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Data Article

Dataset on the piezo-spectroscopic behaviour of hydroxylapatite: Effect of mechanical stress on the Raman and Infrared vibrational bands from *ab initio* quantum mechanical simulations

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ABSTRACT

This article reports data on the vibrational (Raman and Infrared) behavior of hydroxylapatite [OHAp, $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$, space group $P6_3$] under mechanical stress, which were discussed in details in the work of Ulian and Valdrè (2017) [1]. 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.

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Specifications Table

Subject area	Physics
More specific subject area	Vibrational spectroscopy (Raman and IR) of biomaterials
Type of data	Tables
How data was acquired	

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	<i>Quantum mechanical simulations at the Density Functional Theory (DFT)/B3LYP level of theory, including dispersive forces contributions (CRYSTAL14 code)</i>
Data format	<i>Raw, analyzed</i>
Theoretical factors	<i>Starting geometry taken from previous DFT simulations [2].</i>
Theoretical features	<i>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 with and without applied strains.</i>
Data source location	<i>Bologna, P. Porta San Donato 1, Italy</i>
Data accessibility	<i>Data is displayed within this article.</i>
Related research article	<i>This Data in Brief article is submitted as a companion paper to: Ulian, G. & Valdrè, G. (2017) Effect of mechanical stress on the Raman and Infrared bands of hydroxylapatite: a quantum mechanical first principle investigation. Journal of the Mechanical Behavior of Biomedical Materials, in press.</i>

Value of the data

- Geometries of hydroxylapatite [OHAp, Ca₁₀(PO₄)₆(OH)₂, space group P6₃] at both equilibrium and stressed conditions.
 - Vibrational analysis (Raman and IR) of each hydroxylapatite geometry.
 - Vibrational spectra (Raman and IR) of each hydroxylapatite geometry up to 4000 cm⁻¹, which could be employed for comparison with experimental data.
 - Results 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.
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1. Data

1.1. Hydroxylapatite geometry at equilibrium and under mechanical stress

Equilibrium and deformed (strained) OHAp models were realized and geometrically optimized, and the stress for each deformation was calculated according to stress-strain formulations.

Hydroxylapatite (OHAp, s.g. P6₃) was optimized to take into account the effect of dispersive force contribution in the final unit cell and internal geometries (Table 1). Then, it was deformed according to the three symmetry-independent strains related to the P6₃ space group [1]:

$$\varepsilon_1 = \delta \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \varepsilon_3 = \delta \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \varepsilon_4 = \delta \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad (1)$$

where ε_1 and ε_3 are normal strains (uniaxial) perpendicular to the (100) and (001) surfaces of the hexagonal unit cell and ε_4 is a shear stress parallel to the (001) surface. The unit cell data (lattice parameters and atomic coordinates) for ε_1 , ε_3 and ε_4 deformed OHAp are reported in Tables 2–4, respectively. In Eq. (1), δ represents a multiplicative factor used to control the compressive ($\delta > 0$) or tensile ($\delta < 0$) deformation of the OHAp unit cell. Four unit cell configurations (two in expansion, $\delta = -0.04$ and $\delta = -0.02$, and two in compression, $\delta = +0.02$ and $\delta = +0.04$) were geometrically optimized for each considered strain (ε_1 , ε_3 , ε_4), resulting in twelve deformed structures of OHAp. In the case of normal strain (ε_1 and ε_3), the unit cell was expanded/contracted by $\pm 4\%$ and $\pm 2\%$, with

Table 1

Simulated OHAp lattice parameters (a , b and c reported in Å; α , β and γ in degrees) and internal coordinates of each irreducible atom (relative to s.g. $P6_3$) at equilibrium.

