

data_fe2o3_frd

start Validation Reply Form

_vrf_PUBL004_GLOBAL

;

PROBLEM: The contact author's name and address are missing,

RESPONSE: ...

;

_vrf_PUBL005_GLOBAL

;

PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and

RESPONSE: ...

;

_vrf_PUBL006_GLOBAL

;

PROBLEM: _publ_requested_journal is missing

RESPONSE: ...

;

_vrf_PUBL008_GLOBAL

;

PROBLEM: _publ_section_title is missing. Title of paper.

RESPONSE: ...

;

_vrf_PUBL009_GLOBAL

;

PROBLEM: _publ_author_name is missing. List of author(s) name(s).

RESPONSE: ...

;

_vrf_PUBL010_GLOBAL

;

PROBLEM: _publ_author_address is missing. Author(s) address(es).

RESPONSE: ...

;

_vrf_PUBL012_GLOBAL

;

PROBLEM: _publ_section_abstract is missing.

RESPONSE: ...

;

_vrf_SYMM001_fe2o3_frd

;

PROBLEM: _symmetry_cell_setting is missing

RESPONSE: ...

;

_vrf_EXPT005_fe2o3_frd

;

PROBLEM: _exptl_crystal_description is missing

RESPONSE: ...

;

_vrf_DIFF005_fe2o3_frd

;

PROBLEM: _diffrn_measurement_method is missing

RESPONSE: ...

;

_vrf_DIFF019_fe2o3_frd
;
PROBLEM: _diffrn_standards_number is missing
RESPONSE: ...
;
_vrf_DIFF020_fe2o3_frd
;
PROBLEM: _diffrn_standards_interval_count and
RESPONSE: ...
;
_vrf_DIFF022_fe2o3_frd
;
PROBLEM: _diffrn_standards_decay_% is missing
RESPONSE: ...
;
end Validation Reply Form

#Added by publCIF (Mon Dec 27 15:55:58 2010)

start Validation Reply Form

_vrf_ABSTY01_fe2o3_frd
;
PROBLEM: The absorption correction should be one of the following
RESPONSE: No absorption correction applied, the sample had thickness of approximately 15 μm and was located in a diamond anvil cell. Synchrotron measurements were performed with a beamsize of roughly 5 x 5 μm . Total thickness of diamonds amounted to roughly 4-4.5 mm. It was assumed that an absorption correction would certainly not improve the data. The in house measurement was conducted on the same sample and DAC and thus was also not corrected.
;
_vrf_PLAT940_fe2o3_frd
;
PROBLEM: F**2 Refinement with I.GT. n * Sigma(I) only .. ?
RESPONSE: The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement.
;
_vrf_PLAT052_fe2o3_frd
;
PROBLEM: (Proper) Absorption Correction Method Missing .. ?
RESPONSE: No absorption correction applied, the sample had thickness of approximately 15 μm and was located in a diamond anvil cell. Synchrotron measurements were performed with a beamsize of roughly 5 x 5 μm . Total thickness of diamonds amounted to roughly 4-4.5 mm. It was assumed that an absorption correction would certainly not improve the data. The in house measurement was conducted on the same sample and DAC and thus was also not corrected.
;
end Validation Reply Form

#Added by publCIF (Mon Dec 27 15:36:10 2010)

_audit_update_record

;
2010-12-27 # Formatted by publCIF
;

_audit_creation_method SHELXL-97
_chemical_name_systematic
?
_chemical_name_common Hematite
_chemical_melting_point ?
_chemical_formula_moiety ?
_chemical_formula_sum
'Fe2 O3'
_chemical_formula_weight 159.70

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scatter_dispersion_real
_atom_type_scatter_dispersion_imag
_atom_type_scatter_source
'O' 'O' 0.0106 0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Fe' 'Fe' 0.3463 0.8444
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting ?
_symmetry_space_group_name_H-M 'R -3 c'

loop_
_symmetry_equiv_pos_as_xyz
'x, y, z'
'-y, x-y, z'
'y, x, -z+1/2'
'-x+y, -x, z'
'-x, -x+y, -z+1/2'
'x-y, -y, -z+1/2'
'x+2/3, y+1/3, z+1/3'
'-y+2/3, x-y+1/3, z+1/3'
'y+2/3, x+1/3, -z+5/6'
'-x+y+2/3, -x+1/3, z+1/3'
'-x+2/3, -x+y+1/3, -z+5/6'
'x-y+2/3, -y+1/3, -z+5/6'
'x+1/3, y+2/3, z+2/3'
'-y+1/3, x-y+2/3, z+2/3'
'y+1/3, x+2/3, -z+7/6'
'-x+y+1/3, -x+2/3, z+2/3'
'-x+1/3, -x+y+2/3, -z+7/6'
'x-y+1/3, -y+2/3, -z+7/6'
'-x, -y, -z'
'y, -x+y, -z'
'-y, -x, z-1/2'
'x-y, x, -z'
'x, x-y, z-1/2'
'-x+y, y, z-1/2'

