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data_Wadsleyite
_audit_creation_method 'Created with CONVERT.DLL (www.crystalimpact.com)'
_audit_creation_date 2011-09-04
_audit_update_record 2011-09-04
_journal_coden_ASTM ?
_journal_year ?
_journal_volume ?
_journal_page_first ?
_journal_page_last ?
_publ_author_name '?,'
_publ_section_title
;
'297'
;
_chemical_formula_sum 'Mg2 Si O4'
_chemical_formula_structural 'Mg16Si8O32'
_chemical_formula_analytical 'Mg2SiO4'
_chemical_name_common
;
wadsleyite
;
_chemical_compound_source
;
Multianvil facility at BGI
;
_chemical_formula_weight 140.693
_cell_length_a 5.7016(1)
_cell_length_b 11.4427(2)
_cell_length_c 8.2491(1)
_cell_angle_alpha 90.000
_cell_angle_beta 90.000
_cell_angle_gamma 90.000
_cell_volume 538.2(0)
_cell_formula_units_Z 8
_symmetry_int_tables_number 74
_symmetry_space_group_name_H-M 'I m m a'
_symmetry_space_group_name_Hall '-I_2b_2'

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loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 -x,0.500-y,z
3 x,-y,-z
4 -x,0.500+y,-z
5 -x,-y,-z
6 x,0.500+y,-z
7 -x,y,z
8 x,0.500-y,z
9 0.500+x,0.500+y,0.500+z
10 0.500-x,1.000-y,0.500+z
11 0.500+x,0.500-y,0.500-z
12 0.500-x,1.000+y,0.500-z

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13 0.500-x,0.500-y,0.500-z
14 0.500+x,1.000+y,0.500-z
15 0.500-x,0.500+y,0.500+z
16 0.500+x,1.000-y,0.500+z

loop_
_atom_type_symbol
_atom_type_oxidation_number
_atom_type_radius_bond
Mg ? 1.200
Si ? 1.200
O ? 1.200

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_symbol
_atom_site_attached_hydrogens
_atom_site_calc_flag
_atom_site_thermal_displace_type
_atom_site_u_iso_or_equiv
Mg1 Mg 0.0000 0.0000 0.0000 1.000 4 a ? d Biso 0.12(4)
Mg2 Mg 0.0000 0.2500 0.9726(4) 1.000 4 e ? d Biso 0.12(4)
Mg3 Mg 0.2500 0.1286(4) 0.2500 1.000 8 g ? d Biso 0.12(4)
Si1 Si 0.0000 0.1187(3) 0.6175(4) 1.000 8 h ? d Biso 0.12(4)
O1 O 0.0000 0.2500 0.2177(9) 1.000 4 e ? d Uiso 0.12(4)
O2 O 0.0000 0.2500 0.7179(9) 1.000 4 e ? d Uiso 0.12(4)
O3 O 0.0000 0.9929(4) 0.2548(9) 1.000 8 h ? d Uiso 0.12(4)
O4 O 0.2624(5) 0.1227(12) 0.9945(4) 1.000 16 j ? d Uiso 0.12(4)