

Jacobi matrix :

| # | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|----|--------------|----------------|---------------|---------------|----------------|----------------|---------|---|---|---|
| 0 | 2320686.0 | | | | | | | | | |
| 1 | -262581.88 | 168950.53 | | | | | | | | |
| 2 | 3143.5862 | -1370.233 | 84.62642 | | | | | | | |
| 3 | 273744.34 | -159814.53 | 7357.566 | 767545.8 | | | | | | |
| 4 | 2.8672342E7 | -2.0313818E7 | 767288.3 | 8.8052696E7 | 1.06934487E10 | | | | | |
| 5 | 3.43803341E9 | -2.68978381E9 | 8.8050472E7 | 1.06967747E10 | 1.34933434E12 | 1.7497564 | | | | |
| 6 | 4.4736204E11 | -3.64749292E11 | 1.07021066E10 | 1.35045487E12 | 1.75066541E14 | 2.317603 | | | | |
| 7 | 23945.014 | 4539.197 | 353.83246 | 37082.43 | 4332892.0 | 5.3905677E8 | 6.9724 | | | |
| 8 | -79474.06 | 21824.637 | 1284.4181 | 153846.28 | 1.9657404E7 | 2.5996521E9 | 3.514 | | | |
| 9 | -8.5784456E7 | 5.8210344E7 | -1991996.1 | -2.25563616E8 | -2.81015194E10 | -3.65983826E | | | | |
| 10 | -3.7030036E7 | 2.455478E7 | -903614.94 | -9.9202624E7 | -1.21169439E10 | -1.55553536E | | | | |
| 11 | -114.087654 | 44.869938 | -0.7661285 | -48.95486 | -3433.2485 | -230361.03 | -1.034 | | | |
| 12 | -16.78297 | 6.918435 | -0.016203362 | 0.024353728 | 83.07221 | 12534.051 | 14923 | | | |
| 13 | 36.55929 | -13.96271 | 0.18642646 | 11.579822 | 722.8468 | 33614.816 | -128827 | | | |
| 14 | -2.9410696 | 1.0083505 | -0.16400796 | -13.825074 | -1241.1654 | -111997.12 | -9643 | | | |
| 15 | -15.253112 | 5.5158334 | -0.051348887 | -2.3128111 | -41.07314 | 14220.74 | 37061 | | | |
| 16 | -2816028.2 | 2282897.5 | -77247.94 | -9658187.0 | -1.18573811E9 | -1.4681591E11 | -1. | | | |
| 17 | -1585278.1 | 1382046.8 | -45096.336 | -5211590.0 | -6.3129709E8 | -7.8119617E10 | -9. | | | |
| 18 | -3252852.5 | 1640191.1 | -52131.074 | -6886291.5 | -8.5368672E8 | -1.06331193E11 | -1. | | | |
| 19 | -5167346.0 | 5502417.0 | -188254.62 | -2.2970382E7 | -2.80263066E9 | -3.45988366E11 | | | | |
| 20 | -3723578.5 | 3798363.8 | -152885.94 | -1.969012E7 | -2.44086477E9 | -3.04725262E11 | | | | |
| 21 | -83694.71 | 21596.66 | -1596.6995 | -180274.33 | -2.2053726E7 | -2.82023552E9 | -3.7 | | | |
| 22 | 426859.47 | -699259.25 | -2487.6494 | -238594.77 | -2.5100858E7 | -2.82739277E9 | -3. | | | |
| 23 | -54.95011 | 47.811386 | -0.26626024 | -20.060003 | -1734.1344 | -167712.14 | -1.761 | | | |
| 24 | 5.4453926 | -1.1807307 | -0.019931033 | -1.8552476 | -166.49065 | -15117.154 | -139 | | | |
| 25 | -37525.01 | 2342795.8 | -8470.878 | -857312.1 | -9.1435784E7 | -1.01562491E10 | -1.1 | | | |
| 26 | 108569.164 | 586334.5 | -1803.0104 | -193674.77 | -2.197125E7 | -2.60300288E9 | -3.1 | | | |

Correlation matrix:

| # | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|----|-------------|-------------|-------------|-------------|------------|------------|---------|---|---|---|
| 0 | 1.0 | | | | | | | | | |
| 1 | 1.1172022 | 1.0 | | | | | | | | |
| 2 | -1.4306132 | -2.108188 | 1.0 | | | | | | | |
| 3 | 1.1017957 | 1.0000435 | -2.048964 | 1.0 | | | | | | |
| 4 | 0.07571307 | -0.42965126 | -1.1765563 | -0.40272415 | -1.0 | | | | | |
| 5 | 0.7435833 | 1.181598 | -0.15749966 | 1.256491 | 0.0040128 | 1.0 | | | | |
| 6 | -0.8987394 | -1.1615773 | 0.6495925 | -1.114463 | 0.1519316 | -1.0103989 | 1.0 | | | |
| 7 | -0.80029196 | -0.65634733 | 1.7443758 | -0.71994203 | 0.5490073 | -1.2364945 | 1.145 | | | |
| 8 | -1.1640744 | -1.0438722 | 2.240625 | -1.0696719 | 0.49525458 | -1.3600948 | 1.3112 | | | |
| 9 | -1.2458993 | -1.1564342 | 2.2168732 | -1.1265858 | 0.3382199 | -1.0518703 | 1.0150 | | | |
| 10 | 1.1864697 | 1.155508 | -2.1739879 | 1.2146904 | -0.3807976 | 1.0660706 | -1.0211 | | | |
| 11 | 0.64939964 | 0.788152 | -0.7221152 | 0.73158807 | 0.26388425 | 0.09264239 | -0.25 | | | |

