

data_BREARL

_ccdc_journal_manuscript_code 3755

_publ_contact_author_name 'Chi Ma'

_publ_contact_author_address

'Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 9112'

_publ_contact_author_email chi@gps.caltech.edu

_publ_contact_author_phone '626 395 6253 '

_publ_contact_author_fax '(626) 568-0935'

loop_

_publ_author_name

_publ_author_address

'Ma, Chi'

'Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 9112, USA'

'Connolly, Harold C.'

;Department of Physical Sciences, Kingsborough Community College of CUNY, Brooklyn, NY 11235 and Earth and Environmental Sciences, The Graduate Center of CUNY, New York, NY 10024, USA;

Department of Earth and Planetary Sciences, American Museum of Natural History, New York, NY 10024, USA;

Lunar and Planetary Laboratory, University of Arizona, Tucson, AZ 85721, USA;

;

'Beckett, John R.'

'Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125, USA'

'Tschauner, Oliver'

'Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125, USA;

High Pressure Science and Engineering Center and Department of Geoscience, University of Nevada, Las Vegas, NV 89154, USA'

'Rossman, George R.'

'Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA 91125, USA'

'Kampf, Anthony R.'

'Mineral Sciences Department, Natural History Museum of Los Angeles County, Los Angeles, CA 90007, '

'Zega, Thomas J.'

'Materials Science and Technology Division, Naval Research Laboratory, Washington, DC 20375, USA'

'Sweeney Smith, Stuart A.'

;Department of Earth and Planetary Sciences, American Museum of Natural History, New York, NY 10024, USA;

Department of Geology, Carleton College, Northfield, MN 55057, USA

;

'Schrader, Devin L.'

'Lunar and Planetary Laboratory, University of Arizona, Tucson, AZ 85721, USA'

_audit_creation_method 'Created with Endeavour Version 1.7e'

_audit_creation_date 2011-01-10

_audit_update_record 2011-01-10

_chemical_name_systematic Tridecacalciumtetradecaluminatedichloride

_chemical_name_common Brearleyite

_chemical_formula_moiety 'Ca_{26.64} Al_{27.998} O_{63.998} Cl_{4.44}'

_chemical_formula_sum 'Ca_{26.64} Al_{27.998} O_{63.998} Cl_{4.44}'

_chemical_compound_source 'Allende Meteorite'

_chemical_formula_weight 3004.463

_cell_length_a 11.979

_cell_length_b 11.979

_cell_length_c 11.979

_cell_angle_alpha 90.000

_cell_angle_beta 90.000

_cell_angle_gamma 90.000

_cell_volume 1719.1

_symmetry_cell_setting cubic
_symmetry_space_group_name_H-M 'I -4 3 d'
_symmetry_int_tables_number 220
_chemical_absolute_configuration ?
_symmetry_space_group_name_Hall I_-4bd_2c_3

loop_
_symmetry_equiv_pos_site_id
_symmetry_equiv_pos_as_xyz
1 x,y,z
2 0.250+y,0.750-x,0.250-z
3 -x,0.500-y,z
4 0.250-y,0.250+x,0.750-z
5 0.250-x,0.250+z,0.750-y
6 x,-y,0.500-z
7 0.750-x,0.250-z,0.250+y
8 0.750-z,0.250-y,0.250+x
9 0.500-x,y,-z
10 0.250+z,0.750-y,0.250-x
11 z,x,y
12 y,z,x
13 -y,0.500-z,x
14 z,-x,0.500-y
15 0.500-y,z,-x
16 -z,0.500-x,y
17 0.500-z,x,-y
18 y,-z,0.500-x
19 0.750-y,0.250-x,0.250+z
20 0.250+y,0.250+x,0.250+z
21 0.250+x,0.750-z,0.250-y
22 0.250+x,0.250+z,0.250+y
23 0.250-z,0.250+y,0.750-x
24 0.250+z,0.250+y,0.250+x

loop_
_atom_type_symbol
_atom_type_oxidation_number
_atom_type_radius_bond
Ca ? 1.200
Al ? 1.200
O ? 1.200
Cl ? 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
Ca1 Ca 0.6150 0.0000 0.2500 0.770 24 d ? d ? ?
Ca2 Ca 0.5550 0.0000 0.2500 0.340 24 d ? d ? ?
Al1 Al 0.0130 0.0130 0.0130 1.000 16 c ? d ? ?
Al2 Al 0.8750 0.0000 0.2500 1.000 12 b ? d ? ?
O1 O 0.7920 0.0950 0.3000 ? 48 e ? d ? ?
O2 O 0.1700 0.1700 0.1700 1.000 16 c ? d ? ?
Cl Cl 0.3750 0.0000 0.2500 0.370 12 a ? d ? ?
_diffrn_radiation_probe      electron
_diffrn_radiation_wavelength 0.06199
_diffrn_source                'electron microscope'
_diffrn_source_type           'JEOL 2200FS transmission electron microscope'

```