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Blue spinel crystals in the $MgAl_2O_4$-$CoAl_2O_4$ series: Part II. Cation ordering over short-range and long-range scales

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Abstract

Optical absorption spectroscopy and X-ray structural refinements were used to characterize short-range and long-range structures of 10 gem-quality, blue spinel single crystals synthesized on the $(Mg_{1-x}Co_x)Al_2O_4$ solid solution (x = 0.07–1.00). The site distributions of Mg, Co^{2+}, and Al show that the tetrahedrally coordinated site (T) is mainly populated by Mg and Co^{2+}, with a marked preference of Co^{2+} for tetrahedral coordination with respect to Mg, while the octahedrally coordinated site (M) is dominated by Al. Crystals also show a certain degree of inversion, i.e., occurrence of Al at T counterbalanced by the occurrence of divalent cations at M, which decreases from 0.24 to 0.13 with increasing Co^{2+} content.

Short-range information based on the crystal field splitting parameter Dq derived from single-crystal optical spectra suggests that the local Co^{2+}-O bond length at the T-site may increase marginally at increasing Co^{2+} content. An almost constant value for the Racah B-parameter, also derived from optical spectra, for tetrahedrally coordinated Co^{2+} suggests that any influence of substitutional second nearest neighbor cations on the ionicity of Co^{2+}-O bonds at the T-site is very small. Long-range information shows that variations in the unit-cell parameter from 8.084 to 8.105 Å along the solid-solution series are mainly related to the ordering of Al at the M site as a result of the replacement of Mg by Co^{2+}. Therefore, the spinel structure responds to the chemical variation by ordering of Al in such a manner that M-O remains almost constant and T-O increases. In this way, the lengths of shared octahedral edges are reduced and the destabilization effect due to the increased octahedral cation-cation repulsion is minimized. In line with other studies, the importance of steric factors for controlling the cation distributions in the spinel structure has also been shown to be valid in the $MgAl_2O_4$-$CoAl_2O_4$ solid-solution series.

Keywords: Cobalt spinel, optical absorption spectroscopy, X-ray diffraction, cation ordering, ionic potential

Introduction

Many substances crystallize in the spinel type structure, most of which are oxides, in addition to sulfides (e.g., $ZnAl_2S_4$), selenides (e.g., $CuCr_2Se_4$), halides (e.g., Li_2NiF_4), and pseudohalides [e.g., $ZnK(CN)_4$]. In spinel oxides, steric factors are important for the cation distribution among the structural sites, as exemplified by, e.g., $FeAl_2O_4$, $CuAl_2O_4$, and $CoAl_2O_4$ spinels (Harrison et al. 1998; O'Neill 1994; O'Neill et al. 2005), in which the small Al^{3+} cation prefers the octahedrally coordinated (M) sites to the tetrahedrally coordinated (T) ones. In these spinels, cation size and crystal field stabilization energy suggest that Fe^{2+}, Cu^{2+}, and Co^{2+} should prefer the octahedra, but the presence of Al obviously counteracts this behavior. They are in fact (almost) normal spinels with the divalent cations ordered at T and Al^{3+} cations ordered at the M sites in the slightly distorted cubic close-packed array of oxygen atoms. Moreover, it has been shown on a limited number of spinel solid-solution series that the average structure determined from diffraction data often differs from the local structure retrieved by spectroscopic methods; this means that Vegard's rule is not obeyed at the atomic scale due to lattice relaxation during atomic substitution (Galoisy 1996; Hålenius et al. 2010, 2011).

As comprehensively described in the part I of the present study (D'Ippolito et al. 2012, this issue), $CoAl_2O_4$ oxide is rarely found as a mineral but is widely used, since the discovery of its industrial synthesis route, as a pigment for the coloration of a large range of materials (e.g., ceramics, and many others). This is due to its peculiar and highly efficient optical absorption in the red-yellow region, which gives the typical, highly saturated blue color in daylight and violet in tungsten light (Dharmaratne 1993). In addition to that, Co-bearing materials with spinel structure exhibit many other remarkable properties (e.g., catalytic activity, Fierro et al. 2005 and references therein) and are extensively investigated because of that. However, in spite of the interest due to physical properties, very little information is available in the literature on $CoAl_2O_4$ (and Co-bearing materials) crystal chemistry, and many aspects regarding electronic structure and cation distribution are not well understood or even unknown. Previous studies on $CoAl_2O_4$ include investigations of electron density (Toriumi et al. 1978), crystal field transitions (e.g., Kuleshov et al. 1993) and cation distribution as a function of temperature (O'Neill 1994; Nakatsuka et al. 2003). In particular, the latter authors highlighted that at high temperatures, limited fractions of the Co^{2+} and Al^{3+} ions may interchange their structural positions. Nevertheless, systematic investigation of the structural variations all along the entire $(Mg_{1-x}Co_x)Al_2O_4$ solid-solution series is missing.

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In the present work, we investigated through a combined crystallographic and spectroscopic approach spinel single crystals belonging to the $(Mg_{1-x}Co_x)Al_2O_4$ series, produced by flux growth and chemically characterized by D'Ippolito et al. (2012, this issue), to reveal structural details and improve our understanding of factors that affect cation distribution and influences some of the physical properties (e.g., color).

Experimental methods

Optical absorption spectroscopy

Ten representative crystal fragments were selected along the $MgAl_2O_4$-$CoAl_2O_4$ series. Nonpolarized room-temperature optical absorption spectra were recorded in the UV/VIS to NIR spectral range (330–2000 nm) on double-sided polished single crystals ranging in thickness from 13 to 390 µm with a Zeiss MPM800 microscope spectrometer equipped with Ultrafluar 10× objective and condensor lenses, Xenon arc 75W and Halogen 100 W light sources, blazed concave monochromators and photomultiplier and photoconductive PbS-cell detectors. The spectra were recorded at the Mineralogy Department, Naturhistoriska Riksmuseet, Stockholm, using a spot with a measured diameter of 40 µm during three cycles at a resolution of 1 and 5 nm in the UV/VIS (330–800 nm) and NIR (800–2000 nm) spectral regions, respectively. The accuracy of determined absorption band energies in the UV/VIS-NIR region is estimated on the basis of measured Ho_2O_3-doped and Pr_2O_3/Nd_2O_3-doped calibration standards (Hellma glass filters 666-F1 and 666-F7) to be better than 60 cm^{-1}. In the MIR range (2000–4000 nm) spectra were collected on the same single-crystal absorbers as above during 128 cycles using a square-shaped 40 × 40 µm aperture at a spectral resolution of 4 cm^{-1} with a Bruker Equinox 55S FTIR microscope spectrometer equipped with a glowbar source, KBr beamsplitter and a MCT-detector. Recorded spectra were fitted using the peak resolution program Jandel PeakFit 4.0 assuming Gaussian absorption bands.

Single-crystal structural refinement

X-ray diffraction measurements were performed at the Earth Sciences Department, Sapienza University of Rome, with a Bruker KAPPA APEX-II single-crystal diffractometer, equipped with CCD area detector (6.2 × 6.2 cm^2 active detection area, 512 × 512 pixels) and a graphite crystal monochromator, using Mo$K\alpha$ radiation from a fine-focus sealed X-ray tube. The sample-to-detector distance was 4 cm. A total of about 5000 exposures per sample (step = 0.2°, time/step = 10 s) covering a full reciprocal sphere were collected. The orientation of the crystal lattice was determined from 500 to 1000 strong reflections ($I > 100\ \sigma_I$) evenly distributed in the reciprocal space, and used for subsequent integration of all recorded intensities. Final unit-cell parameters were refined by means of the Bruker AXS SAINT program from ca. 2300 recorded reflections with $I > 10\ \sigma_I$ in the range $8° < 2\theta < 90°$. The intensity data were processed and corrected for Lorentz, polarization, and background effects with APEX2 software program of Bruker AXS. The data were corrected for absorption using multi-scan method (SADABS). The absorption correction led to a significant improvement in R_{int}. No violation of $Fd\bar{3}m$ symmetry was noted. Sporadic appearance of forbidden space-group reflections was recognized as double reflections by their anomalously narrow reflection profiles.

Structural refinements were carried out with the SHELXL program (Sheldrick 2008). Setting the origin at $\bar{3}m$, initial atomic positions for oxygen atoms were taken from the structure of spinel (Fregola et al. 2011). Variable parameters were overall scale factor, extinction coefficient, atomic coordinates, site-scattering values expressed as mean atomic number (m.a.n.), and atomic displacement factors. No chemical constraint was applied during the refinement. To obtain the best values of statistical indexes ($R1$ and $wR2$) the oxygen site was modeled with neutral vs. full, ionized oxygen scattering curves, while neutral curves were used for the cation sites. In detail, the T site was modeled considering the presence of Mg and Co scattering factors, whereas the M site was modeled with the Al scattering factor. Three full-matrix refinement cycles with isotropic displacement parameters for all atoms were followed by anisotropic cycles until convergence was attained, that is, when the shifts in all refined parameters were less than their estimated standard deviation. No correlation over 0.7 between parameters was observed at the end of refinement. Table 1 summarizes structural parameters and refinement details. (CIFs available on deposit[1].)

[1] Deposit item AM-12-084, CIFs. Deposit items are available two ways: For a paper copy contact the Business Office of the Mineralogical Society of America (see inside front cover of recent issue) for price information. For an electronic copy visit the MSA web site at http://www.minsocam.org, go to the *American Mineralogist* Contents, find the table of contents for the specific volume/issue wanted, and then click on the deposit link there.

