Crystal-chemical and structural data related to the equation of state and second-order elastic constants of portlandite \( \text{Ca(OH)}_2 \) and brucite \( \text{Mg(OH)}_2 \)

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Abstract

This data article reports crystal-chemical and structural data (unit cell parameters and internal coordinates) of two hydroxyl minerals, namely brucite [magnesium hydroxide, \( \text{Mg(OH)}_2 \)] and portlandite [calcium hydroxide, \( \text{Ca(OH)}_2 \)], which were calculated and employed to derive the mechanical behavior of these solid phases under hydrostatic compression (Ulian and Valdrè, 2018). The dataset has been obtained by \textit{ab initio} quantum mechanical means, by employing Density Functional Theory methods, in particular the B3LYP hybrid functional, all-electron Gaussian-type orbitals basis sets and a correction to take into account the effects of dispersive forces. Equilibrium and expanded/compressed models of both minerals were realized and geometrically optimized within two space group settings, \( P\text{3}m1 \) and \( P\text{3} \).

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Specifications table

| Subject area       | Physics                                                                 |
|--------------------|-------------------------------------------------------------------------|
| More specific subject area | Unit cell and internal geometry of hydroxyl mineral structures used to calculate the equation of state and second order elastic constants |
| Type of data       | Tables, CIF files                                                       |
| How data was acquired | Quantum mechanical simulations at the DFT/B3LYP level of theory, including dispersive forces contributions (CRYSTAL14 code) |
| Data format        | Raw, analyzed                                                           |
| Experimental factors | Initial geometries were taken from experimental data available in literature |
| Experimental features | Quantum mechanical simulations conducted using Density Functional Theory, B3LYP functional and Gaussian-type orbitals basis sets. Inclusion of dispersive forces contribution via DFT-D2 scheme, corrected for the B3LYP functional (B3LYP-D* approach). Geometry optimization of the unit cell under different hydrostatic compression states. |
| Data source location | Bologna, P. Porta San Donato 1, Italy                                  |
| Data accessibility | Data is displayed within this article.                                  |
| Related research article | This Data in Brief article is related to the paper: Ulian, G. & Valdrè, G. (2018) Equation of state and second-order elastic constants of portlandite Ca(OH)2 and brucite Mg(OH)2. Physics and Chemistry of Minerals, in press, DOI:10.1007/s00269-018-0989-3. |

Value of the data

- Geometries of brucite [magnesium hydroxide, Mg(OH)2] and portlandite [calcium hydroxide, Ca (OH)2] in space group $P\bar{3}m1$ (ordered protons) and $P\bar{3}$ (disordered protons), at $T = 0\ \text{K}$ and taking into account the effect of dispersive force on the final geometries [1]. At each unit cell compressive state, the pressure was calculated using a third-order Birch-Murnaghan equation of state formulation:

$$E = E_0 + \frac{9}{16} K_0 V_0 \left\{ K' (\eta^2 - 1)^3 + \left[ (\eta^2 - 1)^2 (6 - 4\eta^2) \right] \right\}$$

$$\eta = \left( \frac{V_0}{V} \right)^{1/3}$$

(1)

The unit cell data for brucite in the both symmetry settings are reported in Table 1 ($P\bar{3}m1$) and Table 2 ($P\bar{3}$), whereas for portlandite the optimization results are reported in Tables 3 and 4 for the $P\bar{3}m1$ and $P\bar{3}$ space groups, respectively.

1. Data

1.1. Brucite and portlandite structure at equilibrium and under hydrostatic compression

Brucite Mg(OH)$_2$ and portlandite Ca(OH)$_2$ were optimized considering two different space group setups, namely $P\bar{3}m1$ (ordered protons) and $P\bar{3}$ (disordered protons), at $T = 0\ \text{K}$ and taking into account the effect of dispersive force on the final geometries [1]. At each unit cell compressive state, the pressure was calculated using a third-order Birch-Murnaghan equation of state formulation:
| Model | P01 | P02 | P03 | P00 | P04 | P05 | P06 | P07 | P08 | P09 | P10 |
|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| \(P\ (\text{GPa})\) | 1.99 | 1.35 | -0.51 | 0.08 | 0.58 | 1.95 | 3.65 | 5.71 | 8.20 | 11.19 | 14.67 |
| \(a\ (\text{Å})\) | 3.155328 | 3.148869 | 3.140127 | 3.133631 | 3.128596 | 3.114591 | 3.098550 | 3.080985 | 3.062159 | 3.042367 | 3.022219 |
| \(c\ (\text{Å})\) | 4.871112 | 4.782579 | 4.701791 | 4.660154 | 4.629442 | 4.564626 | 4.505604 | 4.451461 | 4.409938 | 4.352940 | 4.307592 |
| \(V\ (\text{Å}^3)\) | 41.9998 | 41.0678 | 40.1503 | 39.6302 | 39.2426 | 38.3476 | 37.4628 | 36.5942 | 35.7381 | 34.8928 | 34.0735 |
| \(\rho\ (\text{kg m}^{-3})\) | 2293 | 2345 | 2398 | 2430 | 2454 | 2511 | 2570 | 2631 | 2694 | 2760 | 2826 |
| \(Mg1\ (x/a)\) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| \(O1\ (y/b)\) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| \(Mg1\ (z/c)\) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| \(O1\ (z/c)\) | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 |
| \(H1\ (x/a)\) | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 |
| \(H1\ (y/b)\) | 0.215189 | 0.219210 | 0.222949 | 0.224898 | 0.226318 | 0.229328 | 0.232036 | 0.234477 | 0.236706 | 0.238774 | 0.240683 |
| \(H1\ (z/c)\) | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 |
| \(H1\ (z/c)\) | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 |