Equilibrium					
a		9.38593	α		90
b		9.38593	β		90
c		6.87087	γ		120
Ca1	X	0.333333	O2	X	– 0.412019
	Y	– 0.333333		Y	0.465624
	Z	– 0.000114		Z	0.244387
Ca2	X	– 0.333333	O3	X	0.334650
	Y	0.333333		Y	0.251336
	Z	– 0.001445		Z	0.071593
Ca3	X	0.247056	O4	X	– 0.347179
	Y	– 0.004869		Y	– 0.256809
	Z	0.249398		Z	– 0.065903
P1	X	0.396585	O5	X	0.000000
	Y	0.366658		Y	0.000000
	Z	0.250675		Z	– 0.211631
O1	X	0.324502	H1	X	0.000000
	Y	0.483345		Y	0.000000
	Z	0.252703		Z	– 0.070371

resulting applied stress in the range ± 9 GPa. Symmetry analysis conducted on the deformed geometries revealed that for strain ε_1 the OHAp unit cell belongs to space group $P2_1$, for strain ε_3 to $P6_3$ and ε_4 to space group $P1$ (absence of symmetry).

1.2. Vibrational frequencies

For each optimized hydroxylapatite model, both at equilibrium ($\delta = + 0.00$) and at strained configurations ($\delta = \pm 0.02$ and $\delta = \pm 0.04$), vibrational frequencies (Raman and IR) were obtained by means of finite displacements method. In the OHAp unit cell, there are 44 atoms, resulting in 132 degrees of freedom (129 with vibrational character) [1]. The calculated frequencies for ε_1 , ε_3 and ε_4 deformed OHAp are reported in Tables S1–S3 (Supplementary material), respectively. To aid the comparison between the peak positions, for the strains ε_1 and ε_4 the normal modes of the non-deformed hydroxylapatite were calculated with the symmetry of the strained cells ($P2_1$ and $P1$, respectively).

1.3. Vibrational intensities

Vibrational intensities were calculated within the Placzek approximation (Raman, partial derivatives of the polarizability tensor with respect to atomic positions) [3–5] and analytically through Coupled-Perturbed Kohn–Sham approach (Infrared) [6–9]. The intensity of each normal mode, IR and Raman, was calculated for each OHAp model and reported in the Supplementary material section (Tables S1–S3).

Table 2

Simulated OHP lattice parameters (a , b and c reported in Å; α , β and γ in degrees) and internal coordinates of each irreducible atom (relative to s.g. $P2_1$) under the effect of strain ε_1 .

