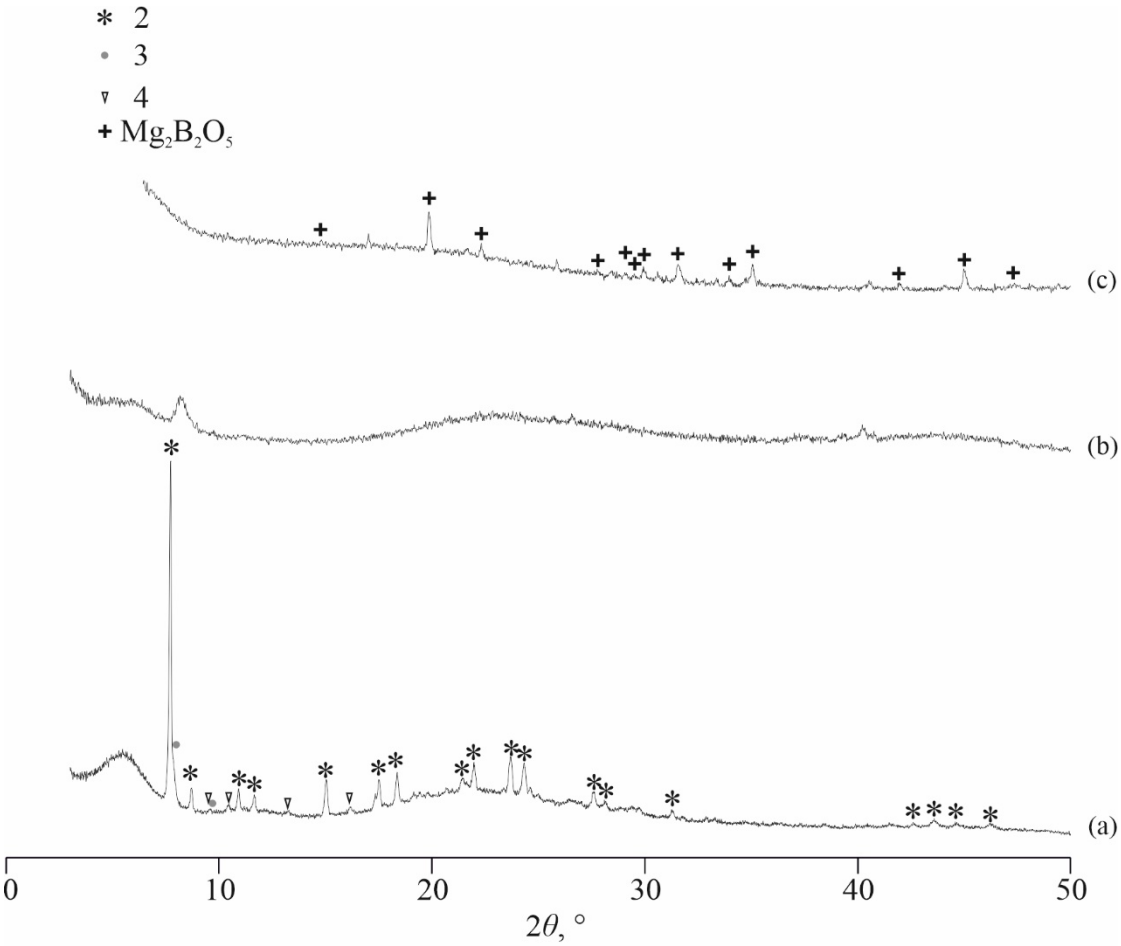


Figure S2. (a) X-ray diffraction patterns of sample of **2**. The sample was heat treated at (b) 300 °C for 2 h and (c) 800 °C for 86 h.

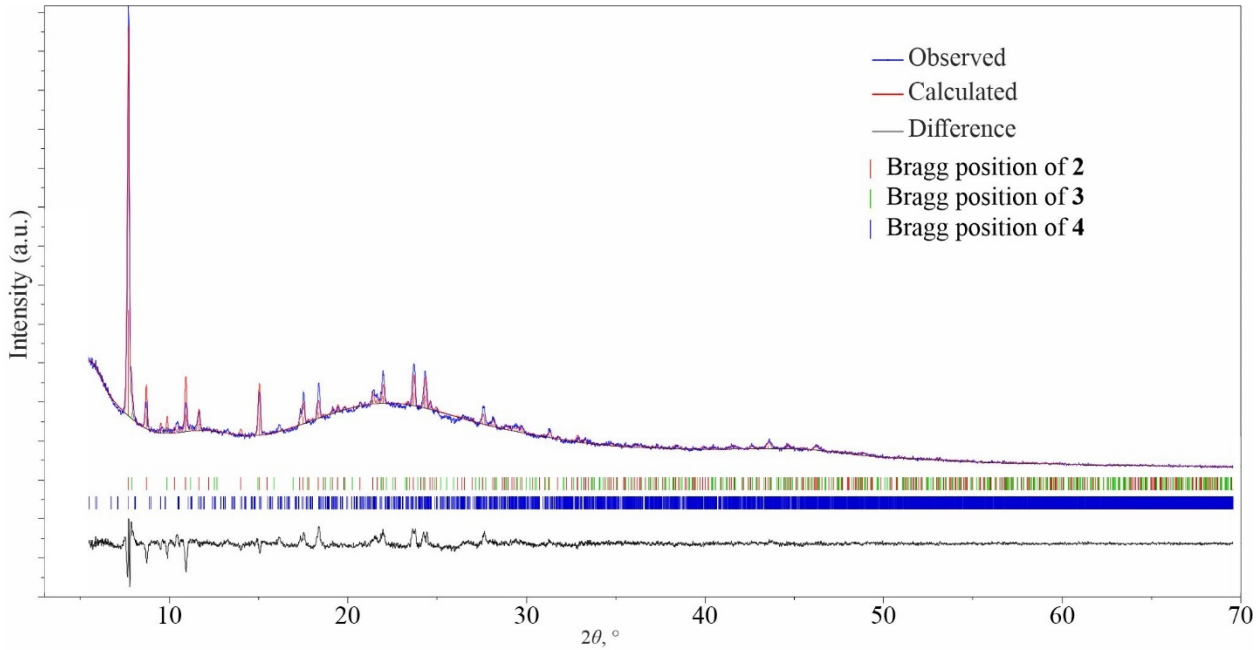


Figure S3. Intensity profiles for the powder X-ray Rietveld refinement of **2**. The observed and calculated profiles are represented in blue and red lines, respectively. The difference profile is plotted at the bottom. Vertical bars indicate the positions of the Bragg reflections.

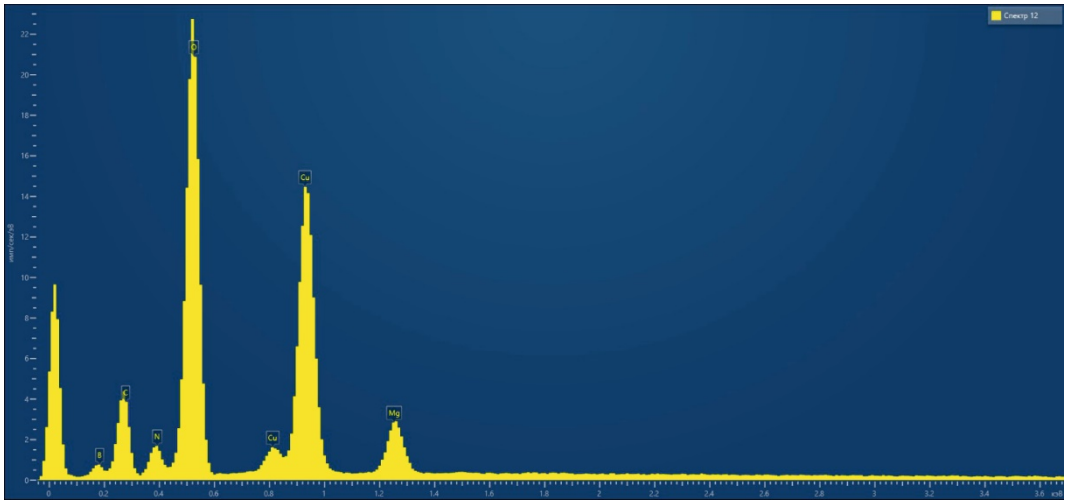


Figure S4. EDX spectrum of **2**.

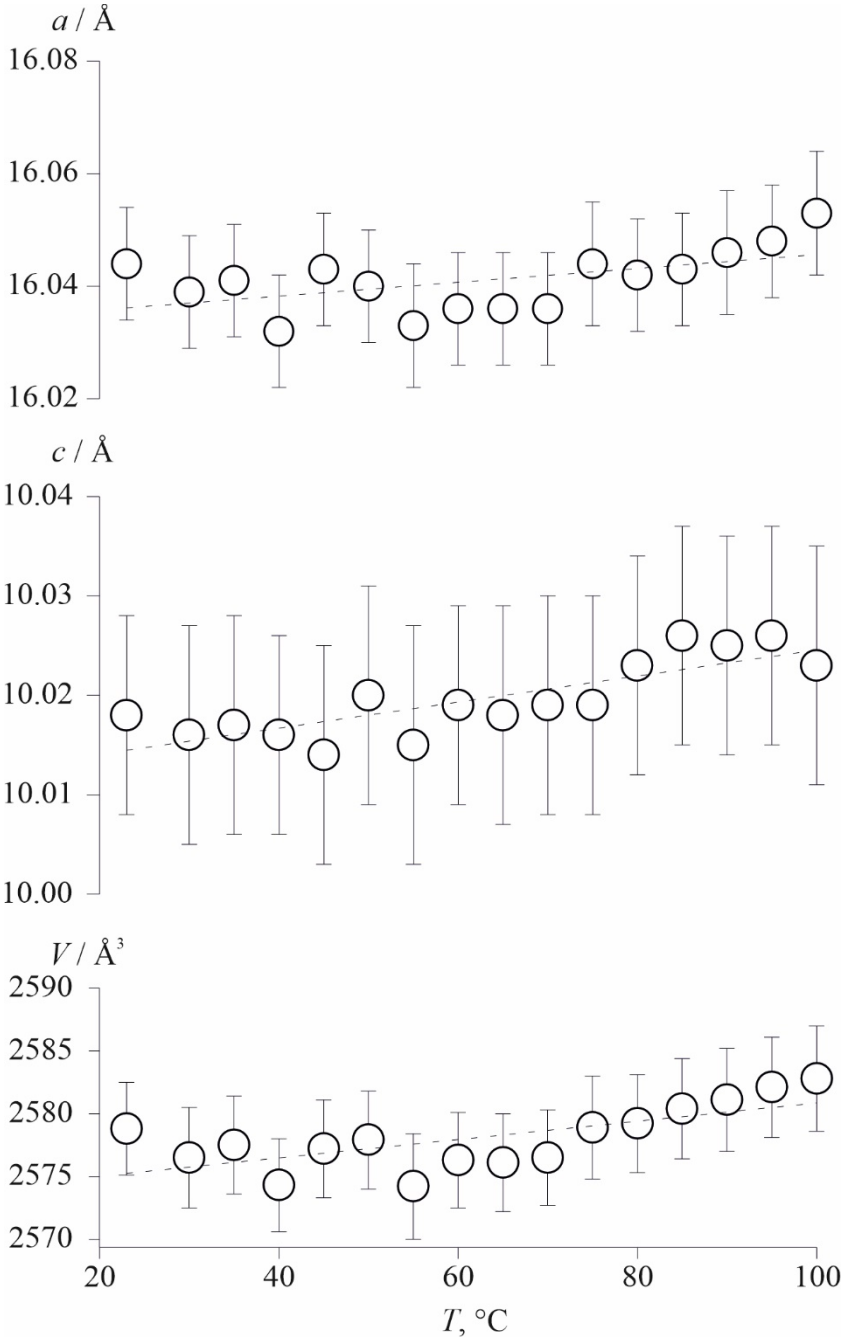


Figure S5. Temperature dependences of the unit-cell parameters and volume for **2**.

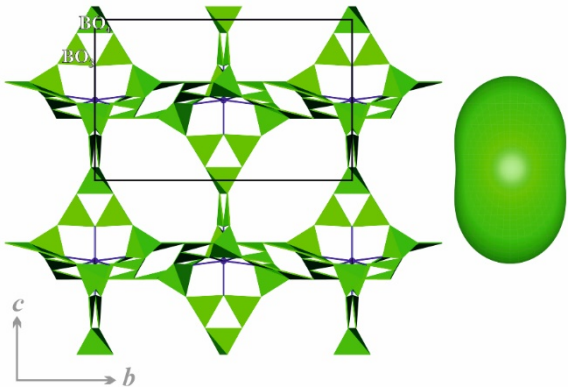


Figure S6. Projections of the crystal structure of **2** onto the *bc* plane in comparison to the thermal expansion tensor at 50 °C.

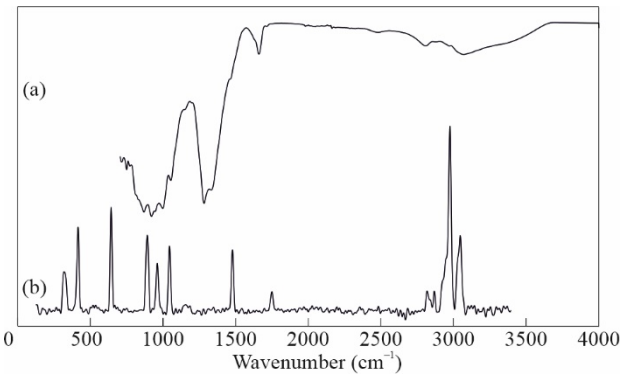


Figure S7. The (a) IR and (b) Raman spectra of **2**.