Table 1
Simulated brucite (s.g. \(P\overline{3}m1\)) lattice parameters, unit cell volume, density and internal coordinates of each irreducible atom at different hydrostatic compression values.
Table 2
Simulated brucite (s.g. \(P\bar{3}\)) lattice parameters, unit cell volume, density and internal coordinates of each irreducible atom at different hydrostatic compression values.

| Model | P01 | P02 | P03 | P00 | P04 | P05 | P06 | P07 | P08 | P09 | P10 |
|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| \(P\) (GPa) | -1.73 | -1.37 | -0.63 | -0.04 | 0.48 | 1.94 | 3.75 | 5.87 | 8.30 | 11.03 | 14.00 |
| \(a\) (Å) | 5.457850 | 5.448528 | 5.431555 | 5.419010 | 5.410109 | 5.383694 | 5.354487 | 5.323469 | 5.291050 | 5.257357 | 5.223264 |
| \(a/\sqrt{3}\) (Å) | 3.151091 | 3.145709 | 3.135910 | 3.128667 | 3.123528 | 3.108277 | 3.091415 | 3.073506 | 3.057489 | 3.035337 | 3.015653 |
| \(c\) (Å) | 4.823064 | 4.770027 | 4.698890 | 4.657285 | 4.629417 | 4.565066 | 4.505499 | 4.451049 | 4.401053 | 4.353352 | 4.308918 |
| \(V\) (Å\(^3\)) | 124.4219 | 122.6337 | 120.0533 | 118.4413 | 117.3462 | 114.5878 | 111.8689 | 109.2402 | 106.7016 | 104.2052 | 101.8082 |
| \(V/3\) (Å\(^3\)) | 41.4740 | 40.8779 | 40.0178 | 39.4804 | 39.1154 | 38.1959 | 37.2896 | 36.4134 | 35.5672 | 34.7351 | 33.9361 |
| \(\rho\) (kg m\(^{-3}\)) | 2322 | 2356 | 2406 | 2439 | 2462 | 2521 | 2582 | 2645 | 2707 | 2772 | 2838 |
| \(Mg1\) (x/a) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| \(Mg1\) (y/b) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| \(Mg1\) (z/c) | 0.012533 | 0.013765 | 0.014899 | 0.014865 | 0.014835 | 0.015002 | 0.014868 | 0.014868 | 0.014868 | 0.014868 | 0.014868 |
| \(O1\) (x/a) | 0.004323 | 0.004665 | 0.004954 | 0.004938 | 0.004927 | 0.004917 | 0.004907 | 0.004907 | 0.004907 | 0.004907 | 0.004907 |
| \(O1\) (y/b) | 0.335505 | 0.335673 | 0.335822 | 0.335816 | 0.335816 | 0.335816 | 0.335816 | 0.335816 | 0.335816 | 0.335816 | 0.335816 |
| \(O1\) (z/c) | 0.217662 | 0.220196 | 0.223642 | 0.225615 | 0.226931 | 0.230049 | 0.232910 | 0.23504 | 0.237858 | 0.240124 | 0.242250 |
| \(H1\) (x/a) | 0.033005 | 0.036912 | 0.041444 | 0.042531 | 0.043311 | 0.046943 | 0.049180 | 0.051679 | 0.054312 | 0.057579 | 0.061439 |
| \(H1\) (y/b) | 0.349532 | 0.351391 | 0.353461 | 0.353991 | 0.354371 | 0.355728 | 0.356838 | 0.357857 | 0.358915 | 0.360210 | 0.361716 |
| \(H1\) (z/c) | 0.415044 | 0.419293 | 0.425094 | 0.428690 | 0.431100 | 0.436498 | 0.441527 | 0.446091 | 0.450175 | 0.453903 | 0.457173 |
| Model | P01  | P02  | P03  | P00  | P04  | P05  | P06  | P07  | P08  | P09  | P10  |
|-------|------|------|------|------|------|------|------|------|------|------|------|
| $P$ (GPa) | -1.29 | -0.80 | -0.20 | 0.05 | 0.54 | 1.43 | 2.49 | 3.76 | 5.24 | 6.97 | 8.96 |
| $a$ (Å)   | 3.610971 | 3.600982 | 3.589831 | 3.582472 | 3.576342 | 3.562471 | 3.546410 | 3.528975 | 3.510193 | 3.490606 | 3.470128 |
| $c$ (Å)   | 5.068373 | 4.983721 | 4.902409 | 4.858831 | 4.827818 | 4.754439 | 4.686310 | 4.622658 | 4.562908 | 4.506061 | 4.452422 |
| $V$ ($Å^3$) | 57.2331 | 55.9663 | 54.7127 | 54.0043 | 53.4761 | 52.2556 | 51.0434 | 49.8562 | 48.6894 | 47.5477 | 46.4321 |
| $ρ$ (kg m$^{-3}$) | 2146 | 2195 | 2245 | 2274 | 2297 | 2351 | 2406 | 2464 | 2523 | 2583 | 2645 |
| Ca1 (x/a) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Ca1 (y/b) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Ca1 (z/c) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| O1 (x/a) | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 |
| O1 (y/b) | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 |
| O1 (z/c) | 0.228797 | 0.232582 | 0.236315 | 0.238368 | 0.239877 | 0.243346 | 0.246629 | 0.249679 | 0.252516 | 0.255147 | 0.257563 |
| H1 (x/a) | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 |
| H1 (y/b) | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 |
| H1 (z/c) | 0.418805 | 0.425818 | 0.432753 | 0.436560 | 0.439335 | 0.445858 | 0.452046 | 0.457868 | 0.463356 | 0.468555 | 0.473426 |