Table 1. Selected X-ray diffraction data of the analyzed spinels along $(Mg_{1-x}Co_x)Al_2O_4$

Crystal	CoAl0.5	CoAl1	CoAl10	CoAl14	CoAl20	CoAl34	CoAl45	CoAl50	CoAl67	CoAl100
Crystal sizes (mm)	0.20×0.20×0.12	0.22×0.21×0.18	0.22×0.20×0.15	0.20×0.20×0.16	0.20×0.20×0.20	0.30×0.25×0.20	0.20×0.20×0.20	0.16×0.16×0.10	0.16×0.14×0.09	0.19×0.19×0.12
a (Å)	8.0851(3)	8.0848(4)	8.0840(3)	8.0875(4)	8.0902(3)	8.0914(4)	8.0943(3)	8.0957(3)	8.1010(5)	8.1047(4)
u	0.26209(4)	0.26216(5)	0.26216(5)	0.26242(4)	0.26249(5)	0.26281(5)	0.26308(5)	0.26251(6)	0.26321(4)	0.26355(5)
T-O (Å)	1.9198(6)	1.9207(7)	1.9206(6)	1.9250(6)	1.9266(7)	1.9314(7)	1.9359(7)	1.9282(9)	1.9392(6)	1.9449(7)
M-O (Å)	1.9285(3)	1.9279(4)	1.9277(3)	1.9267(3)	1.9268(4)	1.9248(3)	1.9235(3)	1.9280(5)	1.9242(3)	1.9226(4)
T-m.a.n.	13.06(6)	13.24(7)	13.48(7)	15.71(7)	16.91(8)	18.91(9)	20.34(10)	20.11(12)	22.10(11)	25.28(8)
M-m.a.n.	12.82(4)	12.86(5)	12.89(4)	13.03(4)	13.17(4)	13.26(4)	13.37(4)	13.75(5)	13.53(4)	13.88(5)
T-U^{11} (Å^2)	0.0048(2)	0.0046(2)	0.0047(2)	0.0049(1)	0.0050(1)	0.0052(1)	0.0048(1)	0.0056(2)	0.00543(9)	0.00524(8)
M-U^{11} (Å^2)	0.0045(1)	0.0043(2)	0.0045(1)	0.0043(1)	0.0043(1)	0.0044(1)	0.0039(1)	0.0045(2)	0.0045(1)	0.0040(1)
M-U^{12} (Å^2)	–0.00013(4)	–0.00013(4)	–0.00011(4)	–0.00016(4)	–0.00018(5)	–0.00021(5)	–0.00020(5)	–0.00021(6)	–0.00027(5)	–0.00028(6)
O-U^{11} (Å^2)	0.0078(1)	0.0076(2)	0.0076(2)	0.0076(1)	0.0076(1)	0.0078(1)	0.0071(1)	0.0088(2)	0.0078(1)	0.0074(1)
O-U^{12} (Å^2)	0.00021(7)	0.00017(8)	0.00017(8)	0.00015(8)	0.0002(1)	0.0002(1)	0.0001(1)	0.0002(1)	–0.00003(9)	–0.0002(1)
Reciprocal space range *hkl*										
	$-15 \le h \le 15$	$-14 \le h \le 15$	$-15 \le h \le 13$	$-15 \le h \le 14$	$-16 \le h \le 12$	$-9 \le h \le 15$	$-11 \le h \le 15$	$-13 \le h \le 16$	$-10 \le h \le 15$	$-14 \le h \le 15$
	$-15 \le k \le 14$	$-15 \le k \le 15$	$-15 \le k \le 15$	$-16 \le k \le 16$	$-16 \le k \le 16$	$-14 \le k \le 10$	$-15 \le k \le 16$	$-14 \le k \le 11$	$-16 \le k \le 16$	$-15 \le k \le 15$
	$-15 \le l \le 13$	$-11 \le l \le 16$	$-9 \le l \le 15$	$-15 \le l \le 8$	$-15 \le l \le 6$	$-16 \le l \le 16$	$-15 \le l \le 13$	$-13 \le l \le 16$	$-15 \le l \le 7$	$-15 \le l \le 7$
EXTI	0.164(7)	0.22(1)	0.195(9)	0.090(3)	0.073(3)	0.045(2)	0.045(2)	0.23(1)	0.024(1)	0.026(1)
Set of read reflections	2552	2490	2452	2492	2465	2471	2460	2567	2445	2484
Unique reflections	132	132	130	133	132	129	132	133	133	131
R int. (%)	2.57	2.08	1.46	2.26	1.87	2.58	4.49	1.86	1.55	2.40
*R*1 (%) all reflections	1.56	2.11	1.86	1.28	1.49	1.49	1.36	1.98	1.06	1.11
*wR*2 (%) all reflections	3.56	4.57	4.13	3.17	3.48	3.39	3.50	4.48	2.65	2.45
GooF	1.239	1.322	1.330	1.178	1.293	1.376	1.244	1.286	1.153	1.286
Diff. peaks (±*e*/Å^3)	–0.36; 0.23	–0.53; 0.49	–0.50; 0.55	–0.37; 0.23	–0.36; 0.27	–0.56; 0.32	–0.30; 0.30	–0.70; 0.29	–0.30; 0.25	–0.28; 0.33

Notes: *a* = unit-cell parameter; *u* = oxygen fractional coordinate; T-O and M-O = tetrahedral and octahedral bond lengths, respectively; T- and M-m.a.n.. = T- and M-mean atomic number, i.e., number of electrons at site; U^{11} = atomic displacement parameter; $U^{11} = U^{22} = U^{33}$ and $U^{12} = U^{13} = U^{23}$ (=0 for *T*-site due to symmetry reasons); EXTI = extinction parameter; *R* int. = merging residual value; *R*1 = discrepancy index, calculated from *F*-data; *wR*2 = weighted discrepancy index, calculated from F^2-data; GooF = goodness of fit; Diff. peaks = maximum and minimum residual electron density. Radiation, Mo$K\alpha$ = 0.71073 Å. Data collection temperature = 293 K. Total number of frames ~5000. Range for data collection $8 < °2\theta < 91$. Origin fixed at $\bar{3}m$. Space group $Fd\bar{3}m$. $Z = 8$. Spinel structure has cations at Wyckoff positions 8*a* ≡ T (1/8, 1/8, 1/8) and 16*d* ≡ M (1/2, 1/2, 1/2), and oxygen anions at 32*e* (*u*, *u*, *u*).

Cation distribution

The intracrystalline cation distribution was obtained by an optimization program applying a minimization function in which both structural and chemical data (such as bond lengths and site-scattering in terms of equivalent electrons, i.e., mean atomic number) are taken into account. The minimization procedure has been presented and discussed previously (Carbonin et al. 1996; Andreozzi et al. 2001; Lavina et al. 2002; Bosi et al. 2004; Lenaz and Princivalle 2011; Della Giusta et al. 2011). Octahedral and tetrahedral bond lengths (M-O and T-O, respectively) were calculated as the linear contribution of each cation multiplied by its specific bond length, the latter refined on the basis of analysis of more than 250 spinel structural data from the literature (Lavina et al. 2002). However, using the bond length of 1.972(2) Å reported for $^{T}Co^{2+}$-O in Lavina et al. (2002), low values in the minimization function were obtained only for the Co-rich terms. Best fits for all examined crystals were obtained using variable $^{T}Co^{2+}$-O bond lengths, ranging from 1.966 Å in the Co-poor terms to 1.972 Å in the Co-rich terms. The final cation distribution was obtained by using the average value of 1.969(3) Å for $^{T}Co^{2+}$-O along the entire solid-solution series (Table 2).

Results and discussion

The synthetic $(Mg_{1-x}Co_x)Al_2O_4$ spinel crystals are characterized by the $Co^{2+} \rightarrow Mg$ substitution with x ranging from 0.07 to 1 (D'Ippolito et al. 2012, this issue). The site distribution of Mg, Co^{2+}, and Al shows that the M site is dominated by Al and the T site is mainly populated by Mg and Co^{2+}, with a marked preference of Co^{2+} for the tetrahedral coordination with respect to Mg. Accordingly, the degree of cation inversion, expressed as the occurrence of Al at T sites, decreases from 0.24 to 0.13 with increasing Co^{2+} content (Table 2).

Short-range structure

Recorded optical absorption spectra show three regions of absorption at ca. 4000, 7000, and 17 000 cm^{-1} caused by the spin-allowed electronic d-d transitions $^4A_2(F) \rightarrow {}^4T_2(F)$, $^4A_2(F) \rightarrow {}^4T_1(F)$, and $^4A_2(F) \rightarrow {}^4T_1(P)$ in tetrahedrally coordinated Co^{2+} (Figs. 1 and 2). Each of the three observed band regions are split in three absorption peaks due to first-order spin orbit coupling effects. Additional absorption bands caused by spin-forbidden transitions to the $^2T_1(G)$ and $^2A_1(G)$ levels in tetrahedrally coordinated Co^{2+} are observed (at ca. 15 700 and 18 300 cm^{-1}, respectively) close to the split spin-allowed $^4A_2(F) \rightarrow {}^4T_1(P)$ band. The absorbance in the three band regions vary greatly, with absorption caused by the split $^4A_2(F) \rightarrow {}^4T_1(P)$ transition displaying a linear absorption coefficient ca. 2 orders of magnitude stronger than for the $^4A_2(F) \rightarrow {}^4T_2(F)$ transition. The reason for the observed low intensity for bands caused by the latter transition is that they represent electric-dipole forbidden transitions.

In spectra of the sample CoAl0.5 it was not possible to record bands caused by the $^4A_2(F) \rightarrow {}^4T_2(F)$ transition due to their low intensity in combination with low Co-concentration and small crystal sizes. On the contrary, in spectra of the sample CoAl100, corresponding to the end-member $CoAl_2O_4$, it was impossible to observe peak positions of the strong bands caused by the split $^4A_2(F) \rightarrow {}^4T_1(F)$ transition due to very high absorption coefficients in combination with high Co-concentrations and difficulties to prepare sufficiently thin double-sided polished sections (thickness ≤8 µm would have been required). For the same reasons, peak positions of the extremely strong bands caused by the split $^4A_2(F) \rightarrow {}^4T_1(P)$ transition could not be determined from spectra of the samples spanning from CoAl34 to CoAl100.

Energies of the observed bands caused by the three split spin-allowed transitions as determined from the peak fitting procedure are summarized in Table 3. It is evident from the peak positions

Table 2. Structural formulae of the analyzed spinels along $(Mg_{1-x}Co_x)Al_2O_4$

Sample	Formula
CoAl0.5	$^{T}(Co_{0.06}Mg_{0.70}Al_{0.24})^{M}(Co_{0.01}Mg_{0.23}Al_{1.76})O_4$
CoAl1	$^{T}(Co_{0.07}Mg_{0.69}Al_{0.23})^{M}(Co_{0.01}Mg_{0.22}Al_{1.77})O_4$
CoAl10	$^{T}(Co_{0.09}Mg_{0.68}Al_{0.23})^{M}(Co_{0.02}Mg_{0.21}Al_{1.77})O_4$
CoAl14	$^{T}(Co_{0.23}Mg_{0.55}Al_{0.22})^{M}(Co_{0.02}Mg_{0.20}Al_{1.78})O_4$
CoAl20	$^{T}(Co_{0.31}Mg_{0.48}Al_{0.21})^{M}(Co_{0.03}Mg_{0.18}Al_{1.79})O_4$
CoAl34	$^{T}(Co_{0.44}Mg_{0.37}Al_{0.19})^{M}(Co_{0.04}Mg_{0.15}Al_{1.81})O_4$
CoAl45	$^{T}(Co_{0.54}Mg_{0.30}Al_{0.17})^{M}(Co_{0.05}Mg_{0.11}Al_{1.83})O_4$
CoAl50	$^{T}(Co_{0.52}Mg_{0.27}Al_{0.21})^{M}(Co_{0.11}Mg_{0.10}Al_{1.79})O_4$
CoAl67	$^{T}(Co_{0.67}Mg_{0.17}Al_{0.16})^{M}(Co_{0.09}Mg_{0.08}Al_{1.84})O_4$
CoAl100	$^{T}(Co_{0.87}Mg_{0.00}Al_{0.13})^{M}(Co_{0.13}Mg_{0.00}Al_{1.87})O_4$

Note: T = tetrahedrally coordinated site; M = octahedrally coordinated site.