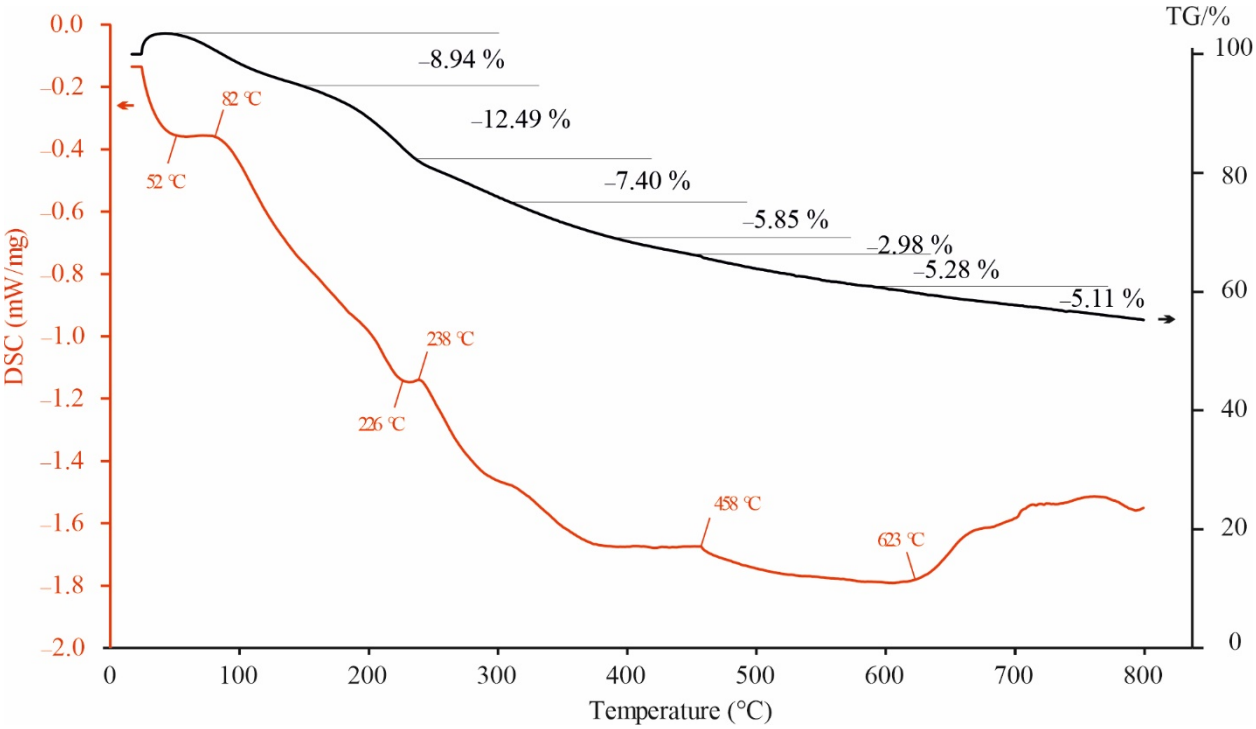


Figure S8. DSC and TG data for **2**.

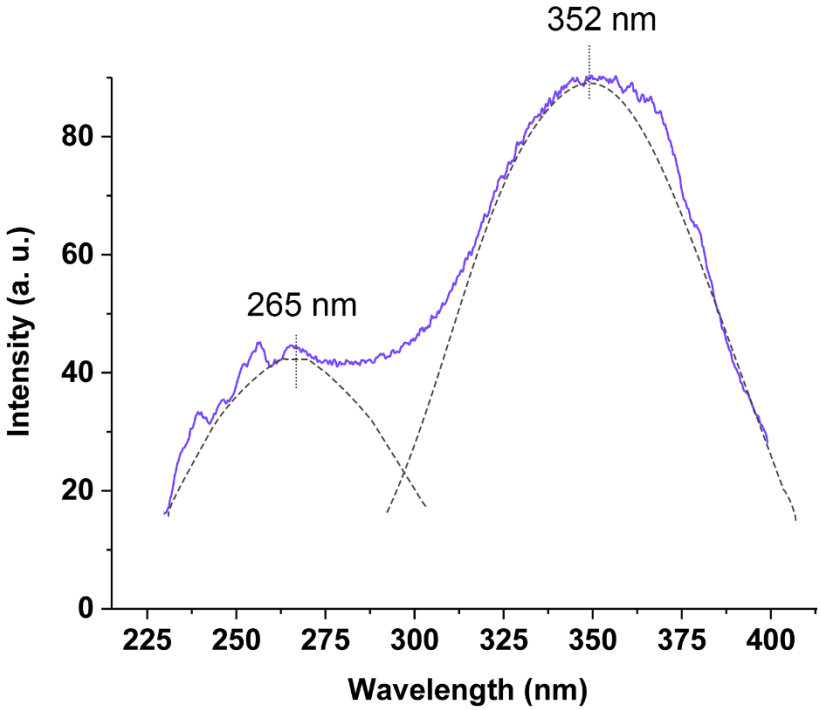


Figure S9. PLE spectra of **2** at λ_{em} = 425 nm.

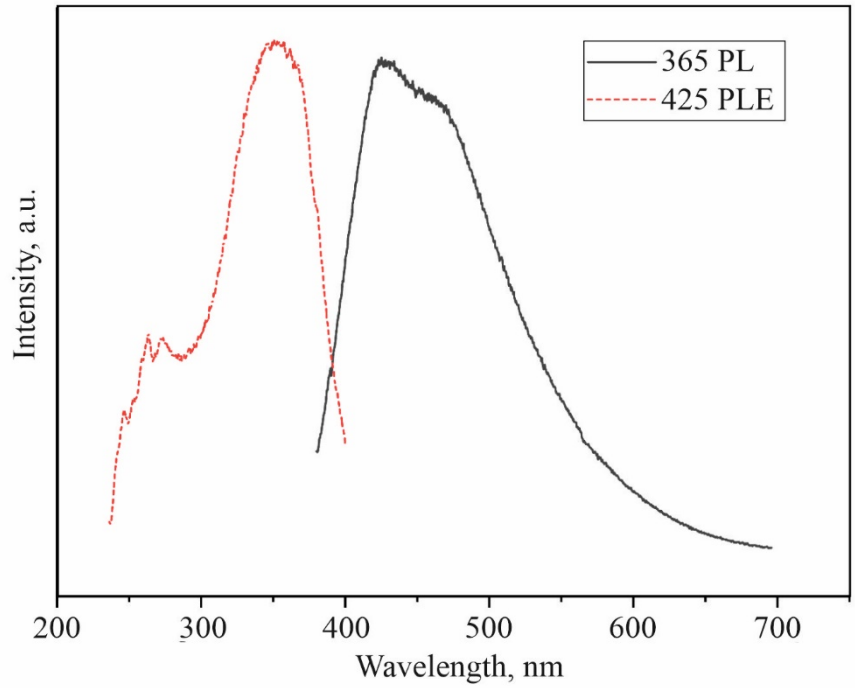


Figure S10. Excitation (PLE) and emission (PL) spectra of the synthesized sample at λ_{em} = 425 and λ_{ex} = 365 nm, respectively.

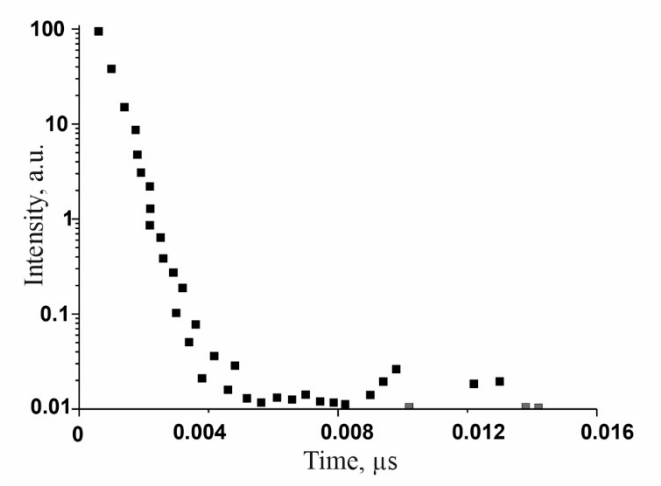


Figure S11. Luminescence decay curve of **2**.

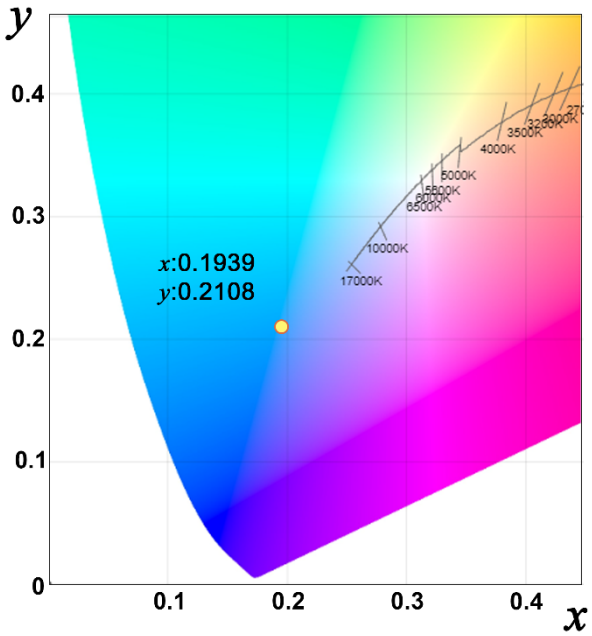
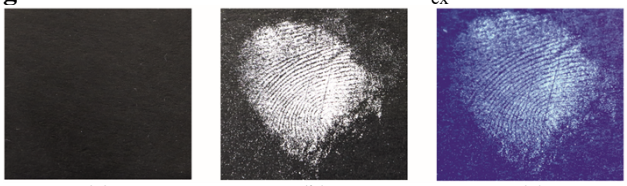


Figure S12. CIE coordinates for **2** at λ_{ex} = 352 nm.



(a) (b) (c)

Figure S13. Luminescence image of a fingerprint on a black paper: (a) untreated surface, (b) surface under natural light and (c) surface under UV light

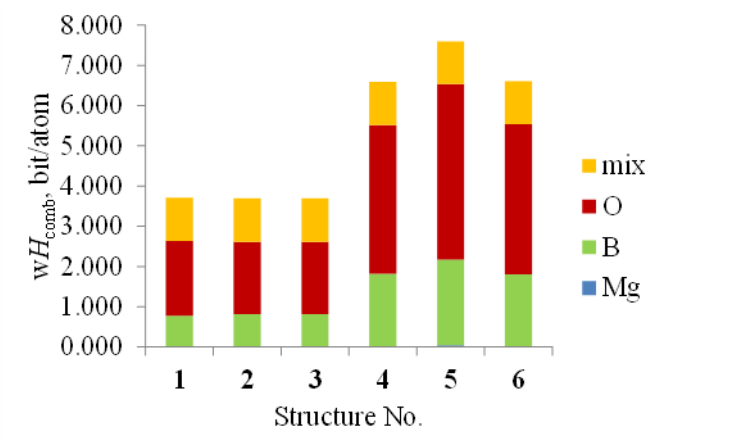


Figure S14. The weighted contribution of H_{comb}(Mg), H_{comb}(B), H_{comb}(O), and H_{comb}^{mix} for compounds **1**–**6**.

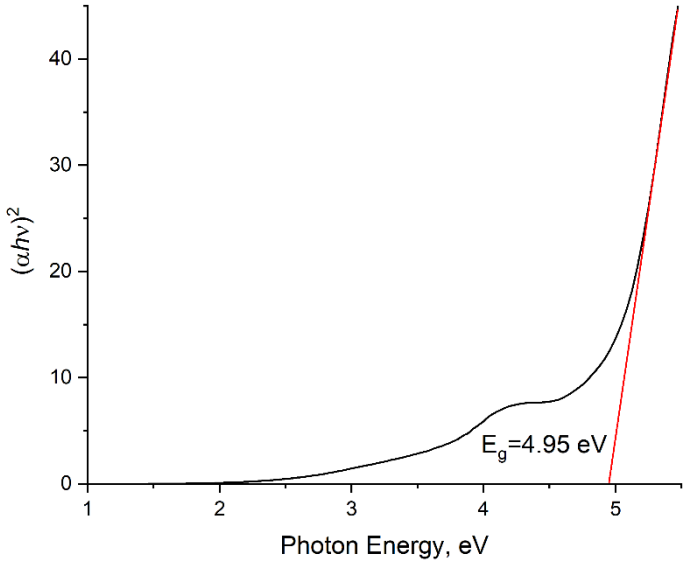


Figure S15. Tauc plot of absorbance spectra for **2**.

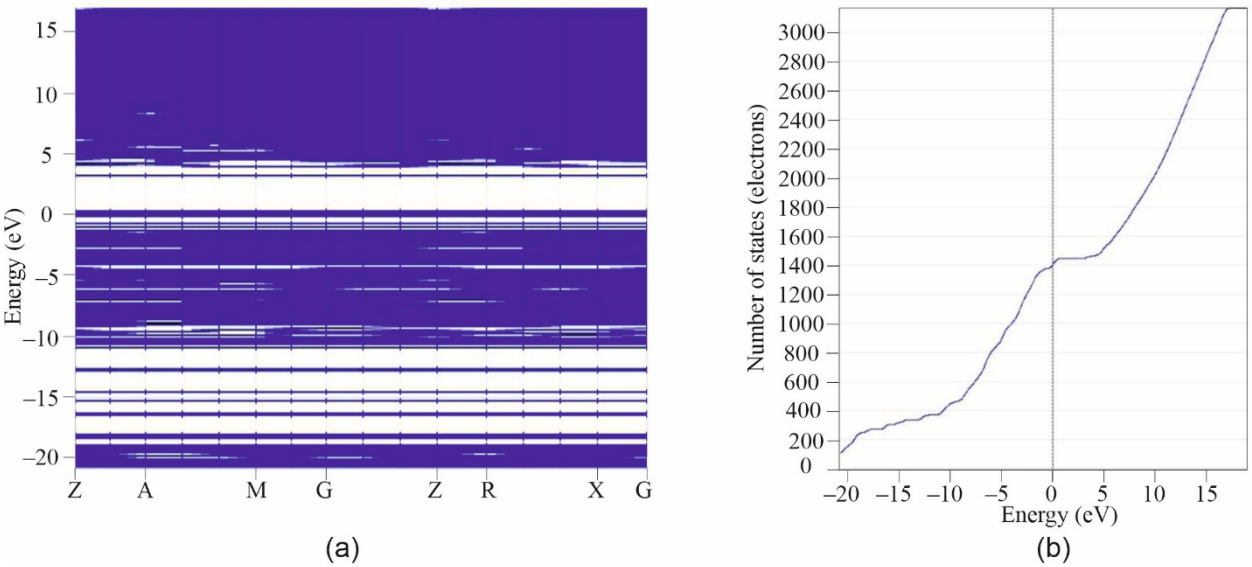


Figure S16. (a) Band Structure and (b) electron energy distribution function for **2**.

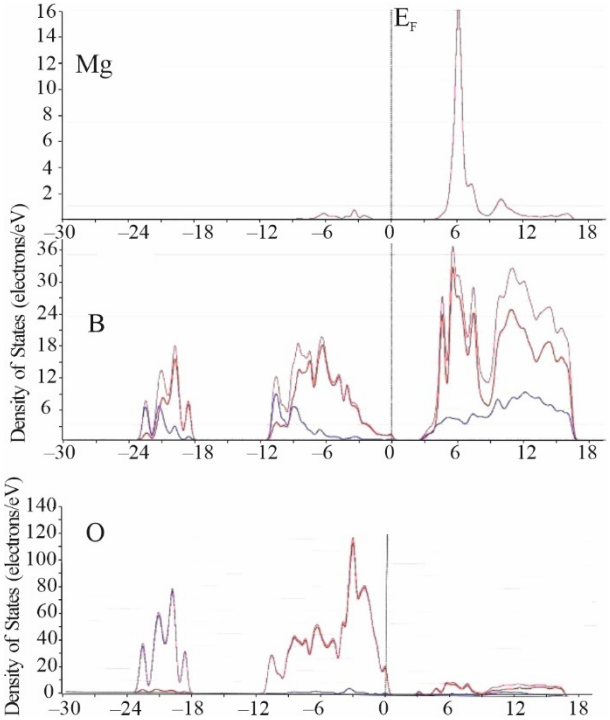


Figure S17. Element-wise density of states for **2:** blue – density of *s*-states, red - density of *p*-states, black - full density of states.