	$\delta = + 0.04$	$\delta = + 0.02$	$\delta = + 0.02$	$\delta = + 0.04$		$\delta = + 0.04$	$\delta = + 0.02$	$\delta = + 0.02$	$\delta = + 0.04$
a	9.10581	9.2455	9.52707	9.66888	α	90.00	90.00	90.00	90.00
b	9.38593	9.38593	9.38593	9.38593	β	90.00	90.00	90.00	90.00
c	6.87087	6.87087	6.87087	6.87087	γ	120.50	120.50	119.51	119.04
Ca1	X 0.334810 Y - 0.331032 Z - 0.002772	0.334094 - 0.332457 - 0.001538	0.332927 - 0.333257 0.000396	0.332281 - 0.333138 0.001281	O4	X - 0.407217 Y 0.464545 Z 0.240659	- 0.409670 0.465670 0.242976	- 0.414299 0.464858 0.245895	- 0.416287 0.463486 0.247193
Ca2	X - 0.335426 Y 0.331427 Z - 0.002140	- 0.334529 0.332667 - 0.001585	- 0.332699 0.333309 - 0.001351	- 0.331698 0.333293 - 0.001216	O5	X - 0.469999 Y 0.117859 Z 0.239863	- 0.467559 0.120143 0.242299	- 0.464408 0.123902 0.245715	- 0.463039 0.125989 0.247234
Ca3	X 0.238849 Y - 0.012941 Z 0.247401	0.243491 - 0.008877 0.248632	0.249691 - 0.001104 0.249881	0.252164 0.002777 0.250231	O6	X - 0.120787 Y 0.410566 Z 0.240694	- 0.121688 0.411251 0.242877	- 0.123114 0.412787 0.245898	- 0.123577 0.413645 0.247425
Ca4	X 0.012074 Y 0.254700 Z 0.248849	0.008724 0.253625 0.249276	0.000618 0.250064 0.249949	- 0.004550 0.247442 0.250410	O7	X 0.326445 Y 0.246297 Z 0.073655	0.331460 0.249132 0.072288	0.337021 0.253683 0.071044	0.338766 0.255873 0.070760
Ca5	X - 0.256111 Y - 0.248862 Z 0.249720	- 0.253600 - 0.247339 0.249546	- 0.250597 - 0.247559 0.249725	- 0.249725 - 0.248625 0.249876	O8	X - 0.245517 Y 0.085670 Z 0.069842	- 0.248248 0.084471 0.070934	- 0.254588 0.082113 0.072006	- 0.258257 0.080969 0.072041
P1	X 0.395158 Y 0.364127 Z 0.250976	0.395861 0.365397 0.250771	0.397267 0.368077 0.250699	0.398207 0.369622 0.250741	O9	X - 0.082900 Y - 0.333158 Z 0.073071	- 0.083337 - 0.334300 0.072278	- 0.082818 - 0.334646 0.071116	- 0.082408 - 0.334680 0.070702
P2	X - 0.364316 Y 0.030767 Z 0.248902	- 0.365317 0.030307 0.249928	- 0.368288 0.029306 0.251094	- 0.370176 0.028805 0.251384	O10	X - 0.346732 Y - 0.255203 Z - 0.064935	- 0.347075 - 0.255916 - 0.065518	- 0.346556 - 0.257720 - 0.066304	- 0.345796 - 0.258815 - 0.066697
P3	X - 0.029861 Y - 0.397445 Z 0.250235	- 0.029834 - 0.396998 0.250525	- 0.029849 - 0.396220 0.250926	- 0.029788 - 0.395826 0.251265	O11	X 0.253804 Y - 0.095908 Z - 0.066095	0.255077 - 0.092927 - 0.065884	0.259281 - 0.087972 - 0.065922	0.261861 - 0.085534 - 0.066167
O1	X 0.324735 Y 0.482800 Z 0.254065	0.323687 0.482319 0.253318	0.326660 0.485632 0.252327	0.330157 0.488963 0.251940	O12	X 0.093661 Y 0.352673 Z - 0.065452	0.091860 0.349651 - 0.065756	0.088316 0.344521 - 0.065818	0.086403 0.342029 - 0.065559
O2	X - 0.479400 Y - 0.160573 Z 0.252610	- 0.481514 - 0.159795 0.252714	- 0.484890 - 0.158046 0.252693	- 0.486650 - 0.156986 0.252461	O13	X 0.004396 Y 0.000806 Z - 0.203916	0.001682 0.000320 - 0.208469	- 0.000994 - 0.000271 - 0.214420	- 0.001575 - 0.000473 - 0.217080
O3	X 0.166247 Y - 0.319183 Z 0.252679	0.162538 - 0.321969 0.252709	0.155331 - 0.327414 0.252524	0.151899 - 0.330061 0.252451	H1	X 0.002633 Y - 0.000019 Z - 0.062913	0.000802 - 0.000395 - 0.067321	- 0.000841 0.000372 - 0.073074	- 0.001210 0.001256 - 0.075674

Table 3

Simulated OHAp lattice parameters (a , b and c reported in Å; α , β and γ in degrees) and internal coordinates of each irreducible atom (relative to s.g. $P6_3$) under the effect of strain ϵ_3 .