| | | | | | | | |
|----|-------------|-------------|--------------|-------------|--------------|-------------|--------|
| 12 | 0.4176235 | 0.66122466 | -0.080595136 | 0.57855755 | 0.5593096 | -0.33516228 | 0.1 |
| 13 | 0.96166843 | 0.9480173 | -1.6030025 | 0.9245425 | -0.15376365 | 0.73813933 | -0.77 |
| 14 | 0.9186794 | 0.9382405 | -1.460842 | 0.9113212 | -0.07349816 | 0.6004678 | -0.690 |
| 15 | 0.7125633 | 0.65450597 | -1.2438524 | 0.6170209 | -0.16437864 | 0.41070652 | -0.37 |
| 16 | -0.36467668 | -0.58940166 | -0.10231407 | -0.435021 | -0.6812386 | 0.92630345 | -0.7 |
| 17 | -0.17412207 | -0.04218333 | 0.06942157 | 0.21034205 | -0.19401489 | 0.3392057 | -0.3 |
| 18 | 0.83249617 | 1.1418967 | 0.18373576 | 0.61035955 | 1.4950699 | -2.1078734 | 1.82 |
| 19 | 0.28975978 | 0.5640442 | 0.105304584 | 0.52527976 | 0.57012075 | -0.73993826 | 0.5 |
| 20 | -0.33532614 | -0.85898775 | -0.18405274 | -0.98935753 | -0.73250353 | 0.88130915 | -0. |
| 21 | -0.30360427 | -0.55457044 | -0.10155178 | -0.4818411 | -0.58676165 | 0.77466923 | -0. |
| 22 | -0.3679621 | -0.9680177 | -0.20037152 | -1.1375841 | -0.8033701 | 0.9556078 | -0.70 |
| 23 | -0.3599482 | -0.09981872 | 1.2580613 | -0.18148325 | 0.73363626 | -1.1818405 | 0.99 |
| 24 | 1.8247024 | 1.8267995 | -2.8970602 | 1.7341024 | -0.14597592 | 1.3259907 | -1.455 |
| 25 | -0.0814266 | -0.06590362 | 0.17292151 | -0.06900434 | 0.050831053 | -0.10665317 | 0.0 |
| 26 | 0.035204194 | 0.026945353 | -0.07861243 | 0.028723478 | -0.025714995 | 0.046321698 | |

Correlation matrix from Choleski decomposition :

| # | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|----|-------------|-------------|--------------|-------------|--------------|-------------|---------|---|---|---|
| 0 | 1.0 | | | | | | | | | |
| 1 | 1.1172022 | 1.0 | | | | | | | | |
| 2 | -1.4306132 | -2.108188 | 1.0 | | | | | | | |
| 3 | 1.1017957 | 1.0000435 | -2.048964 | 1.0 | | | | | | |
| 4 | 0.07571307 | -0.42965126 | -1.1765563 | -0.40272415 | -1.0 | | | | | |
| 5 | 0.7435833 | 1.181598 | -0.15749966 | 1.256491 | 0.0040128 | 1.0 | | | | |
| 6 | -0.8987394 | -1.1615773 | 0.6495925 | -1.114463 | 0.1519316 | -1.0103989 | 1.0 | | | |
| 7 | -0.80029196 | -0.65634733 | 1.7443758 | -0.71994203 | 0.5490073 | -1.2364945 | 1.145 | | | |
| 8 | -1.1640744 | -1.0438722 | 2.240625 | -1.0696719 | 0.49525458 | -1.3600948 | 1.3112 | | | |
| 9 | -1.2458993 | -1.1564342 | 2.2168732 | -1.1265858 | 0.3382199 | -1.0518703 | 1.0150 | | | |
| 10 | 1.1864697 | 1.155508 | -2.1739879 | 1.2146904 | -0.3807976 | 1.0660706 | -1.0211 | | | |
| 11 | 0.64939964 | 0.788152 | -0.7221152 | 0.73158807 | 0.26388425 | 0.09264239 | -0.25 | | | |
| 12 | 0.4176235 | 0.66122466 | -0.080595136 | 0.57855755 | 0.5593096 | -0.33516228 | 0.1 | | | |
| 13 | 0.96166843 | 0.9480173 | -1.6030025 | 0.9245425 | -0.15376365 | 0.73813933 | -0.77 | | | |
| 14 | 0.9186794 | 0.9382405 | -1.460842 | 0.9113212 | -0.07349816 | 0.6004678 | -0.690 | | | |
| 15 | 0.7125633 | 0.65450597 | -1.2438524 | 0.6170209 | -0.16437864 | 0.41070652 | -0.37 | | | |
| 16 | -0.36467668 | -0.58940166 | -0.10231407 | -0.435021 | -0.6812386 | 0.92630345 | -0.7 | | | |
| 17 | -0.17412207 | -0.04218333 | 0.06942157 | 0.21034205 | -0.19401489 | 0.3392057 | -0.3 | | | |
| 18 | 0.83249617 | 1.1418967 | 0.18373576 | 0.61035955 | 1.4950699 | -2.1078734 | 1.82 | | | |
| 19 | 0.28975978 | 0.5640442 | 0.105304584 | 0.52527976 | 0.57012075 | -0.73993826 | 0.5 | | | |
| 20 | -0.33532614 | -0.85898775 | -0.18405274 | -0.98935753 | -0.73250353 | 0.88130915 | -0. | | | |
| 21 | -0.30360427 | -0.55457044 | -0.10155178 | -0.4818411 | -0.58676165 | 0.77466923 | -0. | | | |
| 22 | -0.3679621 | -0.9680177 | -0.20037152 | -1.1375841 | -0.8033701 | 0.9556078 | -0.70 | | | |
| 23 | -0.3599482 | -0.09981872 | 1.2580613 | -0.18148325 | 0.73363626 | -1.1818405 | 0.99 | | | |
| 24 | 1.8247024 | 1.8267995 | -2.8970602 | 1.7341024 | -0.14597592 | 1.3259907 | -1.455 | | | |
| 25 | -0.0814266 | -0.06590362 | 0.17292151 | -0.06900434 | 0.050831053 | -0.10665317 | 0.0 | | | |
| 26 | 0.035204194 | 0.026945353 | -0.07861243 | 0.028723478 | -0.025714995 | 0.046321698 | | | | |

Analysis title: Put a title here

Refined parameters:

0 SB-G65-after:SB-G65-After:layer1:_pd_phase_atom_%1 value:0.056937348 error:0.002968641
1 SB-G65-after:SB-G65-After:layer1:_pd_phase_atom_%2 value:0.27427205 error:0.02639672
2 SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol0 value:133.51048 error:3.8
3 SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol1 value:-3.8674955 error:0.1
4 SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol2 value:0.0564561 error:0.0
5 SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol3 value:-3.7068027E-4 erro
6 SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol4 value:8.240464E-7 error:3
7 SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:_pd_proc_intensity_incident val
8 SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:_riet_par_2-theta_offset0 value:
9 SB-G65-after:SB-G65-After:Martensite:_cell_length_a value:2.8919082 error:9.551888E-4
10 SB-G65-after:SB-G65-After:Martensite:_cell_length_c value:2.8588412 error:0.0024356034
11 SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size0 value:672.3011
12 SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size1 value:-454.3521
13 SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size2 value:1101.7301
14 SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size3 value:-273.7166
15 SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size4 value:-126.0619
16 SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain0 value:0.00521
17 SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain1 value:0.01711
18 SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain2 value:-0.01268
19 SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain3 value:-0.01420
20 SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain4 value:0.01104
21 SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv value:-
22 SB-G65-after:SB-G65-After:Ferrite:_cell_length_a value:2.8739357 error:4.390898E-4
23 SB-G65-after:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size0 value:345.56393 erro
24 SB-G65-after:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size1 value:-160.28221 er
25 SB-G65-after:SB-G65-After:Ferrite:Popa rules:_riet_par_aniso_microstrain0 value:-0.00385935
26 SB-G65-after:SB-G65-After:Ferrite:Popa rules:_riet_par_aniso_microstrain1 value:0.00116872

Refinement final output indices:

Global Rwp: 0.19905752

Global Rp: 0.118245184

Global Rwpb (no background): 7.5018306

Global Rpb (no background): 0.12342153

Total Energy: 0.0

Refinement final output indices for single samples:

Sample SB-G65-After :

Sample Rwp: 0.19905752

Sample Rp: 0.118245184

Sample Rwpb (no background): 7.5018306

Sample Rpb (no background): 0.12342153

Refinement final output indices for single datasets:

DataSet SB-G65-after :

DataSet Rwp: 0.19905752

DataSet Rp: 0.118245184

DataSet Rwpb (no background): 7.5018306

DataSet Rpb (no background): 0.12342153

Refinement final output indices for single spectra:

Datafile SB-G65.xrdml(0) : Rwp: 0.19905752, Rp: 0.118245184, Rwpb: 7.5018306, Rpb: 0.123421

Sample:SB-G65-After

Phases:

Martensite

Density: 7.757471646904133

Qc: 0.05531834991659745

Austenite

Density: 7.8298424756303495

Qc: 0.055575788236870996

Ferrite

Density: 7.81354455522871

Qc: 0.05551791723819582

Object tree full informations

Object: SB-G65-after

String informations (CIF term, value) :

_audit_creation_date, Mon Oct 12 15:11:53 PDT 1998

_audit_creation_method, Maud, version 2.33

_audit_update_record, Last update Thu May 09 15:33:24 BST 2013

_computing_structure_refinement, Maud, version 2.33

_refine_ls_R_factor_all, 0.118245184

_refine_ls_wR_factor_all, 0.19905752

_refine_ls_goodness_of_fit_all, 0.10654729

_publ_contact_author_name, Luca Lutterotti

_publ_section_title, Put a title here

_pd_proc_ls_extract_int, end of iteration

_pd_proc_ls_texture_comp, end of iteration

_computing_reduce_memory_occ, true

_pd_proc_ls_theoretical_weight, false

_pd_proc_ls_extract_pos, end of iteration

_pd_proc_ls_strain_comp, end of iteration

_pd_proc_ls_extract_Fhkl, end of iteration

_pd_proc_ls_Fhkl_comp, end of iteration

_pd_proc_ls_weight_scheme, sqrt

_refine_ls_weighting_scheme, WgtSS

_refine_ls_WSS_factor, 16439.678

_maud_store_spectra_with_analysis, false

_riet_remove_phases_under, 0.001

_riet_refine_cell_over, 0.1

_riet_refine_sizestrain_over, 0.1

_riet_refine_crystal_structure_over, 0.1

_riet_refine_texture_over, 0.15
_riet_refine_strain_over, 0.25
_pd_proc_ls_interpolation_comp, end of iteration

Subordinate objects :

Subordinate object number 0 :

Object: Marqardt Least Squares

String informations (CIF term, value) :

_refine_ls_number_iteration, 5
_riet_refine_ls_precision, 0.00000001
_riet_refine_ls_derivative_step, 0.0001
_riet_refine_ls_double_derivative, false

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: SB-G65-After

String informations (CIF term, value) :

_pd_spec_description, Sample description
_riet_thin_film_phase_refinement, films

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:_pd_spec_orientation_omega Value: 0, minimum: 0.0, maximum: 360.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_orientation_chi Value: 0, minimum: 0.0, maximum: 90.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_orientation_phi Value: 0, minimum: 0.0, maximum: 360.0
- Parameter: SB-G65-after:SB-G65-After:_riet_par_spec_displac_x Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_riet_par_spec_displac_y Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_riet_par_spec_displac_z Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_size_axial Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_size_equat Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_size_thick Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_size_radius Value: 0, minimum: 0.0, maximum: 0.0
- Parameter: SB-G65-after:SB-G65-After:_pd_spec_size_radius_y Value: 0, minimum: 0.0, maximum: 0.0

Subordinate objects :

Subordinate object number 0 :

Object: flat_sheet

Subordinate object number 1 :

Object: None Layer workout

Subordinate object number 2 :

Object: No precession

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: layer1

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:layer1:_riet_par_spec_layer_thickness Value: 1.0E7, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:_reflectivity_layer_critical_qc Value: 0.04, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:_reflectivity_layer_absorption Value: 2.0E-7, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:_reflectivity_layer_roughness Value: 2.0, minimum

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after:SB-G65-After:layer1:_pd_phase_atom_%0 Value: 0.6687906, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:_pd_phase_atom_%1 Value: 0.056937348, minimum
- Parameter: SB-G65-after:SB-G65-After:layer1:_pd_phase_atom_%2 Value: 0.27427205, minimum

Object loop number 1 :

Object number 0 :

Object: SB-G65-after

String informations (CIF term, value) :

_pd_meas_datetime_initiated, Date/time meas
_pd_meas_info_author_name,
_riet_meas_datafile_format,
_pd_proc_ls_background_function,
_pd_proc_ls_profile_function,
_pd_proc_ls_peak_cutoff, 30
_pd_proc_2theta_range_min, 0
_pd_proc_2theta_range_max, 0
_pd_proc_2theta_range_inc,
_diffrn_ambient_pressure,
_diffrn_ambient_temperature,
_riet_lorentz_restricted, true
_riet_par_background_interpolated, false
_riet_par_background_interpolation_range, 10
_riet_meas_dataset_compute, true
_riet_meas_datafile_replace, false
_riet_meas_dataset_random_texture, false