Table S1. X-ray Rietveld refinement of the structure of **2**.

Chemical formula	$MgB_{17}O_{28}[NH(CH_3)_3][NH_2(CH_3)_2]_2[NH(CH_3)_2]_6$
Temperature (°C)	23(2)
Crystal system, space group	Tetragonal, $P\bar{4}2_1m$
a (Å), c (Å)	16.15577(39), 10.11458(63)
V (Å^3)	2640.00(29)
Z	2
Radiation type	Cu Kα
Data collection	
Diffractometer	Rigaku Miniflex II
θ-range	2.5–35, Step size (°) 0.02
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.372
Refinement	
	R_{wp} 0.056 R_p 0.040 R_{Bragg} 0.032
S	1.77
No. of parameters	42

Computer program: *RietveldToThensor*.[27]

Table S2. Assignment of the vibrational bands observed in the infrared and Raman spectra for **2**.

IR peak, cm^{-1}	Raman peak, cm^{-1}	Assignment
	315	Lattice
	415	Lattice
	641	δs (BO_3)
810		$\nu_s(B_{[4]}O)$
870	893	ν_s (CNC)
920		$\nu_s(B_{[3]}O)$
950	961	ρ(CH_3)
1000		$\nu_{as}(B_{[4]}O)$
1055	1044	ρ(CH_3), ν_{as}(CNC)
1280		ν_a(CN)
1340		$\delta_s(CH_3)$
1470	1478	$\nu_{as}(BO_3)$, $\delta_a(CH_3)$
1630		δ(NH_2)
2475		ρ(NH_2), δ(NH_2)
2805	2820, 2839, 2870	$\nu_s(CH_3)$
	2924,2976	$\nu_s(CH_3)N$
3070	3028, 3047	ν(NH_2), $\nu_{as}(CH_3)$
3350		ν(NH_2)

Table S3. The data on PL/PLE spectra of different organically templated borates

Compound	PLE maxima, nm	PL maxima, nm	Ref.
$[Zn(dap)_2]$-$[AlB_5O_{10}]$	327	420	[28]
$B_6O_9(en)_2@(H_2en)Cl_2$	367	457	[29]
$Na_2B_{10}O_{17}\cdot H_2en$	*na*	432	[30]

$[Cd@B_{14}O_{20}(OH)_6]^{2-}$	360	430	[31]
$(H_2en)_2(Hen)_2B_{16}O_{27}$	353	428	[32]
$Mg_7@[B_{69}O_{108}(OH)_{18}]$	249	423	[33]

* dap = 1,3-diaminopropane, en = ethylenediamine

Table S4. Structural schemes for the different types of $\{Mg@[B_{18}O_n(OH)_m]\}$ clusters in the crystal structures of **1**–**6**

Type of the cluster	Formula	Structural scheme
A	$\{Mg@[B_{18}O_{34}]\}$ $\{Mg@[B_{18}O_{32}(OH)_2]\}$ $\{Mg@[B_{18}O_{30}(OH)_4]\}$	18B : 12Δ6□ : <2Δ□><<2Δ□><2Δ□><2Δ□><2Δ□>><2Δ□>
B	$\{Mg@[B_{18}O_{31}(OH)_4]\}$	18B : 10Δ8□ : <2Δ□><<2□Δ><2Δ□><2Δ□><2Δ□>><2□Δ>
B’	$\{Mg@[B_{18}O_{31}(OH)_4]\}$	18B : 10Δ8□ : <2Δ□><<2□Δ><□2Δ><□2Δ><□2Δ>><2□Δ>
C	$\{Mg@[B_{18}O_{31}(OH)_4]\}$	18B : 10Δ8□ : <2Δ□><<2□Δ><2Δ□><2Δ□><2Δ□>><2□Δ>
C’	$\{Mg@[B_{18}O_{31}(OH)_4]\}$	18B : 10Δ8□ : <2Δ□><<□2Δ><□2Δ><□2Δ><Δ2□>><2□Δ>

Table S5. Topological types and other characteristics of nets formed solely by condensed oligoborate clusters (1 cluster in each vertex of the net).

Compound	Dimensionality of the net	Topological type	Descriptor of the borate framework	TD_{10}	Infimal v'', e'' (transitivity)	Observed v'', e''
1	1D	**2C1**	18 : ∞^1 [A]	21	1,1	1,1
2	3D	**pcu**	18 : ∞^3 [A]	1561	1,1	1,2
3	3D	**bsn**	18 : ∞^3 [A]	1941	1,2	1,2
4	2D	**2,4L3**	34 : ∞^2 [2A+B+B’]	219	2,1	2,3
5	1D	**2C1**	68 : ∞^1 [2A+2C]	21	1,1	2,2 x2
6	1D	**2C1**	34 : ∞^1 [A+C’]	21	1,1	1,1 x2

Table S6. The combinatorial complexities (bit/atom): H_{comb}(Mg) for Mg^{2+} substructure, H_{comb}(Mg, B) for Mg^{2+} implemented in polyborate net of boron polyhedral centers, and H_{comb}(Mg, B, O) for the latter substructure complemented by covalently bound oxygen atoms.

Compound	H_{comb}(Mg)	H_{comb}(Mg, B)	H_{comb}(Mg, B, O)
1	0	2.392	3.710
2	0	2.392	3.697
3	0	2.392	3.697
4	1.000	5.170	6.585
5	2.000	6.170	7.600
6	1.000	5.170	6.600

Table S7. Summary of the solvent masking result for solvated structures.

Name	Masked volume V (Å^3)	Number of masked electrons	e Å^{-3}
1	798	267	0.3346
2	1729	516	0.2984
3	3230	1244	0.3851
4	3436	1107	0.3222
5	4446	1405	0.3160
6	2008	581	0.2893

Table S8. Experimental details for single-crystal X-ray diffraction studies.

Crystal data	**1**	**2**	**3**	**4**	**5**	**6**
Chemical formula	$MgB_{17}O_{30}C_{12}N_4H_{43}$	$MgB_{17}O_{28}C_{19}N_9H_{68}$	$MgB_{17}O_{30}C_{24}N_9H_{82}$	$MgB_{17}O_{31.5}C_9N_{4.5}H_{41}$	$MgB_{17}O_{32}C_{11.75}N_5H_{49.5}$	$MgB_{17}O_{31.5}C_{11}N_{4.5}H_{41.5}$
M_r	1435.8	1078.863	1125.9	924.5	981.1	949.52
Crystal system, space group	Tetragonal, $P4_2/n$	Tetragonal, $P\bar{4}2_1m$	Tetragonal, $I\bar{4}2d$	Monoclinic, $P2_1/c$	Monoclinic, Pc	Monoclinic, $P2_1$
Temperature (°C)	23	23	23	−173	−173	23
Unit-cell parameters	a = 14.0492 (4) Å c = 10.1802 (3) Å	a = 16.1163 (6) Å c = 10.0685 (6) Å	a = 22.4695 (3) Å c = 10.1408 (5) Å	a = 19.6909 (10) Å b = 15.9750 (8) Å c = 22.8241 (10) Å β = 90.418 (4) °	a = 19.5105 (10) Å b = 19.9572 (8) Å c = 21.3269 (11) Å β = 91.091 (5) °	a = 14.33587 (19) b = 19.9667 (3) c = 14.4962 (2) β = 94.5979 (13)
V (Å^3)	2009.37 (12)	2615.1 (2)	5119.9 (3)	7179.4 (6)	8302.6 (7)	4136.05 (10)
Z	2	2	4	8	8	4
Radiation type	Mo $K\alpha$	Mo $K\alpha$	Cu $K\alpha$	Mo $K\alpha$	Mo $K\alpha$	Cu $K\alpha$
μ (mm^{-1})	0.15	0.12	0.11	0.17	0.15	0.15
Crystal size (mm)	0.17 × 0.12 × 0.09	0.05 × 0.14 × 0.14	0.04 × 0.10 × 0.30	0.06 × 0.10 × 0.16	0.08 × 0.15 × 0.17	0.19 × 0.21 × 0.30
Data collection						
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix	XtaLAB Synergy, Single source at home/near, HyPix	XtaLAB Synergy, Dualflex, HyPix	XtaLAB Synergy, Single source at home/near, HyPix	XtaLAB Synergy, Single source at home/near, HyPix	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Gaussian *CrysAlis PRO* 1.171.41.93a (Rigaku Oxford Diffraction, 2020) Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Gaussian *CrysAlis PRO* 1.171.41.93a (Rigaku Oxford Diffraction, 2020) Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	For a sphere *CrysAlis PRO* 1.171.41.93a (Rigaku Oxford Diffraction, 2020) Spherical absorption correction using equivalent radius and absorption coefficient. Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan *CrysAlis PRO* 1.171.41.93a (Rigaku Oxford Diffraction, 2020) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Multi-scan *CrysAlis PRO* 1.171.41.93a (Rigaku Oxford Diffraction, 2020) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.	Gaussian *CrysAlis PRO* 1.171.41.93a (Rigaku Oxford Diffraction, 2020) Numerical absorption correction based on gaussian integration over a multifaceted crystal model Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min}, T_{max}	0.918, 1.000	0.988, 1.000	0.571, 0.604	0.143, 1.000	0.502, 1.000	0.483, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28549, 1630, 1364	25772, 2278, 1783	25273, 2775, 2159	56873, 5346, 4651	72918, 25415, 12696	43527, 15771, 14747
R_{int}	0.122	0.133	0.083	0.121	0.134	0.057
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.578	0.582	0.638	0.455	0.602	0.639
Refinement						
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.059, 0.169, 1.14	0.034, 0.082, 0.90	0.031, 0.086, 0.98	0.100, 0.264, 1.20	0.099, 0.297, 0.96	0.055, 0.158, 1.02
No. of reflections	1630	2278	2775	5346	25415	15771
No. of parameters	111	106	105	861	696	874
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.43, -0.28	0.22, -0.22	0.14, -0.12	0.61, -0.28	0.02, -0.02	0.35, -0.41

Computer programs: Computer programs: *CrysAlis PRO* 1.171.41.93a (Rigaku OD, 2020), *SHELXD* (Sheldrick, 2008), *SHELXL* 2019/3 (Sheldrick, 2015), Jana2020 (Petříček, V., *et al*., 2023), Olex2 1.5-alpha (Dolomanov *et al.*, 2009).

Table S9. Fractional atomic coordinates, site-occupancy factors (SOFs) and isotropic or equivalent isotropic displacement parameters (Å^2) in the structure of **1**.

Atom	SOF	x	y	z	U_{eq}
Mg1	1	0.25	0.25	0.25	0.0264(4)
O1	1	0.0699(2)	–0.14041(17)	0.1028(3)	0.0620(10)
O2	1	0.25	0.25	0.0351(3)	0.0329(9)
O3	1	0.18874(15)	0.11544(14)	0.22284(19)	0.0322(7)
O4	1	0.39555(15)	0.33819(16)	0.02635(19)	0.0395(7)
O5	1	0.05316(16)	0.02419(16)	0.1391(2)	0.0456(8)
O6	1	0.32848(17)	0.02550(16)	0.2669(2)	0.0433(8)
O7	1	0.20016(19)	–0.05073(17)	0.1739(3)	0.0562(9)
O8	1	0.32555(18)	0.2890(2)	–0.1680(2)	0.0543(9)

B1	1	0.3248(3)	0.2938(3)	–0.0363(3)	0.0353(11)
B2	1	0.2395(3)	0.0314(3)	0.2226(3)	0.0369(11)
B3	1	0.1058(3)	–0.0540(3)	0.1350(4)	0.0480(14)
B4	1	0.4073(3)	0.3814(3)	0.1561(3)	0.0350(11)
B5	1	0.25	0.25	–0.25	0.0480(17)

Table S10. Atomic displacement parameters (Å^2) in the structure of **1**.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0323(7)	0.0323(7)	0.0147(9)	0	0	0
O1	0.0680(18)	0.0341(14)	0.084(2)	–0.0073(12)	–0.0233(15)	–0.0063(13)
O2	0.0402(17)	0.0407(17)	0.0177(14)	0.0009(13)	0	0
O3	0.0383(12)	0.0339(12)	0.0244(11)	–0.0029(9)	–0.0050(9)	–0.0028(9)
O4	0.0400(13)	0.0527(14)	0.0258(11)	–0.0045(10)	0.0059(10)	0.0005(10)
O5	0.0464(14)	0.0400(14)	0.0504(14)	–0.0062(11)	–0.0107(11)	–0.0065(11)
O6	0.0484(14)	0.0375(13)	0.0441(13)	0.0051(10)	–0.0169(11)	–0.0058(10)
O7	0.0612(17)	0.0380(14)	0.0695(18)	–0.0002(12)	–0.0243(14)	–0.0120(13)
O8	0.0564(16)	0.090(2)	0.0164(11)	–0.0135(14)	0.0064(10)	–0.0002(12)
B1	0.039(2)	0.045(2)	0.0219(17)	0.0057(16)	0.0044(15)	0.0037(15)
B2	0.051(2)	0.033(2)	0.0266(18)	–0.0034(16)	–0.0029(17)	–0.0005(15)
B3	0.060(3)	0.038(2)	0.046(2)	–0.0042(19)	–0.015(2)	0.0031(18)
B4	0.0362(19)	0.039(2)	0.0298(18)	–0.0048(15)	0.0041(15)	0.0030(15)
B5	0.063(3)	0.063(3)	0.018(3)	0	0	0

Table S11. Selected bond lengths (Å) in the structure of **1**.

Bond	Length	Bond	Length
Mg1—O2^{i}	2.187 (3)	O4—B1	1.336 (4)
Mg1—O2	2.187 (3)	O4—B4	1.463 (4)
Mg1—O3^{i}	2.095 (2)	O5—B3	1.325 (5)
Mg1—O3^{ii}	2.095 (2)	O5—B4^{iii}	1.449 (4)
Mg1—O3	2.095 (2)	O6—B2	1.332 (5)
Mg1—O3^{iii}	2.095 (2)	O6—B4^{i}	1.434 (4)
O1—B3	1.355 (5)	O7—B2	1.373 (4)
O2—B1^{iii}	1.419 (4)	O7—B3	1.385 (5)
O2—B1	1.419 (4)	O8—B1	1.342 (4)
O3—B2	1.379 (4)	O8—B5	1.457 (2)
O3—B4^{iii}	1.511 (4)		

Symmetry code(s): (i) y, $-x+1/2$, $-z+1/2$; (ii) $-y+1/2$, x, $-z+1/2$; (iii) $-x+1/2$, $-y+1/2$, z.

