Jacobi matrix :

#	0	1	2	3	4	5	6	7
0	306991.22							
1	-37762.793	6050.4243						
2	1213.8352	-210.73676	84.6361					
3	130212.805	-22256.162	7362.3223	768440.0				
4	-14650.236	2279.1206	-214.66757	-25126.363	2115.3306			
5	20230.773	4532.519	-446.51218	-76706.92	2030.9542	6985861.0		
6	42.958508	-4.7918453	-0.09633363	-7.159875	-1.7184876	-9.593055	0.01719	
7	-1472465.4	131675.16	5666.7812	634316.6	83176.19	389889.12	-823.033	

Correlation matrix:

#	0	1	2	3	4	5	6	7
0	-1.0							
1	-2.7379484	1.0						
2	-0.58195037	1.8944004	1.0					
3	-2.623144	0.86356336	11.093933	-1.0				
4	-3.6574423	0.17640617	1.4654853	-1.1007534	-1.0			
5	0.27840868	3.0100083	0.6166852	-1.6003472	-2.56908	1.0		
6	-1.9371381	1.1806421	1.159257	0.97736293	0.60518795	-2.3171697	1.0	
7	0.31172383	-2.4336932	-0.983239	-3.4154925	-2.5617738	1.2808795	-2594.6	

Correlation matrix from Choleski decomposition :

#	0	1	2	3	4	5	6	7
0	-1.0							
1	-2.7379484	1.0						
2	-0.58195037	1.8944004	1.0					
3	-2.623144	0.86356336	11.093933	-1.0				
4	-3.6574423	0.17640617	1.4654853	-1.1007534	-1.0			
5	0.27840868	3.0100083	0.6166852	-1.6003472	-2.56908	1.0		
6	-1.9371381	1.1806421	1.159257	0.97736293	0.60518795	-2.3171697	1.0	
7	0.31172383	-2.4336932	-0.983239	-3.4154925	-2.5617738	1.2808795	-2594.6	

Analysis title: Put a title here

Refined parameters:

0 paramete.sav:SB-G65-After:layer1:Volume fraction of Fe4.00 value:0.09879181 error:0.008199
1 paramete.sav:SB-G65-After:layer1:Volume fraction of ferrite value:0.79759556 error:0.0575263
2 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol0 value:120.63882 error:0.5
3 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol1 value:-2.6130648 error:0.
4 paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv value:-1
5 paramete.sav:SB-G65-After:Austenite:_cell_length_a value:3.6190095 error:7.486679E-4
6 paramete.sav:SB-G65-After:Austenite:Isotropic:_riet_par_cryst_size value:238.97253 error:28.9
7 paramete.sav:SB-G65-After:Austenite:Isotropic:_riet_par_rs_microstrain value:0.0040923166 er

Refinement final output indices:
Global Rwp: 0.21008857
Global Rp: 0.13301754
Global Rwpb (no background): 8.265378
Global Rpb (no background): 0.14447562
Total Energy: 0.0

Refinement final output indices for single samples:
Sample SB-G65-After :
Sample Rwp: 0.21008857
Sample Rp: 0.13301754
Sample Rwpb (no background): 8.265378
Sample Rpb (no background): 0.14447562

Refinement final output indices for single datasets:
DataSet SB-G65-after :
DataSet Rwp: 0.21008857
DataSet Rp: 0.13301754
DataSet Rwpb (no background): 8.265378
DataSet Rpb (no background): 0.14447562

Refinement final output indices for single spectra:
Datafile SB-G65.xrdml(0) : Rwp: 0.21008857, Rp: 0.13301754, Rwpb: 8.265378, Rpb: 0.1444756

Sample:SB-G65-After

Phases:
Martensite
Density: 7.56187773695375
Qc: 0.054616509880306766
Austenite
Density: 7.826003915737813
Qc: 0.05556216362404908
Ferrite
Density: 7.787271858628547
Qc: 0.05542450037886537