	$\delta = + 0.04$	$\delta = + 0.02$	$\delta = + 0.02$	$\delta = + 0.04$		$\delta = + 0.04$	$\delta = + 0.02$	$\delta = + 0.02$	$\delta = + 0.04$
a	9.38593	9.38593	9.38593	9.38593	α	90.00	90.00	90.00	90.00
b	9.38593	9.38593	9.38593	9.38593	β	90.00	90.00	90.00	90.00
c	6.59603	6.73345	7.00828	7.1457	γ	120.00	120.00	120.00	120.00
Ca1	X 0.333333 Y - 0.333333 Z - 0.000031	0.333333 - 0.333333 - 0.000278	0.333333 - 0.333333 - 0.000904	0.333333 - 0.333333 - 0.001605	O2	X - 0.409655 Y 0.466622 Z 0.244320	- 0.410986 0.465970 0.244309	- 0.412928 0.465637 0.243946	- 0.413543 0.465740 0.243187
Ca2	X - 0.333333 Y 0.333333 Z - 0.003014	- 0.333333 0.333333 - 0.002237	- 0.333333 0.333333 - 0.000716	- 0.333333 0.333333 - 0.000374	O3	X 0.337166 Y 0.252233 Z 0.066124	0.335544 0.251681 0.068984	0.333634 0.250917 0.074434	0.332652 0.250429 0.077408
Ca3	X 0.247451 Y 0.000046 Z 0.248920	0.247081 - 0.002840 0.249246	0.246898 - 0.006431 0.249385	0.246772 - 0.007450 0.249155	O4	X - 0.348993 Y - 0.257121 Z - 0.061829	- 0.347836 - 0.256932 - 0.063824	- 0.347275 - 0.256962 - 0.067928	- 0.347891 - 0.257259 - 0.069991
P1	X 0.399551 Y 0.369103 Z 0.250104	0.397883 0.367792 0.250441	0.395473 0.365772 0.250902	0.394719 0.365044 0.251102	O5	X 0.000000 Y 0.000000 Z - 0.208776	0.000000 0.000000 - 0.210548	0.000000 0.000000 - 0.211885	0.000000 0.000000 - 0.211451
O1	X 0.329540 Y 0.486221 Z 0.251860	0.326911 0.484797 0.252352	0.322026 0.481844 0.253216	0.319982 0.480488 0.253807	H1	X 0.000000 Y 0.000000 Z - 0.061677	0.000000 0.000000 - 0.066456	0.000000 0.000000 - 0.073360	0.000000 0.000000 - 0.075575

2. Theoretical design, materials, and methods

The data here presented was obtained by first principle simulations on periodic systems, using the CRYSTAL14 code [10], which implements the Hartree–Fock and Kohn–Sham self-consistent field method.

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 were chosen among previously adopted ones for [2,11–13].

2.2. Hamiltonian and computational parameters

The Becke [14] three-parameter (B3LYP) hybrid exchange functional in combination with the gradient-corrected correlation functional of Lee et al. [15] 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 [16]. The tolerance thresholds that control accuracy of the Coulomb and exchange integrals were set to 10^{-7} and 10^{-16} , respectively [10]. The Hamiltonian matrix has been diagonalized using a shrinking factor that leads to 12 reciprocal lattice points (k-points). 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.

Table 4

Simulated OHAp lattice parameters (a , b and c reported in Å; α , β and γ in degrees) and internal coordinates of each irreducible atom (relative to s.g. $P1$) under the effect of strain ε_4 .