Table S12. Fractional atomic coordinates, site–occupancy factors (SOFs) and isotropic or equivalent isotropic displacement parameters (Å^2) in the structure of **2**.

Atom	SOF	x	y	z	U_{eq}
Mg1	1	0.5	0.5	0.5	0.0285(3)
O1	1	0.14877(9)	0.64877(9)	0.6117(2)	0.0412(7)
O2	1	0.38152(8)	0.55512(9)	0.52283(13)	0.0344(5)
O3	1	0.5	0.5	0.71338(16)	0.0285(7)
O4	1	0.42425(8)	0.69401(9)	0.48503(16)	0.0401(5)
O5	1	0.64725(9)	0.52520(10)	0.72250(14)	0.0437(6)
O6	1	0.23982(9)	0.53831(9)	0.60850(16)	0.0433(5)
O7	1	0.29158(10)	0.67070(10)	0.55159(19)	0.0577(7)
O8	1	0.57168(10)	0.51740(10)	0.91755(14)	0.0533(7)
B1	1	0.57143(19)	0.51439(16)	0.7812(2)	0.0423(10)
B2	1	0.67947(15)	0.50440(17)	0.5903(2)	0.0320(8)
B3	1	0.22713(17)	0.61808(14)	0.5914(3)	0.0388(9)
B4	1	0.36863(15)	0.63850(14)	0.5221(2)	0.0273(8)
B5	1	0.5	0.5	1	0.0356(13)

Table S13. Atomic displacement parameters (Å^2) in the structure of **2**.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0276(4)	0.0276(4)	0.0304(7)	0	0	0
O1	0.0196(7)	0.0196(7)	0.0844(17)	0.0138(9)	0.0106(8)	0.0106(8)

O2	0.0355(8)	0.0313(8)	0.0365(8)	–0.0001(6)	–0.0026(7)	0.0031(7)
O3	0.0296(12)	0.0275(12)	0.0285(10)	0.0011(12)	0	0
O4	0.0272(8)	0.0370(9)	0.0562(10)	0.0053(7)	0.0066(8)	–0.0046(8)
O5	0.0382(9)	0.0568(12)	0.0362(8)	–0.0024(8)	–0.0014(8)	–0.0119(7)
O6	0.0363(9)	0.0362(9)	0.0573(10)	0.0074(7)	–0.0017(8)	0.0018(8)
O7	0.0370(10)	0.0317(9)	0.1045(16)	0.0009(8)	0.0322(9)	0.0087(8)
O8	0.0638(12)	0.0648(13)	0.0312(9)	0.0034(10)	–0.0082(8)	–0.0054(8)
B1	0.063(2)	0.0295(16)	0.0343(14)	0.0083(14)	0.0120(14)	–0.0075(12)
B2	0.0358(14)	0.0368(14)	0.0233(13)	0.0104(12)	–0.0067(11)	–0.0138(13)
B3	0.0426(17)	0.0110(13)	0.0628(18)	0.0023(12)	–0.0117(15)	0.0008(12)
B4	0.0373(15)	0.0224(13)	0.0221(13)	0.0049(10)	0.0012(11)	0.0066(11)
B5	0.0369(17)	0.0369(17)	0.033(3)	0	0	0

Table S14. Selected bond lengths (Å) in the structure of **2**.

Bond	Length	Bond	Length
Mg1—O2^{i}	2.1185 (14)	O3—B1	1.359 (3)
Mg1—O2^{ii}	2.1185 (14)	O4—B2^{iii}	1.397 (3)
Mg1—O2	2.1185 (14)	O4—B4	1.320 (3)
Mg1—O2^{iii}	2.1185 (14)	O5—B1	1.368 (3)
Mg1—O3	2.1484 (17)	O5—B2	1.468 (3)
Mg1—O3^{iii}	2.1484 (17)	O6—B2^{i}	1.483 (3)
O1—B3^{iv}	1.372 (3)	O6—B3	1.313 (3)
O1—B3	1.372 (3)	O7—B3	1.400 (3)
O2—B2^{i}	1.532 (3)	O7—B4	1.378 (3)
O2—B4	1.360 (3)	O8—B1	1.374 (3)
O3—B1^{i}	1.359 (3)	O8—B5^{v}	1.4500 (16)

Symmetry code(s): (i) –*x*+1, –*y*+1, *z*; (ii) *y*, –*x*+1, –*z*+1; (iii) –*y*+1, *x*, –*z*+1; (iv) *y*–1/2, *x*+1/2, *z*; (v) –*y*+1, *x*, –*z*+2.

Table S15. Fractional atomic coordinates, site–occupancy factors (SOFs) and isotropic or equivalent isotropic displacement parameters (Å^2) in the structure of **3**.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Mg1	1	0.5	0.5	0.5	0.03837(19)
O1	1	0.46380(4)	0.58501(4)	0.52511(11)	0.0452(3)
O2	1	0.47837(4)	0.68586(5)	0.61035(15)	0.0665(4)
O3	1	0.36329(4)	0.55775(4)	0.47926(16)	0.0690(4)
O4	1	0.5	0.5	0.71427(14)	0.0574(5)
O5	1	0.51805(6)	0.60453(6)	0.72553(14)	0.0770(5)
O6	1	0.39485(7)	0.75	0.625	0.1022(11)
O7	1	0.38171(5)	0.65180(5)	0.5587(2)	0.1096(7)
O8	1	0.51200(11)	0.55272(9)	0.91728(15)	0.1251(9)
B1	1	0.50406(7)	0.62827(6)	0.5958(2)	0.0526(5)
B2	1	0.40285(7)	0.59712(8)	0.5190(3)	0.0582(7)
B3	1	0.5	0.5	1	0.1053(16)
B4	1	0.50927(12)	0.55380(12)	0.7851(2)	0.0777(8)
B5	1	0.42067(6)	0.69761(9)	0.5930(3)	0.0751(8)

Table S16. Atomic displacement parameters (Å^2) in the structure of **3**.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0287(2)	0.0287(2)	0.0577(5)	0	0	0
O2	0.0315(4)	0.0296(4)	0.0746(7)	0.0020(3)	0.0074(4)	–0.0106(4)
O3	0.0293(4)	0.0465(6)	0.1236(11)	–0.0023(4)	0.0074(6)	–0.0304(6)
O4	0.0420(5)	0.0308(5)	0.1341(11)	0.0019(4)	–0.0236(7)	–0.0205(6)
O5	0.0570(8)	0.0655(9)	0.0497(8)	–0.0155(8)	0	0
O6	0.0937(10)	0.0624(7)	0.0748(8)	–0.0165(7)	–0.0158(7)	–0.0111(7)
O7	0.0467(8)	0.0340(8)	0.226(3)	0	0	–0.0381(12)
O8	0.0480(6)	0.0368(6)	0.244(2)	–0.0011(5)	–0.0121(9)	–0.0580(9)
O9	0.184(2)	0.1336(16)	0.0577(9)	–0.0135(16)	–0.0078(11)	–0.0222(9)
B1	0.0355(7)	0.0327(7)	0.0897(12)	–0.0046(6)	0.0074(10)	–0.0166(8)
B2	0.0310(7)	0.0452(9)	0.0985(16)	0.0034(6)	–0.0086(9)	–0.0217(10)
B3	0.131(3)	0.131(3)	0.054(2)	0	0	0
B4	0.0858(16)	0.0829(15)	0.0644(13)	–0.0082(13)	–0.0144(12)	–0.0135(11)

B5	0.0190(7)	0.0523(10)	0.154(2)	0.0007(6)	0.0019(9)	–0.0309(13)

Table S17. Selected bond lengths (Å) in the structure of **3**.

Bond	Length	Bond	Length
Mg1—O2	2.0916 (8)	O4—B2	1.317 (2)
Mg1—O2^{i}	2.0916 (8)	O5—B4	1.421 (3)
Mg1—O2^{ii}	2.0916 (8)	O5—B4^{i}	1.421 (3)
Mg1—O2^{iii}	2.0916 (8)	O6—B1	1.454 (3)
Mg1—O5	2.1729 (14)	O6—B4	1.305 (3)
Mg1—O5^{ii}	2.1729 (14)	O7—B5	1.3520 (19)
O2—B1	1.5093 (19)	O7—B5^{iv}	1.3520 (19)
O2—B2	1.3976 (17)	O8—B2	1.3774 (19)
O3—B1	1.4245 (19)	O8—B5	1.395 (2)
O3—B5	1.3348 (19)	O9—B4	1.342 (3)
O4—B1^{iii}	1.439 (2)	O9—B3^{v}	1.476 (2)

Symmetry code(s): (i) –*x*+1, –*y*+1, *z*; (ii) *y*, –*x*+1, –*z*+1; (iii) –*y*+1, *x*, –*z*+1; (iv) *x*, –*y*+3/2, –*z*+5/4; (v) *y*, –*x*+1, –*z*+2.

Table S18. Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2) in the structure of **4**.

Atom	SOF	*x*	*y*	*z*	U_{eq}
Mg1	1	0.88085(13)	0.76090(15)	0.38385(10)	0.0441(10)
Mg2	1	0.38883(13)	0.73677(15)	0.36190(11)	0.0434(10)
O1	1	0.4979(3)	0.9243(4)	0.2599(2)	0.062(2)
O2	1	0.3377(3)	0.7714(4)	0.5459(3)	0.064(3)
O3	1	0.3781(2)	0.7846(3)	0.44827(19)	0.0357(17)
O4	1	0.4260(3)	0.8505(3)	0.3313(2)	0.0463(19)
O5	1	0.3750(2)	0.6114(3)	0.3920(2)	0.0400(17)
O6	1	0.8924(3)	0.6374(3)	0.3574(2)	0.049(2)
O7	1	0.4311(3)	0.8131(4)	0.2304(2)	0.056(2)
O8	1	0.3746(2)	0.6976(3)	0.2763(2)	0.0404(19)
O9	1	0.0867(3)	0.8350(4)	0.3171(3)	0.070(3)
O10	1	0.8534(3)	0.8825(3)	0.4114(2)	0.0439(19)
O11	1	0.3992(3)	0.9297(3)	0.4167(3)	0.060(2)
O12	1	0.4932(3)	0.7054(3)	0.3717(2)	0.0403(17)
O13	1	0.2629(3)	0.6472(3)	0.2953(2)	0.049(2)
O14	1	0.9092(4)	0.3926(4)	0.3106(3)	0.087(3)
O15	1	0.3906(3)	0.5136(3)	0.4734(2)	0.046(2)
O16	1	0.8906(3)	0.4893(4)	0.3836(4)	0.076(3)
O17	1	0.8768(3)	0.8051(3)	0.2982(2)	0.0517(19)
O18	1	0.3571(3)	0.5520(3)	0.2979(2)	0.045(2)
O19	1	0.2814(3)	0.7631(3)	0.3566(2)	0.0456(19)
O20	1	0.9219(3)	0.5865(4)	0.4578(3)	0.067(3)
O21	1	0.8456(3)	0.7885(4)	0.1967(3)	0.072(3)
O22	1	0.3751(3)	0.7156(4)	0.1716(3)	0.063(3)
O23	1	0.2877(3)	0.8765(4)	0.4246(3)	0.062(3)
O24	1	0.7765(3)	0.7286(3)	0.3948(2)	0.053(2)
O25	1	0.3543(3)	0.9056(3)	0.5094(2)	0.049(2)
O26	1	0.8810(3)	0.9526(4)	0.3229(3)	0.059(2)
O27	1	0.1857(3)	0.8480(4)	0.3792(3)	0.072(3)
O28	1	0.4709(3)	0.6196(3)	0.4558(2)	0.045(2)
O29	1	0.1043(3)	0.7450(4)	0.4020(3)	0.073(3)
O30	1	0.8945(3)	0.9193(3)	0.2271(2)	0.059(2)
O31	1	0.3302(3)	0.6068(4)	0.1091(3)	0.068(3)
O32	1	0.8746(3)	0.5304(4)	0.2840(3)	0.065(2)
O33	1	0.8524(4)	0.8963(4)	0.1292(3)	0.085(3)
O34	1	0.8455(3)	0.8480(4)	0.5132(2)	0.056(2)
O35	1	0.3732(3)	0.4629(3)	0.3763(2)	0.059(3)
O36	1	0.3763(4)	0.3676(4)	0.4553(2)	0.072(3)
O37	1	0.5273(3)	0.7871(4)	0.2908(3)	0.064(2)
O38	1	0.6100(3)	0.7140(5)	0.3410(3)	0.079(3)
O39	1	0.3618(3)	0.6517(4)	0.4932(2)	0.052(2)

