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1 data_CHA
2 #*****
3 #
4 # CIF taken from the IZA-SC Database of Zeolite Structures
5 # Ch. Baerlocher and L.B. McCusker
6 # Database of Zeolite Structures: http://www.iza-structure.org/databases/
7 #
8 # The atom coordinates and the cell parameters were optimized with DLS76
9 # assuming a pure SiO2 composition.
10 #
11 #*****
12
13 _cell_length_a          13.6750 (0)
14 _cell_length_b          13.6750 (0)
15 _cell_length_c          14.7670 (0)
16 _cell_angle_alpha       90.0000 (0)
17 _cell_angle_beta        90.0000 (0)
18 _cell_angle_gamma       120.0000 (0)
19
20 _symmetry_space_group_name_H-M      'R -3 m'
21 _symmetry_Int_Tables_number        166
22 _symmetry_cell_setting              trigonal
23
24 loop_
25 _symmetry_equiv_pos_as_xyz
26 '+x,+y,+z'
27 '2/3+x,1/3+y,1/3+z'
28 '1/3+x,2/3+y,2/3+z'
29 '-y,+x-y,+z'
30 '2/3-y,1/3+x-y,1/3+z'
31 '1/3-y,2/3+x-y,2/3+z'
32 '-x+y,-x,+z'
33 '2/3-x+y,1/3-x,1/3+z'
34 '1/3-x+y,2/3-x,2/3+z'
35 '-y,-x,+z'
36 '2/3-y,1/3-x,1/3+z'
37 '1/3-y,2/3-x,2/3+z'
38 '-x+y,+y,+z'
39 '2/3-x+y,1/3+y,1/3+z'
40 '1/3-x+y,2/3+y,2/3+z'
41 '+x,+x-y,+z'
42 '2/3+x,1/3+x-y,1/3+z'
43 '1/3+x,2/3+x-y,2/3+z'
44 '-x,-y,-z'
45 '2/3-x,1/3-y,1/3-z'
46 '1/3-x,2/3-y,2/3-z'
47 '+y,-x+y,-z'
48 '2/3+y,1/3-x+y,1/3-z'
49 '1/3+y,2/3-x+y,2/3-z'
50 '+x-y,+x,-z'
51 '2/3+x-y,1/3+x,1/3-z'
52 '1/3+x-y,2/3+x,2/3-z'
53 '+y,+x,-z'
54 '2/3+y,1/3+x,1/3-z'
55 '1/3+y,2/3+x,2/3-z'
56 '+x-y,-y,-z'
57 '2/3+x-y,1/3-y,1/3-z'
58 '1/3+x-y,2/3-y,2/3-z'
59 '-x,-x+y,-z'
60 '2/3-x,1/3-x+y,1/3-z'
61 '1/3-x,2/3-x+y,2/3-z'
62
63 loop_
64 _atom_site_label
65 _atom_site_type_symbol
66 _atom_site_fract_x
67 _atom_site_fract_y
68 _atom_site_fract_z
69 O1 O 0.9020 0.0980 0.1227
70 O2 O 0.9767 0.3101 0.1667
71 O3 O 0.1203 0.2405 0.1315
72 O4 O 0.0000 0.2577 0.0000
73 T1 Si 0.9997 0.2264 0.1051

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