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_exp_shift Value: 0,
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_exp_thermal_shift
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_pd_spec_orientation_omega Value: 0, m
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_pd_spec_orientation_chi Value: 0, minim
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_pd_spec_orientation_phi Value: 0, minim

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol0 Value: 133.51
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol1 Value: -3.867
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol2 Value: 0.0564
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol3 Value: -3.706
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:_riet_par_background_pol4 Value: 8.2404

Subordinate objects :

Subordinate object number 0 :

Object: Le Bail

String informations (CIF term, value) :

_riet_lebail_iteration_max, 5
_riet_lebail_error_max, 0.0050
_riet_lebail_range_factor, 0.05
_riet_lebail_use_bkg, true
_riet_lebail_use_hkl, true
_riet_lebail_summation_delta, 1.0E-4

Subordinate object number 1 :

Object: none pe

Subordinate object number 2 :

Object: none reflectivity

Subordinate object number 3 :

Object: Diffraction Instrument

String informations (CIF term, value) :

_diffrn_measurement_device_type, Diffraction Instrument

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:_pd_proc_intensity_

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:_riet_par_2-theta_of

Subordinate objects :

Subordinate object number 0 :

Object: none cal

Subordinate object number 1 :

Object: Instrument disalignment

Subordinate object number 2 :

Object: Bragg-Brentano

String informations (CIF term, value) :

_diffrn_radiation_monochromator, Filtered

_pd_instr_2theta_monochr_post, 0

_pd_instr_dist_src/samp, 175.0

_pd_instr_monochr_pre_spec, none

_pd_instr_2theta_monochr_pre, 0

_pd_instr_divg_ax_src/samp, 0.0

_pd_instr_divg_slit_auto, false

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Bragg-Brentano:_dif

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Bragg-Brentano:_dif

Subordinate object number 3 :

Object: Theta-2Theta

Subordinate object number 4 :

Object: X-ray tube

Subordinate object number 5 :

Object: Scintillation

Subordinate object number 6 :

Object: Caglioti PV

String informations (CIF term, value) :

_riet_caglioti_d_dep, true
_riet_asymmetry_tan_dep, false
_riet_omega/chi_broadening_convolutd, false
_riet_par_asymmetry_truncation, 0.4

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa

Parameter loop number : 1

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa

Parameter loop number : 2

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa

Subordinate object number 7 :

Object: none abs

Loops of subordinate objects :

Subordinate object number 4 :

Object: none fluorescence

Loops of subordinate objects :

Object loop number 2 :

Object number 0 :

Object: SB-G65.xrdml(0)

String informations (CIF term, value) :

_riet_meas_datafile_format,
_pd_meas_orientation_omega, 0.0
_pd_meas_orientation_chi, 0.0
_pd_meas_orientation_phi, 0.0
_pd_meas_orientation_eta, 0.0
_riet_meas_datafile_compute, true
_riet_meas_datafile_fitting, false
_pd_meas_detector_id, none
_pd_meas_step_count_time, 10.00

_pd_meas_units_of_intensity, counts
 _riet_meas_datafile_as_background, false
 _riet_meas_data_group_count, 1
 _riet_datafile_type, 0
 _riet_datafile_save_custom,
 _pd_meas_image_id, -1
 _riet_background_interpolated_manual, false

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):_pd_meas_counts_moni
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):_riet_par_spec_displac_
- Parameter: SB-G65-after:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):_riet_par_spec_displac_

Parameter loop informations :

Object loop number 2 :

Object number 0 :

Object: Martensite

General position

- 1) +x | +y | +z
- 2) +y | -x | -z
- 3) -x | -y | +z
- 4) -y | +x | -z
- 5) +x+0.5 | +y+0.5 | +z+0.5
- 6) +y+0.5 | -x+0.5 | -z+0.5
- 7) -x+0.5 | -y+0.5 | +z+0.5
- 8) -y+0.5 | +x+0.5 | -z+0.5

Atom list

n label symbol quantity occupancy x y z multiplicity B radius weighth neutron scattering neu

1) Fe Fe 2.0 1.0 0 0 0 2 -0.5939843 1.27 55.847

Atomic #, atom #, isotope #, weight, radius, symbol for tables: 26, 54, 80, 55.847, 1.27, Fe

Neutron sf: 9.45

Magnetic sf: 0.0706 35.0085 0.3589 15.3583 0.5819 5.5606 -0.0114

Electron sf: 0.1929 0.8239 1.8689 2.3694 1.906 0.1087 1.0806 4.7637 22.85

Neutron abs: 0.525525525525254

Electron abs: 0.0

X-ray sf: 0.493002 0.322912 0.140191 0.04081 10.5109 26.1257 3.14236 57.7997 0.003038 0.48

X-ray disp and abs: 0.0 0.0 0.0 0.0 0.002 0.002 0.008 0.008 0.018 0.035 0.0 0.059 0.09 0.09 0.09

Reflection list

n h k l multiplicity meanFhkl crystallite(Angstrom) microstrain

1) 1 1 0 4 5094.882412809033 1244.1353817627619 0.008177597333938618

2) 1 0 1 8 10142.696724020227 203.6147026192553 0.004504781159019493
 3) 2 0 0 4 3631.842231344322 1086.3471853154338 0.005210699
 4) 0 0 2 2 1791.6637247684773 1318.080429462003 0.016729969880883596
 5) 1 2 1 8 5612.159111682829 744.4890212870919 0.01228494307500575
 6) 2 1 1 8 5612.159111682829 517.8480037782318 0.0032250490279108553
 7) 1 1 2 8 5568.8383106837 376.96355577590424 0.005674087966230884
 8) 2 2 0 4 2308.4961109016585 1244.1353817627619 0.008177597333938618
 9) 2 0 2 8 4579.9507976260675 203.6147026192553 0.004504781159019493
 10) 1 3 0 4 1979.1435104886164 1307.600500515134 0.011124340626119942
 11) 3 1 0 4 1979.1435104886164 978.7013715578097 0.010505050942351643
 12) 3 0 1 8 3952.0775307313575 743.3133859963503 0.0033645443591046797
 13) 1 0 3 8 3903.411526082905 941.9401286348459 0.01389909709615408
 14) 2 2 2 8 3498.3750584735994 338.15180019066105 0.00924380722733438
 15) 2 3 1 8 3210.6460806465066 1052.732924722315 0.0120453537009035
 16) 3 2 1 8 3210.6460806465066 843.6712936490825 0.0019280543601993883
 17) 1 3 2 8 3202.11811311386 440.6717148446274 0.010950751888032205
 18) 3 1 2 8 3202.11811311386 275.07502759170666 0.0014314090170158104
 19) 1 2 3 8 3188.160665746065 357.10439197236855 0.003017522355603804
 20) 2 1 3 8 3188.160665746065 316.38032861042467 0.006171905267640922
 21) 4 0 0 4 1504.7474519661382 1086.3471853154338 0.005210699
 22) 0 0 4 2 744.9684543317587 1318.080429462003 0.016729969880883596

