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Interlayer Interactions in $M(OH)_2$: A Neutron Diffraction Study of $Mg(OH)_2$

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Abstract

Magnesium hydroxide, $Mg(OH)_2$: $M_r = 58.3$, trigonal, $P\bar{3}m1$, $a = 3.148(1)$, $c = 4.779(2)$ Å, $V = 41.015$ Å^3, $D_x = 2.36$ g cm^{-3} at room temperature; $a = 3.145(1)$, $c = 4.740(2)$ Å, $V = 40.602$ Å^3, $D_x = 2.39$ g cm^{-3} at 70 K; $Z = 1$, $\lambda = 0.8330(5)$ Å, $\mu = 1.78$ cm^{-1}, $F(000) = 9.503$ fm; final $R = 2.42$, $wR = 2.40$, $S = 3.22$ for 82 unique reflections at room temperature; $R = 1.84$, $wR = 1.82$, $S = 2.54$ for 81 unique reflections at 70 K. Refinements have been carried out using anisotropic thermal coefficients for all atoms. To interpret the very large thermal motion of the H atom, subsequent refinements have been carried out with an anharmonic model and with a three-site split-atom model, and results are compared with those previously reported for $Ca(OH)_2$. By comparing the interatomic distances O···O, H···H and H···O in the interlayer spacing of $Mg(OH)_2$ and $Ca(OH)_2$, as well as their temperature dependence, the nature and the strength of interlayer interactions in both compounds are discussed.

1. Introduction

Brucite $Mg(OH)_2$ belongs to the family of divalent metal hydroxides $M(OH)_2$, with M = Mg, Ca, Ni, Co, Fe, Mn or Cd, which are isostructural with the layered compound CdI_2 (space group $P\bar{3}m1$). In $M(OH)_2$ compounds the layers are built with distorted edge-sharing MO_6 octahedra, the M cation planes being situated between alternate pairs of O planes which form an almost hexagonal close-packed array. The hydroxyl groups (OH), which are directed along the threefold axes, are bonded to three M cations and in interlayer spacings they are surrounded by three other (OH) groups belonging to the adjacent layer (Fig. 1).

Hydroxides $M(OH)_2$ are of special interest for studying the influence of the cation M (nature, ionic radius) on structural packing and IR (OH) stretching frequencies in solids, owing to their crystalline structure which is comparatively simple (Brindley & Kao, 1984). On the other hand, the nature of the interactions between adjacent layers has been the subject of controversy in the literature; recently, Krüger, Williams & Jeanioz (1989) reported the presence of hydrogen bonding in $Mg(OH)_2$ and $Ca(OH)_2$ from IR spectroscopy experiments under pressure.

An early structural study of an hydroxide $M(OH)_2$, by single-crystal neutron diffraction, was carried out by Busing & Levy (1957) on $Ca(OH)_2$. They reported an unusual thermal motion for the H atom; it is very large and anisotropic at room temperature as well as low temperature (130 K). The authors suggested that the H atom undergoes a 'riding' motion and proposed a mathematical expression, based on an umbrella-shaped distribution for the H atom, to calculate the actual O—H bond length. This unusual thermal behavior has since been revealed in other hydroxides: $Mg(OH)_2$ (Zigan & Rothbauer, 1967) and $Ni(OH)_2$ (Greaves & Thomas, 1986). In a recent study (Desgranges *et al.*, 1993), we analyzed more precisely the thermal motion of the H atom in $Ca(OH)_2$ using more accurate and more fully extended neutron data sets collected at 80 K and room temperature. Thus, for the first time, refinements with an anharmonic thermal motion model for the H atom could be performed. Comparison between 80 K and room temperature results led us to propose a three-site split-atom model for the H atom, which enables to describe more satisfactorily the H-atom thermal motion.

The crystal structure of $Mg(OH)_2$ was first refined by Zigan & Rothbauer (1967), but in this work the calculated value for the O—H bond length is much

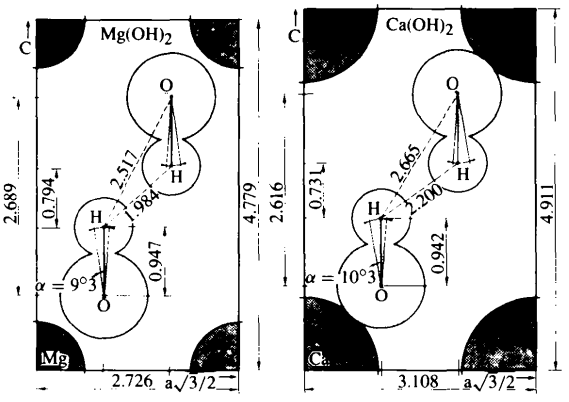

Fig. 1. Structure of $Mg(OH)_2$ and $Ca(OH)_2$ in projection in the plane $(\mathbf{a} + \mathbf{b}/2, \mathbf{c})$. Numerical values correspond to the room temperature results.

