Jacobi matrix :

#	0	1	2	3	4	5	6	7	8	9
0	2229416.8									
1	-211736.25	62829.38								
2	3608.1316	-1349.3416	84.71496							
3	340480.4	-147319.38	7364.1616	768114.9						
4	3.7932676E7	-1.7805968E7	768153.94	8.813816E7	1.07062733E10					
5	4.7110118E9	-2.26964429E9	8.8097048E7	1.07007457E10	1.35014344E12	1.7497576E				
6	6.2321145E11	-2.99028972E11	1.07033907E10	1.35041109E12	1.75100783E14	2.31666				
7	19837.484	-1944.6616	246.28918	25097.02	2868668.8	3.50601504E8	4.472			
8	-98475.23	26894.525	683.8913	74726.22	8972828.0	1.13392269E9	1.4818			
9	-5.1037372E7	2.1347046E7	-1136398.4	-1.12110512E8	-1.27310592E10	-1.54780081E				
10	-2.3856654E7	1.0203337E7	-566836.5	-5.4717888E7	-6.0981499E9	-7.288699E11				
11	-93.52664	25.227657	-0.615061	-40.162838	-2686.9434	-148838.92	-38306			
12	-14.406687	3.7492359	-0.021735672	-0.7747224	-21.786205	-1011.6334	-272			
13	30.034193	-8.047814	0.17753483	11.054225	684.5496	30111.66	-16554			
14	-2.1436465	1.4069729	-0.15158452	-12.638912	-1104.4781	-94667.05	-7350			
15	-12.861102	3.2488122	-0.057953935	-3.2325842	-160.80576	-1303.001	1661			
16	-4297631.5	167701.28	6975.6006	1133798.6	1.53930768E8	1.86885939E10	2.			
17	-1784312.1	953217.7	-34976.668	-4089508.2	-4.87909312E8	-5.9093574E10	-7.			
18	-5943556.5	-1934113.6	112347.79	1.3990598E7	1.72170637E9	2.09859461E11				
19	-6865141.5	2906928.8	-111424.055	-1.2618282E7	-1.47316966E9	-1.76535683E11				
20	-7726428.0	-411908.84	36551.016	4710519.5	5.8614502E8	6.8374045E10	7.3			
21	-95584.85	29337.459	-1297.5474	-143706.47	-1.7384776E7	-2.20526438E9	-2.8			
22	405735.9	-425573.03	-2241.58	-210502.7	-2.1796992E7	-2.42550989E9	-2.84			
23	-59.682182	32.157406	-0.29220596	-21.517406	-1822.7766	-173276.11	-1.79			
24	6.187418	-1.0612355	-0.019833282	-1.8986312	-171.84586	-15629.131	-1445			
25	10050.366	1337945.4	-14219.573	-1179817.2	-1.04760736E8	-9.9957053E9	-1.			
26	67977.12	158504.31	-681.3834	-74672.33	-8549153.0	-1.01587763E9	-1.246			
27	752.86285	-3348.6794	-118.476425	-12300.315	-1358680.5	-1.56595152E8	-1.8			

Correlation matrix:

#	0	1	2	3	4	5	6	7	8	9
0	1.0									
1	0.28317118	-1.0								
2	0.40395924	-0.8031095	-1.0							
3	-0.64525306	-1.2466481	-0.7853578	-1.0						
4	0.6271497	-0.6292195	-1.0060226	-0.6524996	-1.0					
5	0.11504606	3.4942248	3.6067724	3.620772	0.88701665	1.0				
6	-0.61251307	-2.6776247	-2.5688002	-2.4491284	-0.3040602	-1.1340234	1.0			
7	0.24393786	-0.04643079	-0.14085808	-0.13104339	-0.1470407	0.8049159	-0.68			
8	-3.3144026	-1.4605658	-0.0110524325	-0.12361315	0.17889169	-1.7136948	1.29			
9	-3.9388425	-2.0688694	-0.30781808	-0.46219563	-0.058489952	-0.6312107	0.40			
10	4.606639	2.745153	0.3744012	1.12114	-0.08744915	1.1847738	-0.76697			