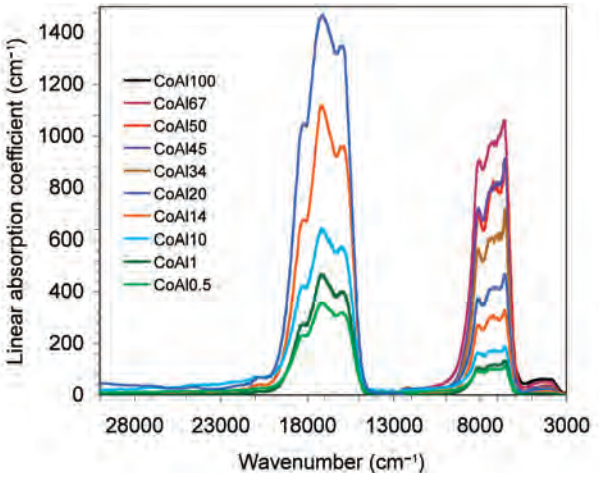

Figure 1. Nonpolarized single-crystal absorption spectra of the $(Mg_{1-x}Co_x)Al_2O_4$ series. Complete spectra into the UV-region could not be recorded for the high-Co crystals CoAl34 to CoAl100 because of difficulties to prepare sufficiently thin absorbers (≤8 µm).

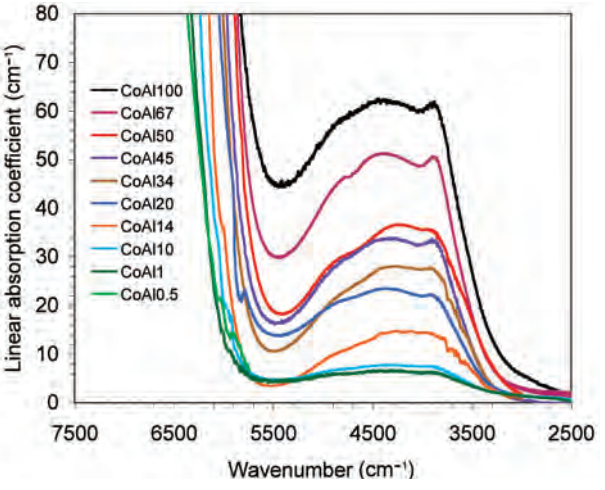

Figure 2. Nonpolarized single-crystal absorption spectra of the split $^4A_2(F) \rightarrow {}^4T_2(F)$ transition in tetrahedrally coordinated Co^{2+} in the $(Mg_{1-x}Co_x)Al_2O_4$ spinel series. Low Co-content in combination with limited crystal size and low molar absorption coefficient precluded recordings of this transition in sample CoAl0.5.

of the fitted spectra that energies of all the observed main bands caused by electronic transitions in tetrahedrally coordinated Co^{2+} display only very marginal energy shifts with progressive Co^{2+}-Mg substitution at the T site (Table 3, Figs. 1 and 2).

The observed behavior has practical consequences because, together with the increase of absorption band intensity as a function of Co^{2+} content, it is the reason for both the absence of color shift and the perceived intensification of blue color of the crystals along the series (D'Ippolito et al. 2012, this issue). Notably, this is significantly different from what is observed in $MgAl_2O_4$-$FeAl_2O_4$ and in $MgAl_2O_4$-$MgCr_2O_4$ spinel solid-solution series, where a marked color shift (and absorption intensification) from pale lilac to dark green and from light red to dark green was observed as a function of Fe^{2+} and of Cr^{3+} content, respectively (Hålenius et al. 2002, 2010).

The crystal field splitting parameter *Dq*, the Racah *B*-parameter and spin-orbit coupling λ-parameters for Co^{2+} at the T site may be calculated from the energies of the observed spin-allowed d-d transitions applying the Tanabe-Sugano equations (e.g., Oh et al. 2000; Pappalardo and Dietz 1961)

$^4A_2$ (F) → $^4T_2$(F) [ν_1]: $10Dq + 5/2\ |\lambda_0|$
$10Dq + |\lambda_0|$
$10Dq - 3/2\ |\lambda_0|$.
$^4A_2$(F) → $^4T_1$ (F) [ν_2]: $18Dq + 9/4\ |\lambda_1|$
$18Dq - 6/4\ |\lambda_1|$
$18Dq - 15/4\ |\lambda_1|$.
$^4A_2$(F) → $^4T_1$ (P) [ν_3]: $15B + 12Dq + 5/2\ |\lambda_2|$
$15B + 12Dq + |\lambda_2|$
$15B + 12Dq - 3/2\ |\lambda_2|$.

Table 4 summarizes the parameters resulting from best fits of the energies of the spin-allowed transitions observed in our spectra for tetrahedrally coordinated Co^{2+}. Our obtained *Dq* values are very similar (416–421 cm^{-1}) and compare very well with the range of *Dq*-values between 370–420 cm^{-1} that were determined by optical absorption spectroscopy for a large range of Co^{2+}-doped spinel compounds by Hochu and Lenglet (1998) and those reported for low Co^{2+} contents in $MgAl_2O_4$ (400 cm^{-1}, Weakliem 1962; Kuleshov et al. 1993) and in $ZnGa_2O_4$ (403 cm^{-1}, Abritta and Blak 1991). Moreover, our calculated *Dq* values compare very well with the value of 390 cm^{-1} determined for $CoAl_2O_4$ from magnetic neutron scattering experiments by Winkler et al. (1997). The presently obtained values for the Racah *B*-parameter (799–808 cm^{-1}), though limited to low-Co samples due to the above mentioned spectra limitations, are very close to each other and compare very well with those (790–815 cm^{-1}) calculated by Hochu and Lenglet (1998) for a range of aluminate spinels. Finally, the presently calculated spin-orbit coupling parameters (257–318 cm^{-1}) are relatively high, a fact that has been frequently observed in spectral studies of several other Co-bearing compounds (e.g., Pappalardo and Dietz 1961) and also commented on (e.g., Wildner 1996) but not been resolved. Pappalardo and Dietz (1961) suggested that anomalously high λ-value for the $^4A_2$(F) → $^4T_1$(P) transition may be due to strong spin-orbit mixing with the doublet terms derived from the ^{2}G-state.

It is notable that the crystal field splitting parameter *Dq* as well as the Racah *B*-parameter for tetrahedrally coordinated Co^{2+} show only insignificant changes within the present spinel series. As a consequence of the $Dq \approx 1/R^5$ ligand field relation-

TABLE 3. Energies (cm^{-1}) of absorption bands caused by spin orbit coupling split spin-allowed transitions in tetrahedrally coordinated Co^{2+} for analyzed spinels along $(Mg_{1-x}Co_x)Al_2O_4$

Sample	CoAl0.5	CoAl1	CoAl10	CoAl14	CoAl20	CoAl34	CoAl45	CoAl50	CoAl67	CoAl100
Transition										
$^4A_2$ (F)-$^4T_2$(F)		4927	4916	4962	4913	4989	4891	4865	4886	4959
		4388	4360	4374	4344	4417	4346	4364	4320	4315
		3842	3834	3807	3799	3838	3839	3857	3833	3812
$^4A_2$ (F)-$^4T_1$(F)	8196	8156	8153	8164	8149	8152	8161	8152	8103	
	7178	7170	7212	7179	7187	7151	7195	7163	7276	
	6512	6515	6509	6514	6512	6510	6524	6460	6579	
$^4A_2$ (F)-$^4T_1$(P)	17834	17802	17865	17813	17762					
	17315	17394	17337	17406	17314					
	16606	16782	16614	16743	16755					

Note: Estimated relative standard uncertainties in band energies are 0.5%.

TABLE 4. Energies (cm^{-1}) of spin-allowed $^T Co^{2+}$-bands, crystal field splitting, repulsion, spin orbit coupling parameters, and calculated local $^T Co^{2+}$-O (Å) distances for analyzed spinels along $(Mg_{1-x}Co_x)Al_2O_4$

Sample	ν_{1soc}*	ν_{2soc}*	ν_{3soc}*	*Dq*	*B*	λ_0	λ_1	λ_2	Local $^T Co^{2+}$-O
^{T}Co-O									
CoAl0.5		7578	17044	421	799		–283	–312	1.967
CoAl1	4197	7556	17154	420	808	–283	–276	–257	1.968
CoAl10	4181	7570	17060	419	802	–284	–279	–318	1.969
CoAl14	4179	7563	17142	419	808	–303	–278	–268	1.969
CoAl20	4157	7559	17105	418	806	–292	–276	–258	1.970
CoAl34	4215	7546	no	420		–300	–275		1.968
CoAl45	4174	7570	no	419		–276	–276		1.969
CoAl50	4187	7544	no	419		–263	–286		1.969
CoAl67	4161	7581	no	419		–278	–261		1.969
CoAl100	4158	no	no	416		–306			1.972

Notes: Estimated relative standard uncertainties in band energies are 0.5%; estimated errors in *Dq*, *B*, and λ values are ±2 cm^{-1}; estimated standard uncertainty in the calculated local ^{T}Co-O distance is 0.002 Å. no = not observed due to limitations in sample preparation.
* Band energies without spin orbit coupling effects.

ship, this demonstrates that the local Co^{2+}-O bond distance at the T-site only marginally increases with increasing Co-content in the $(Mg_{1-x}Co_x)Al_2O_4$-series (Table 4). In addition, the almost constant Racah *B*-parameter for tetrahedrally coordinated Co^{2+} in this series suggests that any influence of substitutional next nearest neighbor cations on the ionicity of Co^{2+}-O bonds at the T-site is very small. Constant Racah *B*-parameters for tetrahedrally coordinated Mn^{2+} and hence comparable insensitivity to next-nearest neighbor effects on bond ionicity were also observed for $^{T}Mn^{2+}$-O bonds in the $MgAl_2O_4$-$MnAl_2O_4$ spinel solid-solution series (Hålenius et al. 2011).

Co^{2+}-O tetrahedral bond length variation

Variation in $^{T}Co^{2+}$-O has been shown to occur in the normal spinel of the binary join $Co^{2+}(Co^{3+}_{2-x}Cr_x)O_4$ by O'Neill (2003): $^{T}Co^{2+}$-O increases, from ~1.93 Å in Co_3O_4 to ~1.97 Å in $CoCr_2O_4$, with increasing M-O from ~1.92 to ~1.99 Å.