larger than in $Ca(OH)_2$ and $Ni(OH)_2$. Recently, the crystal structure of deuterated brucite $Mg(OD)_2$ has been refined at room temperature from time-of-flight powder neutron diffraction data (Partin, O'Keeffe & Von Dreele, 1994). The calculated O—D bond length, corrected for 'riding' motion (0.956 Å), agrees well with the O—H bond in $Ca(OH)_2$ and $Ni(OH)_2$.

The aim of this study is to improve the description of H-atom thermal motion in $Mg(OH)_2$ from single-crystal neutron diffraction data collected at room temperature and 70 K. Structural refinements were carried out, using the same thermal motion models as for $Ca(OH)_2$, and the results are discussed and compared.*

2. Experimental

An untwinned part was cut from a natural crystal of $Mg(OH)_2$. The unit-cell parameters and the orientation matrix were refined using 20 centered reflections. Bragg intensities were measured normally for three symmetry-equivalent reflections, with $\lambda = 0.8330$ (5) Å, on a neutron four-circle P110 diffractometer at the Orphee Reactor (CEN–Saclay). For the data collections, ω scans ($3 \le 2\theta \le 75°$) and ω–2θ scans ($75 \le 2\theta \le 77.6°$) were used; 41 steps, 2.5–5 s per step as a function of $I/\sigma(I)$ of scan widths according to the instrumental resolution $(195–658\ \mathrm{tg}\theta + 1072\ \mathrm{tg}^2\theta)°$.

The sample was mounted in a He cryostat and two data sets were collected at room temperature (324 reflections measured, $\sin\theta/\lambda \le 0.763$, good stability of the standard reflections 004 and $\bar{2}\bar{1}\bar{2}$) and 70 K (202 reflections measured, $\sin\theta/\lambda \le 0.716$).

The integrated intensities were determined from resolution-adapted profile measurement of the peaks. The background was calculated from an average of the first and last steps of each side of the reflections: Lorentz–polarization and absorption corrections were performed; no extinction correction was applied because of the large mosaic spread of the used crystal.

Refinements were performed on a SUN 4-370 computer, using the full-matrix least-squares method based on F, with the program *PROMETHEUS* (Zucker, Perenthaler, Kuhs, Backmann & Schulz, 1983). The neutron scattering lengths for Mg, O and H were taken as $b_{Mg} = 5.375$, $b_O = 5.805$ and $b_H = -3.741$ fm (Delapalme, 1985). Table 1 provides full experimental details.

3. Refinements

The atomic positions of Mg, O and H in the space group $P\bar{3}m1$ are, respectively, 1(*a*) (0,0,0), 2(*d*) $(\frac{1}{3}, \frac{2}{3}, z)$ and 2(*d*) $(\frac{1}{3}, \frac{2}{3}, z)$. There are two independent anisotropic thermal coefficients, u_{11} and u_{33}, for all the atoms in an harmonic model of thermal motion. As for $Ca(OH)_2$, refinements have also been carried out with an anharmonic model and with a three-site split-atom model for the H atom.

Results of refinements with a harmonic thermal motion model (nine parameters refined) are given in Table 2 and compared with those of $Ca(OH)_2$. The values of u_{ij} coefficients are very close for both compounds; however, for $Mg(OH)_2$ thermal motion is slightly less anisotropic for Mg and H, but is more anisotropic for O.

In the anharmonic thermal motion model, the coefficients were developed in a Gram–Charlier expansion up to fourth order. Since the site symmetry of the H atom is 3*m*, there are three third-order and four fourth-order independent anharmonic coefficients. The total number of refined parameters is 16. Results are given in Table 3. Unlike $Ca(OH)_2$, all the anharmonic coefficients are below 3σ and consequently their values are not statistically meaningful. This result could be due to data sets which are less $\sin\theta/\lambda$ extended for $Mg(OH)_2$: 72 and 57 reflections, with $F^2 > 2.5\sigma(F^2)$, at room temperature and 70 K, respectively, against 188 and 88, with $F^2 > 3\sigma(F^2)$, for $Ca(OH)_2$.