Object tree full informations

Object: paramete.sav

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 09:25:58 BST 2013
_computing_structure_refinement, Maud, version 2.33
_refine_ls_R_factor_all, 0.13301754

_refine_ls_wR_factor_all, 0.21008857
_refine_ls_goodness_of_fit_all, 0.10676198
_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, 18312.217
_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: paramete.sav:SB-G65-After:_pd_spec_orientation_omega Value: 0, minimum: 0.0, r

- Parameter: paramete.sav:SB-G65-After:_pd_spec_orientation_chi Value: 0, minimum: 0.0, maxi
- Parameter: paramete.sav:SB-G65-After:_pd_spec_orientation_phi Value: 0, minimum: 0.0, maxi
- Parameter: paramete.sav:SB-G65-After:_riet_par_spec_displac_x Value: 0, minimum: 0.0, maxi
- Parameter: paramete.sav:SB-G65-After:_riet_par_spec_displac_y Value: 0, minimum: 0.0, maxi
- Parameter: paramete.sav:SB-G65-After:_riet_par_spec_displac_z Value: 0, minimum: 0.0, maxi
- Parameter: paramete.sav:SB-G65-After:_pd_spec_size_axial Value: 0, minimum: 0.0, maximum
- Parameter: paramete.sav:SB-G65-After:_pd_spec_size_equat Value: 0, minimum: 0.0, maximum
- Parameter: paramete.sav:SB-G65-After:_pd_spec_size_thick Value: 0, minimum: 0.0, maximum
- Parameter: paramete.sav:SB-G65-After:_pd_spec_size_radius Value: 0, minimum: 0.0, maximu
- Parameter: paramete.sav:SB-G65-After:_pd_spec_size_radius_y Value: 0, minimum: 0.0, maxim

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: paramete.sav:SB-G65-After:layer1:_riet_par_spec_layer_thickness Value: 1.0E7, m
- Parameter: paramete.sav:SB-G65-After:layer1:_reflectivity_layer_critical_qc Value: 0.04, minim
- Parameter: paramete.sav:SB-G65-After:layer1:_reflectivity_layer_absorption Value: 2.0E-7, min
- Parameter: paramete.sav:SB-G65-After:layer1:_reflectivity_layer_roughness Value: 2.0, minimu

Parameter loop informations :
Parameter loop number : 0
- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of Fe2.00 Value: 0.10361261, m
- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of Fe4.00 Value: 0.09879181, m
- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of ferrite Value: 0.79759556, mi

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

Parameter loop informations :
Parameter loop number : 0
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol0 Value: 120.63
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol1 Value: -2.613
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol2 Value: 0.032
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol3 Value: -2.078
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol4 Value: 5.602

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: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:_pd_proc_intensity_

Parameter loop informations :
Parameter loop number : 0
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:_riet_par_2-theta_o

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: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Bragg-Brentano:_di
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Bragg-Brentano:_di

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_convoluted, false
_riet_par_asymmetry_truncation, 0.4

Parameter loop informations :
Parameter loop number : 0
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa

Parameter loop number : 1
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa

Parameter loop number : 2
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:Caglioti PV:_riet_pa
- Parameter: paramete.sav: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: paramete.sav:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):_pd_meas_counts_moni
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:SB-G65.xrdml(0):_riet_par_spec_displac_
- Parameter: paramete.sav: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 weigth neutron scattering neu
1) Fe Fe 2.0 1.0 0 0 0 2 -1.1149117 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: 0.5255255255255254
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 5446.462153690649 184.77011 0.004382993
2) 1 0 1 8 10871.662698426388 184.77011 0.004382993
3) 2 0 0 4 4138.590050693494 184.77011 0.004382993
4) 0 0 2 2 2058.3448697657027 184.77011 0.004382993
5) 1 2 1 8 6820.043884326234 184.77011 0.004382993
6) 2 1 1 8 6820.043884326234 184.77011 0.004382993
7) 1 1 2 8 6800.837803824398 184.77011 0.004382993
8) 2 2 0 4 2979.3107731533296 184.77011 0.004382993
9) 2 0 2 8 5943.007063765376 184.77011 0.004382993
10) 1 3 0 4 2715.4924334862403 184.77011 0.004382993
11) 3 1 0 4 2715.4924334862403 184.77011 0.004382993
12) 3 0 1 8 5428.631076516575 184.77011 0.004382993
13) 1 0 3 8 5410.066816404758 184.77011 0.004382993
14) 2 2 2 8 5119.934387965842 184.77011 0.004382993
15) 2 3 1 8 4976.54557439149 184.77011 0.004382993
16) 3 2 1 8 4976.54557439149 184.77011 0.004382993
17) 1 3 2 8 4975.1237090022605 184.77011 0.004382993
18) 3 1 2 8 4975.1237090022605 184.77011 0.004382993
19) 1 2 3 8 4972.835567033542 184.77011 0.004382993
20) 2 1 3 8 4972.835567033542 184.77011 0.004382993
21) 4 0 0 4 2475.0848261170077 184.77011 0.004382993
22) 0 0 4 2 1238.243919268576 184.77011 0.004382993

String informations (CIF term, value) :
_chemical_name_common, Martensite
_chemical_formula_sum, Phase unknown
_symmetry_cell_setting, tetragonal
_symmetry_Int_Tables_number, 82
_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: paramete.sav:SB-G65-After:Martensite:_cell_length_a Value: 2.9111097, minimum:
- Parameter: paramete.sav:SB-G65-After:Martensite:_cell_length_b Value: 2.9111097, minimum:
- Parameter: paramete.sav:SB-G65-After:Martensite:_cell_length_c Value: 2.894226, minimum: 5
- Parameter: paramete.sav:SB-G65-After:Martensite:_cell_angle_alpha Value: 90, minimum: 90.0
- Parameter: paramete.sav:SB-G65-After:Martensite:_cell_angle_beta Value: 90, minimum: 90.0,
- Parameter: paramete.sav:SB-G65-After:Martensite:_cell_angle_gamma Value: 90, minimum: 90
- Parameter: paramete.sav:SB-G65-After:Martensite:_riet_par_strain_thermal Value: 0, minimum
- Parameter: paramete.sav:SB-G65-After:Martensite:_exptl_absorpt_cryst_size Value: 0, minimun
- Parameter: paramete.sav:SB-G65-After:Martensite:_riet_par_phase_scale_factor Value: 1.0, mi

Subordinate objects :
 Subordinate object number 0 :

Object: none tex

 Subordinate object number 1 :

Object: Delf

 Subordinate object number 2 :

Object: Isotropic

Parameter informations :
- Parameter: paramete.sav:SB-G65-After:Martensite:Isotropic:_riet_par_cryst_size Value: 184.77
- Parameter: paramete.sav:SB-G65-After:Martensite:Isotropic:_riet_par_rs_microstrain Value: 0.0

 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, d

Parameter informations :
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_occupancy
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_fract_x Valu
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_fract_y Valu

- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_fract_z Valu
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_B_iso_or_e
  Parameters bounded to this parameter:
    paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv

- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_aniso_B_11
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_aniso_B_22
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_aniso_B_33
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_aniso_B_23
- Parameter: paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_aniso_B_13
- Parameter: paramete.sav: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 | +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 | +y | -x
9) -x | +y | -z
10) -z | +y | +x
11) +z | +x | +y
12) +y | +z | +x
13) -y | -z | +x
14) +z | -x | -y
15) -y | +z | -x
16) -z | -x | +y
17) -z | +x | -y
18) +y | -z | -x
19) +y | +x | -z
20) -y | -x | -z
21) -x | +z | +y
22) -x | -z | -y
23) +z | -y | +x
24) -z | -y | -x
25) -x | -y | -z
26) +y | -x | -z
27) +x | +y | -z
28) -y | +x | -z
29) -x | +z | -y
30) -x | +y | +z
31) -x | -z | +y
32) -z | -y | +x
33) +x | -y | +z
34) +z | -y | -x
35) -z | -x | -y
36) -y | -z | -x
37) +y | +z | -x
38) -z | +x | +y
39) +y | -z | +x
40) +z | +x | -y
41) +z | -x | +y
42) -y | +z | +x
43) -y | -x | +z
44) +y | +x | +z

45) +x | -z | -y
46) +x | +z | +y
47) -z | +y | -x
48) +z | +y | +x
49) +x | +y+0.5 | +z+0.5
50) -y | +x+0.5 | +z+0.5
51) -x | -y+0.5 | +z+0.5
52) +y | -x+0.5 | +z+0.5
53) +x | -z+0.5 | +y+0.5
54) +x | -y+0.5 | -z+0.5
55) +x | +z+0.5 | -y+0.5
56) +z | +y+0.5 | -x+0.5
57) -x | +y+0.5 | -z+0.5
58) -z | +y+0.5 | +x+0.5
59) +z | +x+0.5 | +y+0.5
60) +y | +z+0.5 | +x+0.5
61) -y | -z+0.5 | +x+0.5
62) +z | -x+0.5 | -y+0.5
63) -y | +z+0.5 | -x+0.5
64) -z | -x+0.5 | +y+0.5
65) -z | +x+0.5 | -y+0.5
66) +y | -z+0.5 | -x+0.5
67) +y | +x+0.5 | -z+0.5
68) -y | -x+0.5 | -z+0.5
69) -x | +z+0.5 | +y+0.5
70) -x | -z+0.5 | -y+0.5
71) +z | -y+0.5 | +x+0.5
72) -z | -y+0.5 | -x+0.5
73) -x | -y+0.5 | -z+0.5
74) +y | -x+0.5 | -z+0.5
75) +x | +y+0.5 | -z+0.5
76) -y | +x+0.5 | -z+0.5
77) -x | +z+0.5 | -y+0.5
78) -x | +y+0.5 | +z+0.5
79) -x | -z+0.5 | +y+0.5
80) -z | -y+0.5 | +x+0.5
81) +x | -y+0.5 | +z+0.5
82) +z | -y+0.5 | -x+0.5
83) -z | -x+0.5 | -y+0.5
84) -y | -z+0.5 | -x+0.5
85) +y | +z+0.5 | -x+0.5
86) -z | +x+0.5 | +y+0.5
87) +y | -z+0.5 | +x+0.5
88) +z | +x+0.5 | -y+0.5
89) +z | -x+0.5 | +y+0.5
90) -y | +z+0.5 | +x+0.5
91) -y | -x+0.5 | +z+0.5
92) +y | +x+0.5 | +z+0.5

