This article reports data on the vibrational (Raman and Infrared) behavior of hydroxylapatite [OHAp, Ca_{10}(PO_4)_6(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 \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.

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Quantum mechanical simulations at the Density Functional Theory (DFT)/B3LYP level of theory, including dispersive forces contributions (CRYSTAL14 code)

Data format
Raw, analyzed

Theoretical factors
Starting geometry taken from previous DFT simulations [2].

Theoretical 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 with and without applied strains.

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 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.

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.

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]:

\[
\begin{align*}
\epsilon_1 &= \delta \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
\epsilon_3 &= \delta \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\
\epsilon_4 &= \delta \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}
\end{align*}
\] (1)

where \(\epsilon_1\) and \(\epsilon_3\) are normal strains (uniaxial) perpendicular to the (100) and (001) surfaces of the hexagonal unit cell and \(\epsilon_4\) is a shear stress parallel to the (001) surface. The unit cell data (lattice parameters and atomic coordinates) for \(\epsilon_1\), \(\epsilon_3\) and \(\epsilon_4\) deformed OHAp are reported in Tables 2–4, respectively. In Eq. (1), \(\delta\) 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 (\(\epsilon_1\), \(\epsilon_3\), \(\epsilon_4\)), resulting in twelve deformed structures of OHAp. In the case of normal strain (\(\epsilon_1\) and \(\epsilon_3\)), the unit cell was expanded/contracted by \(\pm 4\%\) and \(\pm 2\%, with
resulting applied stress in the range $\pm$ 9 GPa. Symmetry analysis conducted on the deformed geometries revealed that for strain $\varepsilon_1$ the OHAp unit cell belongs to space group $P\overline{2}1$, for strain $\varepsilon_3$ to $P\overline{6}_3$ and $\varepsilon_4$ 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 ($\delta = 0.02$ and $\delta = 0.04$), 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 $\varepsilon_1$, $\varepsilon_3$ and $\varepsilon_4$ deformed OHAp are reported in Tables S1–S3 (Supplementary material), respectively. To aid the comparison between the peak positions, for the strains $\varepsilon_1$ and $\varepsilon_4$ the normal modes of the non-deformed hydroxylapatite were calculated with the symmetry of the strained cells ($P\overline{2}1$ 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 1

Simulated OHAp lattice parameters ($a$, $b$ and $c$ reported in Å; $\alpha$, $\beta$ and $\gamma$ in degrees) and internal coordinates of each irreducible atom (relative to s.g. $P\overline{6}_3$) at equilibrium.

|     | $a$     | $\alpha$ | $b$     | $\beta$ | $c$     | $\gamma$ |
|-----|---------|-----------|---------|--------|---------|----------|
| $\delta$ | 9.38593 | 90        | 9.38593 | 90     | 6.87087 | 120      |
| $\delta$ | 0.33333 | O2        | X       | -0.412019 |
| Y     | -0.33333 | Y         | 0.465624 |
| Z     | -0.001445 | Z         | 0.244387 |
| $\delta$ | X       | -0.33333 | O3      | X     |
| Y     | 0.33333 | Y         | 0.251336 |
| Z     | -0.001445 | Z         | 0.071593 |
| $\delta$ | X       | 0.247056 | O4      | X     |
| Y     | -0.004869 | Y         | -0.347179 |
| Z     | 0.249398 | Z         | -0.065903 |
| $\delta$ | X       | 0.396585 | O5      | X     |
| Y     | 0.366658 | Y         | 0.000000 |
| Z     | 0.250675 | Z         | -0.211631 |
| $\delta$ | X       | 0.324502 | H1      | X     |
| Y     | 0.483345 | Y         | 0.000000 |
| Z     | 0.252703 | Z         | -0.070371 |
Table 2
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 e.g. P2₁) under the effect of strain e₁.