In the three-site split-atom model, each H atom $(\frac{1}{3}, \frac{2}{3}, z)$ is split into three positions 6(*i*) $(x, \bar{x}, z)$ with an equal occupation rate. The number of refined parameters is 12, of which four are anisotropic thermal coefficients for the H atom in a harmonic model. Results are given in Table 4. In this model the O—H direction makes an angle α with the threefold *c* axis (Fig. 1). The calculated values are 7.8 (2) and 9.3 (2)° at 70 K and room temperature, respectively, and are very close to those of $Ca(OH)_2$, 9.9 and 10.3° at 80 K and room temperature, respectively.

4. Discussion

The bond lengths Mg—O and O—H, interatomic distances O···O, H···H and H···O, bond angle β = O—*M*—O and the valence angle γ = O—H···O, as well as the *a* and *c* unit-cell parameters of $Mg(OH)_2$ are given in Table 5 with the corresponding values for $Ca(OH)_2$. The values of the distances O—H, H···H and H···O and of the angle γ are given both for the harmonic one-site model (1) and the three-site model (3).

For both compounds the cation–oxygen distance (*M*—O) is exactly equal to the sum of the effective ionic radii for cations M^{VI} in sixfold coordination and oxygen ions O^{IV} in fourfold coordination [2.10 Å for Mg—O and 2.38 Å for Ca—O, from Shannon (1974)]. The bond angle β = O—*M*—O in the octahedral sheets, where the O ions are in the same plane, is almost constant for all the $M(OH)_2$ structures with an average value $\beta = 97.4(4)°$; it results that the *a* unit-cell

* The numbered intensity of each measured point on the profile has been deposited with the IUCr (Reference: DU0401). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Experimental details*

	Room temperature data	Data at 70 K
Crystal data		
Chemical formula	H_2MgO_2	H_2MgO_2
Chemical formula weight	58.3	58.3
Cell setting	Trigonal	Trigonal
Space group	$P\bar{3}m1$	$P\bar{3}m1$
a (Å)	3.148 (1)	3.145 (1)
c (Å)	4.779 (2)	4.740 (2)
V (Å^3)	41.015	40.602
Z	1	1
D_x (Mg m^{-3})	2.36	2.39
Radiation type	Neutron	Neutron
Wavelength (Å)	0.8330 (5)	0.8330 (5)
No. of reflections for cell parameters	20	20
θ range (°)	12–30	12–30
μ (mm^{-1})	0.178	0.178
Temperature (K)	298	70
Crystal form	Platelet	Platelet
Crystal size (mm)	5.6 × 5.4 × 0.6	5.6 × 5.4 × 0.6
Crystal color	Colorless	Colorless
Data Collection		
Diffractometer	P110 Canal 5C2	P110 Canal 5C2
Data collection method	ω–2θ	ω–2θ
Absorption correction	Empirical	Empirical
T_{min}	0.5401	0.5414
T_{max}	0.8979	0.8979
No. of measured reflections	324	202
No. of independent reflections	82	81
No. of observed reflections	72	57
Criterion for observed reflections	$F^2 > 2.5\sigma(F^2)$	$F^2 > 2.5\sigma(F^2)$
R_{int}	0.044	0.046
θ_{max} (°)	33.46	36.61
Range of h, k, l	$0 \rightarrow h \rightarrow 4$	$0 \rightarrow h \rightarrow 4$
	$0 \rightarrow k \rightarrow 4$	$0 \rightarrow k \rightarrow 4$
	$0 \rightarrow l \rightarrow 7$	$0 \rightarrow l \rightarrow 7$
No. of standard reflections	2	2
Frequency of standard reflections	Every 2 h	Every 2 h
Intensity decay (%)	1	1
Refinement		
Refinement on	F	F
R	2.42	1.84
wR	2.40	1.82
S	3.22	2.54
No. of reflections used in refinement	82	81
No. of parameters used	12	12
H-atom treatment	See text	See text
Weighting scheme	$w = 1/\sigma^2$	$w = 1/\sigma^2$
$(\Delta/\sigma)_{max}$	0.0	0.0
$\Delta\rho_{max}$ (e Å^{-3})	0.612	0.447
$\Delta\rho_{min}$ (e Å^{-3})	−0.334	−0.423
Extinction method	None	None
Source of atomic scattering factors	Delapalme (1985)	Delapalme (1985)