O40	1	0.7474(3)	0.8482(4)	0.4519(2)	0.054(2)
O41	1	0.7960(3)	0.9708(4)	0.4855(2)	0.054(2)
O42	1	0.9150(4)	0.7724(5)	0.5732(2)	0.079(3)
O43	1	0.9061(3)	0.7345(4)	0.4694(2)	0.059(2)
O44	1	0.9912(3)	0.7840(3)	0.3733(2)	0.0474(19)
O45	1	0.6641(3)	0.7539(4)	0.4295(3)	0.065(3)
O46	1	0.9740(3)	0.6482(4)	0.5388(3)	0.071(3)
O47	1	0.9860(3)	0.7036(4)	0.6384(3)	0.075(3)
O48	1	0.8627(4)	0.6711(4)	0.2570(2)	0.080(3)
O49	1	1.0157(3)	0.6794(4)	0.4466(2)	0.061(2)
O50	1	0.7802(3)	0.6136(4)	0.3228(3)	0.066(3)
O51	1	0.9819(3)	0.8823(4)	0.2961(3)	0.064(3)
O52	1	0.6892(3)	0.6215(3)	0.3894(3)	0.058(2)
O53	1	0.3164(3)	0.6002(3)	0.2087(2)	0.052(2)
O54	1	0.4579(4)	0.9926(4)	0.3434(3)	0.087(3)
O55	1	0.5187(5)	1.0675(5)	0.2756(4)	0.115(4)
O56	1	0.8028(4)	1.1187(4)	0.4749(3)	0.077(3)
O57	1	0.5819(3)	0.6463(3)	0.4318(2)	0.057(3)
O58	1	0.8419(3)	1.0308(4)	0.4000(3)	0.063(2)
O59	1	0.8038(3)	0.5892(4)	0.4254(3)	0.071(3)
O60	1	0.1725(3)	0.7305(4)	0.3158(3)	0.065(3)
B1	1	0.2527(5)	0.8297(7)	0.3861(4)	0.045(4)
B2	1	0.9085(5)	0.8906(6)	0.2869(4)	0.043(4)
B3	1	0.8894(6)	0.4729(6)	0.3297(7)	0.061(5)
B4	1	0.8847(7)	0.7851(9)	0.5176(5)	0.070(5)
B5	1	0.7297(6)	0.7753(6)	0.4291(5)	0.061(5)
B6	1	0.9540(5)	0.6622(7)	0.4778(4)	0.050(4)
B7	1	0.4276(6)	0.9255(7)	0.3632(5)	0.056(3)
B8	1	0.4902(6)	0.9933(7)	0.2916(5)	0.056(3)
B9	1	0.3591(5)	0.7322(8)	0.4930(5)	0.052(4)
B10	1	0.3415(6)	0.8561(8)	0.5536(6)	0.067(6)
B11	1	1.0370(6)	0.7350(6)	0.4064(5)	0.053(4)
B12	1	1.0196(5)	0.8352(7)	0.3273(5)	0.049(4)
B13	1	0.3662(6)	0.5442(6)	0.3547(5)	0.055(4)
B14	1	0.8108(5)	1.0373(9)	0.4547(6)	0.068(5)
B15	1	0.1375(6)	0.7910(7)	0.3503(6)	0.067(4)
B16	1	0.3568(6)	0.8752(8)	0.4502(5)	0.066(5)
B17	1	0.3799(5)	0.4510(6)	0.4348(5)	0.052(4)
B18	1	0.4680(6)	0.8457(6)	0.2764(4)	0.054(4)
B19	1	0.8603(5)	0.9525(6)	0.3757(6)	0.055(5)
B20	1	0.8096(6)	0.8835(7)	0.4672(4)	0.050(4)
B21	1	0.8811(6)	0.5778(9)	0.4079(8)	0.096(7)
B22	1	0.8643(7)	0.8726(7)	0.1839(6)	0.069(5)
B23	1	0.9608(6)	0.7041(10)	0.5838(6)	0.083(6)
B24	1	0.8527(6)	0.6141(6)	0.3067(4)	0.052(4)
B25	1	0.3966(5)	0.7424(7)	0.2265(4)	0.042(4)
B26	1	0.4020(5)	0.5987(6)	0.4524(4)	0.041(4)
B27	1	0.6382(5)	0.6827(6)	0.3994(4)	0.047(4)
B28	1	0.2406(5)	0.7133(6)	0.3209(5)	0.048(4)
B29	1	0.3280(5)	0.6266(6)	0.2684(4)	0.051(4)
B30	1	0.8616(7)	0.7533(8)	0.2527(6)	0.077(6)
B31	1	0.5428(6)	0.7363(7)	0.3345(5)	0.060(5)
B32	1	0.5146(6)	0.6564(7)	0.4216(4)	0.049(4)
B33	1	0.7591(6)	0.6374(7)	0.3818(5)	0.064(5)
B34	1	0.3396(6)	0.6396(8)	0.1627(5)	0.059(5)

Table S19. Atomic displacement parameters (Å^2) in the structure of **4**.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.0534(19)	0.0436(17)	0.0354(17)	0.0092(12)	0.0080(12)	0.0001(12)
Mg2	0.0469(18)	0.0404(17)	0.0430(17)	0.0020(12)	–0.0008(12)	0.0062(12)
O1	0.070(4)	0.062(4)	0.054(4)	–0.029(3)	–0.010(3)	0.013(3)

O2	0.078(4)	0.055(5)	0.060(4)	0.015(3)	0.011(3)	0.014(3)
O3	0.055(3)	0.033(3)	0.019(3)	–0.003(3)	–0.004(2)	0.017(2)
O4	0.062(4)	0.040(3)	0.037(3)	–0.008(3)	0.013(3)	0.006(3)
O5	0.046(3)	0.037(3)	0.037(3)	0.000(2)	–0.006(2)	0.000(3)
O6	0.050(4)	0.042(3)	0.056(4)	0.003(3)	0.022(3)	0.027(3)
O7	0.052(4)	0.055(4)	0.062(4)	–0.019(3)	–0.007(3)	0.010(3)
O8	0.043(3)	0.027(3)	0.051(4)	–0.010(3)	–0.010(3)	0.014(3)
O9	0.048(5)	0.069(4)	0.093(5)	0.011(3)	0.003(4)	0.004(4)
O10	0.049(3)	0.041(4)	0.042(3)	0.015(3)	0.016(3)	0.005(3)
O11	0.074(4)	0.039(3)	0.066(4)	–0.028(3)	–0.004(4)	0.009(3)
O12	0.048(3)	0.045(3)	0.028(3)	0.000(3)	0.008(3)	0.013(3)
O13	0.048(4)	0.052(4)	0.046(3)	–0.002(3)	–0.006(3)	0.009(3)
O14	0.097(5)	0.052(5)	0.112(5)	0.010(4)	0.009(4)	0.039(4)
O15	0.057(4)	0.044(4)	0.037(3)	–0.001(3)	0.000(2)	0.016(3)
O16	0.078(5)	0.068(5)	0.081(6)	–0.003(3)	–0.015(4)	0.006(4)
O17	0.080(4)	0.033(3)	0.042(3)	–0.006(3)	–0.004(3)	0.006(3)
O18	0.072(4)	0.047(4)	0.017(4)	–0.007(3)	–0.007(2)	0.017(3)
O19	0.055(4)	0.032(3)	0.050(3)	0.010(3)	0.012(3)	–0.005(3)
O20	0.064(4)	0.073(5)	0.064(4)	0.005(4)	–0.002(4)	0.011(3)
O21	0.080(5)	0.080(5)	0.056(4)	–0.008(4)	0.004(3)	0.023(4)
O22	0.068(4)	0.059(4)	0.061(5)	–0.001(3)	0.013(3)	0.023(3)
O23	0.066(5)	0.066(4)	0.053(4)	0.012(3)	–0.001(4)	–0.006(3)
O24	0.055(4)	0.041(3)	0.063(4)	0.005(3)	0.009(3)	0.014(3)
O25	0.088(4)	0.029(3)	0.031(4)	0.010(3)	0.007(3)	0.003(3)
O26	0.079(4)	0.062(4)	0.035(4)	0.012(3)	0.022(3)	0.006(3)
O27	0.054(5)	0.080(4)	0.081(5)	–0.004(4)	0.005(3)	–0.005(4)
O28	0.051(5)	0.046(3)	0.037(3)	–0.008(3)	0.002(3)	0.001(3)
O29	0.044(5)	0.103(5)	0.071(4)	0.018(4)	0.005(3)	0.022(4)
O30	0.098(5)	0.044(3)	0.035(4)	–0.018(3)	–0.007(3)	–0.004(3)
O31	0.103(5)	0.080(4)	0.022(4)	–0.026(4)	0.004(3)	0.005(4)
O32	0.075(4)	0.058(4)	0.063(4)	–0.009(3)	0.003(3)	–0.015(4)
O33	0.124(6)	0.080(5)	0.050(5)	0.015(4)	–0.012(4)	0.008(4)
O34	0.068(4)	0.058(4)	0.042(4)	0.030(4)	–0.004(3)	0.004(3)
O35	0.097(5)	0.049(4)	0.031(4)	–0.006(3)	0.006(3)	0.009(3)
O36	0.110(5)	0.050(4)	0.055(4)	0.005(3)	–0.009(3)	0.003(3)
O37	0.042(4)	0.090(4)	0.061(4)	0.007(3)	0.006(3)	0.027(4)
O38	0.051(5)	0.134(6)	0.052(4)	0.004(4)	–0.002(3)	0.045(4)
O39	0.063(4)	0.046(4)	0.048(4)	0.004(3)	0.002(3)	–0.003(3)
O40	0.046(4)	0.043(4)	0.073(4)	0.000(3)	0.013(3)	0.005(3)
O41	0.069(4)	0.046(4)	0.046(3)	0.009(3)	0.014(3)	–0.001(3)
O42	0.097(5)	0.102(5)	0.037(4)	0.041(4)	–0.014(3)	0.004(3)
O43	0.051(4)	0.084(4)	0.041(4)	0.021(3)	0.004(3)	0.007(3)
O44	0.047(4)	0.053(3)	0.042(3)	0.005(3)	–0.010(3)	0.002(3)
O45	0.034(4)	0.062(4)	0.098(5)	–0.011(3)	0.010(3)	–0.005(4)
O46	0.075(5)	0.082(4)	0.056(5)	0.034(3)	0.008(3)	–0.008(4)
O47	0.080(5)	0.074(4)	0.070(5)	–0.005(3)	–0.010(4)	–0.006(3)
O48	0.141(7)	0.063(5)	0.036(4)	–0.036(4)	–0.010(3)	0.003(3)
O49	0.043(4)	0.089(4)	0.052(4)	0.016(3)	0.007(3)	0.018(4)
O50	0.062(5)	0.057(4)	0.079(5)	0.004(3)	0.001(3)	–0.010(3)
O51	0.052(5)	0.059(4)	0.081(4)	0.002(3)	0.004(3)	0.018(3)
O52	0.046(4)	0.047(4)	0.082(4)	–0.009(3)	0.008(3)	0.002(3)
O53	0.073(4)	0.049(3)	0.033(4)	–0.016(3)	0.006(3)	0.007(3)
O54	0.117(6)	0.064(4)	0.080(5)	–0.034(4)	0.024(4)	0.013(4)
O55	0.155(8)	0.092(6)	0.097(6)	–0.034(5)	0.033(5)	0.026(5)
O56	0.101(5)	0.044(4)	0.087(5)	0.003(3)	0.015(4)	–0.015(3)
O57	0.055(5)	0.055(4)	0.061(4)	0.006(3)	–0.010(3)	0.006(3)
O58	0.072(4)	0.057(4)	0.059(4)	0.012(3)	0.023(3)	0.011(3)
O59	0.087(5)	0.053(4)	0.074(4)	–0.004(3)	–0.007(4)	0.004(3)
O60	0.045(5)	0.057(4)	0.094(5)	0.001(3)	0.001(3)	–0.015(3)
B1	0.031(7)	0.079(8)	0.026(5)	–0.014(6)	–0.003(5)	0.017(6)
B2	0.044(7)	0.052(7)	0.032(6)	0.006(5)	0.018(5)	–0.005(5)
B3	0.072(8)	0.012(6)	0.100(11)	0.009(5)	0.001(7)	0.020(7)
B4	0.087(9)	0.084(9)	0.040(8)	0.021(8)	0.019(7)	0.043(7)

B5	0.067(10)	0.018(6)	0.098(9)	0.001(6)	0.036(7)	0.003(6)
B6	0.057(7)	0.059(7)	0.033(6)	0.003(6)	–0.002(5)	0.001(5)
B7	0.064(5)	0.063(6)	0.042(5)	–0.016(4)	0.020(4)	0.023(5)
B8	0.064(5)	0.063(6)	0.042(5)	–0.016(4)	0.020(4)	0.023(5)
B9	0.048(6)	0.057(9)	0.052(8)	0.035(6)	–0.011(5)	–0.026(7)
B10	0.062(8)	0.046(9)	0.094(12)	0.011(6)	–0.033(7)	0.009(8)
B11	0.063(9)	0.050(6)	0.045(7)	–0.001(6)	0.004(6)	–0.009(6)
B12	0.033(8)	0.048(6)	0.065(7)	0.010(6)	0.000(6)	0.012(6)
B13	0.080(8)	0.024(6)	0.061(9)	–0.007(5)	0.024(6)	–0.009(7)
B14	0.032(6)	0.096(12)	0.077(9)	–0.002(6)	0.004(6)	0.013(9)
B15	0.049(7)	0.052(7)	0.101(9)	–0.017(7)	–0.010(7)	–0.005(7)
B16	0.053(8)	0.085(10)	0.061(9)	0.043(7)	–0.021(6)	0.005(7)
B17	0.064(7)	0.029(7)	0.064(9)	–0.010(5)	0.002(5)	0.007(6)
B18	0.064(7)	0.046(6)	0.052(7)	–0.027(6)	–0.012(6)	0.003(5)
B19	0.042(6)	0.028(7)	0.094(11)	0.006(5)	0.007(6)	0.000(7)
B20	0.052(7)	0.060(7)	0.039(6)	–0.009(6)	0.006(6)	0.023(6)
B21	0.051(8)	0.088(11)	0.149(15)	0.009(7)	–0.033(9)	–0.042(11)
B22	0.090(9)	0.060(8)	0.056(10)	0.005(7)	0.030(7)	–0.004(7)
B23	0.063(8)	0.128(12)	0.059(10)	0.019(8)	0.010(7)	0.047(9)
B24	0.080(9)	0.031(6)	0.044(7)	0.005(5)	0.013(6)	–0.004(5)
B25	0.044(6)	0.063(8)	0.018(6)	0.020(6)	–0.012(5)	0.006(6)
B26	0.041(7)	0.038(6)	0.044(7)	–0.013(5)	–0.003(5)	–0.003(5)
B27	0.027(6)	0.052(7)	0.062(7)	0.004(6)	0.001(5)	–0.005(6)
B28	0.039(8)	0.033(6)	0.072(7)	0.024(6)	0.001(6)	–0.016(6)
B29	0.063(8)	0.061(7)	0.028(7)	0.000(6)	0.009(5)	0.019(5)
B30	0.104(10)	0.047(9)	0.081(11)	–0.028(7)	0.022(8)	–0.012(8)
B31	0.061(9)	0.055(7)	0.065(8)	0.007(6)	0.000(7)	0.015(7)
B32	0.034(8)	0.070(7)	0.044(7)	–0.008(6)	–0.012(6)	–0.006(6)
B33	0.060(9)	0.059(8)	0.072(9)	–0.003(6)	–0.013(6)	0.005(6)
B34	0.063(7)	0.071(8)	0.043(9)	–0.001(7)	–0.011(6)	0.008(7)

Table S20. Selected bond lengths (Å) in the structure of **4**.