| Parameter | δ = + 0.04 | δ = + 0.02 | δ = + 0.04 | δ = + 0.04 | δ = + 0.02 | δ = + 0.04 |
|-----------|-------------|-------------|-------------|-------------|-------------|-------------|
| a         | 9.10581     | 9.2455      | 9.52707     | 9.66888     | 9.00000     | 9.00000     |
| b         | 9.38593     | 9.38593     | 9.38593     | 9.38593     | 9.00000     | 9.00000     |
| c         | 6.87087     | 6.87087     | 6.87087     | 6.87087     | 120.50000   | 120.50000   |
| Ca¹       | 0.334810    | 0.334094    | 0.332927    | 0.332281    | 0.470718    | 0.409670    |
|           | -0.332457   | -0.333257   | -0.333138   | Y           | 0.464545    | 0.465670    |
|           | 0.002772    | 0.001538    | 0.000936    | 0.001281    | Z           | 0.240659    |
|           | 0.249691    | 0.252164    | 0.250410    | 0.249881    | 0.250231    | 0.249409    |
| Ca²       | 0.335426    | 0.334529    | 0.332699    | 0.331698    | 0.001104    | 0.000777    |
|           | 0.332667    | 0.333099    | 0.332939    | Y           | 0.410566    | 0.411251    |
|           | -0.001585   | -0.001351   | -0.001216   | Z           | 0.239863    | 0.242299    |
|           | 0.243491    | 0.246961    | 0.249949    | 0.249881    | 0.250231    | 0.249409    |
| Ca³       | 0.012074    | 0.008724    | 0.000618    | -0.004550   | 0.326445    | 0.331460    |
|           | 0.254700    | 0.253625    | 0.250664    | 0.247442    | 0.246297    | 0.249132    |
|           | 0.248849    | 0.249276    | 0.249949    | 0.250410    | 0.073655    | 0.072288    |
|           | 0.249720    | 0.249546    | 0.249725    | 0.249878    | 0.069842    | 0.070934    |
|           | 0.395158    | 0.395861    | 0.397267    | 0.398207    | 0.082900    | 0.083337    |
|           | 0.364127    | 0.365397    | 0.368077    | 0.369622    | 0.083337    | 0.082818    |
|           | 0.250976    | 0.250771    | 0.250699    | 0.250741    | 0.082818    | 0.082818    |
| P1        | 0.0012074   | 0.008724    | 0.000618    | -0.004550   | 0.326445    | 0.331460    |
|           | 0.254700    | 0.253625    | 0.250664    | 0.247442    | 0.246297    | 0.249132    |
|           | 0.248849    | 0.249276    | 0.249949    | 0.250410    | 0.073655    | 0.072288    |
|           | 0.249720    | 0.249546    | 0.249725    | 0.249878    | 0.069842    | 0.070934    |
| P2        | 0.395158    | 0.395861    | 0.397267    | 0.398207    | 0.082900    | 0.083337    |
|           | 0.364127    | 0.365397    | 0.368077    | 0.369622    | 0.083337    | 0.082818    |
|           | 0.250976    | 0.250771    | 0.250699    | 0.250741    | 0.082818    | 0.082818    |
| P3        | 0.0012074   | 0.008724    | 0.000618    | -0.004550   | 0.326445    | 0.331460    |
|           | 0.254700    | 0.253625    | 0.250664    | 0.247442    | 0.246297    | 0.249132    |
|           | 0.248849    | 0.249276    | 0.249949    | 0.250410    | 0.073655    | 0.072288    |
|           | 0.249720    | 0.249546    | 0.249725    | 0.249878    | 0.069842    | 0.070934    |
|           | 0.395446    | 0.395861    | 0.397267    | 0.398207    | 0.082900    | 0.083337    |
|           | Y 0.082900  | 0.083337    | 0.082818    | 0.082818    | 0.082818    | 0.082818    |
|           | 0.364127    | 0.365397    | 0.368077    | 0.369622    | 0.083337    | 0.082818    |
|           | 0.250976    | 0.250771    | 0.250699    | 0.250741    | 0.082818    | 0.082818    |
| P4        | 0.395158    | 0.395861    | 0.397267    | 0.398207    | 0.082900    | 0.083337    |
|           | 0.364127    | 0.365397    | 0.368077    | 0.369622    | 0.083337    | 0.082818    |
|           | 0.250976    | 0.250771    | 0.250699    | 0.250741    | 0.082818    | 0.082818    |

Notes:
- Y = 0.464408 – 0.463039
- Z = 0.070934 – 0.070702
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 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 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 3

Simulated OHAp lattice parameters ($a$, $b$ and $c$ reported in Å; $\alpha$, $\beta$ and $\gamma$ in degrees) and internal coordinates of each irreducible atom (relative to s.g. $P6_3$) under the effect of strain $\varepsilon$.