parameter of these compounds is linearly related to the (M—O) bond length (Brindley & Kao, 1984). Likewise, the thickness of the octahedral sheets c_o (distance between the oxygen planes, Table 5 and Fig. 1) is fully determined by the (M—O) bond length and the angle β (Brindley & Kao, 1984). On the other hand, the plot of the interlayer distance c_i ($c = c_o + c_i$, Fig. 1) *versus* M—O provides evidence for two distinct groups for the $M(OH)_2$ compounds: one for the rare gas-type cation Mg^{2+} and Ca^{2+} and the other for the transition metal cations (Brindley & Kao, 1984). Using an O—H distance of 0.995 Å in $Mg(OH)_2$ and of 0.936 Å in $Ca(OH)_2$, the authors interpreted the decrease in c_i from $Mg(OH)_2$ to $Ca(OH)_2$ ($\Delta c_i = 0.073$ Å at room temperature) by the O—H bond length. Our results disagree with this interpretation because these bond lengths are equal, taking into account the standard deviation, for $Mg(OH)_2$ and $Ca(OH)_2$, both for the one-site (1) and the three-site (3) models (Table 5).

Although the distance c_i and, consequently, the distance between H planes, are slightly longer for $Mg(OH)_2$, the interatomic distances H···H and H···O are much shorter (Table 5), for example, 1.984 against 2.200 Å for the H···H distance in the one-site model (1) at room temperature. This results from the distance between O—H groups in octahedral sheets, which is shorter in the $Mg(OH)_2$ structure [3.148 against 3.589 Å for $Ca(OH)_2$]. In the three-site model (3) each H atom is

Table 2. *Results of the refinements with a harmonic thermal motion model and comparison with $Ca(OH)_2$ (from Desgranges et al., 1993)*

		70 K $Mg(OH)_2$	80 K $Ca(OH)_2$	Room temperature $Mg(OH)_2$	Room temperature $Ca(OH)_2$
	z_O	−0.2195 (2)	−0.2341 (1)	−0.2187 (2)	−0.2337 (1)
	z_H	−0.4205 (5)	−0.4285 (3)	−0.4169 (5)	−0.4256 (2)
M	u_{11}	47 (4)	16 (2)	61 (4)	42 (1)
	u_{33}	100 (7)	62 (4)	165 (8)	145 (2)
	B_{eq}	0.51	0.25	0.75	0.60
O	u_{11}	48 (3)	32 (2)	74 (3)	82 (2)
	u_{33}	98 (6)	49 (3)	133 (5)	106 (2)
	B_{eq}	0.51	0.30	0.74	0.71
H	u_{11}	347 (8)	346 (4)	484 (10)	510 (5)
	u_{33}	145 (10)	107 (5)	181 (11)	157 (3)
	B_{eq}	2.21	2.10	3.03	3.10
	R	0.019	0.019	0.025	0.028
	wR	0.020	0.020	0.025	0.029

Thermal coefficients u_{ij} are given in $Å^2 \times 10^4$ and equivalent isotropic parameters B_{eq} in $Å^2$.

Table 3. *Results of the refinements with an anharmonic thermal motion model for the H atom*

		70 K	Room temperature
	z_O	−0.2190 (4)	−0.2189 (3)
	z_H	−0.4222 (13)	−0.4167 (12)
Mg	u_{11}	41 (4)	59 (4)
	u_{33}	104 (7)	166 (8)
	B_{eq}	0.49	0.75
O	u_{11}	50 (3)	75 (3)
	u_{33}	74 (9)	128 (8)
	B_{eq}	0.46	0.73
H	u_{11}	359 (22)	467 (27)
	u_{33}	161 (41)	237 (36)
	c_{111}	−0.0012 (8)	−0.021 (11)
	c_{333}	−0.0011 (5)	−0.0003 (3)
	c_{113}	0.0012 (4)	0.0011 (5)
	d_{1111}	0.0002 (5)	−0.0003 (7)
	d_{3333}	0.00006 (11)	0.00015 (9)
	d_{1113}	0.00010 (11)	0.00011 (14)
	d_{1133}	0.00013 (7)	0.00002 (9)
	B_{eq}	2.31	3.08
	R	0.017	0.022
	wR	0.016	0.022

Thermal coefficients u_{ij} are given in $Å^2 \times 10^4$ and equivalent isotropic parameters B_{eq} in $Å^2$.

moved towards one O—H group of the adjacent layer such that there are one H···H distance and one H···O distance shorter and two distances longer (Table 5).