String informations (CIF term, value) :

_chemical_name_common, Martensite
 _chemical_formula_sum, Phase unknown
 _symmetry_cell_setting, tetragonal
 _symmetry_Int_Tables_number, triclinic
 _symmetry_space_group_name_sch, 1
 _symmetry_space_group_name_H-M, I-4
 _symmetry_space_group_name_Hall, P1
 _cell_formula_units_Z, 1
 _refine_ls_d_res_low, 0
 _refine_ls_d_res_high, 5000
 _reflns_d_resolution_low, 0.7
 _reflns_d_resolution_high, 50

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:Martensite:_cell_length_a Value: 2.8919082, minimum:
 - Parameter: SB-G65-after:SB-G65-After:Martensite:_cell_length_b Value: 2.8919082, minimum:
 - Parameter: SB-G65-after:SB-G65-After:Martensite:_cell_length_c Value: 2.8588412, minimum:
 - Parameter: SB-G65-after:SB-G65-After:Martensite:_cell_angle_alpha Value: 90, minimum: 90.0
 - Parameter: SB-G65-after:SB-G65-After:Martensite:_cell_angle_beta Value: 90, minimum: 90.0,
 - Parameter: SB-G65-after:SB-G65-After:Martensite:_cell_angle_gamma Value: 90, minimum: 90
 - Parameter: SB-G65-after:SB-G65-After:Martensite:_riet_par_strain_thermal Value: 0, minimum:
 - Parameter: SB-G65-after:SB-G65-After:Martensite:_exptl_absorpt_cryst_size Value: 0, minimum:
 - Parameter: SB-G65-after:SB-G65-After:Martensite:_riet_par_phase_scale_factor Value: 1.2227

Subordinate objects :

Subordinate object number 0 :

Object: none tex

Subordinate object number 1 :

Object: Delf

Subordinate object number 2 :

Object: Popa rules

String informations (CIF term, value) :

_rita_harmonic_expansion_degree, 4

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size0 Value
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size1 Value
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size2 Value
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size3 Value
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size4 Value

Parameter loop number : 1

- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain0 Val
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain1 Val
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain2 Val
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain3 Val
- Parameter: SB-G65-after:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain4 Val

Subordinate object number 3 :

Object: none abm

Subordinate object number 4 :

Object: none pd

Subordinate object number 5 :

Object: no magnetic

Subordinate object number 6 :

Object: no strain

Subordinate object number 7 :

Object: No microabsorption

Subordinate object number 8 :

Object: Atomic Structure

String informations (CIF term, value) :

_riet_structure_quantity_from_occupancy, true
_refine_ls_energy_weight, 1.0

Subordinate objects :

Subordinate object number 0 :

Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

_riet_ga_population_size, 500
_riet_ga_generations_number, 20
_riet_ga_mutation_prob, 0.01
_riet_ga_permutation_prob, 0.01

Subordinate object number 1 :

Object: No force field

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: Fe

String informations (CIF term, value) :

_atom_site_type_symbol, Fe
_atom_site_constraints,
_atom_type_number_in_cell, 2.0
_atom_site_calc_flag, .

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_occupancy
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_fract_x Valu
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_fract_y Valu
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_fract_z Valu
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_B_iso_or_eo

Parameters bounded to this parameter:

SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv
SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv

- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_aniso_B_11
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_aniso_B_22
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_aniso_B_33
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_aniso_B_23
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_aniso_B_13
- Parameter: SB-G65-after:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_aniso_B_12

Subordinate object number 9 :

Object: atomic standard model

Subordinate object number 10 :

Object: Le Bail

String informations (CIF term, value) :

_riet_lebail_iteration_max, 5
 _riet_lebail_error_max, 0.005
 _riet_lebail_range_factor, 0.05
 _riet_lebail_use_bkg, true
 _riet_lebail_summation_delta, 1.0E-4
 _riet_lebail_use_previous_factors, true

Subordinate object number 11 :

Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

_riet_ga_population_size, 500
 _riet_ga_generations_number, 20
 _riet_ga_mutation_prob, 0.01
 _riet_ga_permutation_prob, 0.01

Subordinate object number 12 :

Object: None TDS

Loops of subordinate objects :

Object number 1 :

Object: Austenite

General position

- 1) $+x \mid +y \mid +z$
- 2) $-y \mid +x \mid +z$
- 3) $-x \mid -y \mid +z$
- 4) $+y \mid -x \mid +z$
- 5) $+x \mid -z \mid +y$
- 6) $+x \mid -y \mid -z$
- 7) $+x \mid +z \mid -y$
- 8) $+z \mid +y \mid -x$
- 9) $-x \mid +y \mid -z$
- 10) $-z \mid +y \mid +x$
- 11) $+z \mid +x \mid +y$
- 12) $+y \mid +z \mid +x$
- 13) $-y \mid -z \mid +x$
- 14) $+z \mid -x \mid -y$
- 15) $-y \mid +z \mid -x$
- 16) $-z \mid -x \mid +y$
- 17) $-z \mid +x \mid -y$
- 18) $+y \mid -z \mid -x$
- 19) $+y \mid +x \mid -z$
- 20) $-y \mid -x \mid -z$
- 21) $-x \mid +z \mid +y$
- 22) $-x \mid -z \mid -y$
- 23) $+z \mid -y \mid +x$
- 24) $-z \mid -y \mid -x$
- 25) $-x \mid -y \mid -z$
- 26) $+y \mid -x \mid -z$
- 27) $+x \mid +y \mid -z$
- 28) $-y \mid +x \mid -z$
- 29) $-x \mid +z \mid -y$
- 30) $-x \mid +y \mid +z$
- 31) $-x \mid -z \mid +y$
- 32) $-z \mid -y \mid +x$
- 33) $+x \mid -y \mid +z$
- 34) $+z \mid -y \mid -x$
- 35) $-z \mid -x \mid -y$
- 36) $-y \mid -z \mid -x$
- 37) $+y \mid +z \mid -x$
- 38) $-z \mid +x \mid +y$
- 39) $+y \mid -z \mid +x$
- 40) $+z \mid +x \mid -y$
- 41) $+z \mid -x \mid +y$
- 42) $-y \mid +z \mid +x$
- 43) $-y \mid -x \mid +z$
- 44) $+y \mid +x \mid +z$
- 45) $+x \mid -z \mid -y$
- 46) $+x \mid +z \mid +y$
- 47) $-z \mid +y \mid -x$
- 48) $+z \mid +y \mid +x$