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

|   | δ = + 0.04 | δ = + 0.02 | δ = + 0.02 | δ = + 0.04 |
|---|-----------|-----------|-----------|-----------|
| a | 9.38781   | 9.38640   | 9.38640   | 9.38781   |
| b | 9.39344   | 9.38781   | 9.39344   | 9.39344   |
| c | 6.87636   | 6.87224   | 6.87224   | 6.87636   |
| Ca1 | 0.317777  | 0.325394  | 0.345306  | 0.350730  |
| Y  | -0.335664 | -0.339535 | -0.318267 | -0.308686 |
| Z  | -0.004382 | -0.000749 | 0.000061  | 0.003185  |
| Ca2 | 0.350739  | 0.345318  | 0.325344  | 0.317811  |
| Y  | 0.308678  | 0.318245  | 0.339541  | 0.335575  |
| Z  | -0.496843 | -0.499870 | 0.499292  | 0.495590  |
| Ca3 | 0.316706  | 0.322659  | 0.347882  | 0.353545  |
| Y  | 0.339178  | 0.343603  | 0.315378  | 0.307537  |
| Z  | 0.003451  | 0.000631  | 0.000976  | 0.003025  |
| Ca4 | 0.353566  | 0.347874  | 0.322603  | 0.316635  |
| Y  | -0.307562 | -0.315382 | -0.346304 | -0.339244 |
| Z  | 0.497034  | 0.498979  | 0.499305  | 0.496550  |
| Ca5 | 0.238172  | 0.244317  | 0.240684  | 0.235374  |
| Y  | -0.007066 | 0.005546  | 0.007533  | 0.008280  |
| Z  | 0.263515  | 0.255414  | 0.243789  | 0.236597  |
| Ca6 | 0.235385  | 0.240627  | 0.244328  | 0.238180  |
| Y  | 0.008264  | 0.007666  | 0.005526  | 0.007063  |
| Z  | 0.263314  | 0.256208  | 0.244574  | 0.236824  |
| Ca7 | 0.011899  | 0.008172  | 0.004476  | 0.007596  |
| Y  | 0.255380  | 0.254440  | 0.255109  | 0.256278  |
| Z  | 0.245777  | 0.250077  | 0.248823  | 0.252624  |
| Ca8 | 0.255123  | 0.252422  | 0.253419  | 0.257677  |
| Y  | -0.251298 | -0.247303 | -0.247645 | -0.252167 |
| Z  | 0.238718  | 0.243382  | 0.256264  | 0.261076  |
| Ca9 | 0.257719  | 0.253400  | 0.252409  | 0.255165  |
| Y  | 0.252215  | 0.247583  | 0.247319  | 0.251278  |
| Z  | 0.238915  | 0.243751  | 0.256553  | 0.261272  |
| Ca10| -0.007549 | -0.004481 | -0.008189 | -0.011967 |
| Y  | -0.256235 | -0.255130 | -0.254376 | -0.255382 |
| Z  | -0.247446 | -0.251170 | -0.249952 | -0.254167 |
| P1 | 0.387784  | 0.392693  | 0.394568  | 0.389046  |
| Y  | 0.363307  | 0.365549  | 0.365743  | 0.363954  |
| Z  | 0.259845  | 0.257975  | 0.243578  | 0.241845  |
| P2 | -0.389017 | -0.394562 | -0.392695 | -0.387777 |
| Y  | -0.363976 | -0.365739 | -0.365717 | -0.363317 |
| Z  | -0.258135 | -0.256412 | -0.242030 | -0.240183 |

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

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

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

(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 \( C_i^d \) 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 \( \delta \) 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 \( s_0 \) 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 \( \Gamma \) point are evaluated diagonalising the central zone \((k = 0)\) mass-weighted Hessian matrix:

\[
W_{ij}(k = 0) = \sum_G \frac{H_{ij}^{0G}}{\sqrt{M_i M_j}}
\]

(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 \((u_i = x_i - x_i^0)\) and displacement of atom B in cell G \((u_j = x_j - x_j^0)\) from their equilibrium position \( x_i^0, x_j^0 \):

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

(4)

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

\[
\Phi_j = \sum_G \nu_j^G = \sum_G \frac{\partial E}{\partial u_j^G} \quad j = 1, \ldots, 3N
\]

(5)

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

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

(6)

The Hessian matrix eigenvalues provide the normal harmonic frequencies \( \omega_h \) 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

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.
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