'-x+2/3, -y+1/3, -z+1/3'
'y+2/3, -x+y+1/3, -z+1/3'
'-y+2/3, -x+1/3, z-1/6'
'x-y+2/3, x+1/3, -z+1/3'
'x+2/3, x-y+1/3, z-1/6'
'-x+y+2/3, y+1/3, z-1/6'
'-x+1/3, -y+2/3, -z+2/3'
'y+1/3, -x+y+2/3, -z+2/3'
'-y+1/3, -x+2/3, z+1/6'
'x-y+1/3, x+2/3, -z+2/3'
'x+1/3, x-y+2/3, z+1/6'
'-x+y+1/3, y+2/3, z+1/6'

_cell_length_a 5.0354(17)
_cell_length_b 5.0354(17)
_cell_length_c 13.748(5)
_cell_angle_alpha 90.00
_cell_angle_beta 90.00
_cell_angle_gamma 120.00
_cell_volume 301.88(18)
_cell_formula_units_Z 6
_cell_measurement_temperature 293(2)
_cell_measurement_reflms_used 82
_cell_measurement_theta_min 3
_cell_measurement_theta_max 27

_exptl_crystal_description ?
_exptl_crystal_colour black
_exptl_crystal_size_max 0.040
_exptl_crystal_size_mid 0.02
_exptl_crystal_size_min 0.015
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 5.271
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000 456
_exptl_absorpt_coefficient_mu 14.067
_exptl_absorpt_correction_type ?
_exptl_absorpt_correction_T_min ?
_exptl_absorpt_correction_T_max ?
_exptl_absorpt_process_details ?

_exptl_special_details
?

_diffn_ambient_temperature 293(2)
_diffn_radiation_wavelength 0.71065
_diffn_radiation_type MoK\alpha
_diffn_radiation_source 'fine-focus sealed tube'
_diffn_radiation_monochromator graphite
_diffn_measurement_device_type DAC
_diffn_measurement_method ?
_diffn_detector_area_resol_mean ?
_diffn_standards_number ?
_diffn_standards_interval_count ?

```

_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%       ?
_diffrn_reflns_number           387
_diffrn_reflns_av_R_equivalents 0.0672
_diffrn_reflns_av_sigmaI/netI   0.0596
_diffrn_reflns_limit_h_min      -4
_diffrn_reflns_limit_h_max      6
_diffrn_reflns_limit_k_min      -6
_diffrn_reflns_limit_k_max      6
_diffrn_reflns_limit_l_min      -15
_diffrn_reflns_limit_l_max      17
_diffrn_reflns_theta_min        5.53
_diffrn_reflns_theta_max        27.85
_reflns_number_total            82
_reflns_number_gt               82
_reflns_threshold_expression     >2sigma(I)

```

```

_computing_data_collection      ?
_computing_cell_refinement      ?
_computing_data_reduction       ?
_computing_structure_solution   ?
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics   ?
_computing_publication_material ?

```

```
_refine_special_details
```

```
;
```

Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2 , conventional R-factors R are based on F, with F set to zero for negative F^2 . The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

```
;
```

```

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type          full
_refine_ls_weighting_scheme     calc
_refine_ls_weighting_details
'calc w=1/[\s^2*(Fo^2)+(0.0688P)^2+0.1327P] where P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary    direct
_atom_sites_solution_secondary  difmap
_refine_ls_number_reflns       82
_refine_ls_number_parameters    6
_refine_ls_number_restraints    0
_refine_ls_R_factor_all        0.0391
_refine_ls_R_factor_gt         0.0391
_refine_ls_wR_factor_ref       0.1007
_refine_ls_wR_factor_gt       0.1007
_refine_ls_goodness_of_fit_ref 1.002
_refine_ls_restrained_S_all    1.002
_refine_ls_shift/su_max        0.000
_refine_ls_shift/su_mean       0.000

```

```

loop_
  _atom_site_label
  _atom_site_type_symbol
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_U_iso_or_equiv
  _atom_site_adp_type
  _atom_site_occupancy
  _atom_site_symmetry_multiplicity
  _atom_site_calc_flag
  _atom_site_refinement_flags
  _atom_site_disorder_assembly
  _atom_site_disorder_group
Fe Fe 0.0000 0.0000 0.35523(7) 0.0106(11) Uani 1 3 d S . .
O O 0.3059(5) 0.0000 0.2500 0.0132(13) Uani 1 2 d S . .