49) $+x \mid +y+0.5 \mid +z+0.5$
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175) $-x+0.5 \mid -z+0.5 \mid +y$
176) $-z+0.5 \mid -y+0.5 \mid +x$
177) $+x+0.5 \mid -y+0.5 \mid +z$
178) $+z+0.5 \mid -y+0.5 \mid -x$
179) $-z+0.5 \mid -x+0.5 \mid -y$
180) $-y+0.5 \mid -z+0.5 \mid -x$
181) $+y+0.5 \mid +z+0.5 \mid -x$
182) $-z+0.5 \mid +x+0.5 \mid +y$
183) $+y+0.5 \mid -z+0.5 \mid +x$
184) $+z+0.5 \mid +x+0.5 \mid -y$
185) $+z+0.5 \mid -x+0.5 \mid +y$
186) $-y+0.5 \mid +z+0.5 \mid +x$
187) $-y+0.5 \mid -x+0.5 \mid +z$
188) $+y+0.5 \mid +x+0.5 \mid +z$
189) $+x+0.5 \mid -z+0.5 \mid -y$
190) $+x+0.5 \mid +z+0.5 \mid +y$
191) $-z+0.5 \mid +y+0.5 \mid -x$
192) $+z+0.5 \mid +y+0.5 \mid +x$

Atom list

n label symbol quantity occupancy x y z multiplicity B radius weight neutron scattering neu
1) Fe Fe 4.0 1.0 0 0 0 4 -0.5939843 1.27 55.847
Atomic #, atom #, isotope #, weight, radius, symbol for tables: 26, 54, 80, 55.847, 1.27, Fe
Neutron sf: 9.45
Magnetic sf: 0.0706 35.0085 0.3589 15.3583 0.5819 5.5606 -0.0114
Electron sf: 0.1929 0.8239 1.8689 2.3694 1.906 0.1087 1.0806 4.7637 22.85
Neutron abs: 0.525525525525254
Electron abs: 0.0
X-ray sf: 0.493002 0.322912 0.140191 0.04081 10.5109 26.1257 3.14236 57.7997 0.003038 0.48
X-ray disp and abs: 0.0 0.0 0.0 0.0 0.002 0.002 0.008 0.008 0.018 0.035 0.0 0.059 0.09 0.09 0.09

Reflection list

n h k l multiplicity meanFhkl crystallite(Angstrom) microstrain
1) 1 1 1 8 41451.91123610173 156.13226340182888 0.0011898097855989414
2) 2 0 0 6 27522.037707515003 127.14182989696118 0.0020608109999999999
3) 2 2 0 12 37514.093045765934 148.88465502642458 0.0014572134328438302
4) 3 1 1 24 60629.49391403588 140.79848039106793 0.0017068074304245398
5) 2 2 2 8 19026.22816978255 156.13226340182888 0.0011898097855989414
6) 4 0 0 6 11702.07042796694 127.14182989696118 0.0020608109999999999
7) 3 3 1 24 41888.405280312945 150.9926851633674 0.0013847722918190607
8) 4 2 0 24 40612.00521613274 141.05723797981776 0.0016993882854869512
9) 4 2 2 24 36827.14867841135 148.88465502571046 0.00145721343284383

String informations (CIF term, value) :

_chemical_name_common, Austenite
_chemical_formula_sum, Phase unknown
_symmetry_cell_setting, cubic
_symmetry_Int_Tables_number, triclinic
_symmetry_space_group_name_sch, 1
_symmetry_space_group_name_H-M, Fm-3m
_symmetry_space_group_name_Hall, P1
_cell_formula_units_Z, 1
_refine_ls_d_res_low, 0
_refine_ls_d_res_high, 5000
_reflns_d_resolution_low, 0.7
_reflns_d_resolution_high, 50

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:Austenite:_cell_length_a Value: 3.618418, minimum: 5.
- Parameter: SB-G65-after:SB-G65-After:Austenite:_cell_length_b Value: 3.618418, minimum: 5.
- Parameter: SB-G65-after:SB-G65-After:Austenite:_cell_length_c Value: 3.618418, minimum: 5.
- Parameter: SB-G65-after:SB-G65-After:Austenite:_cell_angle_alpha Value: 90, minimum: 90.0,
- Parameter: SB-G65-after:SB-G65-After:Austenite:_cell_angle_beta Value: 90, minimum: 90.0, n
- Parameter: SB-G65-after:SB-G65-After:Austenite:_cell_angle_gamma Value: 90, minimum: 90.0
- Parameter: SB-G65-after:SB-G65-After:Austenite:_riet_par_strain_thermal Value: 0, minimum: -
- Parameter: SB-G65-after:SB-G65-After:Austenite:_exptl_absorpt_cryst_size Value: 0.42649165

- Parameter: SB-G65-after:SB-G65-After:Austenite:_riet_par_phase_scale_factor Value: 4.06760

Subordinate objects :

Subordinate object number 0 :

Object: none tex

Subordinate object number 1 :

Object: Delf

Subordinate object number 2 :

Object: Popa rules

String informations (CIF term, value) :

_rita_harmonic_expansion_degree, 4

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after:SB-G65-After:Austenite:Popa rules:_riet_par_anisocryst_size0 Value:

- Parameter: SB-G65-after:SB-G65-After:Austenite:Popa rules:_riet_par_anisocryst_size1 Value:

Parameter loop number : 1

- Parameter: SB-G65-after:SB-G65-After:Austenite:Popa rules:_riet_par_aniso_microstrain0 Valu

- Parameter: SB-G65-after:SB-G65-After:Austenite:Popa rules:_riet_par_aniso_microstrain1 Valu

Subordinate object number 3 :

Object: none abm

Subordinate object number 4 :

Object: none pd

Subordinate object number 5 :

Object: no magnetic

Subordinate object number 6 :

Object: no strain

Subordinate object number 7 :

Object: No microabsorption

Subordinate object number 8 :

Object: Atomic Structure

String informations (CIF term, value) :

_riet_structure_quantity_from_occupancy, true
_refine_ls_energy_weight, 1.0

Subordinate objects :

Subordinate object number 0 :

Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

_riet_ga_population_size, 500
_riet_ga_generations_number, 20
_riet_ga_mutation_prob, 0.01
_riet_ga_permutation_prob, 0.01

Subordinate object number 1 :

Object: No force field

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: Fe

String informations (CIF term, value) :

_atom_site_type_symbol, Fe
_atom_site_constraints,
_atom_type_number_in_cell, 4.0
_atom_site_calc_flag, .