	$\delta = + 0.04$	$\delta = + 0.02$	$\delta = + 0.02$	$\delta = + 0.04$		$\delta = + 0.04$	$\delta = + 0.02$	$\delta = + 0.02$	$\delta = + 0.04$
a	9.38781	9.38640	9.38640	9.38781	α	94.58	92.29	92.29	94.58
b	9.39344	9.38781	9.38781	9.39344	β	87.71	88.85	88.85	87.71
c	6.87636	6.87224	6.87224	6.87636	γ	120.02	120.01	120.01	120.02
Ca1	X 0.317777 Y - 0.335664 Z - 0.004382	0.325394 - 0.339535 - 0.000749	0.345306 - 0.318267 0.000061	0.350730 - 0.308686 0.003185	O7	X - 0.424147 Y 0.460737 Z 0.220911	- 0.416872 0.464704 0.236204	- 0.414115 0.464319 0.253665	- 0.421470 0.459810 0.272171
Ca2	X - 0.350739 Y 0.308678 Z - 0.496843	- 0.345318 0.318245 - 0.499870	- 0.325344 0.339541 0.499292	- 0.317811 0.335575 0.495590	O8	X 0.421491 Y - 0.459857 Z - 0.227839	0.414110 - 0.464346 - 0.246542	0.416883 - 0.464694 - 0.263921	0.424165 - 0.460757 - 0.279192
Ca3	X - 0.316706 Y 0.339178 Z 0.003451	- 0.322659 0.343603 - 0.000631	- 0.347882 0.315378 - 0.000976	- 0.353545 0.307537 - 0.003025	O9	X - 0.471770 Y 0.114190 Z 0.225423	- 0.467099 0.120651 0.226771	- 0.471200 0.116920 0.263951	- 0.475702 0.111324 0.268135
Ca4	X 0.353566 Y - 0.307562 Z 0.497034	0.347874 - 0.315382 0.498979	0.322603 - 0.343604 0.499305	0.316635 - 0.339244 - 0.496550	O10	X - 0.121780 Y 0.416154 Z 0.280222	- 0.122116 0.414081 0.268411	- 0.122702 0.416816 0.221001	- 0.122305 0.419510 0.212080
Ca5	X 0.238172 Y - 0.007066 Z 0.263151	0.244317 - 0.005546 0.255414	0.240684 - 0.007633 0.243789	0.235374 - 0.008280 0.236597	O11	X 0.122281 Y - 0.419475 Z - 0.287908	0.122688 - 0.416855 - 0.279002	0.122093 - 0.414034 - 0.231674	0.121789 - 0.416116 - 0.219790
Ca6	X - 0.235385 Y 0.008264 Z - 0.263314	- 0.240627 0.007666 - 0.256208	- 0.244328 0.005526 - 0.244574	- 0.238180 0.007063 - 0.236824	O12	X 0.475653 Y - 0.111372 Z - 0.231836	0.471260 - 0.116880 - 0.236129	0.467054 - 0.120669 - 0.273243	0.471780 - 0.114178 - 0.274632
Ca7	X 0.011899 Y 0.255380 Z 0.245777	0.008172 0.254440 0.250077	0.004476 0.255109 0.248823	0.007596 0.256278 0.252624	O13	X 0.294097 Y 0.232824 Z 0.092206	0.314600 0.243480 0.083082	0.348475 0.256793 0.062531	0.357871 0.264575 0.058012
Ca8	X - 0.255123 Y - 0.251298 Z 0.238718	- 0.252422 - 0.247303 0.243382	- 0.253419 - 0.247645 0.256264	- 0.257677 - 0.252167 0.261076	O14	X - 0.357847 Y - 0.264600 Z - 0.441962	- 0.348406 - 0.256753 - 0.437439	- 0.314463 - 0.243430 - 0.416837	- 0.293989 - 0.232812 - 0.407743
Ca9	X 0.257719 Y 0.252215 Z - 0.238915	0.253400 0.247583 - 0.243751	0.252409 0.247319 - 0.256653	0.255165 0.251278 - 0.261272	O15	X - 0.239997 Y 0.089710 Z 0.067441	- 0.241474 0.085247 0.071672	- 0.265029 0.085724 0.071015	- 0.269416 0.085911 0.074323
Ca10	X - 0.007549 Y - 0.256235 Z - 0.247446	- 0.004481 - 0.255130 - 0.251170	- 0.008189 - 0.254376 - 0.249952	- 0.011967 - 0.255382 - 0.254167	O16	X - 0.091499 Y - 0.367644 Z 0.065286	- 0.090552 - 0.357511 0.064135	- 0.070627 - 0.305906 0.081394	- 0.068819 - 0.295881 0.080736
P1	X 0.387784 Y 0.363307 Z 0.259845	0.392693 0.365549 0.257975	0.394568 0.365743 0.243578	0.389046 0.363954 0.241845	O17	X 0.068879 Y 0.295981 Z - 0.419296	0.070548 0.305844 - 0.418581	0.090518 0.357462 - 0.435836	0.091524 0.367689 - 0.434678
P2	X - 0.389017 Y - 0.363976 Z - 0.258135	- 0.394562 - 0.365739 - 0.256412	- 0.392695 - 0.365571 - 0.242030	- 0.387777 - 0.363317 - 0.240183	O18	X 0.269374 Y - 0.085944 Z - 0.425671	0.265004 - 0.085783 - 0.428976	0.241449 - 0.085235 - 0.428328	0.239960 - 0.089713 - 0.432568

Table 4 (continued)