11	3.3729405	2.1122072	0.38396105	0.9000333	0.04205235	0.88555807	-0.80	
12	1.9286962	0.89161354	0.065028824	0.0904278	-0.03934627	0.8588433	-0.7	
13	2.9429858	1.9816883	0.40521184	0.96917623	0.06774128	0.62920517	-0.5	
14	1.0192261	0.6399249	0.18838668	0.20313704	0.12208611	-0.08698139	-0.1	
15	-4.399012	-2.3244693	-0.21692435	-0.668466	0.1393051	-1.6917347	1.2711	
16	-2.202517	-1.1546304	-0.13632149	-0.29132536	0.026500707	-1.049706	0.896	
17	-4.014488	-2.8684397	-0.5301827	-1.6473007	0.03580179	-1.5329397	1.4028	
18	0.60103035	1.0292603	0.54890794	0.8764145	0.3838002	-1.5106722	1.024	
19	3.8493042	2.805574	0.5403357	1.6485775	-0.015669206	1.3751875	-1.279	
20	-3.4007382	-2.9835317	-0.7778237	-2.0807543	-0.16895835	-0.3002597	0.492	
21	-1.7521019	-2.1689603	-1.1600344	-1.4724355	-0.90132606	3.2152882	-2.170	
22	-2.5278132	-2.2458518	-0.5513547	-1.6247442	-0.06923238	-0.42510727	0.515	
23	4.9424667	3.2325294	0.65181094	1.482027	0.12083186	1.0560944	-1.057	
24	-1.6525245	-0.029153874	0.59005886	0.62517554	0.6132096	-2.877833	2.10	
25	1.6256633	0.7230407	-0.016048912	0.09489431	-0.12736462	1.2527578	-1.0	
26	-4.3252296	-1.9554428	0.033859536	-0.30148926	0.34204462	-3.297509	2.64	
27	4.2245293	1.9006656	-0.040561557	0.28501394	-0.34050426	3.2532725	-2.6	

Correlation matrix from Choleski decomposition :

#	0	1	2	3	4	5	6	7	8	9
0	1.0									
1	0.28317118	-1.0								
2	0.40395924	-0.8031095	-1.0							
3	-0.64525306	-1.2466481	-0.7853578	-1.0						
4	0.6271497	-0.6292195	-1.0060226	-0.6524996	-1.0					
5	0.11504606	3.4942248	3.6067724	3.620772	0.88701665	1.0				
6	-0.61251307	-2.6776247	-2.5688002	-2.4491284	-0.3040602	-1.1340234	1.0			
7	0.24393786	-0.04643079	-0.14085808	-0.13104339	-0.1470407	0.8049159	-0.68			
8	-3.3144026	-1.4605658	-0.0110524325	-0.12361315	0.17889169	-1.7136948	1.29			
9	-3.9388425	-2.0688694	-0.30781808	-0.46219563	-0.058489952	-0.6312107	0.40			
10	4.606639	2.745153	0.3744012	1.12114	-0.08744915	1.1847738	-0.76697			
11	3.3729405	2.1122072	0.38396105	0.9000333	0.04205235	0.88555807	-0.80			
12	1.9286962	0.89161354	0.065028824	0.0904278	-0.03934627	0.8588433	-0.7			
13	2.9429858	1.9816883	0.40521184	0.96917623	0.06774128	0.62920517	-0.5			
14	1.0192261	0.6399249	0.18838668	0.20313704	0.12208611	-0.08698139	-0.1			
15	-4.399012	-2.3244693	-0.21692435	-0.668466	0.1393051	-1.6917347	1.2711			
16	-2.202517	-1.1546304	-0.13632149	-0.29132536	0.026500707	-1.049706	0.896			
17	-4.014488	-2.8684397	-0.5301827	-1.6473007	0.03580179	-1.5329397	1.4028			
18	0.60103035	1.0292603	0.54890794	0.8764145	0.3838002	-1.5106722	1.024			
19	3.8493042	2.805574	0.5403357	1.6485775	-0.015669206	1.3751875	-1.279			
20	-3.4007382	-2.9835317	-0.7778237	-2.0807543	-0.16895835	-0.3002597	0.492			
21	-1.7521019	-2.1689603	-1.1600344	-1.4724355	-0.90132606	3.2152882	-2.170			
22	-2.5278132	-2.2458518	-0.5513547	-1.6247442	-0.06923238	-0.42510727	0.515			
23	4.9424667	3.2325294	0.65181094	1.482027	0.12083186	1.0560944	-1.057			
24	-1.6525245	-0.029153874	0.59005886	0.62517554	0.6132096	-2.877833	2.10			
25	1.6256633	0.7230407	-0.016048912	0.09489431	-0.12736462	1.2527578	-1.0			
26	-4.3252296	-1.9554428	0.033859536	-0.30148926	0.34204462	-3.297509	2.64			
27	4.2245293	1.9006656	-0.040561557	0.28501394	-0.34050426	3.2532725	-2.6			

