Jacobi matrix :

#	0	1	2	3	4	5	6	7	8	9
0	76289.19									
1	-76307.94	1429351.6								
2	-27797.53	-89986.84	20384.576							
3	1084.8103	1756.8812	-642.68304	84.64521						
4	138423.4	122545.54	-73147.875	7359.519	767779.25					
5	4526.418	5320.7144	-2502.5122	113.45912	11280.298	1299.6965				
6	-61132.184	-130054.336	38887.168	37.98319	5163.184	-477.12354	677594			
7	849608.75	599117.9	-435204.97	-2573.1875	-223642.6	1897.1298	-789013			
8	-16.725811	-120.68188	18.078701	-0.52258486	-35.026913	2.673837	18.249			
9	-0.7794647	14.717323	-0.93805695	-0.018772243	-2.2871065	0.020816306	1.46			
10	-528189.0	74294.15	232466.12	-1825.7523	-193868.83	5627.0366	-40955.			
11	-460762.8	156393.9	194939.62	-1915.4133	-212164.77	5379.027	-52779.2			

Correlation matrix:

#	0	1	2	3	4	5	6	7	8	9
0	1.0									
1	-1.0576816	1.0								
2	-1.0900635	-1.2873312	1.0							
3	-1.2307396	1.5764332	3.6688137	1.0						
4	-0.10103819	-0.17593877	0.076434724	25.19288	1.0					
5	0.17397144	-0.7593415	-1.2271056	-0.6188008	-3.112748	-1.0				
6	0.10107788	-0.02548505	0.15464588	-0.17826833	-0.1968477	1.012194	-1.0			
7	0.069633745	-0.2168203	0.01270721	-0.0042098416	0.08631411	-0.93510777	-0			
8	0.5030971	0.4583249	0.04598755	-1.3634825	0.8886687	1.3540202	-0.916			
9	0.022591498	0.04650142	0.09506539	-0.07622326	0.15144613	0.37380663	-0.			
10	-0.012108134	0.06262338	0.06513416	0.014862346	0.24253394	0.08535216	-0			
11	-0.010353442	0.069391765	0.025627911	-0.010443795	0.14931893	0.063513465				

Correlation matrix from Choleski decomposition :

#	0	1	2	3	4	5	6	7	8	9
0	1.0									
1	-1.0576816	1.0								
2	-1.0900635	-1.2873312	1.0							
3	-1.2307396	1.5764332	3.6688137	1.0						
4	-0.10103819	-0.17593877	0.076434724	25.19288	1.0					
5	0.17397144	-0.7593415	-1.2271056	-0.6188008	-3.112748	-1.0				
6	0.10107788	-0.02548505	0.15464588	-0.17826833	-0.1968477	1.012194	-1.0			
7	0.069633745	-0.2168203	0.01270721	-0.0042098416	0.08631411	-0.93510777	-0			
8	0.5030971	0.4583249	0.04598755	-1.3634825	0.8886687	1.3540202	-0.916			
9	0.022591498	0.04650142	0.09506539	-0.07622326	0.15144613	0.37380663	-0.			
10	-0.012108134	0.06262338	0.06513416	0.014862346	0.24253394	0.08535216	-0			
11	-0.010353442	0.069391765	0.025627911	-0.010443795	0.14931893	0.063513465				

Analysis title: Put a title here

Refined parameters:

0 paramete.sav:SB-G65-After:layer1:Volume fraction of Fe2.00 value:0.29344478 error:0.7835961
1 paramete.sav:SB-G65-After:layer1:Volume fraction of Fe4.00 value:0.056580514 error:0.15098
2 paramete.sav:SB-G65-After:layer1:Volume fraction of ferrite value:0.6499747 error:1.7327243
3 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol0 value:127.55769 error:0.5
4 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol1 value:-3.0465617 error:0.
5 paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:_pd_proc_intensity_incident val
6 paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:_riet_par_2-theta_offset0 value
7 paramete.sav:SB-G65-After:Ferrite:_cell_length_a value:2.8728325 error:4.8002214E-4
8 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size0 value:254.46109 erro
9 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size1 value:-97.37789 error
10 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_aniso_microstrain0 value:-0.0019117
11 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_aniso_microstrain1 value:-0.0024406

Refinement final output indices:
Global Rwp: 0.21160439
Global Rp: 0.13416685
Global Rwpb (no background): 8.691372
Global Rpb (no background): 0.14555074
Total Energy: 0.0

Refinement final output indices for single samples:
Sample SB-G65-After :
Sample Rwp: 0.21160439
Sample Rp: 0.13416685
Sample Rwpb (no background): 8.691372
Sample Rpb (no background): 0.14555074

Refinement final output indices for single datasets:
DataSet SB-G65-after :
DataSet Rwp: 0.21160439
DataSet Rp: 0.13416685
DataSet Rwpb (no background): 8.691372
DataSet Rpb (no background): 0.14555074

Refinement final output indices for single spectra:
Datafile SB-G65.xrdml(0) : Rwp: 0.21160439, Rp: 0.13416685, Rwpb: 8.691372, Rpb: 0.1455507

Sample:SB-G65-After

Phases:
Martensite
Density: 7.731316112748702
Qc: 0.055225013923017034
Austenite
Density: 7.830600750084675

Qc: 0.05557847926675985
Ferrite
Density: 7.822549479375717
Qc: 0.055549899565310444

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 13:05:17 BST 2013
_computing_structure_refinement, Maud, version 2.33
_refine_ls_R_factor_all, 0.13416685
_refine_ls_wR_factor_all, 0.21160439
_refine_ls_goodness_of_fit_all, 0.10671681
_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, 18577.42
_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, maximur
- 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, maxir

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: 0.29344478, m
- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of Fe4.00 Value: 0.056580514,
- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of ferrite Value: 0.6499747, mini