In the present solid solution, we also observe a small variation in $^{T}Co^{2+}$-O from 1.966 to 1.972 Å derived from optical spectra and optimization of site occupancies of cations, which, however, appears to be inversely related to M-O: i.e., $^{T}Co^{2+}$-O increases with decreasing M-O. This is reflected by the correlation between T-O and ^{T}Al (Fig. 3), from which the value of $^{T}Co^{2+}$-O = 1.974(1) Å is retrieved for an ideal, fully ordered $^{T}(Co)^{M}(Al)_2O_4$ spinel (which would have ^{M}Al-O ~1.91 Å). Such a decreasing trend is confirmed in a study on the binary join Co_2GeO_4-Co_2TiO_4, by Hirota et al. (1990), in which they recorded $^{T}Co^{2+}$-O ~1.90 Å at a concomitant M-O ~2.07 Å.

This dual behavior of $^{T}Co^{2+}$-O could be explained by considering that the series $Co^{2+}(Co^{3+}_{2-x}Cr_x)O_4$ is characterized by a high degree of covalent bonding and Co^{3+} in the low-spin state, whereas the series $(Mg_{1-x}Co_x)Al_2O_4$ and the term $^{T}(Co^{2+})^{M}(Co^{2+}Ti)O_4$ are ionically bonded with all cations in their high-spin states.

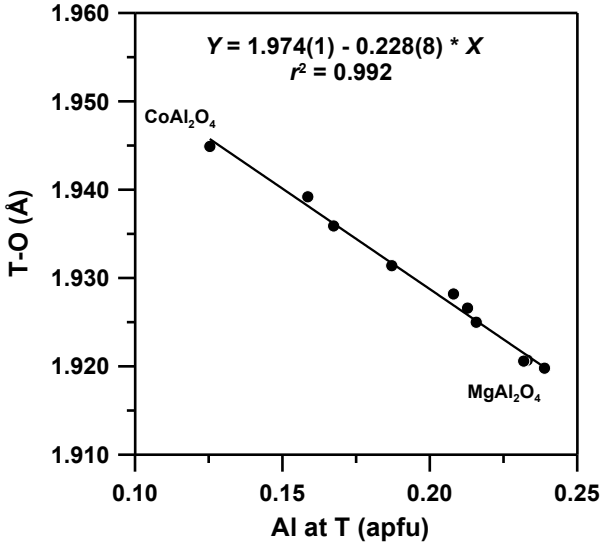

FIGURE 3. Variation in tetrahedral bond length (T-O) as a function of Al content at the T site. Symbol size is proportional to the analytical error.

Long-range structure

The observed variation of the unit-cell parameter *a* from 8.084 to 8.105 Å (D'Ippolito et al. 2012, this issue), is mainly related to the strong variations in the tetrahedral bond length from 1.920 to 1.945 Å rather than to the considerably more limited variations in the octahedral bond length from 1.923 to 1.929 Å (Fig. 4). Although the increments in both *a*-parameter and the T-O distance directly reflect an increase in the Co-spinel component ($r^2 = 0.88$ and $r^2 = 0.92$, respectively), the ultimate cause of the geometrical variations is related to variations in Al content at the T site. In fact, the substitution $Co^{2+} \rightarrow Mg$ at the T site is not expected to cause any T-O bond distance change because the two cations have been shown to have very similar cation radii: as mentioned before, the optimized value for $^{T}Co^{2+}$-O distance equals 1.969(3) Å compared to 1.966(1) Å for $^{T}Mg^{2+}$-O (reported by Lavina et al. 2002). Consequently, any increase in T-O distance with increased incorporation of Co in the structure must be mainly ascribed to a decrease in Al content at the T site (Fig. 3). In Figure 4, sample CoAl50 plots off the regression line because its subsolidus equilibrium temperature was higher (ca. 1000 °C) than that of the other samples (ca. 800 °C). Such a temperature difference affects the cation ordering as well as the bond distances T-O and M-O, but not the *a*-parameter (see D'Ippolito et al. 2012, this issue).

As a consequence of $Co^{2+} \rightarrow Mg$, the inversion degree decreases and the Al occupancy at the M-site increases (Fig. 5). The studied spinels contain only two types of divalent cations (Mg and Co^{2+}) and only one type of trivalent cation (Al). We

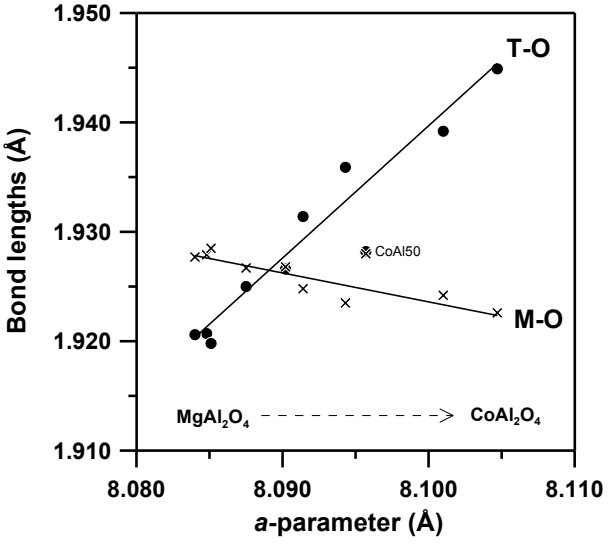

FIGURE 4. Relationship between unit-cell parameter (*a*) and tetrahedral (filled circles) and octahedral (black crosses) bond lengths in the synthesized crystals. The linear fit and the determination coefficient ($r^2 = 0.97$ and 0.83 for T-O and M-O, respectively) are calculated by using all points except for that of sample CoAl50. This latter plots off the regression line because its subsolidus equilibrium temperature was higher (ca. 1000 °C) than that of the other samples (ca. 800 °C). Such a temperature affects the cation ordering as well as the structural parameters (see D'Ippolito et al. 2012, this issue). Symbol size is proportional to the analytical error.

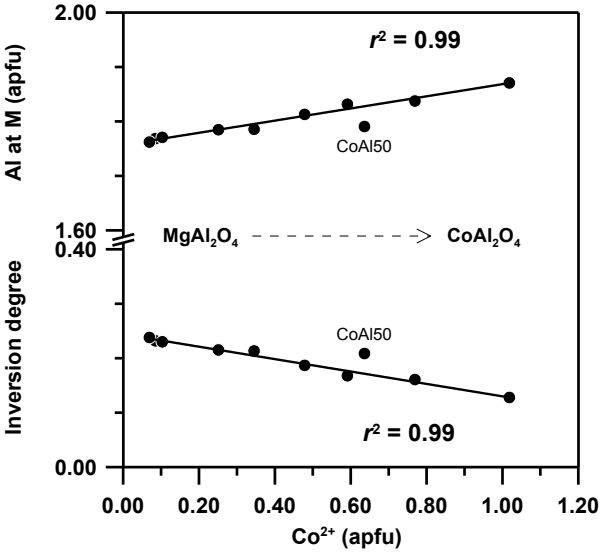

FIGURE 5. Linear relationship of inversion parameter and ^{M}Al against Co content showing the progressive structural ordering of Al from $MgAl_2O_4$ to $CoAl_2O_4$. Sample CoAl50 plots off the regression line because of its higher subsolidus equilibrium temperature and was then excluded from the correlation analysis (see also caption to Fig. 4). Symbol size is proportional to the analytical error.

know that the size of Mg and Co^{2+} at the T site is very similar. Consequently, the only steric effect that may account for variations in Al ordering must be related to the cation occupancy of the M site. Noteworthy, Mg and Co^{2+} at the M site yield significantly different bond distances: $^{M}Mg^{2+}$-O = 2.082(1) Å and $^{M}Co^{2+}$-O = 2.11(1) Å (Lavina et al. 2002). To show how such steric effect drives the Al ordering at M, we may consider a theoretical case in which the inversion degree is assumed to be constant. In this case, as a result of the substitution $Co^{2+} \rightarrow$ Mg we would expect no variation in T-O bond length and an increase in M-O bond length due to the larger $^{M}Co^{2+}$-O value. Such a situation would lead to a reduction in both the octahedral distortion and oxygen fractional coordinate (Bosi et al. 2010). This means that the shared octahedral edges, $^{M}(O\text{-}O)_{shared}$, would become larger. In this way, the enlargement in $^{M}(O\text{-}O)_{shared}$ would result in a diminishing oxygen shielding effect to the octahedral cation-cation repulsion, leading to energetic destabilization of the spinel structure, as previously discussed by Lavina et al. (2003) and Nakatsuka et al. (2003). Consequently, this case must be ruled out because the more Co^{2+} enters the solid solution, the more unstable it would become. However, in the present solid-solution series an opposite behavior is observed: i.e., a variation in the inversion degree is connected with a slight variation in M-O distances, a significant increase in T-O distances and a decrease in $^{M}(O\text{-}O)_{shared}$ at increasing $CoAl_2O_4$ component (Table 1). To describe in numerical terms the electrostatic cation-cation repulsion across $^{M}(O\text{-}O)_{shared}$ in the spinel structure, the ionic potential at M, ^{M}IP, may be useful (Bosi et al. 2011). ^{M}IP is calculated as the ratio of the aggregate formal valence of the cations occupying the M site to aggregate cation radius at M obtained by M-O distance minus 1.38 Å (i.e., the ionic radius of oxygen in fourfold coordination). Since ^{M}IP is proportional to the charge density at M (i.e., the electrostatic charge on the cation surface), an increase in ^{M}IP leads to a decrease in $^{M}(O\text{-}O)_{shared}$, which provides a better oxygen shielding effect to the octahedral cation-cation repulsion. This effect was demonstrated for the ^{T}Zn-spinels characterized by the substitutions of Al^{3+}, Cr^{3+}, Ga^{3+}, V^{3+}, Fe^{3+}, and Mn^{3+} at the M site (Bosi et al. 2011), and a very similar correlation has been obtained for the present ^{T}Co-spinels as well as for the $Co^{2+}(Co^{3+}_{2-x}Cr_x)O_4$ series and the $^{T}(Co^{2+})^{M}(Co^{2+}Ti)O_4$ term (O'Neill 2003; Hirota et al. 1990) (Fig. 6). All data follow a similar quadratic trend probably ascribable to the soft behavior of $^{T}Co^{2+}$- and $^{T}Zn^{2+}$-cations, which yields variation in $^{T}Co^{2+}$-O and $^{T}Zn^{2+}$-O bond length (O'Neill 2003 and Bosi et al. 2011).

In summary, in the studied $MgAl_2O_4$-$CoAl_2O_4$ series, due to the very similar size of Co^{2+} and Mg at the T site and the larger size of Co^{2+} with respect to Mg at the M site, the spinel structure responds to the $Co^{2+} \rightarrow$ Mg substitution by increasing the ordering of Al in such a manner that M-O remains almost constant and T-O increases. In this way, $^{M}(O\text{-}O)_{shared}$ distances are reduced and the destabilization effect due to the increased octahedral cation-cation repulsion is minimized.

