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Data Article

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



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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, $\text{Mg}(\text{OH})_2$] and portlandite [calcium hydroxide, $\text{Ca}(\text{OH})_2$], 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 *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, $P\bar{3}m1$ and $P\bar{3}$.

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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 $\text{Ca}(\text{OH})_2$ and brucite $\text{Mg}(\text{OH})_2$. <i>Physics and Chemistry of Minerals</i> , in press, DOI:10.1007/s00269-018-0989-3.

Value of the data

- Geometries of brucite [magnesium hydroxide, $\text{Mg}(\text{OH})_2$] and portlandite [calcium hydroxide, $\text{Ca}(\text{OH})_2$] in space group $P\bar{3}m1$ and $P\bar{3}$ settings at both equilibrium and stressed conditions, useful for structural and mechanical applications of these mineral phases.
- The present data could be helpful for researchers involved in the crystal-chemical properties of hydroxyl phases under the effect of applied pressure, for example, for geological and building/cement applications.
- The present data were obtained at the Density Functional Theory (DFT) level, employing hybrid B3LYP functional and including a correction to take into account the contribution of dispersive forces, and could be useful for *ab initio* comparisons of similar materials.

1. Data

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

Brucite $\text{Mg}(\text{OH})_2$ and portlandite $\text{Ca}(\text{OH})_2$ 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:

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

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.

Table 1Simulated brucite (s.g. $P\bar{3}m1$) 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
<i>P</i> (GPa)	−1.99	−1.35	−0.51	0.08	0.58	1.95	3.65	5.71	8.20	11.19	14.67
<i>a</i> (Å)	3.155328	3.148869	3.140127	3.133631	3.128596	3.114591	3.098550	3.080985	3.062159	3.042367	3.022219
<i>c</i> (Å)	4.871112	4.782579	4.701791	4.660154	4.629442	4.564626	4.505604	4.451461	4.400938	4.352940	4.307592
<i>V</i> (Å ³)	41.9998	41.0678	40.1503	39.6302	39.2426	38.3476	37.4628	36.5942	35.7381	34.8928	34.0735
ρ (kg m ^{−3})	2293	2345	2398	2430	2454	2511	2570	2631	2694	2760	2826
<i>Mg1</i> (<i>x/a</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>Mg1</i> (<i>y/b</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>Mg1</i> (<i>z/c</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>O1</i> (<i>x/a</i>)	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333
<i>O1</i> (<i>y/b</i>)	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667
<i>O1</i> (<i>z/c</i>)	0.215189	0.219210	0.222949	0.224898	0.226318	0.229328	0.232036	0.234477	0.236706	0.238774	0.240683
<i>H1</i> (<i>x/a</i>)	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333
<i>H1</i> (<i>y/b</i>)	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667
<i>H1</i> (<i>z/c</i>)	0.412508	0.420222	0.427445	0.431226	0.434014	0.439947	0.445365	0.450322	0.454925	0.459268	0.463346

Table 2Simulated 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
<i>P</i> (GPa)	−1.73	−1.37	−0.63	−0.04	0.48	1.94	3.75	5.87	8.30	11.03	14.00
<i>a</i> (Å)	5.457850	5.448528	5.431555	5.419010	5.410109	5.383694	5.354487	5.323469	5.291050	5.257357	5.223264
<i>a</i> /√3 (Å)	3.151091	3.145709	3.135910	3.128667	3.123528	3.108277	3.091415	3.073506	3.054789	3.035337	3.015653
<i>c</i> (Å)	4.823064	4.770027	4.698890	4.657285	4.629417	4.565066	4.505499	4.451049	4.401053	4.353352	4.308918
<i>V</i> (Å ³)	124.4219	122.6337	120.0533	118.4413	117.3462	114.5878	111.8689	109.2402	106.7016	104.2052	101.8082
<i>V</i> /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
ρ (kg m ^{−3})	2322	2356	2406	2439	2462	2521	2582	2645	2707	2772	2838
<i>Mg1</i> (<i>x/a</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>Mg1</i> (<i>y/b</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>Mg1</i> (<i>z/c</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>Mg2</i> (<i>x/a</i>)	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333
<i>Mg2</i> (<i>y/b</i>)	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667
<i>Mg2</i> (<i>z/c</i>)	−0.012533	−0.013765	−0.014899	−0.014865	−0.014835	−0.015002	−0.014868	−0.014522	−0.014110	−0.013815	−0.013656
<i>O1</i> (<i>x/a</i>)	0.004323	0.004665	0.004954	0.004938	0.004927	0.004957	0.004911	0.004791	0.004644	0.004499	0.004401
<i>O1</i> (<i>y/b</i>)	0.335505	0.335673	0.335822	0.335816	0.335814	0.335855	0.335813	0.335756	0.335675	0.335611	0.335585
<i>O1</i> (<i>z/c</i>)	0.217662	0.220196	0.223642	0.225615	0.226931	0.230049	0.232910	0.235504	0.237858	0.240124	0.242250
<i>H1</i> (<i>x/a</i>)	0.033005	0.036912	0.041444	0.042531	0.043311	0.046493	0.049180	0.051679	0.054312	0.057579	0.061439
<i>H1</i> (<i>y/b</i>)	0.349532	0.351391	0.353461	0.353991	0.354371	0.355728	0.356838	0.357857	0.358915	0.360210	0.361716
<i>H1</i> (<i>z/c</i>)	0.415044	0.419293	0.425094	0.428690	0.431100	0.436498	0.441527	0.446091	0.450175	0.453903	0.457173