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: 127.5
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol1 Value: -3.046

- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol2 Value: 0.040
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol3 Value: -2.499
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol4 Value: 5.940

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 -1.8361543 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 5912.805446792312 618.8043630293826 0.008173502011128354
2) 1 0 1 8 11795.111850585361 259.58666412553686 0.004202504288741284
3) 2 0 0 4 4890.045883616761 698.2725341148155 0.0035351412
4) 0 0 2 2 2430.818342630723 769.1361706828332 0.011114947572356456
5) 1 2 1 8 8781.654360192462 376.6360147480698 0.01052944826338699
6) 2 1 1 8 8781.654360192462 439.30495191565876 0.002520230716277169
7) 1 1 2 8 8761.543099486593 318.35136708627044 0.0015207469007607246
8) 2 2 0 4 4182.289612798663 618.8043630293826 0.008173502011128354
9) 2 0 2 8 8355.959823547784 259.58666412553686 0.004202504288741284
10) 1 3 0 4 4158.759152444054 624.2303945033185 0.010051592580827814
11) 3 1 0 4 4158.759152444054 715.0975905448007 0.008302441926886981
12) 3 0 1 8 8318.662606077329 531.8423360714523 0.0027851451464778925
13) 1 0 3 8 8328.938251288075 594.1327724147934 0.00906055910261526

14) 2 2 2 8 8582.730828603422 262.72429905007124 0.007870039574929065
15) 2 3 1 8 9089.32837145774 488.2055756507301 0.010716267910786035
16) 3 2 1 8 9089.32837145774 545.985555953098 0.00260043047909996
17) 1 3 2 8 9109.649871622167 290.7277177590609 0.009142459803875147
18) 3 1 2 8 9109.649871622167 336.5448268184494 0.0014544088917155663
19) 1 2 3 8 9144.086956770556 298.9910900016182 0.00334729702225132
20) 2 1 3 8 9144.086956770556 310.2787958289713 0.0031478569890573673
21) 4 0 0 4 4932.279430134307 698.2725341148155 0.0035351412
22) 0 0 4 2 2505.184549435762 769.1361706828332 0.011114947572356456

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: 2.8939567, minimum:
- Parameter: paramete.sav:SB-G65-After:Martensite:_cell_length_b Value: 2.8939567, minimum:
- Parameter: paramete.sav:SB-G65-After:Martensite:_cell_length_c Value: 2.8644533, minimum:
- 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, minimur
- Parameter: paramete.sav:SB-G65-After:Martensite:_riet_par_phase_scale_factor Value: 1.0383

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: paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size0 Value
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size1 Value
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size2 Value
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size3 Value
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size4 Value

Parameter loop number : 1
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain0 Va
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain1 Va
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain2 Va
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain3 Va
- Parameter: paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain4 Va

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: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_eq
- 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 1.0 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 34531.82945956095 196.2523225128317 0.0018667067882022427

2) 2 0 0 6 21573.251667032207 201.34314123080432 0.003233231
3) 2 2 0 12 23050.074220497678 197.52502719218216 0.002286239565242562
4) 3 1 1 24 31034.614923039728 198.9449869586878 0.002677830570139118
5) 2 2 2 8 9163.828570960974 196.2523225128317 0.0018667067882022427
6) 4 0 0 6 4418.100321613788 201.34314123080432 0.003233231
7) 3 3 1 24 13175.108657929923 197.15484993086605 0.0021725857935785643
8) 4 2 0 24 12019.252848385626 198.89954824608614 0.002666190585004284
9) 4 2 2 24 8543.627937890753 197.52502719230756 0.0022862395652425626

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: 3.6183012, minimum: 5
- Parameter: paramete.sav:SB-G65-After:Austenite:_cell_length_b Value: 3.6183012, minimum: 5
- Parameter: paramete.sav:SB-G65-After:Austenite:_cell_length_c Value: 3.6183012, 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: 0.3087943,
- Parameter: paramete.sav:SB-G65-After:Austenite:_riet_par_phase_scale_factor Value: 3.00423

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: paramete.sav:SB-G65-After:Austenite:Popa rules:_riet_par_anisocryst_size0 Value
- Parameter: paramete.sav:SB-G65-After:Austenite:Popa rules:_riet_par_anisocryst_size1 Value

Parameter loop number : 1
- Parameter: paramete.sav:SB-G65-After:Austenite:Popa rules:_riet_par_aniso_microstrain0 Valu
- Parameter: paramete.sav: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: 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 1.0 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 12533.586271287139 270.19639221209644 0.002192194912019798
2) 2 0 0 6 3673.7416803475544 191.51988116123766 0.0019117347
3) 2 1 1 24 9373.083448837495 270.19639220951234 0.0021921949120197975
4) 2 2 0 12 3169.0952143017425 270.19639221209644 0.002192194912019798
5) 3 1 0 24 4480.8661580514145 219.84342513954684 0.0020171974598587497
6) 2 2 2 8 1094.2734375818252 296.4218958917954 0.0022780214050763348
7) 3 2 1 48 4953.5437648510215 270.1963922108362 0.002192194912019798
8) 4 0 0 6 478.66909772908286 191.51988116123766 0.0019117347

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: 2.8728325, minimum: 5.0
- Parameter: paramete.sav:SB-G65-After:Ferrite:_cell_length_b Value: 2.8728325, minimum: 5.0
- Parameter: paramete.sav:SB-G65-After:Ferrite:_cell_length_c Value: 2.8728325, 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,
- 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: 1.3276076

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: paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size0 Value: 25
- Parameter: paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size1 Value: -9

Parameter loop number : 1

- Parameter: paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_aniso_microstrain0 Value:
- Parameter: paramete.sav: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: 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 :