The single crystals of $Ca(OH)_2$ can be easily cleaved, so Busing & Levy (1957) considered that the interlayer cohesion in this compound would be due to van der Waals interactions. This assumption cannot be applied to $Mg(OH)_2$, because the H···H distance is much too short (1.984 Å at room temperature) compared with the usual value for a van der Waals bond (around 2.4 Å); moreover, the easy cleavage of $Ca(OH)_2$ crystals, due to a weak resistance to shear stress, does not necessarily involve weak interlayer cohesion.

The strength of atomic interactions can be estimated from values of thermal expansion coefficients; a strong ionocovalent interaction leads to low values of thermal

Table 4. *Results of the refinements with a three-site split-atom model for the H atom*

		70 K	Room temperature
	z_O	−0.2194 (2)	−0.2187 (2)
	x_H	0.3569 (9)	0.3616 (9)
	z_H	−0.4195 (6)	−0.4161 (7)
Mg	u_{11}	46 (4)	59 (4)
	u_{33}	99 (7)	164 (7)
	B_{eq}	0.50	0.74
O	u_{11}	50 (3)	75 (3)
	u_{33}	93 (6)	130 (5)
	B_{eq}	0.51	0.73
H	u_{11}	254 (22)	349 (26)
	u_{33}	149 (10)	183 (10)
	u_{12}	112 (39)	163 (45)
	u_{13}	−64 (24)	−41 (25)
	B_{eq}	1.78	2.36
	R	0.018	0.024
	wR	0.018	0.024

Thermal coefficients u_{ij} are given in $Å^2 \times 10^4$ and equivalent isotropic parameters B_{eq} in $Å^2$.

Table 5. *Unit-cell parameters a and c, layer and interlayer thickness c_o and c_i, bond lengths M—O and O—H, interatomic distances O···O, H···H and H···O, valence angle $\beta = O—M—O$ and angles $\alpha = (O—H, c)$ and $\gamma = (O—H···O)$ for $Mg(OH)_2$ and $Ca(OH)_2$, calculated both with a one-site model (1) and a three-site model (3)*

	$Mg(OH)_2$ 70 K	$Mg(OH)_2$ Room temperature	$Ca(OH)_2$ 80 K	$Ca(OH)_2$ Room temperature
a (Å)	3.145 (1)	3.148 (1)	3.583 (9)	3.589 (8)
c (Å)	4.740 (2)	4.779 (2)	4.894 (15)	4.911 (14)
c_o (Å)	2.081	2.090	2.291	2.295
c_i (Å)	2.659	2.689	2.603	2.616
M—O(1)	2.093 (4)	2.097 (3)	2.367 (4)	2.371 (3)
O—H(1)	0.953 (3)	0.947 (3)	0.950 (3)	0.942 (2)
(3)	0.957 (4)	0.956 (4)	0.959 (3)	0.949 (2)
O···O(1)	3.220 (6)	3.245 (4)	3.323 (6)	3.338 (6)
H···H(1)	1.966 (3)	1.984 (3)	2.187 (4)	2.200 (3)
H···H(3)	1.914 (5)	1.921 (5)	2.117 (7)	2.131 (5)
	2.088 (5)	2.128 (5)	2.347 (7)	2.366 (5)
H···H×2	2.100 (5)	2.145 (5)	2.364 (7)	2.384 (5)
H···O(1)	2.492 (5)	2.517 (4)	2.648 (5)	2.665 (3)
H···O(3)	2.404 (5)	2.411 (4)	2.524 (5)	2.541 (4)
H···O×2	2.545 (5)	2.579 (5)	2.179 (6)	2.741 (4)
β (°) (1)	97.4	97.3	98.4	98.4
α (°) (3)	7.8	9.3	9.9	10.3
γ (°) (1)	133.2	133.8	128.4	128.9
(3)	143.0	145.6	140.8	141.7
×2	127.7	127.0	121.6	121.6

expansion (typically around $10 \times 10^{-6}\,K^{-1}$), while a weak van der Waals interaction leads to values typically around $100 \times 10^{-6}\,K^{-1}$ (Krishnan, Srinivasan & Devanarayanan, 1979). For the $Mg(OH)_2$ and $Ca(OH)_2$ compounds, the thermal expansion in the layer planes is very low, 7.8 and $4.2 \times 10^{-6}\,K^{-1}$, respectively, which is due to the strong ionocovalent *M*—O bonds, of which the length decreases very little as temperature is lowered (Table 5). Along the *c* axis, orthogonally to the layers, the thermal expansion α_c is 36 and $16 \times 10^{-6}\,K^{-1}$ for $Mg(OH)_2$ and $Ca(OH)_2$, respectively. In the interlayer spacing, the thermal expansion $\alpha_{c_i} = \Delta c_i / c_i \Delta T$ is directly correlated to the temperature dependence of the