Analysis title: Put a title here

Refined parameters:

0 paramete.sav:SB-G65-After:layer1:Volume fraction of Fe4.00 value:0.053580675 error:0.00309
1 paramete.sav:SB-G65-After:layer1:Volume fraction of ferrite value:0.381175 error:0.054062404
2 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol0 value:132.7425 error:3.38
3 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol1 value:-3.7946684 error:0.
4 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol2 value:0.055272195 error:
5 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol3 value:-3.720835E-4 error
6 paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol4 value:8.960496E-7 error:3
7 paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:_pd_proc_intensity_incident val
8 paramete.sav:SB-G65-After:SB-G65-after:Diffraction Instrument:_riet_par_2-theta_offset0 value
9 paramete.sav:SB-G65-After:Martensite:_cell_length_a value:2.8926795 error:8.5294707E-4
10 paramete.sav:SB-G65-After:Martensite:_cell_length_c value:2.85709 error:0.0021930747
11 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size0 value:677.6747
12 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size1 value:-456.7452
13 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size2 value:1099.3926
14 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size3 value:-274.8138
15 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_anisocryst_size4 value:-125.4320
16 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain0 value:0.00518
17 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain1 value:0.01683
18 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain2 value:-0.0129
19 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain3 value:-0.0141
20 paramete.sav:SB-G65-After:Martensite:Popa rules:_riet_par_aniso_microstrain4 value:0.01096
21 paramete.sav:SB-G65-After:Martensite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv value:
22 paramete.sav:SB-G65-After:Ferrite:_cell_length_a value:2.873945 error:4.7889075E-4
23 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size0 value:327.73447 err
24 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size1 value:-144.6539 erro
25 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_aniso_microstrain0 value:-0.0034314
26 paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_aniso_microstrain1 value:5.52056E-4
27 paramete.sav:SB-G65-After:Ferrite:Atomic Structure:Fe:_atom_site_B_iso_or_equiv value:-0.2

Refinement final output indices:
Global Rwp: 0.19880465
Global Rp: 0.11860305
Global Rwpb (no background): 7.79586
Global Rpb (no background): 0.12368371
Total Energy: 0.0

Refinement final output indices for single samples:
Sample SB-G65-After :
Sample Rwp: 0.19880465
Sample Rp: 0.11860305
Sample Rwpb (no background): 7.79586
Sample Rpb (no background): 0.12368371

Refinement final output indices for single datasets:
DataSet SB-G65-after :

DataSet Rwp: 0.19880465
DataSet Rp: 0.11860305
DataSet Rwpb (no background): 7.79586
DataSet Rpb (no background): 0.12368371

Refinement final output indices for single spectra:
Datafile SB-G65.xrdml(0) : Rwp: 0.19880465, Rp: 0.11860305, Rwpb: 7.79586, Rpb: 0.12368371

Sample:SB-G65-After

Phases:
Martensite
Density: 7.758087577935114
Qc: 0.055320545967936875
Austenite
Density: 7.829752891451307
Qc: 0.05557547030419097
Ferrite
Density: 7.8134687022852285
Qc: 0.055517647756936114

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 13:35:01 BST 2013
_computing_structure_refinement, Maud, version 2.33
_refine_ls_R_factor_all, 0.11860305
_refine_ls_wR_factor_all, 0.19880465
_refine_ls_goodness_of_fit_all, 0.10653598
_publ_contact_author_name, Luca Lutterotti
_publ_section_title, Put a title here
_pd_proc_ls_extract_int, never
_pd_proc_ls_texture_comp, never
_computing_reduce_memory_occ, true
_pd_proc_ls_theoretical_weight, false
_pd_proc_ls_extract_pos, never
_pd_proc_ls_strain_comp, never
_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, 16397.936
_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, m
- 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: 0.5652443, mi
- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of Fe4.00 Value: 0.053580675,
- Parameter: paramete.sav:SB-G65-After:layer1:Volume fraction of ferrite Value: 0.381175, minim

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: 132.74
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol1 Value: -3.794
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol2 Value: 0.055
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol3 Value: -3.720
- Parameter: paramete.sav:SB-G65-After:SB-G65-after:_riet_par_background_pol4 Value: 8.960