The conclusions achieved here are in line with those of previous studies (e.g., Bosi et al. 2007, 2010), and further emphasize the importance of steric factors for controlling the cation distributions in the spinel structure.

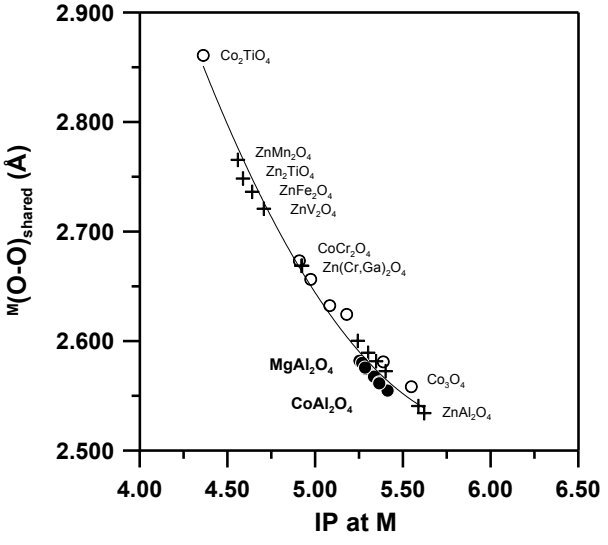

FIGURE 6. Relationship between ionic potential at M (^{M}IP) and octahedral shared edge $^{M}(O\text{-}O)_{shared}$ showing the variation in the shared edge induced by charge density at M. Filled circles represent synthetic crystals from the present study, open circles represent $^{T}Co^{2+}$-spinels from O'Neill (2003) and Hirota et al. (1990), black crosses ^{T}Zn-spinels from Bosi et al. (2011) and Zn_2TiO_4. Note that the data for $CoCr_2O_4$ are averaged from O'Neill (2003), Garcia Casado and Rasines (1986), and Hirota et al. (1990), while data for Zn_2TiO_4 are averaged from Verwey and Heilmann (1947), Bartram and Slepetys (1961), Millard et al. (1995), and Takai et al. (2007). Symbol size for the present crystals is proportional to the analytical error.

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_computing_publication_material   ?

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0231P)^2^+0.3159P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      SHELXL
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O2 0.00779(14) 0.00779(14) 0.00779(14) 0.00022(8) 0.00022(8) 0.00022(8)
O 0.00779(14) 0.00779(14) 0.00779(14) 0.00022(8) 0.00022(8) 0.00022(8)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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AlM O 1.9292(3) 52_455 ?
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AlM O2 1.9292(4) 148_665 ?
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AlM O2 1.9292(4) 75_545 ?
AlM O2 1.9292(3) 171_566 ?
AlM O2 1.9292(3) 52_455 ?
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MgT O 1.9185(7) 27_544 ?
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MgT MgT 3.50104(17) 121 ?
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 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Al'  'Al'   0.0645   0.0514
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Mg'  'Mg'   0.0486   0.0363
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            ?
_symmetry_space_group_name_H-M    ?

loop_
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 'x+1/2, -y+3/4, -z+1/4'
 'z, x, y'
 'z+1/2, -x+3/4, -y+1/4'
 '-z+3/4, -x+1/4, y+1/2'
 '-z+1/4, x+1/2, -y+3/4'
 'y, z, x'
 '-y+1/4, z+1/2, -x+3/4'
 'y+1/2, -z+3/4, -x+1/4'
 '-y+3/4, -z+1/4, x+1/2'
 'y+3/4, x+1/4, -z+1/2'
 '-y, -x, -z'
 'y+1/4, -x+1/2, z+3/4'
 '-y+1/2, x+3/4, z+1/4'
 'x+3/4, z+1/4, -y+1/2'
 '-x+1/2, z+3/4, y+1/4'
 '-x, -z, -y'
 'x+1/4, -z+1/2, y+3/4'
```