Table 3
Simulated portlandite (s.g. P3m1) lattice parameters, unit cell volume, density and internal coordinates of each irreducible atom at different hydrostatic compression values.
Table 4
Simulated portlandite (s.g. $P\overline{3}$) lattice parameters, unit cell volume, density and internal coordinates of each irreducible atom at different hydrostatic compression values.

| Model | P01  | P02  | P03  | P00  | P04  | P05  | P06  | P07  | P08  | P09  | P10  |
|-------|------|------|------|------|------|------|------|------|------|------|------|
| $P$ (GPa) | 1.15 | 0.9  | 0.43 | 0.06 | 0.26 | 1.15 | 2.24 | 3.52 | 4.96 | 6.57 | 8.34 |
| $a$ (Å)  | 6.240742 | 6.231606 | 6.215225 | 6.197545 | 6.187161 | 6.158970 | 6.127688 | 6.094718 | 6.060909 | 6.025379 | 5.988631 |
| $a/\sqrt{3}$ (Å) | 3.603094 | 3.597819 | 3.588362 | 3.578154 | 3.572159 | 3.555883 | 3.537822 | 3.518787 | 3.499267 | 3.478754 | 3.457538 |
| $c$ (Å)  | 5.017526 | 4.981429 | 4.919089 | 4.865425 | 4.830677 | 4.758647 | 4.692959 | 4.639666 | 4.580094 | 4.530007 | 4.482711 |
| $V$ (Å$^3$) | 56.4120 | 55.8423 | 54.8539 | 53.9473 | 53.3827 | 52.1086 | 50.8686 | 49.6901 | 48.5690 | 47.4763 | 46.4093 |
| $\rho$ (kg m$^{-3}$) | 2177 | 2200 | 2239 | 2277 | 2301 | 2357 | 2415 | 2472 | 2529 | 2587 | 2647 |
| Mg1 (x/a) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Mg1 (y/b) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Mg1 (z/c) | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 |
| Mg2 (x/a) | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 | 0.666667 |
| Mg2 (y/b) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| Mg2 (z/c) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| O1 (x/a) | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 | 0.333333 |
| O1 (y/b) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| O1 (z/c) | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 | 0.000000 |
| H1 (x/a) | 0.231412 | 0.230936 | 0.230611 | 0.228979 | 0.224067 | 0.242479 | 0.247697 | 0.250840 | 0.253738 | 0.256580 | 0.259423 |
| H1 (y/b) | 0.000036 | 0.000007 | 0.000143 | 0.028959 | 0.027413 | 0.031681 | 0.035663 | 0.038976 | 0.041216 | 0.046388 | 0.051796 |
| H1 (z/c) | 0.333353 | 0.333388 | 0.333856 | 0.343484 | 0.346536 | 0.348368 | 0.349984 | 0.351193 | 0.352271 | 0.353657 | 0.355305 |
| H1 (x/a) | 0.423348 | 0.426420 | 0.431775 | 0.435716 | 0.438196 | 0.444159 | 0.449564 | 0.454419 | 0.458742 | 0.462387 | 0.465281 |
A total of 44 Crystallographic Interchange Format (CIF) files, one for each optimized structure, are also provided as Supplementary material, in order to ease their employment by other theoretical/experimental researchers.