93) +x | -z+0.5 | -y+0.5
94) +x | +z+0.5 | +y+0.5
95) -z | +y+0.5 | -x+0.5
96) +z | +y+0.5 | +x+0.5
97) +x+0.5 | +y | +z+0.5
98) -y+0.5 | +x | +z+0.5
99) -x+0.5 | -y | +z+0.5
100) +y+0.5 | -x | +z+0.5
101) +x+0.5 | -z | +y+0.5
102) +x+0.5 | -y | -z+0.5
103) +x+0.5 | +z | -y+0.5
104) +z+0.5 | +y | -x+0.5
105) -x+0.5 | +y | -z+0.5
106) -z+0.5 | +y | +x+0.5
107) +z+0.5 | +x | +y+0.5
108) +y+0.5 | +z | +x+0.5
109) -y+0.5 | -z | +x+0.5
110) +z+0.5 | -x | -y+0.5
111) -y+0.5 | +z | -x+0.5
112) -z+0.5 | -x | +y+0.5
113) -z+0.5 | +x | -y+0.5
114) +y+0.5 | -z | -x+0.5
115) +y+0.5 | +x | -z+0.5
116) -y+0.5 | -x | -z+0.5
117) -x+0.5 | +z | +y+0.5
118) -x+0.5 | -z | -y+0.5
119) +z+0.5 | -y | +x+0.5
120) -z+0.5 | -y | -x+0.5
121) -x+0.5 | -y | -z+0.5
122) +y+0.5 | -x | -z+0.5
123) +x+0.5 | +y | -z+0.5
124) -y+0.5 | +x | -z+0.5
125) -x+0.5 | +z | -y+0.5
126) -x+0.5 | +y | +z+0.5
127) -x+0.5 | -z | +y+0.5
128) -z+0.5 | -y | +x+0.5
129) +x+0.5 | -y | +z+0.5
130) +z+0.5 | -y | -x+0.5
131) -z+0.5 | -x | -y+0.5
132) -y+0.5 | -z | -x+0.5
133) +y+0.5 | +z | -x+0.5
134) -z+0.5 | +x | +y+0.5
135) +y+0.5 | -z | +x+0.5
136) +z+0.5 | +x | -y+0.5
137) +z+0.5 | -x | +y+0.5
138) -y+0.5 | +z | +x+0.5
139) -y+0.5 | -x | +z+0.5
140) +y+0.5 | +x | +z+0.5

141) +x+0.5 | -z | -y+0.5
142) +x+0.5 | +z | +y+0.5
143) -z+0.5 | +y | -x+0.5
144) +z+0.5 | +y | +x+0.5
145) +x+0.5 | +y+0.5 | +z
146) -y+0.5 | +x+0.5 | +z
147) -x+0.5 | -y+0.5 | +z
148) +y+0.5 | -x+0.5 | +z
149) +x+0.5 | -z+0.5 | +y
150) +x+0.5 | -y+0.5 | -z
151) +x+0.5 | +z+0.5 | -y
152) +z+0.5 | +y+0.5 | -x
153) -x+0.5 | +y+0.5 | -z
154) -z+0.5 | +y+0.5 | +x
155) +z+0.5 | +x+0.5 | +y
156) +y+0.5 | +z+0.5 | +x
157) -y+0.5 | -z+0.5 | +x
158) +z+0.5 | -x+0.5 | -y
159) -y+0.5 | +z+0.5 | -x
160) -z+0.5 | -x+0.5 | +y
161) -z+0.5 | +x+0.5 | -y
162) +y+0.5 | -z+0.5 | -x
163) +y+0.5 | +x+0.5 | -z
164) -y+0.5 | -x+0.5 | -z
165) -x+0.5 | +z+0.5 | +y
166) -x+0.5 | -z+0.5 | -y
167) +z+0.5 | -y+0.5 | +x
168) -z+0.5 | -y+0.5 | -x
169) -x+0.5 | -y+0.5 | -z
170) +y+0.5 | -x+0.5 | -z
171) +x+0.5 | +y+0.5 | -z
172) -y+0.5 | +x+0.5 | -z
173) -x+0.5 | +z+0.5 | -y
174) -x+0.5 | +y+0.5 | +z
175) -x+0.5 | -z+0.5 | +y
176) -z+0.5 | -y+0.5 | +x
177) +x+0.5 | -y+0.5 | +z
178) +z+0.5 | -y+0.5 | -x
179) -z+0.5 | -x+0.5 | -y
180) -y+0.5 | -z+0.5 | -x
181) +y+0.5 | +z+0.5 | -x
182) -z+0.5 | +x+0.5 | +y
183) +y+0.5 | -z+0.5 | +x
184) +z+0.5 | +x+0.5 | -y
185) +z+0.5 | -x+0.5 | +y
186) -y+0.5 | +z+0.5 | +x
187) -y+0.5 | -x+0.5 | +z
188) +y+0.5 | +x+0.5 | +z