```
'z+3/4, y+1/4, -x+1/2'
'z+1/4, -y+1/2, x+3/4'
'-z+1/2, y+3/4, x+1/4'
'-z, -y, -x'
'x, y+1/2, z+1/2'
'-x+3/4, -y+3/4, z+1'
'-x+1/4, y+1, -z+5/4'
'x+1/2, -y+5/4, -z+3/4'
'z, x+1/2, y+1/2'
'z+1/2, -x+5/4, -y+3/4'
'-z+3/4, -x+3/4, y+1'
'-z+1/4, x+1, -y+5/4'
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'-x, -z+1/2, -y+1/2'
'x+1/4, -z+1, y+5/4'
'z+3/4, y+3/4, -x+1'
'z+1/4, -y+1, x+5/4'
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'-z, -y+1/2, -x+1/2'
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'-z+3/4, x+1/2, -y+5/4'
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'x+5/4, z+1/4, -y+1'
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'z+5/4, y+1/4, -x+1'
'z+3/4, -y+1/2, x+5/4'
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'x+1/2, y+1/2, z'
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'-x+3/4, y+1, -z+3/4'
```

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'x-1/4, -y, z-1/4'
'-x-1/2, y-1/4, z+1/4'
'-z, -x+1/2, -y+1/2'
'-z-1/2, x-1/4, y+1/4'
'z-3/4, x+1/4, -y'
'z-1/4, -x, y-1/4'
'-y, -z+1/2, -x+1/2'
'y-1/4, -z, x-1/4'

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'y-3/4, z+1/4, -x'
'-y-3/4, -x+1/4, z'
'y, x+1/2, z+1/2'
'-y-1/4, x, -z-1/4'
'y-1/2, -x-1/4, -z+1/4'
'-x-3/4, -z+1/4, y'
'x-1/2, -z-1/4, -y+1/4'
'x, z+1/2, y+1/2'
'-x-1/4, z, -y-1/4'
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'z, y+1/2, x+1/2'
'-x+1/2, -y, -z+1/2'
'x-1/4, y-1/4, -z'
'x+1/4, -y-1/2, z-1/4'
'-x, y-3/4, z+1/4'
'-z+1/2, -x, -y+1/2'
'-z, x-3/4, y+1/4'
'z-1/4, x-1/4, -y'
'z+1/4, -x-1/2, y-1/4'
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'y, -x-3/4, -z+1/4'
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'-x+1/4, z-1/2, -y-1/4'
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'z+1/4, -x, y-3/4'
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'-y, z-1/4, x-1/4'
'y-1/4, z+1/4, -x-1/2'
'-y-1/4, -x+1/4, z-1/2'
'y+1/2, x+1/2, z'
'-y+1/4, x, -z-3/4'
'y, -x-1/4, -z-1/4'
'-x-1/4, -z+1/4, y-1/2'

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 'x, -z-1/4, -y-1/4'
 'x+1/2, z+1/2, y'
 '-x+1/4, z, -y-3/4'
 '-z-1/4, -y+1/4, x-1/2'
 '-z+1/4, y, -x-3/4'
 'z, -y-1/4, -x-1/4'
 'z+1/2, y+1/2, x'

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_cell_length_b                    8.0858(5)
_cell_length_c                    8.0858(5)
_cell_angle_alpha                 90.00
_cell_angle_beta                  90.00
_cell_angle_gamma                 90.00
_cell_volume                      528.65(6)
_cell_formula_units_Z             8
_cell_measurement_temperature     293(2)
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_cell_measurement_theta_max       ?

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_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              592
_exptl_absorpt_coefficient_mu     1.314
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_exptl_special_details
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_diffrn_radiation_wavelength      0.71073
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_diffrn_radiation_monochromator   graphite
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_diffrn_measurement_method        ?
_diffrn_detector_area_resol_mean  ?
_diffrn_standards_number          ?
_diffrn_standards_interval_count  ?
_diffrn_standards_interval_time   ?
_diffrn_standards_decay_%         ?
_diffrn_reflns_number             2417
_diffrn_reflns_av_R_equivalents   0.0403
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_diffrn_reflns_limit_k_min        -14
_diffrn_reflns_limit_k_max        11
_diffrn_reflns_limit_l_min        -15
_diffrn_reflns_limit_l_max        13
_diffrn_reflns_theta_min          4.37
_diffrn_reflns_theta_max          45.13
_reflns_number_total              131
_reflns_number_gt                 131
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        ?
_computing_cell_refinement        ?
_computing_data_reduction         ?
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0319P)^2^+0.2177P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.300(18)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          131
_refine_ls_number_parameters      10
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0254
_refine_ls_R_factor_gt            0.0254
_refine_ls_wR_factor_ref          0.0555
_refine_ls_wR_factor_gt           0.0555
_refine_ls_goodness_of_fit_ref    1.350
_refine_ls_restrained_S_all       1.350
_refine_ls_shift/su_max           0.000
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_refine_ls_shift/su_mean          0.000

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 _atom_site_type_symbol
 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
 _atom_site_calc_flag
 _atom_site_refinement_flags
 _atom_site_disorder_assembly
 _atom_site_disorder_group
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MgT Mg 0.1250 0.1250 0.1250 0.0043(2) Uani 1.077(8) 24 d SP . .
O2 O2 0.26208(6) 0.26208(6) 0.26208(6) 0.00780(19) Uani 0.63 6 d SP . .
O O 0.26208(6) 0.26208(6) 0.26208(6) 0.00780(19) Uani 0.37 6 d SP . .

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 _atom_site_aniso_U_11
 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
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MgT 0.0043(2) 0.0043(2) 0.0043(2) 0.000 0.000 0.000
O2 0.00780(19) 0.00780(19) 0.00780(19) 0.00010(9) 0.00010(9) 0.00010(9)
O 0.00780(19) 0.00780(19) 0.00780(19) 0.00010(9) 0.00010(9) 0.00010(9)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
;

loop_
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 _geom_bond_atom_site_label_2
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 _geom_bond_site_symmetry_2
 _geom_bond_publ_flag
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AlM O 1.9287(5) 52_455 ?
AlM O 1.9287(5) 171_566 ?
AlM O 1.9287(5) 75_545 ?
AlM O 1.9287(5) 122_656 ?
```

```
AlM O 1.9287(5) 26_554 ?
AlM O2 1.9287(5) 148_665 ?
AlM O2 1.9287(5) 26_554 ?
AlM O2 1.9287(5) 122_656 ?
AlM O2 1.9287(5) 75_545 ?
AlM O2 1.9287(5) 171_566 ?
AlM O2 1.9287(5) 52_455 ?
MgT O2 1.9197(9) . ?
MgT O 1.9198(9) 76_445 ?
MgT O 1.9198(9) 27_544 ?
MgT O 1.9198(9) 50_454 ?
MgT O2 1.9198(9) 76_445 ?
MgT O2 1.9198(9) 27_544 ?
MgT O2 1.9198(9) 50_454 ?
MgT MgT 3.5013(2) 97 ?
MgT MgT 3.5013(2) 169 ?
MgT MgT 3.5013(2) 145 ?
MgT MgT 3.5013(2) 121 ?
O2 AlM 1.9288(5) 52_455 ?
O2 AlM 1.9288(5) 26_554 ?
O2 AlM 1.9288(5) 75_545 ?

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 _geom_angle_atom_site_label_2
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 _geom_angle_site_symmetry_3
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O AlM O 84.05(3) 148_665 171_566 ?
O AlM O 95.95(3) 52_455 171_566 ?
O AlM O 95.95(3) 148_665 75_545 ?
O AlM O 84.05(3) 52_455 75_545 ?
O AlM O 180.0 171_566 75_545 ?
O AlM O 84.05(3) 148_665 122_656 ?
O AlM O 95.95(3) 52_455 122_656 ?
O AlM O 84.05(3) 171_566 122_656 ?
O AlM O 95.95(3) 75_545 122_656 ?
O AlM O 95.95(3) 148_665 26_554 ?
O AlM O 84.05(3) 52_455 26_554 ?
O AlM O 95.95(3) 171_566 26_554 ?
O AlM O 84.05(3) 75_545 26_554 ?
O AlM O 180.0 122_656 26_554 ?
O AlM O2 0.00(3) 148_665 148_665 ?
O AlM O2 180.0 52_455 148_665 ?
O AlM O2 84.05(3) 171_566 148_665 ?
O AlM O2 95.95(3) 75_545 148_665 ?
O AlM O2 84.05(3) 122_656 148_665 ?
O AlM O2 95.95(3) 26_554 148_665 ?
O AlM O2 95.95(3) 148_665 26_554 ?
O AlM O2 84.05(3) 52_455 26_554 ?
O AlM O2 95.95(3) 171_566 26_554 ?
O AlM O2 84.05(3) 75_545 26_554 ?
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O AlM O2 0.00(6) 26_554 26_554 ?
O2 AlM O2 95.95(3) 148_665 26_554 ?
O AlM O2 84.05(3) 148_665 122_656 ?
O AlM O2 95.95(3) 52_455 122_656 ?
O AlM O2 84.05(3) 171_566 122_656 ?
O AlM O2 95.95(3) 75_545 122_656 ?
O AlM O2 0.00(3) 122_656 122_656 ?
O AlM O2 180.0 26_554 122_656 ?
O2 AlM O2 84.05(3) 148_665 122_656 ?
O2 AlM O2 180.0 26_554 122_656 ?
O AlM O2 95.95(3) 148_665 75_545 ?
O AlM O2 84.05(3) 52_455 75_545 ?
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O2 AlM O2 95.95(3) 148_665 75_545 ?
O2 AlM O2 84.05(3) 26_554 75_545 ?
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O AlM O2 0.00(3) 171_566 171_566 ?
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O2 AlM O2 84.05(3) 148_665 171_566 ?
O2 AlM O2 95.95(3) 26_554 171_566 ?
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O2 AlM O2 180.00(3) 75_545 171_566 ?
O AlM O2 180.0 148_665 52_455 ?
O AlM O2 0.00(3) 52_455 52_455 ?
O AlM O2 95.95(3) 171_566 52_455 ?
O AlM O2 84.05(3) 75_545 52_455 ?
O AlM O2 95.95(3) 122_656 52_455 ?
O AlM O2 84.05(3) 26_554 52_455 ?
O2 AlM O2 180.0 148_665 52_455 ?
O2 AlM O2 84.05(3) 26_554 52_455 ?
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 'Cu'  'Cu'   0.3201   1.2651
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_computing_cell_refinement        ?
_computing_data_reduction         ?
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_computing_molecular_graphics     ?
_computing_publication_material   ?

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.053(2)
_refine_ls_extinction_expression
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_refine_ls_number_parameters      10
_refine_ls_number_restraints      0
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 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
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CuM Cu 0.5000 0.5000 0.5000 0.00478(10) Uani 0.0289(19) 12 d SP . .
MgT Mg 0.1250 0.1250 0.1250 0.00558(14) Uani 0.900(3) 24 d SP . .
CuT Cu 0.1250 0.1250 0.1250 0.00558(14) Uani 0.100(3) 24 d SP . .
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 _atom_site_aniso_U_12
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CuM 0.00478(10) 0.00478(10) 0.00478(10) -0.00021(4) -0.00021(4) -0.00021(4)
MgT 0.00558(14) 0.00558(14) 0.00558(14) 0.000 0.000 0.000
CuT 0.00558(14) 0.00558(14) 0.00558(14) 0.000 0.000 0.000
O2 0.00851(12) 0.00851(12) 0.00851(12) 0.00018(9) 0.00018(9) 0.00018(9)
O 0.00851(12) 0.00851(12) 0.00851(12) 0.00018(9) 0.00018(9) 0.00018(9)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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AlM O 1.9291(3) 26_554 ?
AlM O2 1.9291(3) 148_665 ?
AlM O2 1.9291(3) 52_455 ?
AlM O2 1.9291(3) 171_566 ?
AlM O2 1.9291(3) 75_545 ?
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AlM O2 1.9291(3) 26_554 ?
MgT O2 1.9191(6) . ?
MgT O 1.9191(6) 76_445 ?
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O AlM O 84.08(2) 52_455 75_545 ?
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O AlM O 95.92(2) 75_545 122_656 ?
O AlM O 95.92(2) 148_665 26_554 ?
O AlM O 84.08(2) 52_455 26_554 ?
O AlM O 95.92(2) 171_566 26_554 ?
O AlM O 84.08(2) 75_545 26_554 ?
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O AlM O2 0.00(2) 148_665 148_665 ?
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O2 AlM O2 95.92(2) 52_455 122_656 ?
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O AlM O2 84.08(2) 75_545 26_554 ?
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O AlM O2 0.00(4) 26_554 26_554 ?
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O MgT CuM 80.0 50_454 26_554 ?
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CuM MgT CuM 50.5 26_554 75_545 ?
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MgT O2 AlM 121.175(16) . 75_545 ?
CuM O2 AlM 95.63(2) 52_455 75_545 ?
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AlM O2 AlM 95.63(2) 75_545 52_455 ?
MgT O2 CuM 121.175(16) . 26_554 ?
CuM O2 CuM 95.63(2) 52_455 26_554 ?
AlM O2 CuM 0.0 26_554 26_554 ?
AlM O2 CuM 95.63(2) 75_545 26_554 ?
AlM O2 CuM 95.63(2) 52_455 26_554 ?
MgT O2 CuM 121.175(16) . 75_545 ?
CuM O2 CuM 95.63(2) 52_455 75_545 ?
AlM O2 CuM 95.63(2) 26_554 75_545 ?
AlM O2 CuM 0.0 75_545 75_545 ?
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CuM O2 CuM 95.63(2) 26_554 75_545 ?

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 'Mg'  'Mg'   0.0486   0.0363
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loop_
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 'y+3/4, x+1/4, -z+1/2'
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 'y+1/4, -x+1/2, z+3/4'
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 'x+3/4, z+1/4, -y+1/2'
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_cell_length_c                    8.0867(5)
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_cell_angle_gamma                 90.00
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_reflns_number_gt                 131
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_computing_cell_refinement        ?
_computing_data_reduction         ?
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0101P)^2^+0.7331P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0154(9)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          132
_refine_ls_number_parameters      11
_refine_ls_number_restraints      0
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_refine_ls_R_factor_gt            0.0123
_refine_ls_wR_factor_ref          0.0292
_refine_ls_wR_factor_gt           0.0291
_refine_ls_goodness_of_fit_ref    1.106
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 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
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 _atom_site_symmetry_multiplicity
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 _atom_site_refinement_flags
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MgT Mg 0.1250 0.1250 0.1250 0.00594(13) Uani 0.845(3) 24 d SP . .
CuT Cu 0.1250 0.1250 0.1250 0.00594(13) Uani 0.155(3) 24 d SP . .
O2 O2 0.26204(5) 0.26204(5) 0.26204(5) 0.00873(12) Uani 0.70 6 d SP . .
O O 0.26204(5) 0.26204(5) 0.26204(5) 0.00873(12) Uani 0.30 6 d SP . .

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 _atom_site_aniso_U_22
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 _atom_site_aniso_U_13
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CuM 0.00477(9) 0.00477(9) 0.00477(9) -0.00019(5) -0.00019(5) -0.00019(5)
MgT 0.00594(13) 0.00594(13) 0.00594(13) 0.000 0.000 0.000
CuT 0.00594(13) 0.00594(13) 0.00594(13) 0.000 0.000 0.000
O2 0.00873(12) 0.00873(12) 0.00873(12) 0.00016(9) 0.00016(9) 0.00016(9)
O 0.00873(12) 0.00873(12) 0.00873(12) 0.00016(9) 0.00016(9) 0.00016(9)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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 _geom_bond_atom_site_label_2
 _geom_bond_distance
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AlM O 1.9293(4) 122_656 ?
AlM O 1.9293(4) 26_554 ?
AlM O2 1.9293(4) 148_665 ?
AlM O2 1.9293(4) 52_455 ?
AlM O2 1.9293(4) 171_566 ?
AlM O2 1.9293(4) 75_545 ?
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AlM O2 1.9293(4) 26_554 ?
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MgT O 1.9194(7) 27_544 ?
MgT O 1.9194(7) 50_454 ?
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MgT O2 1.9194(7) 27_544 ?
MgT O2 1.9194(7) 50_454 ?
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MgT CuM 3.3526(2) 52_455 ?
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MgT CuM 3.3526(2) 3_545 ?
O2 CuM 1.9292(4) 52_455 ?
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O2 AlM 1.9292(4) 75_545 ?
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O AlM O 95.92(2) 148_665 75_545 ?
O AlM O 84.08(2) 52_455 75_545 ?
O AlM O 180.0 171_566 75_545 ?
O AlM O 84.08(2) 148_665 122_656 ?
O AlM O 95.92(2) 52_455 122_656 ?
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O AlM O 95.92(2) 75_545 122_656 ?
O AlM O 95.92(2) 148_665 26_554 ?
O AlM O 84.08(2) 52_455 26_554 ?
O AlM O 95.92(2) 171_566 26_554 ?
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O AlM O2 95.92(2) 52_455 171_566 ?
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O AlM O2 84.08(2) 122_656 171_566 ?
O AlM O2 95.92(2) 26_554 171_566 ?
O2 AlM O2 84.08(2) 148_665 171_566 ?
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AlM O2 CuM 0.0 26_554 26_554 ?
AlM O2 CuM 95.63(2) 75_545 26_554 ?
AlM O2 CuM 95.63(2) 52_455 26_554 ?
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_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      SHELXL
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CuT Cu 0.1250 0.1250 0.1250 0.00665(12) Uani 0.260(4) 24 d SP . .
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CuM 0.00523(9) 0.00523(9) 0.00523(9) -0.00024(5) -0.00024(5) -0.00024(5)
MgT 0.00665(12) 0.00665(12) 0.00665(12) 0.000 0.000 0.000
CuT 0.00665(12) 0.00665(12) 0.00665(12) 0.000 0.000 0.000
O2 0.00960(14) 0.00960(14) 0.00960(14) 0.00013(11) 0.00013(11) 0.00013(11)
O 0.00960(14) 0.00960(14) 0.00960(14) 0.00013(11) 0.00013(11) 0.00013(11)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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_diffrn_reflns_limit_k_max        15
_diffrn_reflns_limit_l_min        -16
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_diffrn_reflns_theta_min          4.37
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_reflns_number_gt                 133
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        ?
_computing_data_reduction         ?
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
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_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0048P)^2^+1.0148P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.117(5)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
_refine_ls_number_reflns          133
_refine_ls_number_parameters      10
_refine_ls_number_restraints      0
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_refine_ls_R_factor_gt            0.0171
_refine_ls_wR_factor_ref          0.0350
_refine_ls_wR_factor_gt           0.0350
_refine_ls_goodness_of_fit_ref    1.254
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_refine_ls_shift/su_max           0.000
_refine_ls_shift/su_mean          0.000

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 _atom_site_fract_y
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 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
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 _atom_site_refinement_flags
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CuM Cu 0.5000 0.5000 0.5000 0.00550(14) Uani 0.088(3) 12 d SP . .
MgT Mg 0.1250 0.1250 0.1250 0.00694(17) Uani 0.730(5) 24 d SP . .
CuT Cu 0.1250 0.1250 0.1250 0.00694(17) Uani 0.270(5) 24 d SP . .
O2 O2 0.26200(7) 0.26200(7) 0.26200(7) 0.01018(18) Uani 0.63 6 d SP . .
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 _atom_site_aniso_U_12
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CuM 0.00550(14) 0.00550(14) 0.00550(14) -0.00023(6) -0.00023(6) -0.00023(6)
MgT 0.00694(17) 0.00694(17) 0.00694(17) 0.000 0.000 0.000
CuT 0.00694(17) 0.00694(17) 0.00694(17) 0.000 0.000 0.000
O2 0.01018(18) 0.01018(18) 0.01018(18) 0.00010(13) 0.00010(13) 0.00010(13)
O 0.01018(18) 0.01018(18) 0.01018(18) 0.00010(13) 0.00010(13) 0.00010(13)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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AlM O 1.9290(5) 122_656 ?
AlM O 1.9290(5) 26_554 ?
AlM O2 1.9290(5) 148_665 ?
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AlM O2 1.9290(5) 171_566 ?
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AlM O2 1.9290(5) 122_656 ?
AlM O2 1.9290(5) 26_554 ?
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MgT O2 1.9185(9) . ?
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O AlM O2 0.00(3) 148_665 148_665 ?
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O2 MgT CuM 29.5 50_454 3_545 ?
O2 MgT CuM 121.5 . 3_545 ?
CuM MgT CuM 95.2 26_554 3_545 ?
CuM MgT CuM 144.9 52_455 3_545 ?
CuM MgT CuM 117.0 75_545 3_545 ?
MgT O2 CuM 121.18(2) . 52_455 ?
MgT O2 AlM 121.18(2) . 26_554 ?
CuM O2 AlM 95.61(3) 52_455 26_554 ?
MgT O2 AlM 121.18(2) . 75_545 ?
CuM O2 AlM 95.61(3) 52_455 75_545 ?
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MgT O2 AlM 121.18(2) . 52_455 ?
CuM O2 AlM 0.0 52_455 52_455 ?
AlM O2 AlM 95.61(3) 26_554 52_455 ?
AlM O2 AlM 95.61(3) 75_545 52_455 ?
MgT O2 CuM 121.18(2) . 26_554 ?
CuM O2 CuM 95.61(3) 52_455 26_554 ?
AlM O2 CuM 0.0 26_554 26_554 ?
AlM O2 CuM 95.61(3) 75_545 26_554 ?
AlM O2 CuM 95.61(3) 52_455 26_554 ?
MgT O2 CuM 121.18(2) . 75_545 ?
CuM O2 CuM 95.61(3) 52_455 75_545 ?
AlM O2 CuM 95.61(3) 26_554 75_545 ?
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CuM O2 CuM 95.61(3) 26_554 75_545 ?

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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Al'  'Al'   0.0645   0.0514
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Mg'  'Mg'   0.0486   0.0363
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 'Cu'  'Cu'   0.3201   1.2651
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 'x, -z-1/4, -y-1/4'
 'x+1/2, z+1/2, y'
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 '-z-1/4, -y+1/4, x-1/2'
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 'z+1/2, y+1/2, x'

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_cell_length_b                    8.0857(5)
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_cell_angle_beta                  90.00
_cell_angle_gamma                 90.00
_cell_volume                      528.63(6)
_cell_formula_units_Z             8
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_diffrn_radiation_monochromator   graphite
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_diffrn_reflns_limit_h_max        16
_diffrn_reflns_limit_k_min        -10
_diffrn_reflns_limit_k_max        11
_diffrn_reflns_limit_l_min        -15
_diffrn_reflns_limit_l_max        16
_diffrn_reflns_theta_min          4.37
_diffrn_reflns_theta_max          45.13
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_reflns_number_gt                 132
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        ?
_computing_data_reduction         ?
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0000P)^2^+1.8694P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0107(7)
_refine_ls_extinction_expression
 'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
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_refine_ls_number_parameters      10
_refine_ls_number_restraints      0
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_refine_ls_R_factor_gt            0.0145
_refine_ls_wR_factor_ref          0.0287
_refine_ls_wR_factor_gt           0.0287
_refine_ls_goodness_of_fit_ref    1.108
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_refine_ls_shift/su_max           0.000
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 _atom_site_fract_x
 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
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 _atom_site_refinement_flags
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CuM Cu 0.5000 0.5000 0.5000 0.00604(12) Uani 0.130(5) 12 d SP . .
MgT Mg 0.1250 0.1250 0.1250 0.00790(13) Uani 0.570(6) 24 d SP . .
CuT Cu 0.1250 0.1250 0.1250 0.00790(13) Uani 0.430(6) 24 d SP . .
O2 O2 0.26191(7) 0.26191(7) 0.26191(7) 0.0114(2) Uani 0.64 6 d SP . .
O O 0.26191(7) 0.26191(7) 0.26191(7) 0.0114(2) Uani 0.36 6 d SP . .

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 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
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CuM 0.00604(12) 0.00604(12) 0.00604(12) -0.00027(6) -0.00027(6) -0.00027(6)
MgT 0.00790(13) 0.00790(13) 0.00790(13) 0.000 0.000 0.000
CuT 0.00790(13) 0.00790(13) 0.00790(13) 0.000 0.000 0.000
O2 0.0114(2) 0.0114(2) 0.0114(2) 0.00001(16) 0.00001(16) 0.00001(16)
O 0.0114(2) 0.0114(2) 0.0114(2) 0.00001(16) 0.00001(16) 0.00001(16)

_geom_special_details
;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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 _geom_bond_atom_site_label_2
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AlM O 1.9300(5) 122_656 ?
AlM O 1.9300(5) 26_554 ?
AlM O2 1.9300(5) 148_665 ?
AlM O2 1.9300(5) 52_455 ?
AlM O2 1.9300(5) 171_566 ?
AlM O2 1.9300(5) 75_545 ?
AlM O2 1.9300(5) 122_656 ?
AlM O2 1.9300(5) 26_554 ?
MgT O 1.9173(10) 76_445 ?
MgT O 1.9173(10) 27_544 ?
MgT O 1.9173(10) 50_454 ?
MgT O2 1.9173(10) 76_445 ?
MgT O2 1.9173(10) 27_544 ?
MgT O2 1.9173(10) 50_454 ?
MgT O2 1.9174(10) . ?
MgT CuM 3.3522(2) 26_554 ?
MgT CuM 3.3522(2) 52_455 ?
MgT CuM 3.3522(2) 75_545 ?
MgT CuM 3.3522(2) 3_545 ?
O2 CuM 1.9300(5) 52_455 ?
O2 AlM 1.9300(5) 26_554 ?
O2 AlM 1.9300(5) 75_545 ?
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O2 CuM 1.9300(5) 26_554 ?
O2 CuM 1.9300(5) 75_545 ?

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 _geom_angle_atom_site_label_3
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O AlM O 84.15(4) 148_665 171_566 ?
O AlM O 95.85(4) 52_455 171_566 ?
O AlM O 95.85(4) 148_665 75_545 ?
O AlM O 84.15(4) 52_455 75_545 ?
O AlM O 180.0 171_566 75_545 ?
O AlM O 84.15(4) 148_665 122_656 ?
O AlM O 95.85(4) 52_455 122_656 ?
O AlM O 84.15(4) 171_566 122_656 ?
O AlM O 95.85(4) 75_545 122_656 ?
O AlM O 95.85(4) 148_665 26_554 ?
O AlM O 84.15(4) 52_455 26_554 ?
O AlM O 95.85(4) 171_566 26_554 ?
O AlM O 84.15(4) 75_545 26_554 ?
O AlM O 180.0 122_656 26_554 ?
O AlM O2 0.00(7) 148_665 148_665 ?
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AlM O2 CuM 95.57(3) 75_545 26_554 ?
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_computing_cell_refinement        ?
_computing_data_reduction         ?
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_computing_publication_material   ?

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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_refine_ls_weighting_details
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0412(18)
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CuT Cu 0.1250 0.1250 0.1250 0.00816(15) Uani 0.453(7) 24 d SP . .
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O O 0.26193(8) 0.26193(8) 0.26193(8) 0.0114(2) Uani 0.33 6 d SP . .

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CuM 0.00608(14) 0.00608(14) 0.00608(14) -0.00026(7) -0.00026(7) -0.00026(7)
MgT 0.00816(15) 0.00816(15) 0.00816(15) 0.000 0.000 0.000
CuT 0.00816(15) 0.00816(15) 0.00816(15) 0.000 0.000 0.000
O2 0.0114(2) 0.0114(2) 0.0114(2) 0.00007(17) 0.00007(17) 0.00007(17)
O 0.0114(2) 0.0114(2) 0.0114(2) 0.00007(17) 0.00007(17) 0.00007(17)

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;
 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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AlM O 1.9292(6) 26_554 ?
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AlM O2 1.9292(6) 171_566 ?
AlM O2 1.9292(6) 75_545 ?
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AlM O2 1.9292(6) 26_554 ?
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O AlM O 95.86(4) 75_545 122_656 ?
O AlM O 95.86(4) 148_665 26_554 ?
O AlM O 84.14(4) 52_455 26_554 ?
O AlM O 95.86(4) 171_566 26_554 ?
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O AlM O2 84.14(4) 122_656 171_566 ?
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O2 MgT CuM 29.5 . 75_545 ?
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CuM O2 CuM 95.58(4) 52_455 26_554 ?
AlM O2 CuM 0.0 26_554 26_554 ?
AlM O2 CuM 95.58(4) 75_545 26_554 ?
AlM O2 CuM 95.58(4) 52_455 26_554 ?
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'x-1/4, y+1/4, -z-1/2'
'x+1/4, -y, z-3/4'
'-x, y-1/4, z-1/4'
'-z+1/2, -x+1/2, -y'
'-z, x-1/4, y-1/4'
'z-1/4, x+1/4, -y-1/2'
'z+1/4, -x, y-3/4'
'-y+1/2, -z+1/2, -x'
'y+1/4, -z, x-3/4'
'-y, z-1/4, x-1/4'
'y-1/4, z+1/4, -x-1/2'
'-y-1/4, -x+1/4, z-1/2'
'y+1/2, x+1/2, z'
'-y+1/4, x, -z-3/4'

