Details of crystal structure of diamond monohydride.

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In the main part of article it was mentioned that the DMH can be "obtained" from the diamond structure by a sequence of virtual symmetry breaking operations. In euclidean 3D space geometrically they are described by 4×4 matrix of affine transformation which in block form can be written as:

$$A = \begin{pmatrix} R & T \\ 0 & 1 \end{pmatrix}$$

where R is 3×3 rotation matrix and T – 3 dimensional vector of origin shift.

The sequence is as follows:

1. $Fd\overline{3}m \xrightarrow{(8,1)} R\overline{3}$

$$R_1 = \begin{pmatrix} -1/2 & 0 & 1 \\ 1/2 & -1/2 & 1 \\ 0 & 1/2 & 1 \end{pmatrix} T_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

2. $R\overline{3} \xrightarrow{(1,7)} R\overline{3}$

$$R_2 = \begin{pmatrix} 2 & 1 & 0 \\ -1 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix} T_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

3. $R\overline{3} \xrightarrow{(1,6)} P\overline{3}$

$$R_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} T_3 = \begin{pmatrix} 2/3 \\ 1/3 \\ 5/6 \end{pmatrix}$$

The resulting matrix:

$$A = A_1 \cdot A_2 \cdot A_3 = \begin{pmatrix} -1 & -1/2 & 2 & 0 \\ 3/2 & -1 & 2 & 3/2 \\ -1/2 & 3/2 & 2 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Traditionally in crystallography transformation matrix are acting from the right, so columns in rotational part of A are the coordinates of unit cells vectors of DMH relative to the conventional unit cell of diamond structure. Schematically this transformation is shown in Fig. 1. Detailed crystallographic information about relaxed DMH structure in CIF format are presented in Fig. 2.

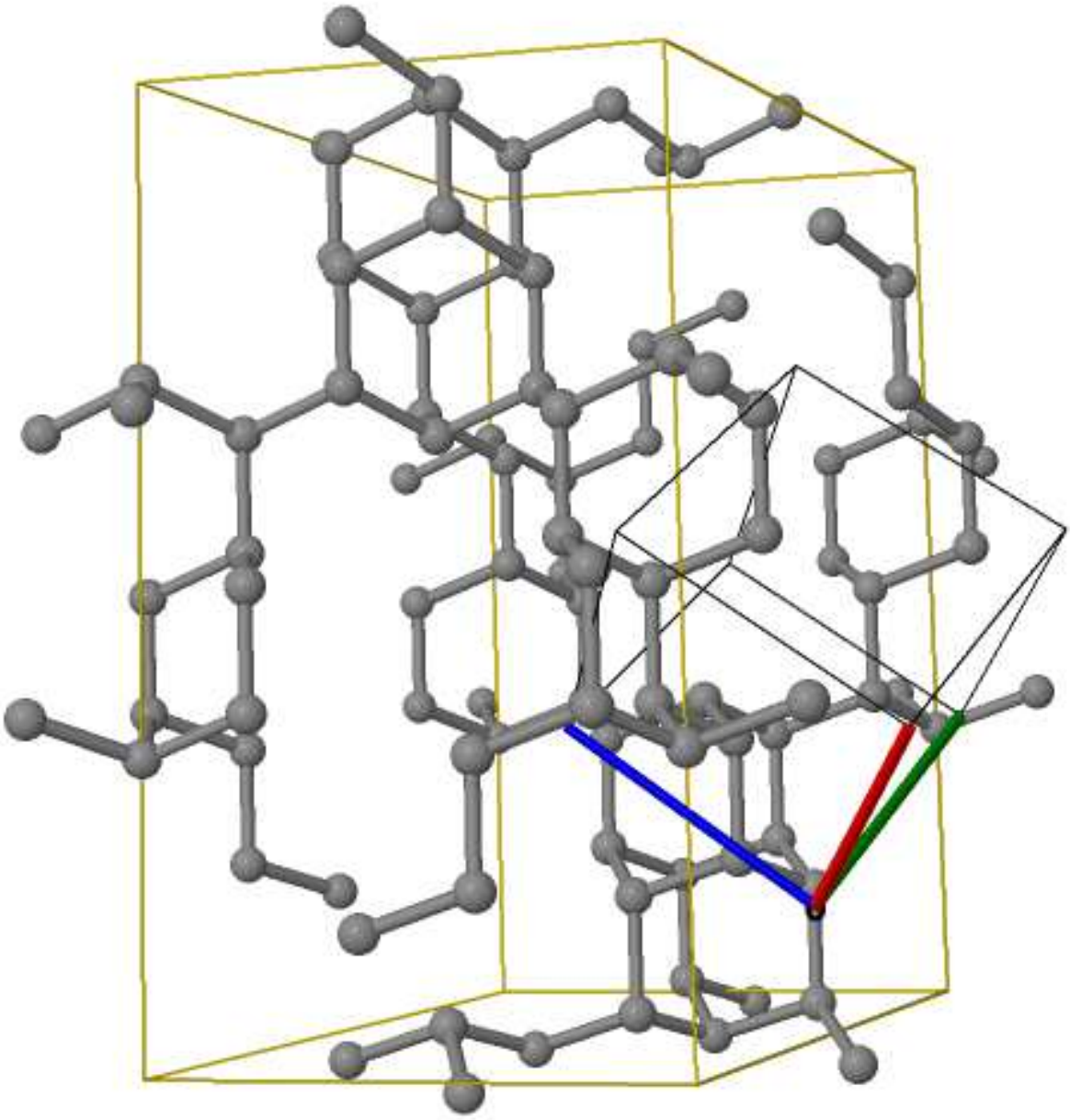

Figure 1: The unit cell of DMH (gold frame) relative to the diamond one (colored cube). Only carbon atoms are shown. Best viewed with AcrobatReader.

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data_global

_cell_length_a 6.926473
_cell_length_b 6.926473
_cell_length_c 12.83020
_cell_angle_alpha 90
_cell_angle_beta 90
_cell_angle_gamma 120
_symmetry_space_group_name_H-M    'P -3'
_symmetry_Int_Tables_number 147

loop_
_atom_site_label
_atom_site_Wyckoff_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
C1   2d     0.333333333   0.666666667   0.652991873
C2   2c     0.000000000   0.000000000   0.680338216
C3   2d     0.666666667   0.333333333   0.986322101
C4   6g     0.566693935   0.835558168   0.812300515
C5   6g     0.766635541   0.831106449   0.521032851
C6   6g     0.900051526   0.502242228   0.145638177
C7   6g     0.569642262   0.843085045   0.691800814
C8   6g     0.763690856   0.823581186   0.641531155
C9   6g     0.902971125   0.509747015   0.025135604
H1   2d     0.333333333   0.666666667   0.567542759
H2   2c    -0.000000000  -0.000000000   0.765789504
H3   2d     0.666666667   0.333333333   0.900880204
H4   6g     0.007808087   0.413550060   0.330108651
H5   6g     0.325523639   0.253115590   1.003226790
H6   6g     0.341140932   0.080216668   0.663440226
H7   6g     0.110353010   0.399959709   0.491271272
H8   6g     0.222982801   0.266707443   0.842060946
H9   6g     0.443681631   0.066615362   0.824605790
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Figure 2: Crystallography Information File of DMH structure.