189) +x+0.5 | -z+0.5 | -y
190) +x+0.5 | +z+0.5 | +y
191) -z+0.5 | +y+0.5 | -x
192) +z+0.5 | +y+0.5 | +x

Atom list

n label symbol quantity occupancy x y z multiplicity B radius weigth neutron scattering neu
1) Fe Fe 4.0 1.0 0 0 0 4 -1.1149117 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: 0.5255255255255254
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 44005.824810054335 238.97253 0.0040923166
2) 2 0 0 6 29805.267250901954 238.97253 0.0040923166
3) 2 2 0 12 43992.6060332299 238.97253 0.0040923166
4) 3 1 1 24 75472.13320270243 238.97253 0.0040923166
5) 2 2 2 8 24159.775315802337 238.97253 0.0040923166
6) 4 0 0 6 16089.648358095024 238.97253 0.0040923166
7) 3 3 1 24 61133.61364889287 238.97253 0.0040923166
8) 4 2 0 24 60460.81843544704 238.97253 0.0040923166
9) 4 2 2 24 59363.33003543833 238.97253 0.0040923166

String informations (CIF term, value) :
_chemical_name_common, Austenite
_chemical_formula_sum, Phase unknown
_symmetry_cell_setting, cubic
_symmetry_Int_Tables_number, 225
_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: paramete.sav:SB-G65-After:Austenite:_cell_length_a Value: 3.6190095, minimum: 5
- Parameter: paramete.sav:SB-G65-After:Austenite:_cell_length_b Value: 3.6190095, minimum: 5
- Parameter: paramete.sav:SB-G65-After:Austenite:_cell_length_c Value: 3.6190095, minimum: 5
- Parameter: paramete.sav:SB-G65-After:Austenite:_cell_angle_alpha Value: 90, minimum: 90.0,

- Parameter: paramete.sav:SB-G65-After:Austenite:_cell_angle_beta Value: 90, minimum: 90.0, r
- Parameter: paramete.sav:SB-G65-After:Austenite:_cell_angle_gamma Value: 90, minimum: 90.
- Parameter: paramete.sav:SB-G65-After:Austenite:_riet_par_strain_thermal Value: 0, minimum:
- Parameter: paramete.sav:SB-G65-After:Austenite:_exptl_absorpt_cryst_size Value: 0.3012927,
- Parameter: paramete.sav:SB-G65-After:Austenite:_riet_par_phase_scale_factor Value: 0.90749

Subordinate objects :
Subordinate object number 0 :

Object: none tex

Subordinate object number 1 :

Object: Delf

Subordinate object number 2 :

Object: Isotropic

Parameter informations :
- Parameter: paramete.sav:SB-G65-After:Austenite:Isotropic:_riet_par_cryst_size Value: 238.972
- Parameter: paramete.sav:SB-G65-After:Austenite:Isotropic:_riet_par_rs_microstrain Value: 0.00

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: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_occupancy V
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_fract_x Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_fract_y Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_fract_z Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_B_iso_or_equ
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_11
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_22
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_33
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_23
- Parameter: paramete.sav:SB-G65-After:Austenite:Atomic Structure:Fe:_atom_site_aniso_B_13
- Parameter: paramete.sav:SB-G65-After:Austenite: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 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 | +y | -x
9) -x | +y | -z
10) -z | +y | +x
11) +z | +x | +y
12) +y | +z | +x