	$\delta = + 0.04$	$\delta = + 0.02$	$\delta = + 0.02$	$\delta = + 0.04$		$\delta = + 0.04$	$\delta = + 0.02$	$\delta = + 0.02$	$\delta = + 0.04$
P3	X - 0.367292	- 0.366735	- 0.368260	- 0.368541	O19	X - 0.302262	- 0.328259	- 0.357389	- 0.364360
	Y 0.028048	0.030259	0.028740	0.027573		Y - 0.236288	- 0.248801	- 0.261053	- 0.266613
	Z 0.235070	0.241021	0.260623	0.267007		Z - 0.086547	- 0.075973	- 0.058820	- 0.056118
P4	X - 0.028723	- 0.028859	- 0.028823	- 0.028992	O20	X 0.364312	0.357338	0.328103	0.302313
	Y - 0.394558	- 0.395317	- 0.393824	- 0.392640		Y 0.266572	0.260987	0.248735	0.236280
	Z 0.257796	0.253098	0.247908	0.243674		Z 0.443890	0.441155	0.423940	0.413440
P5	X 0.028992	0.028805	0.028865	0.028743	O21	X 0.245316	0.247494	0.269866	0.274226
	Y 0.392671	0.393793	0.395355	0.394586		Y - 0.095802	- 0.092378	- 0.090265	- 0.087929
	Z - 0.256317	- 0.252053	- 0.246906	- 0.242159		Z - 0.062120	- 0.065850	- 0.065471	- 0.068438
P6	X 0.368504	0.368268	0.366731	0.367270	O22	X 0.094696	0.094350	0.079329	0.075152
	Y - 0.027606	- 0.028760	- 0.030237	- 0.028078		Y 0.373387	0.365363	0.320241	0.307422
	Z - 0.232990	- 0.239389	- 0.258990	- 0.264961		Z - 0.061900	- 0.060497	- 0.074635	- 0.074407
O1	X 0.316110	0.320362	0.322261	0.318653	O23	X - 0.075131	- 0.079222	- 0.094332	- 0.094689
	Y 0.480524	0.482163	0.482437	0.482438		Y - 0.307374	- 0.320080	- 0.365381	- 0.373399
	Z 0.280226	0.270527	0.235184	0.225712		Z 0.425550	0.425321	0.439479	0.438105
O2	X - 0.318623	- 0.322250	- 0.320379	- 0.316106	O24	X - 0.274193	- 0.269836	- 0.247486	- 0.245369
	Y - 0.482462	- 0.482432	- 0.482195	- 0.480534		Y 0.087944	0.090310	0.092335	0.095788
	Z - 0.274270	- 0.264797	- 0.229445	- 0.219720		Z 0.431558	0.434516	0.434159	0.437889
O3	X - 0.477362	- 0.481229	- 0.479654	- 0.476029	O25	X 0.012018	0.004040	0.002550	0.009398
	Y - 0.162376	- 0.159121	- 0.160975	- 0.162981		Y 0.004631	- 0.000335	- 0.002154	- 0.000222
	Z 0.226760	0.238412	0.266527	0.277438		Z - 0.218148	- 0.213933	- 0.210326	- 0.209714
O4	X 0.159946	0.159757	0.159432	0.159360	O26	X - 0.009426	- 0.002549	- 0.004045	- 0.012063
	Y - 0.321765	- 0.323181	- 0.324593	- 0.322395		Y 0.000251	0.002210	0.000317	- 0.004566
	Z 0.251920	0.248974	0.254990	0.251836		Z 0.290258	0.289557	0.285960	0.281846
O5	X - 0.159362	- 0.159447	- 0.159762	- 0.159926	H1	X 0.000821	- 0.000434	0.004726	0.011511
	Y 0.322395	0.324573	0.323147	0.321769		Y 0.001723	- 0.003302	0.001300	- 0.001104
	Z - 0.248142	- 0.2444909	- 0.250952	- 0.248073		Z - 0.077412	- 0.072863	- 0.069308	- 0.068463
O6	X 0.476043	0.479636	0.481252	0.477346	H2	X - 0.011516	- 0.004702	0.000488	- 0.000875
	Y 0.162940	0.160961	0.159139	0.162351		Y 0.001220	- 0.001243	0.003345	- 0.001712
	Z - 0.222613	- 0.233535	- 0.261582	- 0.273231		Z 0.431514	0.430576	0.427022	0.422587

Van der Waals (dispersive) forces were included with the (DFT+D2 scheme [17]), which adds the following contribution to the calculated DFT energy:

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

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, $R_{vdw}(H)$ to 1.30 and the heavier atom van der Waals radii were scaled by a factor 1.05 (B3LYP-D* approach) [18–23].