Bond	Length	Bond	Length
Mg1—O44	2.218 (6)	O1—B18	1.438 (12)
Mg1—O43	2.054 (6)	O1—B8	1.329 (13)
Mg1—O10	2.113 (5)	O7—B18	1.376 (12)
Mg1—O17	2.079 (5)	O16—B3	1.259 (14)
O24—Mg1	2.134 (6)	O16—B21	1.530 (15)
O6—Mg1	2.076 (6)	O11—B16	1.432 (15)
Mg2—O3	2.126 (5)	O11—B7	1.349 (12)
Mg2—O4	2.081 (5)	O20—B6	1.438 (12)
Mg2—O19	2.160 (6)	O20—B21	1.397 (16)
O5—Mg2	2.135 (5)	O2—B9	1.426 (11)
O8—Mg2	2.069 (6)	O2—B10	1.367 (13)
O12—Mg2	2.126 (5)	O18—B13	1.312 (13)
O5—B26	1.488 (11)	O19—B1	1.383 (12)
O5—B13	1.381 (11)	O35—B13	1.396 (12)
O6—B24	1.442 (12)	O35—B17	1.353 (12)
O6—B21	1.512 (19)	O29—B11^{i}	1.339 (13)
O8—B25	1.414 (11)	O29—B15	1.540 (14)
O8—B29	1.469 (12)	O25—B16	1.436 (13)
O12—B31	1.391 (13)	O25—B10	1.309 (14)
O12—B32	1.442 (12)	O36—B17	1.414 (12)
O13—B28	1.285 (11)	O23—B16	1.477 (13)
O13—B29	1.464 (12)	O23—B1	1.341 (12)
O15—B26	1.458 (11)	O27—B1	1.357 (12)
O15—B17	1.348 (12)	O27—B15	1.468 (13)
O22—B25	1.387 (11)	O14—B3	1.410 (14)
O22—B34	1.415 (13)	O37—B18	1.530 (13)
O24—B33	1.525 (13)	O31—B10^{ii}	1.418 (14)
O24—B5	1.426 (12)	O44—B12	1.447 (12)
O28—B26	1.399 (11)	O44—B11	1.410 (13)

O28—B32	1.306 (12)	O43—B4	1.431 (14)
O32—B24	1.499 (11)	O43—B6	1.502 (12)
O32—B3	1.419 (14)	O10—B19	1.391 (12)
O39—B26	1.490 (12)	O10—B20	1.543 (11)
O39—B9	1.287 (12)	O17—B2	1.525 (11)
O45—B27	1.422 (12)	O21—B22	1.423 (14)
O45—B5	1.336 (13)	O9—B12^{i}	1.343 (12)
O48—B24	1.469 (12)	O9—B15	1.435 (14)
O48—B30	1.316 (14)	O34—B4	1.272 (13)
O50—B24	1.476 (13)	O34—B20	1.383 (12)
O50—B33	1.463 (13)	O26—B2	1.398 (11)
O52—B27	1.420 (11)	O26—B19	1.276 (13)
O52—B33	1.411 (13)	O30—B2	1.463 (11)
O53—B29	1.443 (12)	O30—B22	1.369 (14)
O53—B34	1.309 (12)	O41—B20	1.481 (12)
O57—B27	1.459 (12)	O41—B14	1.308 (14)
O57—B32	1.353 (12)	O40—B20	1.391 (12)
O59—B33	1.532 (13)	O40—B5	1.321 (12)
O59—B21	1.587 (15)	O33—B22	1.324 (14)
B25—O7	1.322 (12)	O42—B4	1.414 (14)
O60—B28	1.371 (12)	O42—B23	1.436 (15)
O60—B15	1.428 (13)	B2—O51	1.466 (12)
B27—O38	1.525 (12)	B19—O58	1.417 (12)
B28—O19	1.390 (12)	O46—B6	1.461 (12)
B29—O18	1.481 (12)	O46—B23	1.386 (17)
B30—O17	1.360 (14)	O47—B23	1.339 (15)
B30—O21	1.431 (15)	B6—O49	1.439 (12)
B31—O38	1.376 (13)	O49—B11	1.347 (12)
B31—O37	1.320 (12)	O58—B14	1.399 (14)
B34—O31	1.342 (13)	O51—B12	1.271 (12)
O3—B16	1.509 (13)	O56—B14	1.390 (15)
O3—B9	1.374 (13)	O54—B7	1.310 (12)
O4—B18	1.509 (12)	O54—B8	1.346 (12)
O4—B7	1.402 (13)	O55—B8	1.362 (13)

Symmetry code(s): (i) *x*–1, *y*, *z*; (ii) *x*, –*y*+3/2, *z*–1/2.

Table S21. Fractional atomic coordinates and isotropic displacement parameters (Å^2) in the structure of **5**.

Atom	SOF	*x*	*y*	*z*	$U_{iso/eq}$
Mg1	1	0.3758(2)	0.86547(17)	0.32076(18)	0.0326(11)
Mg2	1	0.8700(2)	1.13451(19)	0.3330(2)	0.0467(14)
Mg3	1	0.36740(19)	0.36574(16)	0.34012(18)	0.0268(8)
Mg4	1	0.8725(2)	0.63322(18)	0.3276(3)	0.0514(13)
O1	1	0.4624(4)	0.8450(4)	0.4591(4)	0.0386(8)
O2	1	0.4786(4)	0.7919(3)	0.0559(4)	0.0411(10)
O3	1	0.4096(3)	0.8628(3)	0.2263(3)	0.0258(8)
O6	1	0.3999(4)	0.6508(4)	0.3499(4)	0.0337(8)*
O5	1	0.5792(4)	1.0559(4)	0.2302(5)	0.0535(6)
O123	1	0.3628(3)	0.3346(3)	0.5418(3)	0.0268(8)
O7	1	0.3411(3)	0.7680(3)	0.1987(3)	0.0258(8)
O8	1	0.2302(4)	0.8767(4)	0.3885(4)	0.0386(8)
O9	1	0.9555(5)	1.1426(4)	0.4666(4)	0.0475(10)
O10	1	1.0564(5)	1.0939(7)	0.4428(5)	0.0805(14)
O11	1	0.4490(3)	0.3698(3)	0.4775(3)	0.0210(17)
O12	1	0.0826(4)	0.9503(4)	0.2317(4)	0.0393(16)*
O4	1	0.9696(4)	0.7111(4)	0.0606(5)	0.0535(6)
O14	1	0.5542(4)	0.4134(4)	0.4505(4)	0.0408(11)
O15	1	0.7257(5)	1.1170(4)	0.3989(4)	0.0475(10)
O16	1	0.3285(4)	1.2459(4)	0.2405(4)	0.0411(10)
O17	1	0.3962(4)	1.1578(4)	0.3997(4)	0.0411(10)
O18	1	0.4993(4)	0.9762(4)	0.3034(4)	0.0411(10)
O19	1	0.3670(4)	0.7847(4)	0.5115(4)	0.0386(8)
O20	1	0.9931(4)	0.5232(4)	0.3001(5)	0.0535(6)
O21	1	1.0885(4)	0.5759(4)	0.3463(5)	0.0535(6)

O22	1	0.5566(5)	0.9000(4)	0.4373(5)	0.062(3)
O23	1	0.3644(4)	0.4690(4)	0.3162(4)	0.0386(8)
O24	1	0.3044(4)	0.5744(4)	0.3171(4)	0.0337(8)*
O25	1	0.3745(4)	0.7584(4)	0.3053(4)	0.0337(8)*
O26	1	0.2773(3)	0.8811(3)	0.2859(3)	0.0259(11)
O27	1	0.5813(4)	0.4240(4)	0.3438(4)	0.0408(11)
O28	1	0.3787(5)	0.2891(6)	0.1496(4)	0.0716(16)
O29	1	0.3467(4)	0.8417(4)	0.4056(4)	0.0386(8)
O30	1	0.2490(4)	0.3420(3)	0.5054(3)	0.0287(16)
O31	1	0.0819(3)	0.4425(3)	0.2295(3)	0.0252(10)
O32	1	0.6900(5)	1.0900(4)	0.2116(5)	0.0535(6)
O33	1	0.3461(4)	0.6626(3)	0.2453(4)	0.0337(8)*
O34	1	0.5009(3)	0.8291(3)	0.1564(3)	0.0258(8)
O35	1	0.6003(4)	0.9147(4)	0.3367(4)	0.0386(8)
O36	1	0.5872(4)	0.5469(4)	0.2288(4)	0.0417(11)
O37	1	0.1537(3)	0.4210(3)	0.3234(3)	0.0252(10)
O38	1	0.2965(3)	0.8788(3)	0.1743(3)	0.0258(8)
O39	1	0.4843(4)	0.8707(4)	0.3574(4)	0.0386(8)
O40	1	0.9920(5)	1.0246(6)	0.3004(5)	0.0805(14)
O41	1	0.4384(4)	1.0770(4)	0.3385(4)	0.0411(10)
O42	1	0.7517(5)	1.1575(4)	0.5014(4)	0.0475(10)
O43	1	0.2778(4)	0.8639(4)	0.4988(4)	0.0386(8)
O44	1	0.9076(5)	1.1448(6)	0.2308(5)	0.0805(14)
O45	1	0.7662(5)	1.1286(4)	0.2988(5)	0.0535(6)
O46	1	0.8634(4)	1.1649(4)	0.5405(4)	0.0475(10)
O47	1	0.6587(5)	0.5745(5)	0.3172(5)	0.0609(14)
O48	1	0.3687(4)	1.2577(4)	0.3437(4)	0.0411(10)
O49	1	0.1595(3)	0.9261(3)	0.3136(3)	0.0259(11)
O50	1	0.4832(4)	0.4745(4)	0.2970(4)	0.0386(8)
O51	1	0.8715(6)	1.0274(4)	0.3244(5)	0.072(4)
O52	1	0.2204(4)	0.3871(3)	0.4099(3)	0.0287(16)
B1	1	0.3102(7)	0.8185(7)	0.5306(7)	0.0386(8)
O53	1	1.0565(4)	0.5983(4)	0.4423(5)	0.0535(6)
O54	1	0.5312(3)	0.8751(3)	0.2498(3)	0.0258(8)
O55	1	0.3194(4)	1.0714(4)	0.3681(5)	0.062(3)
O56	1	0.2558(4)	0.9879(4)	0.3442(4)	0.038(3)
O57	1	1.0901(5)	1.0824(6)	0.3344(5)	0.0805(14)
B2	1	0.7892(8)	1.1804(8)	0.5393(7)	0.0475(10)
O58	1	0.1863(3)	0.3997(3)	0.2216(3)	0.0252(10)
O59	1	0.4024(5)	0.3410(6)	0.2468(5)	0.0716(16)
O60	1	0.4022(3)	0.2605(3)	0.4550(3)	0.0268(8)
O61	1	0.2655(3)	0.3720(3)	0.3074(3)	0.0252(10)
O62	1	0.9031	0.6469	0.2446	0.0535(6)
O63	1	0.2910(4)	0.8023(4)	0.5933(4)	0.0386(8)
O64	1	0.7246(5)	0.6183(5)	0.4064(5)	0.0609(14)
O65	1	0.7537(5)	1.0160(4)	0.3448(5)	0.0535(6)
O66	1	0.7763(4)	0.6202(4)	0.2959(4)	0.0417(11)
O67	1	0.3855(3)	0.8253(3)	0.1177(3)	0.0258(8)
O68	1	0.4100(4)	0.7413(4)	0.4137(4)	0.0375(16)
O69	1	0.9481(4)	0.6357(4)	0.4749(5)	0.0535(6)
O70	1	0.1979(3)	0.9242(3)	0.2093(3)	0.0259(11)
O71	1	0.4123(4)	0.5658(3)	0.2622(4)	0.0337(8)*
O72	1	0.3339(3)	0.3615(3)	0.4321(3)	0.0268(8)
O73	1	0.6561(4)	1.0792(4)	0.3206(5)	0.0535(6)
O74	1	0.9756(5)	1.1188(6)	0.3707(6)	0.0805(14)
B3	1	0.4883(7)	0.3936(7)	0.4321(7)	0.0408(11)
O75	1	1.0276	0.6259	0.2529	0.0535(6)
O76	1	0.6729(4)	0.9406(4)	0.4181(4)	0.0386(8)
O77	1	0.8901	1.3436	0.3878	0.145(6)*
O78	1	0.8115	1.4277	0.332	0.112(3)*
B4	1	0.3598(7)	0.6108(6)	0.2988(6)	0.034(3)*
O79	1	0.9924	0.6677	0.1555	0.0514(13)
O80	1	0.8449(5)	0.6572(5)	0.4068(5)	0.0609(14)

B5	1	0.3568(5)	0.7235(5)	0.2481(5)	0.018(2)*
O81	1	0.8338(5)	1.1399(4)	0.4294(4)	0.0475(10)
O82	1	0.3165(4)	0.9552(3)	0.4475(4)	0.0375(16)
O83	1	0.2671(3)	0.3074(3)	0.6097(3)	0.0268(8)
O84	1	0.2531(3)	0.4826(3)	0.3536(3)	0.0249(19)
B6	1	0.3026(7)	0.5123(7)	0.3326(7)	0.0386(8)
B7	1	0.4971(7)	0.8611(7)	0.4273(7)	0.0386(8)
O85	1	0.7744(5)	0.6398(5)	0.4998(5)	0.0609(14)
O86	1	1.1685(5)	1.0593(6)	0.4155(5)	0.0805(14)
B8	1	0.2302(6)	0.9084(5)	0.3392(6)	0.0259(11)
B9	1	0.3604(7)	0.8332(6)	0.1811(6)	0.034(3)*
B10	1	0.5972(7)	0.4320(7)	0.4063(7)	0.0408(11)
B11	1	0.6070(7)	0.9175(7)	0.3976(7)	0.0386(8)
B12	1	0.3930(7)	0.7135(6)	0.3644(6)	0.0337(8)*
B13	1	0.2915(6)	0.3236(5)	0.5477(6)	0.0268(8)
B14	1	0.7243(8)	1.0946(7)	0.3473(9)	0.0535(6)
O87	1	0.8738(5)	0.5298(4)	0.3304(5)	0.0535(6)
O88	1	0.8674	1.2428	0.3292	0.123(8)
O89	1	0.7565(4)	0.5148(4)	0.3531(4)	0.0417(11)
O90	1	0.3789(3)	0.9739(3)	0.3342(3)	0.0258(8)
O91	1	1.0209(5)	1.1337(6)	0.2624(5)	0.0805(14)
B15	1	0.8105(8)	0.4910(7)	0.3476(9)	0.0535(6)
B16	1	0.9943(10)	1.1373(12)	0.4300(10)	0.0805(14)
O92	1	1.1590(5)	0.5422(4)	0.4272(4)	0.0475(10)
O93	1	0.9751(5)	0.6201(4)	0.3592(5)	0.0535(6)
O94	1	0.9028	1.2451	0.4406	0.113(7)
B17	1	0.4757(6)	0.8545(5)	0.2081(6)	0.0258(8)
B18	1	0.6332(8)	1.0714(8)	0.2555(9)	0.0535(6)
B19	1	0.3482(7)	1.3106(6)	0.2085(7)	0.036(3)*
B20	1	0.4349(6)	1.0087(5)	0.3326(6)	0.025(2)*
O95	1	0.7967(5)	0.6216(4)	0.1742(4)	0.056(3)
B21	1	0.5150(7)	0.9133(6)	0.3134(7)	0.0375(16)
O96	1	0.4696(4)	0.3861(4)	0.3705(4)	0.0408(11)
B22	1	0.4210(12)	0.4987(12)	0.2817(12)	0.088(3)*
O97	1	0.7779(5)	1.1997(4)	0.6003(4)	0.0475(10)
B23	1	0.9920(8)	0.6105(7)	0.4302(9)	0.0535(6)
B24	1	1.0108(10)	1.0921(12)	0.3160(10)	0.0805(14)
B25	1	0.3477(7)	1.2167(6)	0.2971(7)	0.0411(10)
B26	1	0.1450(7)	0.9416(7)	0.2496(7)	0.0393(16)*
O98	1	0.3557(4)	1.1482(4)	0.3042(4)	0.0411(10)
O99	1	0.6541(4)	0.4667(4)	0.4284(4)	0.0408(11)
O100	1	0.5190(5)	0.3668(6)	0.2690(4)	0.0716(16)
B27	1	0.2162(5)	0.4112(6)	0.3470(6)	0.0252(10)
B28	1	0.3876(6)	0.3315(5)	0.4759(5)	0.0210(17)
O101	1	0.7861(4)	1.1626(4)	0.1997(5)	0.0535(6)
O102	1	0.8087	0.9225	0.3505	0.0535(6)
O103	1	0.9032(4)	0.7648(4)	0.4108(5)	0.0535(6)
O104	1	0.4272(6)	0.4519(6)	0.2285(6)	0.088(3)*
B29	1	0.6476(7)	0.5669(7)	0.2551(7)	0.0417(11)
B30	1	0.5134(7)	0.4206(7)	0.3266(7)	0.0408(11)
B31	1	0.1406(6)	0.4200(6)	0.2643(5)	0.0252(10)
O105	1	0.6955(4)	0.5816(4)	0.2158(4)	0.0417(11)
O106	1	0.2876(4)	1.3360(3)	0.1997(3)	0.034(2)
B32	1	0.2443(5)	1.3686(5)	0.2439(5)	0.019(2)*
B33	1	0.3168(7)	1.0076(6)	0.3643(6)	0.035(3)*
O107	1	0.7760(5)	0.6880(5)	0.6100(5)	0.0609(14)
O108	1	0.8791	0.6822	0.1261	0.0535(6)
B34	1	0.3852(7)	0.8023(6)	0.4472(7)	0.0375(16)
O109	1	0.9151	0.936	0.2653	0.047(3)
B35	1	1.0180(8)	0.5803(7)	0.3215(9)	0.0535(6)
B36	1	1.1083(10)	1.0728(12)	0.4002(10)	0.0805(14)
O110	1	0.8357	0.7323	0.2005	0.0535(6)
O111	1	0.8712	0.7103	0.5102	0.0609(14)