Table 3Simulated portlandite (s.g. $P\bar{3}m1$) 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
<i>P</i> (GPa)	−1.29	−0.80	−0.20	0.05	0.54	1.43	2.49	3.76	5.24	6.97	8.96
<i>a</i> (Å)	3.610971	3.600982	3.589831	3.582472	3.576342	3.562471	3.546410	3.528975	3.510193	3.490606	3.470128
<i>c</i> (Å)	5.068373	4.983721	4.902409	4.858831	4.827818	4.754439	4.686310	4.622658	4.562908	4.506061	4.452422
<i>V</i> (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
<i>Ca1</i> (<i>x/a</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>Ca1</i> (<i>y/b</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>Ca1</i> (<i>z/c</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>O1</i> (<i>x/a</i>)	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333
<i>O1</i> (<i>y/b</i>)	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667
<i>O1</i> (<i>z/c</i>)	0.228797	0.232582	0.236315	0.238368	0.239877	0.243346	0.246629	0.249679	0.252516	0.255147	0.257563
<i>H1</i> (<i>x/a</i>)	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333
<i>H1</i> (<i>y/b</i>)	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667
<i>H1</i> (<i>z/c</i>)	0.418805	0.425818	0.432753	0.436560	0.439335	0.445858	0.452046	0.457868	0.463356	0.468555	0.473426

Table 4Simulated portlandite (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
<i>P</i> (GPa)	−1.15	−0.9	−0.43	−0.06	0.26	1.15	2.24	3.52	4.96	6.57	8.34
<i>a</i> (Å)	6.240742	6.231606	6.215225	6.197545	6.187161	6.158970	6.127688	6.094718	6.060909	6.025379	5.988631
<i>a</i> /√3 (Å)	3.603094	3.597819	3.588362	3.578154	3.572159	3.555883	3.537822	3.518787	3.499267	3.478754	3.457538
<i>c</i> (Å)	5.017526	4.981429	4.919089	4.865425	4.830677	4.758647	4.692959	4.633966	4.580094	4.530007	4.482711
<i>V</i> (Å ³)	169.2360	167.5269	164.5618	161.8418	160.1480	156.3257	152.6057	149.0702	145.7070	142.4289	139.2280
<i>V</i> /3 (Å ³)	56.4120	55.8423	54.8539	53.9473	53.3827	52.1086	50.8686	49.6901	48.5690	47.4763	46.4093
ρ (kg m ^{−3})	2177	2200	2239	2277	2301	2357	2415	2472	2529	2587	2647
<i>Mg1</i> (<i>x/a</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>Mg1</i> (<i>y/b</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>Mg1</i> (<i>z/c</i>)	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
<i>Mg2</i> (<i>x/a</i>)	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333	0.333333
<i>Mg2</i> (<i>y/b</i>)	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667	0.666667
<i>Mg2</i> (<i>z/c</i>)	−0.000016	−0.000004	−0.000476	−0.008984	−0.011583	−0.012343	−0.012705	−0.012249	−0.011311	−0.010156	−0.008533
<i>O1</i> (<i>x/a</i>)	0.333331	0.333333	0.333253	0.332008	0.331688	0.331734	0.331879	0.332180	0.332590	0.333121	0.333835
<i>O1</i> (<i>y/b</i>)	−0.000005	−0.000001	−0.000159	−0.002601	−0.003240	−0.003129	−0.002814	−0.002155	−0.001274	−0.000112	0.001427
<i>O1</i> (<i>z/c</i>)	0.231412	0.233096	0.236011	0.238797	0.240607	0.244279	0.247697	0.250840	0.253738	0.256580	0.259423
<i>H1</i> (<i>x/a</i>)	0.000036	0.000007	0.001043	0.020859	0.027413	0.031681	0.035663	0.038976	0.042116	0.046388	0.051796
<i>H1</i> (<i>y/b</i>)	0.333353	0.333338	0.333856	0.343484	0.346536	0.348368	0.349984	0.351193	0.352271	0.353657	0.355305
<i>H1</i> (<i>z/c</i>)	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 monoelectronic 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 Ca^{2+} and Mg^{2+} 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 $8 \times 8 \times 8$ for the high symmetry models (s.g. $P\bar{3}m1$), whereas a $4 \times 4 \times 4$ grid was employed for the low symmetry (s.g. $P\bar{3}$) 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:

$$E_{DISP} = -s_6 \sum_{\mathbf{g}} \sum_{i \neq j} f_{dump}(R_{ij,\mathbf{g}}^6) \frac{C_6^i C_6^j}{R_{ij,\mathbf{g}}^6} \quad (2)$$

The summation over all atom pairs ij and \mathbf{g} lattice vectors excludes the self-interaction contribution ($i = j$) for every \mathbf{g} . The parameters C_6^i represent the dispersion coefficient for the atom i , $R_{ij,\mathbf{g}}$ is the interatomic distance between atom i in the reference cell and atom j in the neighbouring cells at distance $|\mathbf{g}|$ and s_6 is a functional-dependent scaling factor. The function f_{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 were modified, setting s_6 to 1, $R_{vdw}(\text{H})$ 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 $0.86 \times V_{init}$ and $1.06 \times V_{init}$ (step of $0.02 \times V_{init}$) were considered for both $\text{Ca}(\text{OH})_2$ and $\text{Mg}(\text{OH})_2$, where V_{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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