2.3. Vibrational calculations

In periodic systems and within the harmonic approximation, the phonon frequencies at Γ point are evaluated diagonalising the central zone ($k = 0$) mass-weighted Hessian matrix:

$$W_{ij}(k=0) = \sum_G \frac{H_{ij}^{0G}}{\sqrt{M_i M_j}} \quad (3)$$

H_{ij}^{0G} is the second derivative of the electronic and nuclear repulsion energy E evaluated at equilibrium $\mathbf{u} = \mathbf{0}$ with respect to the displacement of atom A in cell 0 ($u_i = x_i - x_i^*$) and displacement of atom B in cell G ($u_j = x_j - x_j^*$) from their equilibrium position x_i^*, x_j^* :

$$\sum_G H_{ij}^{0G} = \sum_G \left[\frac{\partial^2 E}{\partial u_i^0 \partial u_j^G} \right]_0 \quad i = 1, \dots, 3N; \quad j = 1, \dots, 3N \quad (4)$$

In CRYSTAL14, the calculation of the Hessian at equilibrium is made by the analytical evaluation of the energy first derivatives, Φ_j of E with respect to the atomic displacements:

$$\Phi_j = \sum_G \nu_j^G = \sum_G \frac{\partial E}{\partial u_j^G} \quad j = 1, \dots, 3N \quad (5)$$

while second derivatives at $\mathbf{u} = \mathbf{0}$ (where all first derivatives are zero) are calculated numerically using a "two-point" formula:

$$\left[\frac{\partial \Phi_j}{\partial u_i^0} \right]_0 \approx \frac{\Phi_j(0, \dots, u_i^0, \dots, 0) - \Phi_j(0, \dots, u_i^0, \dots, 0)}{u_i^0} \quad i = 1, \dots, 3N; \quad j = 1, \dots, 3N \quad (6)$$

The Hessian matrix eigenvalues provide the normal harmonic frequencies ω_h and it is obtained with $3N + 1$ SCF and gradient calculation.

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Transparency document. Supplementary material

Supplementary data associated with this article can be found in the online version at <http://dx.doi.org/10.1016/j.dib.2018.03.035>.