B37	1	0.8905	0.702	0.4452	0.0609(14)
B38	1	0.8972	0.7891	0.3516	0.0535(6)
B39	1	0.7488(8)	1.1337(7)	0.2389(9)	0.0535(6)
B40	1	0.8507	0.6722	0.1877	0.0535(6)
B41	1	0.9389(8)	0.6807(7)	0.1129(9)	0.0535(6)
B42	1	0.7231(7)	0.5839(7)	0.3426(7)	0.0417(11)
B43	1	0.4504(7)	0.8171(6)	0.1052(7)	0.0411(10)
B44	1	0.3834(6)	0.2245(5)	0.3998(6)	0.0268(8)
B45	1	0.8559	0.8811	0.2977	0.0417(11)
B46	1	0.2599(6)	0.8887(5)	0.2306(6)	0.0258(8)
B47	1	0.2946(7)	0.8815(6)	0.4431(7)	0.0375(16)
B48	1	1.0999(8)	0.5753(8)	0.4021(7)	0.0475(10)
O112	1	0.4884(5)	0.3048(6)	0.1797(4)	0.0716(16)
O113	1	0.4679(5)	0.2654(6)	0.0794(4)	0.0716(16)
B49	1	0.4427(9)	0.2798(11)	0.1401(8)	0.0716(16)
B50	1	0.8871	1.2763	0.3848	0.105(12)
O114	1	0.8742(4)	0.7404(4)	0.3109(5)	0.0535(6)
O115	1	0.8556	1.3557	0.297	0.112(3)*
O116	1	0.9395	1.4254	0.34	0.112(3)*
B51	1	0.799	0.6749	0.5524	0.0609(14)
B52	1	0.3741(7)	1.1128(7)	0.3627(7)	0.0386(8)
B53	1	0.4757(9)	0.3456(11)	0.2330(8)	0.0716(16)
B54	1	0.9210(7)	1.0024(7)	0.2816(7)	0.0417(11)
B55	1	0.9813	0.6464	0.2228	0.0535(6)
O117	1	0.8448	0.8386	0.2517	0.0535(6)
B56	1	0.8408	0.7619	0.2457	0.0535(6)
B57	1	0.8742	1.391	0.3528	0.112(3)*
B58	1	0.7761(9)	1.1334(8)	0.4422(7)	0.0475(10)
O118	1	0.9968(5)	1.1845(6)	0.1731(5)	0.0805(14)
B59	1	0.9668(10)	1.1620(12)	0.2208(10)	0.0805(14)
B60	1	0.8038(8)	0.9873(7)	0.3437(9)	0.0535(6)
O119	1	0.8845	1.2205	0.1525	0.0805(14)
O120	1	0.8389	1.2595	0.2461	0.104(6)
B61	1	0.9420(10)	1.2263(12)	0.1406(10)	0.0805(14)
B62	1	0.8446	1.281	0.2969	0.102(10)
B63	1	0.2644(6)	0.3664(6)	0.4380(6)	0.0287(16)
B64	1	0.8463	1.2051	0.2017	0.0805(14)
O121	1	0.8951	0.8492	0.3771	0.0535(6)
B65	1	0.7775(9)	0.6238(8)	0.4441(9)	0.0609(14)
B66	1	0.9358(8)	0.4949(7)	0.3255(9)	0.0535(6)
B67	1	0.8852(8)	1.1698(7)	0.4728(7)	0.0475(10)
O122	1	0.9766(5)	1.2186(6)	0.0674(5)	0.0805(14)
B68	1	0.7545(7)	0.6069(7)	0.2283(7)	0.0417(11)

*Atoms refined in isotropic approximation

Table S22. Atomic displacement parameters (Å^2) in the structure of **5**.

Atom	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mg1	0.047(2)	0.0260(18)	0.0242(19)	0.0122(15)	–0.0117(16)	–0.0182(15)
Mg2	0.036(2)	0.037(2)	0.067(3)	–0.0232(17)	0.001(2)	0.032(2)
Mg3	0.0278(13)	0.0227(12)	0.0301(14)	0.0123(9)	0.0092(10)	–0.0061(10)
Mg4	0.050(2)	0.0179(16)	0.085(3)	–0.0093(15)	–0.029(2)	0.0082(18)
O1	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O2	0.0425(17)	0.0277(14)	0.053(2)	0.0027(12)	0.0008(14)	–0.0091(13)
O3	0.0234(13)	0.0226(12)	0.0311(15)	–0.0017(9)	–0.0044(11)	0.0013(10)
O5	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O123	0.0278(13)	0.0227(12)	0.0301(14)	0.0123(9)	0.0092(10)	–0.0061(10)
O7	0.0234(13)	0.0226(12)	0.0311(15)	–0.0017(9)	–0.0044(11)	0.0013(10)
O8	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O9	0.063(2)	0.0517(18)	0.0278(16)	0.0113(14)	–0.0020(14)	–0.0193(13)
O10	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
O11	0.027(3)	0.013(3)	0.023(3)	0.006(2)	0.000(2)	–0.008(2)
O4	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O14	0.0225(17)	0.052(2)	0.048(2)	0.0026(15)	–0.0006(15)	–0.0046(18)

O15	0.063(2)	0.0517(18)	0.0278(16)	0.0113(14)	–0.0020(14)	–0.0193(13)
O16	0.0425(17)	0.0277(14)	0.053(2)	0.0027(12)	0.0008(14)	–0.0091(13)
O17	0.0425(17)	0.0277(14)	0.053(2)	0.0027(12)	0.0008(14)	–0.0091(13)
O18	0.0425(17)	0.0277(14)	0.053(2)	0.0027(12)	0.0008(14)	–0.0091(13)
O19	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O20	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O21	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O22	0.047(4)	0.032(3)	0.107(6)	–0.017(3)	0.019(4)	–0.033(3)
O23	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O26	0.030(2)	0.0207(18)	0.027(2)	0.0121(15)	0.0016(17)	–0.0019(16)
O27	0.0225(17)	0.052(2)	0.048(2)	0.0026(15)	–0.0006(15)	–0.0046(18)
O28	0.052(2)	0.125(4)	0.039(2)	–0.035(2)	0.0297(19)	–0.038(2)
O29	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O30	0.030(3)	0.030(2)	0.026(3)	–0.0076(19)	–0.003(2)	0.0062(19)
O31	0.0134(15)	0.0411(18)	0.0209(17)	0.0041(13)	–0.0065(12)	0.0074(14)
O32	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O34	0.0234(13)	0.0226(12)	0.0311(15)	–0.0017(9)	–0.0044(11)	0.0013(10)
O35	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O36	0.0293(17)	0.052(2)	0.043(2)	–0.0190(14)	–0.0184(15)	0.0246(16)
O37	0.0134(15)	0.0411(18)	0.0209(17)	0.0041(13)	–0.0065(12)	0.0074(14)
O38	0.0234(13)	0.0226(12)	0.0311(15)	–0.0017(9)	–0.0044(11)	0.0013(10)
O39	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O40	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
O41	0.0425(17)	0.0277(14)	0.053(2)	0.0027(12)	0.0008(14)	–0.0091(13)
O42	0.063(2)	0.0517(18)	0.0278(16)	0.0113(14)	–0.0020(14)	–0.0193(13)
O43	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O44	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
O45	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O46	0.063(2)	0.0517(18)	0.0278(16)	0.0113(14)	–0.0020(14)	–0.0193(13)
O47	0.048(2)	0.060(2)	0.074(3)	–0.0075(16)	–0.0173(19)	–0.0320(19)
O48	0.0425(17)	0.0277(14)	0.053(2)	0.0027(12)	0.0008(14)	–0.0091(13)
O49	0.030(2)	0.0207(18)	0.027(2)	0.0121(15)	0.0016(17)	–0.0019(16)
O50	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O51	0.102(8)	0.023(4)	0.093(8)	–0.021(4)	0.077(7)	–0.024(4)
O52	0.030(3)	0.030(2)	0.026(3)	–0.0076(19)	–0.003(2)	0.0062(19)
B1	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O53	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O54	0.0234(13)	0.0226(12)	0.0311(15)	–0.0017(9)	–0.0044(11)	0.0013(10)
O55	0.047(4)	0.032(3)	0.107(6)	–0.017(3)	0.019(4)	–0.033(3)
O56	0.035(4)	0.044(4)	0.036(5)	0.001(3)	0.014(3)	0.006(4)
O57	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
B2	0.063(2)	0.0517(18)	0.0278(16)	0.0113(14)	–0.0020(14)	–0.0193(13)
O58	0.0134(15)	0.0411(18)	0.0209(17)	0.0041(13)	–0.0065(12)	0.0074(14)
O59	0.052(2)	0.125(4)	0.039(2)	–0.035(2)	0.0297(19)	–0.038(2)
O60	0.0278(13)	0.0227(12)	0.0301(14)	0.0123(9)	0.0092(10)	–0.0061(10)
O61	0.0134(15)	0.0411(18)	0.0209(17)	0.0041(13)	–0.0065(12)	0.0074(14)
O62	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O63	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O64	0.048(2)	0.060(2)	0.074(3)	–0.0075(16)	–0.0173(19)	–0.0320(19)
O65	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O66	0.0293(17)	0.052(2)	0.043(2)	–0.0190(14)	–0.0184(15)	0.0246(16)
O67	0.0234(13)	0.0226(12)	0.0311(15)	–0.0017(9)	–0.0044(11)	0.0013(10)
O68	0.042(3)	0.032(2)	0.038(3)	–0.0115(19)	–0.013(2)	0.0029(19)
O69	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O70	0.030(2)	0.0207(18)	0.027(2)	0.0121(15)	0.0016(17)	–0.0019(16)
O72	0.0278(13)	0.0227(12)	0.0301(14)	0.0123(9)	0.0092(10)	–0.0061(10)
O73	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O74	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
B3	0.0225(17)	0.052(2)	0.048(2)	0.0026(15)	–0.0006(15)	–0.0046(18)
O75	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O76	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O79	0.050(2)	0.0179(16)	0.085(3)	–0.0093(15)	–0.029(2)	0.0082(18)
O80	0.048(2)	0.060(2)	0.074(3)	–0.0075(16)	–0.0173(19)	–0.0320(19)