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 -0.8192818 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 5235.039208455003 1249.127682077458 0.008399206813394733
2) 1 0 1 8 10421.522832578366 209.61157533502032 0.004709077012011301
3) 2 0 0 4 3833.9677449085034 1092.1279698148635 0.005187216000000001
4) 0 0 2 2 1891.980526593117 1319.9663126250769 0.016419628217098657
5) 1 2 1 8 6087.304555171236 750.1728262470707 0.012303655023192332
6) 2 1 1 8 6087.304555171236 522.7592971580603 0.002764128871280975
7) 1 1 2 8 6042.843249744045 382.4450154922261 0.005289964128515643
8) 2 2 0 4 2571.958659224493 1249.127682077458 0.008399206813394733
9) 2 0 2 8 5106.375568806001 209.61157533502032 0.004709077012011301
10) 1 3 0 4 2265.1696170009045 1313.7566730543972 0.011118882884590587
11) 3 1 0 4 2265.1696170009045 983.5390594043979 0.010357469725597758
12) 3 0 1 8 4524.208854760251 748.9780431740718 0.0033789451444186836
13) 1 0 3 8 4476.341815315379 945.4713152940873 0.013608157565077399
14) 2 2 2 8 4117.145611945078 343.6192980922281 0.00935679637654439
15) 2 3 1 8 3878.708652249115 1058.1946919876611 0.012110495738690804
16) 3 2 1 8 3878.708652249115 848.348892987839 2.681099652218836E-4
17) 1 3 2 8 3871.5281495237755 446.57502905227625 0.01095850503905244
18) 3 1 2 8 3871.5281495237755 280.4843787452472 0.00198718510065292
19) 1 2 3 8 3859.878687210056 362.7551469921901 0.002355127796091011
20) 2 1 3 8 3859.878687210056 321.9609702890364 0.005837140621937628
21) 4 0 0 4 1866.863518565165 1092.1279698148635 0.005187216000000001

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: 2.8926795, minimum:
- Parameter: paramete.sav:SB-G65-After:Martensite:_cell_length_b Value: 2.8926795, minimum:
- Parameter: paramete.sav:SB-G65-After:Martensite:_cell_length_c Value: 2.85709, 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, minimu

- 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_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 -0.8192818 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 42535.88525596487 156.13226340182888 0.0011898097855989414
2) 2 0 0 6 28485.790669111302 127.14182989696118 0.002060810999999999
3) 2 2 0 12 40187.30771815589 148.88465502642458 0.0014572134328438306
4) 3 1 1 24 66648.16498367739 140.79848039106793 0.0017068074304245403
5) 2 2 2 8 21095.679234461677 156.13226340182888 0.0011898097855989414
6) 4 0 0 6 13429.18349562361 127.14182989696118 0.002060810999999999
7) 3 3 1 24 49327.6207630436 150.9926851633674 0.0013847722918190614
8) 4 2 0 24 48237.77162390221 141.05723797981776 0.0016993882854869512
9) 4 2 2 24 45273.772224189874 148.88465502571046 0.0014572134328438306

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: 3.6184318, minimum: 5
- Parameter: paramete.sav:SB-G65-After:Austenite:_cell_length_b Value: 3.6184318, minimum: 5
- Parameter: paramete.sav:SB-G65-After:Austenite:_cell_length_c Value: 3.6184318, 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: 0.4680186
- Parameter: paramete.sav:SB-G65-After:Austenite:_riet_par_phase_scale_factor Value: 3.1141

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 -0.27031678 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 14624.120379145512 351.10910702138517 0.0023947704090583723
2) 2 0 0 6 5000.619694617719 234.2359219287546 0.0034314161
3) 2 1 1 24 14882.864279630488 351.1091070175466 0.002394770409058372
4) 2 2 0 12 5869.571649794063 351.10910702138517 0.0023947704090583723
5) 3 1 0 24 9680.203744400384 276.31026856210167 0.003098439549388316
6) 2 2 2 8 2757.3244592526007 390.0668353797713 0.0019291694929051046
7) 3 2 1 48 14558.239366367001 351.10910701951315 0.0023947704090583727
8) 4 0 0 6 1640.7918459615798 234.2359219287546 0.0034314161

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: 2.873945, minimum: 5.0,
- Parameter: paramete.sav:SB-G65-After:Ferrite:_cell_length_b Value: 2.873945, minimum: 5.0,
- Parameter: paramete.sav:SB-G65-After:Ferrite:_cell_length_c Value: 2.873945, 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: 1.6610774

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: 32
- Parameter: paramete.sav:SB-G65-After:Ferrite:Popa rules:_riet_par_anisocryst_size1 Value: -1

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 :