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_occupancy Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_fract_x Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_fract_y Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_fract_z Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_B_iso_or_equi Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_11 Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_22 Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_33 Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_23 Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_13 Value
- Parameter: SB-G65-after:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_12 Value

Subordinate object number 9 :

Object: atomic standard model

Subordinate object number 10 :

Object: Le Bail

String informations (CIF term, value) :

_riet_lebail_iteration_max, 5
_riet_lebail_error_max, 0.005
_riet_lebail_range_factor, 0.05
_riet_lebail_use_bkg, true
_riet_lebail_summation_delta, 1.0E-4
_riet_lebail_use_previous_factors, true

Subordinate object number 11 :

Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

_riet_ga_population_size, 500
_riet_ga_generations_number, 20
_riet_ga_mutation_prob, 0.01
_riet_ga_permutation_prob, 0.01

Subordinate object number 12 :

Object: None TDS

Loops of subordinate objects :

Object number 2 :

Object: Ferrite

General position

- 1) +x | +y | +z
- 2) -y | +x | +z
- 3) -x | -y | +z
- 4) +y | -x | +z
- 5) +x | -z | +y
- 6) +x | -y | -z
- 7) +x | +z | -y

- 8) $+z \mid +y \mid -x$
- 9) $-x \mid +y \mid -z$
- 10) $-z \mid +y \mid +x$
- 11) $+z \mid +x \mid +y$
- 12) $+y \mid +z \mid +x$
- 13) $-y \mid -z \mid +x$
- 14) $+z \mid -x \mid -y$
- 15) $-y \mid +z \mid -x$
- 16) $-z \mid -x \mid +y$
- 17) $-z \mid +x \mid -y$
- 18) $+y \mid -z \mid -x$
- 19) $+y \mid +x \mid -z$
- 20) $-y \mid -x \mid -z$
- 21) $-x \mid +z \mid +y$
- 22) $-x \mid -z \mid -y$
- 23) $+z \mid -y \mid +x$
- 24) $-z \mid -y \mid -x$
- 25) $-x \mid -y \mid -z$
- 26) $+y \mid -x \mid -z$
- 27) $+x \mid +y \mid -z$
- 28) $-y \mid +x \mid -z$
- 29) $-x \mid +z \mid -y$
- 30) $-x \mid +y \mid +z$
- 31) $-x \mid -z \mid +y$
- 32) $-z \mid -y \mid +x$
- 33) $+x \mid -y \mid +z$
- 34) $+z \mid -y \mid -x$
- 35) $-z \mid -x \mid -y$
- 36) $-y \mid -z \mid -x$
- 37) $+y \mid +z \mid -x$
- 38) $-z \mid +x \mid +y$
- 39) $+y \mid -z \mid +x$
- 40) $+z \mid +x \mid -y$
- 41) $+z \mid -x \mid +y$
- 42) $-y \mid +z \mid +x$
- 43) $-y \mid -x \mid +z$
- 44) $+y \mid +x \mid +z$
- 45) $+x \mid -z \mid -y$
- 46) $+x \mid +z \mid +y$
- 47) $-z \mid +y \mid -x$
- 48) $+z \mid +y \mid +x$
- 49) $+x+0.5 \mid +y+0.5 \mid +z+0.5$
- 50) $-y+0.5 \mid +x+0.5 \mid +z+0.5$
- 51) $-x+0.5 \mid -y+0.5 \mid +z+0.5$
- 52) $+y+0.5 \mid -x+0.5 \mid +z+0.5$
- 53) $+x+0.5 \mid -z+0.5 \mid +y+0.5$
- 54) $+x+0.5 \mid -y+0.5 \mid -z+0.5$
- 55) $+x+0.5 \mid +z+0.5 \mid -y+0.5$

56) +z+0.5 | +y+0.5 | -x+0.5
 57) -x+0.5 | +y+0.5 | -z+0.5
 58) -z+0.5 | +y+0.5 | +x+0.5
 59) +z+0.5 | +x+0.5 | +y+0.5
 60) +y+0.5 | +z+0.5 | +x+0.5
 61) -y+0.5 | -z+0.5 | +x+0.5
 62) +z+0.5 | -x+0.5 | -y+0.5
 63) -y+0.5 | +z+0.5 | -x+0.5
 64) -z+0.5 | -x+0.5 | +y+0.5
 65) -z+0.5 | +x+0.5 | -y+0.5
 66) +y+0.5 | -z+0.5 | -x+0.5
 67) +y+0.5 | +x+0.5 | -z+0.5
 68) -y+0.5 | -x+0.5 | -z+0.5
 69) -x+0.5 | +z+0.5 | +y+0.5
 70) -x+0.5 | -z+0.5 | -y+0.5
 71) +z+0.5 | -y+0.5 | +x+0.5
 72) -z+0.5 | -y+0.5 | -x+0.5
 73) -x+0.5 | -y+0.5 | -z+0.5
 74) +y+0.5 | -x+0.5 | -z+0.5
 75) +x+0.5 | +y+0.5 | -z+0.5
 76) -y+0.5 | +x+0.5 | -z+0.5
 77) -x+0.5 | +z+0.5 | -y+0.5
 78) -x+0.5 | +y+0.5 | +z+0.5
 79) -x+0.5 | -z+0.5 | +y+0.5
 80) -z+0.5 | -y+0.5 | +x+0.5
 81) +x+0.5 | -y+0.5 | +z+0.5
 82) +z+0.5 | -y+0.5 | -x+0.5
 83) -z+0.5 | -x+0.5 | -y+0.5
 84) -y+0.5 | -z+0.5 | -x+0.5
 85) +y+0.5 | +z+0.5 | -x+0.5
 86) -z+0.5 | +x+0.5 | +y+0.5
 87) +y+0.5 | -z+0.5 | +x+0.5
 88) +z+0.5 | +x+0.5 | -y+0.5
 89) +z+0.5 | -x+0.5 | +y+0.5
 90) -y+0.5 | +z+0.5 | +x+0.5
 91) -y+0.5 | -x+0.5 | +z+0.5
 92) +y+0.5 | +x+0.5 | +z+0.5
 93) +x+0.5 | -z+0.5 | -y+0.5
 94) +x+0.5 | +z+0.5 | +y+0.5
 95) -z+0.5 | +y+0.5 | -x+0.5
 96) +z+0.5 | +y+0.5 | +x+0.5