O81	0.063(2)	0.0517(18)	0.0278(16)	0.0113(14)	–0.0020(14)	–0.0193(13)
O82	0.042(3)	0.032(2)	0.038(3)	–0.0115(19)	–0.013(2)	0.0029(19)
O83	0.0278(13)	0.0227(12)	0.0301(14)	0.0123(9)	0.0092(10)	–0.0061(10)
O84	0.018(3)	0.022(3)	0.035(4)	–0.001(3)	0.008(3)	–0.001(3)
B6	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
B7	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
O85	0.048(2)	0.060(2)	0.074(3)	–0.0075(16)	–0.0173(19)	–0.0320(19)
O86	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
B8	0.030(2)	0.0207(18)	0.027(2)	0.0121(15)	0.0016(17)	–0.0019(16)
B10	0.0225(17)	0.052(2)	0.048(2)	0.0026(15)	–0.0006(15)	–0.0046(18)
B11	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
B13	0.0278(13)	0.0227(12)	0.0301(14)	0.0123(9)	0.0092(10)	–0.0061(10)
B14	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O87	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O88	0.075(9)	0.064(8)	0.23(2)	0.002(6)	–0.027(11)	–0.005(10)
O89	0.0293(17)	0.052(2)	0.043(2)	–0.0190(14)	–0.0184(15)	0.0246(16)
O90	0.0234(13)	0.0226(12)	0.0311(15)	–0.0017(9)	–0.0044(11)	0.0013(10)
O91	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
B15	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B16	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
O92	0.063(2)	0.0517(18)	0.0278(16)	0.0113(14)	–0.0020(14)	–0.0193(13)
O93	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O94	0.095(10)	0.089(10)	0.153(15)	0.010(8)	–0.045(10)	–0.037(9)
B17	0.0234(13)	0.0226(12)	0.0311(15)	–0.0017(9)	–0.0044(11)	0.0013(10)
B18	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O95	0.082(7)	0.032(4)	0.055(6)	0.020(4)	0.000(5)	0.025(4)
B21	0.042(3)	0.032(2)	0.038(3)	–0.0115(19)	–0.013(2)	0.0029(19)
O96	0.0225(17)	0.052(2)	0.048(2)	0.0026(15)	–0.0006(15)	–0.0046(18)
O97	0.063(2)	0.0517(18)	0.0278(16)	0.0113(14)	–0.0020(14)	–0.0193(13)
B23	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B24	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
B25	0.0425(17)	0.0277(14)	0.053(2)	0.0027(12)	0.0008(14)	–0.0091(13)
O98	0.0425(17)	0.0277(14)	0.053(2)	0.0027(12)	0.0008(14)	–0.0091(13)
O99	0.0225(17)	0.052(2)	0.048(2)	0.0026(15)	–0.0006(15)	–0.0046(18)
O100	0.052(2)	0.125(4)	0.039(2)	–0.035(2)	0.0297(19)	–0.038(2)
B27	0.0134(15)	0.0411(18)	0.0209(17)	0.0041(13)	–0.0065(12)	0.0074(14)
B28	0.027(3)	0.013(3)	0.023(3)	0.006(2)	0.000(2)	–0.008(2)
O101	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O102	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O103	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B29	0.0293(17)	0.052(2)	0.043(2)	–0.0190(14)	–0.0184(15)	0.0246(16)
B30	0.0225(17)	0.052(2)	0.048(2)	0.0026(15)	–0.0006(15)	–0.0046(18)
B31	0.0134(15)	0.0411(18)	0.0209(17)	0.0041(13)	–0.0065(12)	0.0074(14)
O105	0.0293(17)	0.052(2)	0.043(2)	–0.0190(14)	–0.0184(15)	0.0246(16)
O106	0.069(5)	0.024(4)	0.008(3)	0.028(3)	–0.001(3)	–0.003(3)
O107	0.048(2)	0.060(2)	0.074(3)	–0.0075(16)	–0.0173(19)	–0.0320(19)
O108	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B34	0.042(3)	0.032(2)	0.038(3)	–0.0115(19)	–0.013(2)	0.0029(19)
O109	0.043(5)	0.039(4)	0.059(6)	0.006(4)	–0.005(4)	0.003(4)
B35	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B36	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
O110	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O111	0.048(2)	0.060(2)	0.074(3)	–0.0075(16)	–0.0173(19)	–0.0320(19)
B37	0.048(2)	0.060(2)	0.074(3)	–0.0075(16)	–0.0173(19)	–0.0320(19)
B38	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B39	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B40	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B41	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B42	0.0293(17)	0.052(2)	0.043(2)	–0.0190(14)	–0.0184(15)	0.0246(16)
B43	0.0425(17)	0.0277(14)	0.053(2)	0.0027(12)	0.0008(14)	–0.0091(13)
B44	0.0278(13)	0.0227(12)	0.0301(14)	0.0123(9)	0.0092(10)	–0.0061(10)
B45	0.0293(17)	0.052(2)	0.043(2)	–0.0190(14)	–0.0184(15)	0.0246(16)
B46	0.0234(13)	0.0226(12)	0.0311(15)	–0.0017(9)	–0.0044(11)	0.0013(10)

B47	0.042(3)	0.032(2)	0.038(3)	–0.0115(19)	–0.013(2)	0.0029(19)
B48	0.063(2)	0.0517(18)	0.0278(16)	0.0113(14)	–0.0020(14)	–0.0193(13)
O112	0.052(2)	0.125(4)	0.039(2)	–0.035(2)	0.0297(19)	–0.038(2)
O113	0.052(2)	0.125(4)	0.039(2)	–0.035(2)	0.0297(19)	–0.038(2)
B49	0.052(2)	0.125(4)	0.039(2)	–0.035(2)	0.0297(19)	–0.038(2)
B50	0.083(16)	0.054(12)	0.18(3)	–0.011(11)	0.026(18)	–0.037(15)
O114	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B51	0.048(2)	0.060(2)	0.074(3)	–0.0075(16)	–0.0173(19)	–0.0320(19)
B52	0.0336(13)	0.0411(12)	0.0413(14)	0.0008(9)	0.0027(10)	0.0089(10)
B53	0.052(2)	0.125(4)	0.039(2)	–0.035(2)	0.0297(19)	–0.038(2)
B54	0.0293(17)	0.052(2)	0.043(2)	–0.0190(14)	–0.0184(15)	0.0246(16)
B55	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O117	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B56	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B58	0.063(2)	0.0517(18)	0.0278(16)	0.0113(14)	–0.0020(14)	–0.0193(13)
O118	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
B59	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
B60	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
O119	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
O120	0.102(10)	0.104(10)	0.107(11)	0.041(8)	0.024(9)	0.014(8)
B61	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
B62	0.11(2)	0.056(13)	0.14(2)	0.036(12)	–0.012(18)	–0.036(14)
B63	0.030(3)	0.030(2)	0.026(3)	–0.0076(19)	–0.003(2)	0.0062(19)
B64	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
O121	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B65	0.048(2)	0.060(2)	0.074(3)	–0.0075(16)	–0.0173(19)	–0.0320(19)
B66	0.0436(10)	0.0409(9)	0.0757(14)	–0.0034(7)	–0.0047(9)	–0.0004(9)
B67	0.063(2)	0.0517(18)	0.0278(16)	0.0113(14)	–0.0020(14)	–0.0193(13)
O122	0.0525(19)	0.121(3)	0.068(2)	–0.0148(18)	0.0004(16)	0.034(2)
B68	0.0293(17)	0.052(2)	0.043(2)	–0.0190(14)	–0.0184(15)	0.0246(16)

Table S23. Selected bond lengths (Å) in the structure of **5**.

Bond	Length	Bond	Length
Mg1—O3	2.133 (8)	O53—B48	1.300 (17)
Mg1—O25	2.162 (8)	O54—B17	1.446 (13)
Mg1—O26	2.071 (8)	O54—B21	1.593 (16)
Mg1—O29	1.966 (9)	O55—B33	1.277 (15)
Mg1—O39	2.245 (9)	O55—B52	1.356 (15)
Mg1—O90	2.183 (7)	O56—B8	1.667 (13)
Mg1—B21	2.885 (14)	O56—B33	1.317 (15)
O1—B7	1.020 (15)	O57—B24	1.60 (2)
O1—B34	1.745 (14)	O57—B36	1.45 (2)
Mg2—O44	2.321 (12)	B2—O97	1.379 (15)
Mg2—O45	2.143 (10)	O58—B31	1.348 (13)
Mg2—O51	2.146 (8)	O58—B32^{i}	1.368 (12)
Mg2—O74	2.220 (11)	O59—B19^{i}	1.457 (16)
Mg2—O81	2.190 (9)	O59—B53	1.468 (18)
Mg2—O88	2.163 (4)	O60—B28	1.515 (11)
Mg2—B24	2.90 (2)	O60—B44	1.421 (14)
O2—B43	1.296 (16)	O61—B27	1.511 (13)
O3—B9	1.471 (15)	O61—B32^{i}	1.409 (13)
O3—B17	1.365 (13)	O62—B40	1.6516 (1)
Mg3—O23	2.123 (8)	O62—B55	1.6031 (1)
Mg3—O48^{i}	2.157 (8)	O64—B42	1.524 (18)
Mg3—O59	2.173 (9)	O64—B65	1.301 (18)
Mg3—O61	2.098 (7)	O65—B14	1.670 (17)
Mg3—O72	2.080 (8)	O65—B60	1.134 (17)
Mg3—O96	2.124 (8)	O66—B42	1.623 (15)
O6—B4	1.549 (15)	O66—B68	1.517 (16)
O6—B12	1.296 (14)	O67—B9	1.457 (15)
O5—B18	1.215 (17)	O67—B43	1.309 (16)
O123—B13	1.416 (14)	O68—B12	1.229 (15)
O123—B28	1.496 (13)	O68—B34	1.497 (16)

O7—B5	1.407 (12)	O69—B23	1.387 (19)
O7—B9	1.408 (14)	O69—B37	1.842 (9)
O8—B8	1.227 (14)	O70—B26	1.400 (16)
O8—B47	1.699 (15)	O70—B46	1.467 (13)
O9—B16	1.10 (2)	O71—B4	1.581 (14)
O9—B67	1.484 (17)	O71—B22	1.41 (2)
O10—B16	1.51 (2)	O72—B28	1.513 (13)
O10—B36	1.44 (2)	O72—B63	1.369 (14)
O11—B3	1.334 (16)	O73—B14	1.469 (18)
O11—B28	1.421 (13)	O73—B18	1.46 (2)
O12—B26	1.281 (15)	O74—B16	1.36 (3)
O4—B41	1.41 (2)	O74—B24	1.47 (3)
Mg4—O62	1.898 (6)	B3—O96	1.364 (17)
Mg4—O66	2.000 (8)	O75—B35	1.735 (18)
Mg4—O80	1.844 (11)	O75—B55	1.1724 (1)
Mg4—O87	2.064 (9)	O76—B11	1.426 (15)
Mg4—O93	2.116 (10)	O77—B50	1.3453 (1)
Mg4—B37	2.875 (5)	O77—B57	1.2426 (1)
Mg4—O114	2.168 (9)	O78—B15^{ii}	1.306 (15)
O14—B3	1.396 (15)	O78—B57	1.4860 (1)
O14—B10	1.326 (16)	O79—B41	1.395 (17)
O15—B14	1.189 (19)	O79—B55	1.5167 (1)
O15—B58	1.374 (17)	O80—B37	1.495 (8)
O16—B19	1.512 (15)	O80—B65	1.69 (2)
O16—B25	1.386 (17)	O81—B58	1.170 (18)
O17—B44^{ii}	1.354 (13)	O81—B67	1.478 (17)
O17—B52	1.264 (16)	O82—B47	1.536 (13)
O18—B20	1.555 (14)	O83—B13	1.451 (14)
O18—B21	1.309 (15)	O84—B6	1.226 (15)
O19—B1	1.366 (15)	O84—B27	1.602 (13)
O19—B34	1.465 (16)	O85—B51	1.399 (9)
O20—B35	1.316 (17)	O85—B65	1.23 (2)
O20—B66	1.373 (18)	O86—B36	1.24 (2)
O21—B35	1.467 (18)	B10—O99	1.383 (15)
O21—B48	1.207 (17)	O87—B15	1.509 (18)
O22—B7	1.409 (16)	O87—B66	1.402 (18)
O22—B11	1.355 (16)	O88—B50	1.4084 (1)
O23—B6	1.530 (15)	O88—B62	1.1154 (1)
O23—B22	1.47 (2)	O89—B15	1.164 (17)
O24—B4	1.366 (15)	O89—B42	1.539 (16)
O24—B6	1.282 (15)	O90—B20	1.295 (13)
O25—B5	1.442 (13)	O90—B33	1.537 (15)
O25—B12	1.584 (15)	O91—B24	1.43 (2)
O26—B8	1.573 (13)	O91—B59	1.48 (2)
O26—B46	1.232 (14)	O92—B48	1.425 (17)
O27—B10	1.373 (17)	O93—B23	1.56 (2)
O27—B30	1.370 (15)	O93—B35	1.417 (19)
O28—B19^{i}	1.465 (16)	O94—B50	1.3733 (1)
O28—B49	1.282 (19)	O94—B67	1.690 (16)
O29—B34	1.395 (15)	B19—O106	1.297 (15)
O29—B47	1.526 (16)	O95—B40	1.483 (10)
O30—B13	1.268 (14)	O95—B68	1.460 (17)
O30—B63	1.552 (14)	O96—B30	1.453 (17)
O31—B31	1.425 (12)	B22—O104	1.48 (3)
O32—B18	1.511 (19)	B25—O98	1.385 (15)
O32—B39	1.546 (17)	O98—B52	1.472 (16)
O33—B4	1.559 (15)	O100—B30	1.638 (17)
O33—B5	1.235 (12)	O100—B53	1.207 (19)
O34—B17	1.317 (14)	O101—B39	1.259 (19)
O34—B43	1.477 (16)	O101—B64	1.450 (8)
O35—B11	1.305 (16)	O102—B45	1.6849 (1)
O35—B21	1.727 (15)	O102—B60	1.304 (15)
O36—B29	1.356 (14)	O103—B37	1.475 (9)

O37—B27	1.325 (12)	O103—B38	1.356 (10)
O37—B31	1.282 (14)	B29—O105	1.299 (16)
O38—B9	1.547 (14)	O105—B68	1.281 (14)
O38—B46	1.421 (14)	O106—B32	1.434 (12)
O39—B7	1.518 (16)	O107—B51	1.341 (10)
O39—B21	1.409 (15)	O108—B40	1.4497 (1)
O40—B24	1.43 (3)	O108—B41	1.206 (16)
O40—B54	1.502 (16)	O109—B45	1.7444 (1)
O41—B20	1.371 (13)	O109—B54	1.374 (15)
O41—B52	1.541 (15)	O110—B40	1.2649 (1)
O42—B2	1.174 (16)	O110—B56	1.1341 (1)
O42—B58	1.441 (15)	O111—B37	1.4520 (1)
O43—B1	1.290 (15)	O111—B51	1.8290 (1)
O43—B47	1.288 (15)	B38—O114	1.373 (9)
O44—B59	1.23 (2)	B38—O121	1.3168 (1)
O44—B64	1.798 (11)	B45—O117	1.3120 (1)
O45—B14	1.493 (19)	B45—O121	1.9519 (1)
O45—B39	1.32 (2)	O112—B49	1.315 (19)
O46—B2	1.480 (18)	O112—B53	1.425 (18)
O46—B67	1.517 (17)	O113—B49	1.422 (16)
O47—B29	1.348 (17)	B50—B62	2.0379 (1)
O47—B42	1.373 (15)	O114—B56	1.583 (10)
O48—B25	1.345 (16)	O115—B57	1.4243 (1)
O48—B44^{ii}	1.393 (15)	O115—B62	1.5046 (1)
O49—B8	1.514 (13)	O116—B57	1.4771 (1)
O49—B26	1.422 (16)	O116—B66^{ii}	1.423 (15)
O50—B22	1.34 (2)	O117—B56	1.5392 (1)
O50—B30	1.374 (16)	O118—B59	1.27 (2)
O51—B54	1.431 (18)	O118—B61	1.51 (2)
O51—B60	1.605 (18)	O119—B61	1.161 (19)
O52—B27	1.425 (13)	O119—B64	1.3349 (1)
O52—B63	1.116 (13)	O120—B62	1.1678 (1)
B1—O63	1.433 (16)	O120—B64	1.4497 (1)
O53—B23	1.303 (17)	B61—O122	1.72 (2)

Symmetry code(s): (i) *x*, *y*–1, *z*; (ii) *x*, *y*+1, *z*.

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