Crystallographic information file (.cif) for Bi_8Te_3

The crystal structure was obtained as follows. We fixed the origin at (0,0,0), i.e, the first atom at (0,0,0) for (x, y, z) fractional coordinates; this atom was assigned to Te. The z coordinate for the second atom was obtained by 1/N = 1/11=0.091, and (x,y)=(0,0). The z coordinates for the remaining atoms were obtained by incremental addition of the smallest z value (0.091), whereas keeping the (x,y) coordinates at (0,0). Atoms of equivalent positions were populated by the software according to the symmetry operations within the $R\bar{3}m$ space group. The z for Bi2 atom separating slabs of 11-atoms was shifted by 0.002 units (0.184 instead of 0.182). The same small shift is reported in ikunolite (Kato 1959), i.e., the z for Bi2 is 0.287 instead of 0.284 = 2 x 0.142 (0.142 is the z for Bi1) for a comparable crystal setting with origin at (0,0,0). The structure reported here requires assessment either by single crystal X-ray methods or *ab initio* calculations using density functional theory.

Kato, A. Ikunolite, a new bismuth mineral from the Ikuno mine, Japan. *Mineral. Journal* **1959**, *2*, 397-407.

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_cell_length_b                    4.400000
_cell_length_c                   63.000000
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_cell_angle_beta                 90.000000
_cell_angle_gamma               120.000000

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loop_
_symmetry_equiv_pos_as_xyz
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_atom_site_fract_y
_atom_site_fract_z
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 Bi1  Bi 1.0  0.0  0.0  0.091
 Bi2  Bi 1.0  0.0  0.0  0.184
 Te2  Te 1.0  0.0  0.0  0.273
 Bi3  Bi 1.0  0.0  0.0  0.364
 Bi4  Bi 1.0  0.0  0.0  0.455
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