```

```

loop_
  _atom_site_aniso_label
  _atom_site_aniso_U_11
  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_23
  _atom_site_aniso_U_13
  _atom_site_aniso_U_12
Fe 0.0088(12) 0.0088(12) 0.0141(16) 0.000 0.000 0.0044(6)
O 0.0111(14) 0.0116(14) 0.0171(18) 0.0015(5) 0.0007(3) 0.0058(7)

```

```

_geom_special_details
;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

```

```

loop_
  _geom_bond_atom_site_label_1
  _geom_bond_atom_site_label_2
  _geom_bond_distance
  _geom_bond_site_symmetry_2
  _geom_bond_publ_flag
Fe O 1.9447(16) 34_445 ?
Fe O 1.9447(16) 32 ?
Fe O 1.9447(16) 31_545 ?
Fe O 2.113(2) 4 ?
Fe O 2.113(2) 2 ?
Fe O 2.113(2) . ?
Fe Fe 2.893(2) 3 ?
Fe Fe 2.9689(10) 31_445 ?
Fe Fe 2.9689(10) 31 ?

```

Fe Fe 2.9689(10) 31_545 ?
O Fe 1.9447(16) 27 ?
O Fe 1.9447(16) 31_545 ?
O Fe 2.113(2) 3 ?

loop_

_geom_angle_atom_site_label_1
_geom_angle_atom_site_label_2
_geom_angle_atom_site_label_3
_geom_angle
_geom_angle_site_symmetry_1
_geom_angle_site_symmetry_3
_geom_angle_publ_flag
O Fe O 102.54(4) 34_445 32 ?
O Fe O 102.54(4) 34_445 31_545 ?
O Fe O 102.54(4) 32 31_545 ?
O Fe O 86.04(3) 34_445 4 ?
O Fe O 162.24(9) 32 4 ?
O Fe O 90.50(6) 31_545 4 ?
O Fe O 90.50(6) 34_445 2 ?
O Fe O 86.04(3) 32 2 ?
O Fe O 162.24(9) 31_545 2 ?
O Fe O 78.28(8) 4 2 ?
O Fe O 162.24(9) 34_445 . ?
O Fe O 90.50(6) 32 . ?
O Fe O 86.04(3) 31_545 . ?
O Fe O 78.28(8) 4 . ?
O Fe O 78.28(8) 2 . ?
O Fe Fe 115.74(3) 34_445 3 ?
O Fe Fe 115.74(3) 32 3 ?
O Fe Fe 115.74(3) 31_545 3 ?
O Fe Fe 46.79(5) 4 3 ?
O Fe Fe 46.79(5) 2 3 ?
O Fe Fe 46.79(5) . 3 ?
O Fe Fe 45.24(6) 34_445 31_445 ?
O Fe Fe 145.09(6) 32 31_445 ?
O Fe Fe 98.53(6) 31_545 31_445 ?
O Fe Fe 40.80(4) 4 31_445 ?
O Fe Fe 82.02(3) 2 31_445 ?
O Fe Fe 118.64(6) . 31_445 ?
Fe Fe Fe 78.30(4) 3 31_445 ?
O Fe Fe 98.54(6) 34_445 31 ?
O Fe Fe 45.24(6) 32 31 ?
O Fe Fe 145.08(6) 31_545 31 ?
O Fe Fe 118.64(6) 4 31 ?
O Fe Fe 40.80(4) 2 31 ?
O Fe Fe 82.02(3) . 31 ?
Fe Fe Fe 78.30(4) 3 31 ?
Fe Fe Fe 116.00(2) 31_445 31 ?
O Fe Fe 145.08(6) 34_445 31_545 ?
O Fe Fe 98.53(6) 32 31_545 ?
O Fe Fe 45.24(6) 31_545 31_545 ?
O Fe Fe 82.02(3) 4 31_545 ?
O Fe Fe 118.64(6) 2 31_545 ?

O Fe Fe 40.80(4) . 31_545 ?
Fe Fe Fe 78.30(4) 3 31_545 ?
Fe Fe Fe 116.00(2) 31_445 31_545 ?
Fe Fe Fe 116.00(2) 31 31_545 ?
Fe O Fe 119.64(14) 27 31_545 ?
Fe O Fe 93.96(3) 27 3 ?
Fe O Fe 131.59(4) 31_545 3 ?
Fe O Fe 131.58(4) 27 . ?
Fe O Fe 93.96(3) 31_545 . ?
Fe O Fe 86.42(11) 3 . ?

_diffn_measured_fraction_theta_max 0.965
_diffn_reflns_theta_full 27.85
_diffn_measured_fraction_theta_full 0.965
_refine_diff_density_max 0.622
_refine_diff_density_min -0.380
_refine_diff_density_rms 0.319