Atom list

n label symbol quantity occupancy x y z multiplicity B radius weighth neutron scattering neu

1) Fe Fe 2.0 1.0 0 0 0 2 -0.5939843 1.27 55.847

Atomic #, atom #, isotope #, weight, radius, symbol for tables: 26, 54, 80, 55.847, 1.27, Fe

Neutron sf: 9.45

Magnetic sf: 0.0706 35.0085 0.3589 15.3583 0.5819 5.5606 -0.0114

Electron sf: 0.1929 0.8239 1.8689 2.3694 1.906 0.1087 1.0806 4.7637 22.85

Neutron abs: 0.525525525525254

Electron abs: 0.0

X-ray sf: 0.493002 0.322912 0.140191 0.04081 10.5109 26.1257 3.14236 57.7997 0.003038 0.48

X-ray disp and abs: 0.0 0.0 0.0 0.0 0.002 0.002 0.008 0.008 0.018 0.035 0.0 0.059 0.09 0.09 0.09

Reflection list

n h k l multiplicity meanFhkl crystallite(Angstrom) microstrain

- 1) 1 1 0 12 15208.533175745644 371.4639470734107 0.0026008320868833386
- 2) 2 0 0 6 5408.285306190056 241.9638617221973 0.0038593502
- 3) 2 1 1 24 16739.433122642826 371.4639470691573 0.0026008320868833377
- 4) 2 2 0 12 6865.612272718317 371.4639470734107 0.0026008320868833386
- 5) 3 1 0 24 11775.412621298357 288.5838924486342 0.0034594351640537973
- 6) 2 2 2 8 3488.175919366101 414.6306421840285 0.0020135148547095216
- 7) 3 2 1 48 19153.065981023025 371.4639470713364 0.0026008320868833377
- 8) 4 0 0 6 2244.9254714698886 241.9638617221973 0.0038593502

String informations (CIF term, value) :

_chemical_name_common, Ferrite

_chemical_formula_sum, Phase unknown

_symmetry_cell_setting, cubic

_symmetry_Int_Tables_number, triclinic

_symmetry_space_group_name_sch, 1

_symmetry_space_group_name_H-M, Im-3m

_symmetry_space_group_name_Hall, P1

_cell_formula_units_Z, 1

_refine_ls_d_res_low, 0

_refine_ls_d_res_high, 5000

_reflns_d_resolution_low, 0.7

_reflns_d_resolution_high, 50

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_length_a Value: 2.8739357, minimum: 5.0,
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_length_b Value: 2.8739357, minimum: 5.0,
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_length_c Value: 2.8739357, minimum: 5.0,
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_angle_alpha Value: 90, minimum: 90.0, ma
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_angle_beta Value: 90, minimum: 90.0, max
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_cell_angle_gamma Value: 90, minimum: 90.0, r
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_riet_par_strain_thermal Value: 0, minimum: -0.1
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_exptl_absorpt_cryst_size Value: 0, minimum: 0.
- Parameter: SB-G65-after:SB-G65-After:Ferrite:_riet_par_phase_scale_factor Value: 2.7407699

Subordinate objects :

Subordinate object number 0 :

Object: none tex

Subordinate object number 1 :

Object: Delf

Subordinate object number 2 :

Object: Popa rules

String informations (CIF term, value) :

_rita_harmonic_expansion_degree, 4

Parameter loop informations :

Parameter loop number : 0

- Parameter: SB-G65-after:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size0 Value: 34

- Parameter: SB-G65-after:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size1 Value: -1

Parameter loop number : 1

- Parameter: SB-G65-after:SB-G65-After:Ferrite:Popa rules:_riet_par_aniso_microstrain0 Value:

- Parameter: SB-G65-after:SB-G65-After:Ferrite:Popa rules:_riet_par_aniso_microstrain1 Value:

Subordinate object number 3 :

Object: none abm

Subordinate object number 4 :

Object: none pd

Subordinate object number 5 :

Object: no magnetic

Subordinate object number 6 :

Object: no strain

Subordinate object number 7 :

Object: No microabsorption

Subordinate object number 8 :

Object: Atomic Structure

String informations (CIF term, value) :

_riet_structure_quantity_from_occupancy, true

_refine_ls_energy_weight, 1.0

Subordinate objects :

Subordinate object number 0 :

Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

_riet_ga_population_size, 500

_riet_ga_generations_number, 20

_riet_ga_mutation_prob, 0.01

_riet_ga_permutation_prob, 0.01

Subordinate object number 1 :

Object: No force field

Loops of subordinate objects :

Object loop number 0 :

Object number 0 :

Object: Fe

String informations (CIF term, value) :

_atom_site_type_symbol, Fe

_atom_site_constraints,

_atom_type_number_in_cell, 2.0

_atom_site_calc_flag, .

Parameter informations :

- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_occupancy Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_fract_x Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_fract_y Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_fract_z Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_11 Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_22 Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_33 Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_23 Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_13 Value: 0
- Parameter: SB-G65-after:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_12 Value: 0

Subordinate object number 9 :

Object: atomic standard model

Subordinate object number 10 :

Object: Le Bail

String informations (CIF term, value) :

_riet_lebail_iteration_max, 5
_riet_lebail_error_max, 0.005
_riet_lebail_range_factor, 0.05
_riet_lebail_use_bkg, true
_riet_lebail_summation_delta, 1.0E-4
_riet_lebail_use_previous_factors, true

Subordinate object number 11 :

Object: Genetic Algorithm SDPD

String informations (CIF term, value) :

_riet_ga_population_size, 500
_riet_ga_generations_number, 20
_riet_ga_mutation_prob, 0.01
_riet_ga_permutation_prob, 0.01

Subordinate object number 12 :

Object: None TDS

Loops of subordinate objects :