2. Experimental design, materials, and methods

The data here presented was obtained by first principle simulations on periodic systems, using both the CRYSTAL14 [2] and CRYSTAL17 codes [3], which implements the Hartree–Fock and Kohn–Sham self-consistent field method. The same approach was employed to investigate the elastic behaviour of other phases containing hydroxyl groups [4].

2.1. Basis set

Multielectron wave functions are constructed as an antisymmetrized product (Slater determinant) of mono electronic crystalline orbitals (CO) that are linear combination of local functions (atomic orbitals, AO) centred on each atom in the system. In turn, atomic orbitals (basis set) are linear combinations of Gaussian-type functions (GTF). The all-electron basis sets employed in the present simulations for Ca²⁺ and Mg²⁺ were a 86–511 G* [1,5] and a 8–511 G* basis sets [1,6]. For O and H atoms, a triple-ζ basis set with polarization from to the work of Ahlrichs et al. [7] has been adopted for both atoms.

2.2. Hamiltonian and computational parameters

The Becke [8] three-parameter (B3LYP) hybrid exchange functional in combination with the gradient-corrected correlation functional of Lee et al. [9] has been adopted for all calculations. The exchange-correlation contribution is performed over a grid of points and is the result of a numerical integration of the electron density and its gradient. The adopted pruned grid is given by 75 points and 974 angular points (XLGRID) and obtained from The Gauss–Legendre quadrature and Lebedev schemes [10]. The tolerance thresholds that control accuracy of the Coulomb and exchange integrals were set to 10⁻⁷ and 10⁻¹⁶, respectively [2]. The Hamiltonian matrix has been diagonalized using a Monkhorst grid of k-points of size 8 × 8 × 8 for the high symmetry models (s.g. P₃m₁), whereas a 4 × 4 × 4 grid was employed for the low symmetry (s.g. P₃) ones. The convergence on total energy was reached when the difference between the energy of two subsequent self-consistent field cycles was less than 10⁻⁸ Hartree.

Van der Waals (dispersive) forces were included with the (DFT + D2) scheme [11], which adds the following contribution to the calculated DFT energy:

\[
E_{\text{DISP}} = -s_6 \sum_{g} \sum_{i \neq j} f_{\text{dump}} \left( R_{ij,g} \right) \frac{C_i^g C_j^g}{R_{ij,g}^6} \quad (2)
\]

The summation over all atom pairs \( ij \) and \( g \) lattice vectors excludes the self- interaction contribution \( (i = j) \) for every \( g \). The parameters \( C_i^g \) represent the dispersion coefficient for the atom \( i \), \( R_{ij,g} \) is the interatomic distance between atom \( i \) in the reference cell and atom \( j \) in the neighbouring cells at distance \( g \) and \( s_6 \) is a functional-dependent scaling factor. The function \( f_{\text{dump}} \) is used to dump the energy correction to avoid double counting of short-range contributions to the energy and depends on the sum of atomic van der Waals radii and on a steepness parameter \( (d = 20) \). Due to the molecular nature of the DFT + D2 scheme, which tends to overestimate cohesive energy in solid crystals, the original B3LYP + D parameters where modified, setting \( s_6 \) to 1, \( R_{vdw}(H) \) to 1.30 and the heavier atom van der Waals radii were scaled by a factor 1.05 (B3LYP-D* approach) [12–17].
2.3. Geometry optimization under hydrostatic compression

The compressional behaviour has been investigated carrying out a symmetry-preserving relaxation procedure by exploring, at selected values of volume ($V$), the minimum energy of the $a/b$ and $c/b$ ratios and internal coordinates [18]. Ten volumes between $0.86 \times V_{\text{init}}$ and $1.06 \times V_{\text{init}}$ (step of $0.02 \times V_{\text{init}}$) were considered for both Ca(OH)$_2$ and Mg(OH)$_2$, where $V_{\text{init}}$ is the volume of the original optimized cell. Each model was then geometrically optimized. This approach has been successfully adopted for other mineral phases [6,19].

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Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.11.059.

Appendix A. Supplementary material

Supplementary data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.11.059.

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