13) -y | -z | +x
14) +z | -x | -y
15) -y | +z | -x
16) -z | -x | +y
17) -z | +x | -y
18) +y | -z | -x
19) +y | +x | -z
20) -y | -x | -z
21) -x | +z | +y
22) -x | -z | -y
23) +z | -y | +x
24) -z | -y | -x
25) -x | -y | -z
26) +y | -x | -z
27) +x | +y | -z
28) -y | +x | -z
29) -x | +z | -y
30) -x | +y | +z
31) -x | -z | +y
32) -z | -y | +x
33) +x | -y | +z
34) +z | -y | -x
35) -z | -x | -y
36) -y | -z | -x
37) +y | +z | -x
38) -z | +x | +y
39) +y | -z | +x
40) +z | +x | -y
41) +z | -x | +y
42) -y | +z | +x
43) -y | -x | +z
44) +y | +x | +z
45) +x | -z | -y
46) +x | +z | +y
47) -z | +y | -x
48) +z | +y | +x
49) +x+0.5 | +y+0.5 | +z+0.5
50) -y+0.5 | +x+0.5 | +z+0.5
51) -x+0.5 | -y+0.5 | +z+0.5
52) +y+0.5 | -x+0.5 | +z+0.5
53) +x+0.5 | -z+0.5 | +y+0.5
54) +x+0.5 | -y+0.5 | -z+0.5
55) +x+0.5 | +z+0.5 | -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 weigth neutron scattering neu
1) Fe Fe 2.0 1.0 0 0 0 2 -0.325792 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: 0.5255255255255254
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	14736.987128626875	271.06784	0.0032012293
2)	2	0	0	6	5075.621924052633	271.06784	0.0032012293
3)	2	1	1	24	15211.994325836982	271.06784	0.0032012293
4)	2	2	0	12	6040.563490949909	271.06784	0.0032012293
5)	3	1	0	24	10029.555501895156	271.06784	0.0032012293
6)	2	2	2	8	2875.9198673229057	271.06784	0.0032012293
7)	3	2	1	48	15284.965154345537	271.06784	0.0032012293
8)	4	0	0	6	1734.041860543989	271.06784	0.0032012293

String informations (CIF term, value) :
_chemical_name_common, Ferrite
_chemical_formula_sum,
_symmetry_cell_setting, cubic
_symmetry_Int_Tables_number, 229
_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: paramete.sav:SB-G65-After:Ferrite:_cell_length_a Value: 2.8771641, minimum: 5.0
- Parameter: paramete.sav:SB-G65-After:Ferrite:_cell_length_b Value: 2.8771641, minimum: 5.0
- Parameter: paramete.sav:SB-G65-After:Ferrite:_cell_length_c Value: 2.8771641, minimum: 5.0,
- Parameter: paramete.sav:SB-G65-After:Ferrite:_cell_angle_alpha Value: 90, minimum: 90.0, ma
- Parameter: paramete.sav:SB-G65-After:Ferrite:_cell_angle_beta Value: 90, minimum: 90.0, max
- Parameter: paramete.sav:SB-G65-After:Ferrite:_cell_angle_gamma Value: 90, minimum: 90.0, r
- Parameter: paramete.sav:SB-G65-After:Ferrite:_riet_par_strain_thermal Value: 0, minimum: -0.
- Parameter: paramete.sav:SB-G65-After:Ferrite:_exptl_absorpt_cryst_size Value: 0, minimum: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:_riet_par_phase_scale_factor Value: 1.0, minim

Subordinate objects :
Subordinate object number 0 :

Object: none tex

Subordinate object number 1 :

Object: Delf

Subordinate object number 2 :

Object: Isotropic

Parameter informations :
- Parameter: paramete.sav:SB-G65-After:Ferrite:Isotropic:_riet_par_cryst_size Value: 271.06784
- Parameter: paramete.sav:SB-G65-After:Ferrite:Isotropic:_riet_par_rs_microstrain Value: 0.0032

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: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_occupancy Valu
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_fract_x Value: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_fract_y Value: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_fract_z Value: 0
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_11 Va
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_22 Va
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_33 Va
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_23 Va
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_13 Va
- Parameter: paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_aniso_B_12 Va

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 :