```
 'y, -x-1/4, -z-1/4'
 '-x-1/4, -z+1/4, y-1/2'
 'x, -z-1/4, -y-1/4'
 'x+1/2, z+1/2, y'
 '-x+1/4, z, -y-3/4'
 '-z-1/4, -y+1/4, x-1/2'
 '-z+1/4, y, -x-3/4'
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_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        ?
_computing_data_reduction         ?
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0053P)^2^+1.8984P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.0193(8)
_refine_ls_extinction_expression
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_refine_ls_number_parameters      11
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_refine_ls_goodness_of_fit_ref    1.162
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CuT Cu 0.1250 0.1250 0.1250 0.00813(13) Uani 0.514(6) 24 d SP . .
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CuM 0.00613(12) 0.00613(12) 0.00613(12) -0.00029(7) -0.00029(7) -0.00029(7)
MgT 0.00813(13) 0.00813(13) 0.00813(13) 0.000 0.000 0.000
CuT 0.00813(13) 0.00813(13) 0.00813(13) 0.000 0.000 0.000
O2 0.0118(2) 0.0118(2) 0.0118(2) -0.00006(18) -0.00006(18) -0.00006(18)
O 0.0118(2) 0.0118(2) 0.0118(2) -0.00006(18) -0.00006(18) -0.00006(18)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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AlM O2 1.9301(6) 171_566 ?
AlM O2 1.9301(6) 75_545 ?
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MgT O 1.9159(11) 76_445 ?
MgT O 1.9159(11) 27_544 ?
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O2 AlM 1.9301(6) 75_545 ?
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'-x+5/4, -y+3/4, z+1/2'
'-x+3/4, y+1, -z+3/4'