interatomic distances H···H and H···O, 50 and $23 \times 3\,10^{-6}\,K^{-1}$, respectively, for $Mg(OH)_2$ and $Ca(OH)_2$. These values show that the interlayer cohesion cannot be considered weak, particularly for $Ca(OH)_2$.

In order to interpret these relatively low values, it can be thought that the interlayer cohesion is realized by electrostatic interactions; in such a case the layer packing results from an equilibrium between the H···H repulsions and the H···O attractions. Results obtained with the three-site split-atom model are in agreement with this assumption, because one H···O distance is decreased [2.411 against 2.517 Å for the one-site model, for $Mg(OH)_2$ at room temperature] and two distances H···H are increased (Table 5). Making the rough approximation that charges for O and H atoms are −2 and +1, respectively, the electrostatic bonding energy between layers can be calculated, considering only the H···H and H···O interactions. The calculated value is slightly lower for $Ca(OH)_2$ (*ca* 2%), which means that the interlayer cohesion should be greater in this compound, in agreement with the experimental results concerning the thermal expansion of the interlayer spacing. However, a purely ionic interaction model must be considered with caution, because the H···O distances are such that a slight overlap of electronic clouds cannot be neglected, which should involve an interaction similar to weak hydrogen bonding.

Kruger, Williams & Jeanioz (1989) reported that the frequency of the IR-active (A_{2u}) mode of $Mg(OH)_2$ and $Ca(OH)_2$ decreases with pressure, by 0.6 and 3.5 cm^{-1} GPa^{-1}, respectively. The authors explained the negative pressure dependence of this mode in terms of compression increasing the hydrogen-bond strength within the hydroxide structure; the hydrogen bonding exists even at zero pressure.

Usually the hydrogen bonding is divided into two classes according to the O···O distance, short (or strong) bonds, between 2.4 and 2.75 Å, which are essentially linear with $\gamma \approx 170°$, and long (or weak) bonds, with a reduced value for γ. In the last case the hydrogen bonding is often bifurcated, *i.e.* the H-atom has two near O in approximatively the same plane (Ceccarelli, Jeffrey & Taylor, 1981). In the $M(OH)_2$ structures, each O—H group is surrounded by three other hydroxyl groups belonging to the adjacent layer; thus, the hydrogen bonding is trifurcated according to the previous terminology. In the one-site model the three distances O—H···O and the three angles γ with the adjacent OH groups are equal; on the other hand, in the three-site model one distance is shortened and the corresponding γ angle is increased (Table 5) which strengthens one hydrogen bonding.

5. Concluding remarks

The temperature dependence of the interatomic distances in $Mg(OH)_2$ and $Ca(OH)_2$ indicates that the interlayer cohesion can be explained by the existence of weak hydrogen bonding and that this bonding is slightly weaker for $Ca(OH)_2$. This result is in agreement with the respective values of frequency changes as a function of pressure reported by Kruger, Williams & Jeanioz (1989) for both compounds. The structural packing along the *c*-axis is determined both by the *M*—O bond length, which fixes the distance between OH groups in an octahedral sheet, and by the strength of interactions in the interlayer spacing.

The values of thermal coefficients u_{ij} of H atoms, calculated in the harmonic one-site model, are almost equal for both compounds (Table 2). The very large value of u_{11} has to be correlated to the existence of three minimum energy positions for the H atom. The deviation from the 2*d* symmetry site is almost equivalent for both compounds ($\bar{\alpha} \approx 9.5°$, Fig. 1). Unlike $Ca(OH)_2$, the refinements with an anharmonic thermal motion for the H atom in $Mg(OH)_2$ are not significant, probably because of data sets which are not sufficiently extended in $\sin\theta/\lambda$. For $Ca(OH)_2$ the results obtained at room temperature show that the maximum probability density for the H atom is situated on the symmetry site; on the other hand, at 80 K thermal energy is much reduced and the occupation rate of three-disordered sites is increased such that the maximum H-atom probability density is no more on the symmetry site (Desgranges *et al.*, 1993).

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