Appendix A. Supplementary material

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References

- [1] G. Ulian, G. Valdrè, Effect of mechanical stress on the Raman and Infrared bands of hydroxylapatite: a quantum mechanical first principle investigation, *J. Mech. Behav. Biomed. Mater.* 77 (2018) 683–692.
- [2] G. Ulian, G. Valdrè, M. Corno, P. Ugliengo, Periodic ab initio bulk investigation of hydroxylapatite and type A carbonated apatite with both pseudopotential and all-electron basis sets for calcium atoms, *Am. Mineral.* 98 (2013) 410–416.
- [3] L. Maschio, B. Kirtman, M. Rerat, R. Orlando, R. Dovesi, Ab initio analytical Raman intensities for periodic systems through a coupled perturbed Hartree–Fock/Kohn–Sham method in an atomic orbital basis. I. Theory, *J. Chem. Phys.* 139 (2013) 164101.
- [4] L. Maschio, B. Kirtman, M. Rerat, R. Orlando, R. Dovesi, Ab initio analytical Raman intensities for periodic systems through a coupled perturbed Hartree–Fock/Kohn–Sham method in an atomic orbital basis. II. Validation and comparison with experiments, *J. Chem. Phys.* 139 (2013) 164102.
- [5] G. Placzek, *Handbuch der Radiologie*, Akademische Verlagsgesellschaft, Leipzig, 1934.
- [6] M. Ferrero, M. Rerat, B. Kirtman, R. Dovesi, Calculation of first and second static hyperpolarizabilities of one- to three-dimensional periodic compounds. Implementation in the CRYSTAL code, *J. Chem. Phys.* 129 (2008).
- [7] M. Ferrero, M. Rerat, R. Orlando, R. Dovesi, The calculation of static polarizabilities of 1–3D periodic compounds. The implementation in the CRYSTAL code, *J. Comput. Chem.* 29 (2008) 1450–1459.
- [8] M. Ferrero, M. Rerat, R. Orlando, R. Dovesi, Coupled perturbed Hartree–Fock for periodic systems: the role of symmetry and related computational aspects, *J. Chem. Phys.* 128 (2008).
- [9] M. Ferrero, M. Rerat, R. Orlando, R. Dovesi, I.J. Bush, Coupled perturbed Kohn–Sham calculation of static polarizabilities of periodic compounds – art. no. 012016, *J. Phys. Conf. Ser.* 117 (2008) (12016–12016).
- [10] R. Dovesi, V.R. Saunders, C. Roetti, R. Orlando, C.M. Zicovich–Wilson, F. Pascale, B. Civalleri, K. Doll, N.M. Harrison, I.J. Bush, M. Llunell, M. Causà, Y. Noël, *CRYSTAL14 User's Manual*, University of Torino, Torino, 2014.
- [11] F. Peccati, M. Corno, M. Delle Piane, G. Ulian, P. Ugliengo, G. Valdrè, CO_3^{2-} mobility in carbonate apatite as revealed by density functional modeling, *J. Phys. Chem. C* 118 (2014) 1364–1369.
- [12] G. Ulian, G. Valdrè, M. Corno, P. Ugliengo, DFT investigation of structural and vibrational properties of type B and mixed A–B carbonated hydroxylapatite, *Am. Mineral.* 99 (2014) 117–127.
- [13] G. Ulian, D. Moro, G. Valdrè, First-principles study of structural and surface properties of (001) and (010) surfaces of hydroxylapatite and carbonated hydroxylapatite, *J. Appl. Crystallogr.* 49 (2016) 1893–1903.
- [14] A.D. Becke, A new mixing of Hartree–Fock and local density-functional theories, *J. Chem. Phys.* 98 (1993) 1372–1377.
- [15] C.T. Lee, W.T. Yang, R.G. Parr, Development of the Colle–Salvetti correlation-energy formula into a functional of the electron-density, *Phys. Rev. B* 37 (1988) 785–789.
- [16] M. Prencipe, F. Pascale, C.M. Zicovich–Wilson, V.R. Saunders, R. Orlando, R. Dovesi, The vibrational spectrum of calcite (CaCO_3): an ab initio quantum-mechanical calculation, *Phys. Chem. Miner.* 31 (2004) 559–564.
- [17] S. Grimme, Semiempirical GGA-type density functional constructed with a long-range dispersion correction, *J. Comput. Chem.* 27 (2006) 1787–1799.
- [18] B. Civalleri, C.M. Zicovich–Wilson, L. Valenzano, P. Ugliengo, B3LYP augmented with an empirical dispersion term (B3LYP-D*) as applied to molecular crystals, *CrystEngComm* 10 (2008) 405–410.
- [19] G. Ulian, D. Moro, G. Valdrè, Probing the interaction of (001) carbonated hydroxylapatite surfaces with water: a density functional investigation, *Micro Nano Lett.* (2017), <http://dx.doi.org/10.1049/mnl.2017.0058>.
- [20] G. Ulian, S. Tosoni, G. Valdrè, Comparison between Gaussian-type orbitals and plane wave ab initio density functional theory modeling of layer silicates: talc $\text{Mg}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$ as model system, *J. Chem. Phys.* 139 (2013).
- [21] G. Ulian, G. Valdrè, Density functional investigation of the thermo-physical and thermo-chemical properties of 2M (1) muscovite, *Am. Mineral.* 100 (2015) 935–944.
- [22] G. Ulian, G. Valdrè, Density functional investigation of the thermophysical and thermochemical properties of talc $\text{Mg}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$, *Phys. Chem. Miner.* 42 (2015) 151–162.
- [23] G. Ulian, G. Valdrè, Structural, vibrational and thermophysical properties of pyrophyllite by semi-empirical density functional modelling, *Phys. Chem. Miner.* 42 (2015) 609–627.