'x+1, -y+5/4, -z+1/4'
'z+1/2, x+1/2, y'
'z+1, -x+5/4, -y+1/4'
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'-z+3/4, x+1, -y+3/4'
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'-x-1/4, z, -y-1/4'
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'y, -x-1/4, -z-1/4'
'-x-1/4, -z+1/4, y-1/2'

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 'x+1/2, z+1/2, y'
 '-x+1/4, z, -y-3/4'
 '-z-1/4, -y+1/4, x-1/2'
 '-z+1/4, y, -x-3/4'
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 'z+1/2, y+1/2, x'

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_cell_length_b                    8.0793(4)
_cell_length_c                    8.0793(4)
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_cell_angle_beta                  90.00
_cell_angle_gamma                 90.00
_cell_volume                      527.38(5)
_cell_formula_units_Z             8
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_exptl_special_details
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_diffrn_reflns_limit_k_max        14
_diffrn_reflns_limit_l_min        -13
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_diffrn_reflns_theta_min          4.37
_diffrn_reflns_theta_max          45.17
_reflns_number_total              132
_reflns_number_gt                 130
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        ?
_computing_data_reduction         ?
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
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_computing_molecular_graphics     ?
_computing_publication_material   ?

_refine_special_details
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0138P)^2^+2.2219P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     mixed
_refine_ls_extinction_method      SHELXL
_refine_ls_extinction_coef        0.035(2)
_refine_ls_extinction_expression
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_refine_ls_number_reflns          132
_refine_ls_number_parameters      10
_refine_ls_number_restraints      0
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_refine_ls_R_factor_gt            0.0186
_refine_ls_wR_factor_ref          0.0424
_refine_ls_wR_factor_gt           0.0423
_refine_ls_goodness_of_fit_ref    1.217
_refine_ls_restrained_S_all       1.217
_refine_ls_shift/su_max           0.000
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_refine_ls_shift/su_mean          0.000

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 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_U_iso_or_equiv
 _atom_site_adp_type
 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
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 _atom_site_refinement_flags
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 _atom_site_disorder_group
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CuM Cu 0.5000 0.5000 0.5000 0.00688(17) Uani 0.169(4) 12 d SP . .
AlT Al 0.1250 0.1250 0.1250 0.00938(16) Uani 0.306(9) 24 d SP . .
CuT Cu 0.1250 0.1250 0.1250 0.00938(16) Uani 0.694(9) 24 d SP . .
O2 O2 0.26167(10) 0.26167(10) 0.26167(10) 0.0131(3) Uani 0.77 6 d SP . .
O O 0.26167(10) 0.26167(10) 0.26167(10) 0.0131(3) Uani 0.23 6 d SP . .

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 _atom_site_aniso_U_22
 _atom_site_aniso_U_33
 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
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CuM 0.00688(17) 0.00688(17) 0.00688(17) -0.00031(8) -0.00031(8) -0.00031(8)
AlT 0.00938(16) 0.00938(16) 0.00938(16) 0.000 0.000 0.000
CuT 0.00938(16) 0.00938(16) 0.00938(16) 0.000 0.000 0.000
O2 0.0131(3) 0.0131(3) 0.0131(3) 0.0001(2) 0.0001(2) 0.0001(2)
O 0.0131(3) 0.0131(3) 0.0131(3) 0.0001(2) 0.0001(2) 0.0001(2)

_geom_special_details
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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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 _geom_bond_atom_site_label_2
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AlM O 1.9301(8) 171_566 ?
AlM O 1.9301(8) 75_545 ?
AlM O 1.9301(8) 122_656 ?
AlM O 1.9301(8) 26_554 ?
AlM O2 1.9301(7) 148_665 ?
AlM O2 1.9301(8) 52_455 ?
AlM O2 1.9301(8) 171_566 ?
AlM O2 1.9301(8) 75_545 ?
AlM O2 1.9301(8) 122_656 ?
AlM O2 1.9301(8) 26_554 ?
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AlT O 1.9126(14) 76_445 ?
AlT O2 1.9126(14) 50_454 ?
AlT O2 1.9126(14) 27_544 ?
AlT O2 1.9126(14) 76_445 ?
AlT O 1.9126(14) 50_454 ?
AlT O 1.9126(14) 27_544 ?
O2 CuM 1.9301(8) 52_455 ?
O2 AlM 1.9301(8) 26_554 ?
O2 AlM 1.9301(8) 75_545 ?
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O AlM O 95.73(5) 52_455 122_656 ?
O AlM O 84.27(5) 171_566 122_656 ?
O AlM O 95.73(5) 75_545 122_656 ?
O AlM O 95.73(5) 148_665 26_554 ?
O AlM O 84.27(5) 52_455 26_554 ?
O AlM O 95.73(5) 171_566 26_554 ?
O AlM O 84.27(5) 75_545 26_554 ?
O AlM O 180.0 122_656 26_554 ?
O AlM O2 0.00(10) 148_665 148_665 ?
O AlM O2 180.0 52_455 148_665 ?
O AlM O2 84.27(5) 171_566 148_665 ?
O AlM O2 95.73(5) 75_545 148_665 ?
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O AlM O2 84.27(5) 26_554 52_455 ?
O2 AlM O2 180.00(5) 148_665 52_455 ?
O AlM O2 84.27(5) 148_665 171_566 ?
O AlM O2 95.73(5) 52_455 171_566 ?
O AlM O2 0.00(10) 171_566 171_566 ?
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O2 AlM O2 84.27(5) 148_665 171_566 ?
O2 AlM O2 95.73(5) 52_455 171_566 ?
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O AlM O2 84.27(5) 52_455 75_545 ?
O AlM O2 180.0 171_566 75_545 ?
O AlM O2 0.00(10) 75_545 75_545 ?
O AlM O2 95.73(5) 122_656 75_545 ?
O AlM O2 84.27(5) 26_554 75_545 ?
O2 AlM O2 95.73(5) 148_665 75_545 ?
O2 AlM O2 84.27(5) 52_455 75_545 ?
O2 AlM O2 180.0 171_566 75_545 ?
O AlM O2 84.27(5) 148_665 122_656 ?
O AlM O2 95.73(5) 52_455 122_656 ?
O AlM O2 84.27(5) 171_566 122_656 ?
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O2 AlM O2 84.27(5) 148_665 122_656 ?
O2 AlM O2 95.73(5) 52_455 122_656 ?
O2 AlM O2 84.27(5) 171_566 122_656 ?
O2 AlM O2 95.73(5) 75_545 122_656 ?
O AlM O2 95.73(5) 148_665 26_554 ?
O AlM O2 84.27(5) 52_455 26_554 ?
O AlM O2 95.73(5) 171_566 26_554 ?
O AlM O2 84.27(5) 75_545 26_554 ?
O AlM O2 180.0 122_656 26_554 ?
O AlM O2 0.00(10) 26_554 26_554 ?
O2 AlM O2 95.73(5) 148_665 26_554 ?
O2 AlM O2 84.27(5) 52_455 26_554 ?
O2 AlM O2 95.73(5) 171_566 26_554 ?
O2 AlM O2 84.27(5) 75_545 26_554 ?
O2 AlM O2 180.0 122_656 26_554 ?
O2 AlT O 109.5 . 76_445 ?
O2 AlT O2 109.5 . 50_454 ?
O AlT O2 109.5 76_445 50_454 ?
O2 AlT O2 109.5 . 27_544 ?
O AlT O2 109.5 76_445 27_544 ?
O2 AlT O2 109.5 50_454 27_544 ?
O2 AlT O2 109.5 . 76_445 ?
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O2 AlT O2 109.5 50_454 76_445 ?
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O2 AlT O 109.5 . 50_454 ?
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AlM O2 CuM 0.0 26_554 26_554 ?
AlM O2 CuM 95.46(5) 75_545 26_554 ?
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