

data\_Po5C\_293K\_Bodenmais

\_audit\_creation\_method SHELXL-97  
\_chemical\_name\_systematic  
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Nonairondecasulfide  
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\_chemical\_name\_common '5C pyrrhotite'  
\_chemical\_melting\_point ?  
\_chemical\_formula\_moiety 'Fe9.02 S10'  
\_chemical\_formula\_sum 'Fe9.02 S10'  
\_chemical\_formula\_weight 824.52

loop\_  
\_atom\_type\_symbol  
\_atom\_type\_description  
\_atom\_type\_scatter\_dispersion\_real  
\_atom\_type\_scatter\_dispersion\_imag  
\_atom\_type\_scatter\_source  
'S' 'S' 0.1246 0.1234  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'  
'Fe' 'Fe' 0.3463 0.8444  
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

\_symmetry\_cell\_setting monoclinic  
\_symmetry\_space\_group\_name\_H-M 'P 21'  
\_symmetry\_space\_group\_name\_Hall 'P 2yb'

loop\_  
\_symmetry\_equiv\_pos\_as\_xyz  
'x, y, z'  
'-x, y+1/2, -z'

\_cell\_length\_a 6.8984(13)  
\_cell\_length\_b 28.695(5)  
\_cell\_length\_c 6.8915(13)  
\_cell\_angle\_alpha 90.00  
\_cell\_angle\_beta 119.956(2)  
\_cell\_angle\_gamma 90.00  
\_cell\_volume 1181.9(4)  
\_cell\_formula\_units\_Z 4  
\_cell\_measurement\_temperature 293(2)  
\_cell\_measurement\_reflns\_used 2625  
\_cell\_measurement\_theta\_min 3.408  
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\_exptl\_crystal\_description irregular-fragment  
\_exptl\_crystal\_colour dark-gray  
\_exptl\_crystal\_size\_max 0.1393  
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\_exptl\_crystal\_density\_meas .

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_exptl_absorpt_correction_type  multi-scan
_exptl_absorpt_correction_T_min 0.310
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_exptl_absorpt_process_details  'SADABS (Bruker, 2001)'

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_diffn_radiation_monochromator  graphite
_diffn_measurement_device_type  'Bruker (Siemens) P4'
_diffn_measurement_method       '\f and \w scans'
_diffn_detector                 'SMART 1000 CCD'
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_reflns_number_total             3419
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_computing_data_collection       'SMART (Bruker, 2001)'
_computing_cell_refinement       'SAINT (Bruker, 2001)'
_computing_data_reduction        SAINT
_computing_structure_solution    'SHELXTL (Bruker, 2001)'
_computing_structure_refinement
;SHELXTL and SHELXL-97 (Sheldrick, 2008)
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_computing_molecular_graphics    ?
_computing_publication_material SHELXL-97

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

_refine_ls_structure_factor_coef Fsqd
_refine_ls_matrix_type full
_refine_ls_weighting_scheme calc
_refine_ls_weighting_details
'calc w=1/[\s^2^(Fo^2^)+(0.0421P)^2^+1.0584P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
_refine_ls_extinction_method SHELXL
_refine_ls_extinction_coef 0.00021(7)
_refine_ls_extinction_expression
'Fc*^=kFc[1+0.001xFc^2^/l^3^/sin(2\q)]^-1/4^'
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'Flack H D (1983), Acta Cryst. A39, 876-881'
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_refine_ls_number_restraints 1
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_refine_ls_R_factor_gt 0.0383
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_refine_ls_wR_factor_gt 0.1021
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_refine_ls_restrained_S_all 1.146
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_refine_ls_shift/su_mean 0.001
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_refine_diff_density_min -0.840
_refine_diff_density_rms 0.217

loop_
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_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
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_atom_site_adp_type
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_atom_site_symmetry_multiplicity
_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly

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Fe2 Fe -0.0013(12) -0.0902(2) 0.7299(13) 0.0138(14) Uani 0.468(6) 1 d P . .  
Fe3 Fe 0.5023(9) 0.11471(12) 0.7378(7) 0.0197(5) Uani 1 1 d . . .  
Fe4 Fe 0.0169(7) -0.08520(10) 0.2739(6) 0.0175(7) Uani 1 1 d . . .  
Fe5 Fe -0.0115(5) 0.01159(9) 0.7638(5) 0.0179(7) Uani 1 1 d . . .  
Fe6 Fe 0.5246(6) 0.31557(10) 0.7491(6) 0.0183(6) Uani 1 1 d . . .  
Fe7 Fe -0.0312(5) 0.01524(10) 0.2148(5) 0.0144(6) Uani 1 1 d . . .  
Fe8 Fe 0.9873(7) 0.31511(11) 0.7594(6) 0.0158(6) Uani 1 1 d . . .  
Fe9 Fe 0.0040(11) -0.18036(19) 0.7728(11) 0.0122(13) Uani 0.484(6) 1 d P . .  
Fe10 Fe -0.4724(5) 0.01479(10) 0.7775(5) 0.0152(6) Uani 1 1 d . . .  
Fe11 Fe 0.4774(6) -0.08521(9) 0.7286(6) 0.0160(6) Uani 1 1 d . . .  
Fe12 Fe 0.5061(5) 0.01973(12) 0.2355(6) 0.0146(8) Uani 0.914(6) 1 d P . .  
Fe13 Fe 0.0084(8) 0.11612(12) 0.2538(9) 0.0199(6) Uani 1 1 d . . .  
Fe14 Fe 0.4979(5) 0.21004(12) 0.2322(7) 0.0160(9) Uani 0.891(6) 1 d P . .  
Fe15 Fe 0.0139(4) 0.21795(10) 0.2767(6) 0.0151(6) Uani 1 1 d . . .  
Fe16 Fe 0.0278(4) 0.21488(9) 0.7464(6) 0.0133(5) Uani 1 1 d . . .  
Fe17 Fe 0.4978(6) -0.18681(10) 0.7408(8) 0.0178(7) Uani 1 1 d . . .  
Fe18 Fe -0.0092(8) 0.11418(11) 0.7426(6) 0.0176(5) Uani 1 1 d . . .  
Fe19 Fe 0.496(3) 0.1140(6) 0.249(2) 0.046(3) Uani 0.285(7) 1 d P . .  
Fe20 Fe -0.5050(6) -0.08340(10) 0.2558(7) 0.0178(7) Uani 1 1 d . . .  
S1 S 0.3321(5) -0.02985(13) 0.4157(5) 0.0080(7) Uani 1 1 d . . .  
S2 S 0.3328(5) -0.03387(13) 0.9166(6) 0.0079(8) Uani 1 1 d . . .  
S3 S -0.1617(5) 0.16582(13) 0.4170(5) 0.0089(8) Uani 1 1 d . . .  
S4 S 0.1646(5) -0.13731(15) 0.5816(6) 0.0088(8) Uani 1 1 d . . .  
S5 S -0.1710(5) -0.04002(13) 0.9160(6) 0.0086(8) Uani 1 1 d . . .  
S6 S -0.1700(5) -0.03363(14) 0.4149(6) 0.0086(8) Uani 1 1 d . . .  
S7 S 0.6695(5) 0.26188(14) 0.5847(5) 0.0103(8) Uani 1 1 d . . .  
S8 S 0.3329(6) 0.16174(14) 0.9116(6) 0.0104(8) Uani 1 1 d . . .  
S9 S 0.1624(6) 0.06589(14) 1.0805(6) 0.0099(8) Uani 1 1 d . . .  
S10 S 0.1650(6) 0.06309(16) 0.5804(5) 0.0095(8) Uani 1 1 d . . .  
S11 S 0.3347(5) 0.16598(15) 0.4160(6) 0.0098(8) Uani 1 1 d . . .  
S12 S 0.6694(6) 0.26559(14) 0.0843(5) 0.0088(7) Uani 1 1 d . . .  
S13 S 1.1690(5) 0.26462(14) 0.0851(5) 0.0079(7) Uani 1 1 d . . .  
S14 S -0.3377(5) -0.13384(14) 0.0818(6) 0.0095(8) Uani 1 1 d . . .  
S15 S 0.1697(5) 0.27155(12) 0.5864(5) 0.0072(8) Uani 1 1 d . . .  
S16 S 0.8358(5) 0.16902(14) 0.9161(5) 0.0074(7) Uani 1 1 d . . .  
S17 S 0.1650(5) -0.13208(15) 0.0833(6) 0.0101(8) Uani 1 1 d . . .  
S18 S -0.3416(5) -0.13414(13) 0.5782(6) 0.0084(8) Uani 1 1 d . . .  
S19 S 0.6670(6) 0.06920(15) 0.0799(6) 0.0107(8) Uani 1 1 d . . .  
S20 S 0.6652(6) 0.06460(15) 0.5811(5) 0.0089(8) Uani 1 1 d . . .

loop\_

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Fe1 0.0165(10) 0.0101(12) 0.0224(10) 0.0008(9) 0.0112(9) 0.0001(10)  
Fe2 0.019(2) 0.008(2) 0.015(2) -0.0014(18) 0.0088(18) 0.0039(17)  
Fe3 0.0334(11) 0.0104(10) 0.0214(12) 0.0019(11) 0.0182(10) 0.0055(8)  
Fe4 0.0284(13) 0.0094(13) 0.0184(13) 0.0021(10) 0.0144(11) 0.0024(9)

Fe5 0.0219(12) 0.0114(15) 0.0178(13) -0.0003(11) 0.0079(10) -0.0002(11)  
 Fe6 0.0195(12) 0.0144(13) 0.0197(11) -0.0019(9) 0.0088(10) -0.0022(9)  
 Fe7 0.0178(12) 0.0099(13) 0.0149(12) 0.0003(10) 0.0078(8) 0.0002(10)  
 Fe8 0.0267(13) 0.0083(12) 0.0150(11) 0.0008(10) 0.0123(10) 0.0004(9)  
 Fe9 0.016(2) 0.009(3) 0.012(2) -0.0013(18) 0.0076(18) -0.0026(17)  
 Fe10 0.0168(12) 0.0099(13) 0.0176(12) 0.0004(10) 0.0077(9) 0.0013(10)  
 Fe11 0.0181(12) 0.0060(12) 0.0257(13) -0.0010(10) 0.0123(10) -0.0005(9)  
 Fe12 0.0120(13) 0.0143(16) 0.0172(14) 0.0005(12) 0.0072(10) -0.0001(11)  
 Fe13 0.0193(10) 0.0142(12) 0.0315(12) 0.0006(11) 0.0167(9) -0.0008(9)  
 Fe14 0.0162(13) 0.0123(17) 0.0217(16) 0.0001(11) 0.0113(11) 0.0013(11)  
 Fe15 0.0134(9) 0.0149(13) 0.0163(12) -0.0028(10) 0.0069(8) -0.0032(10)  
 Fe16 0.0156(10) 0.0065(12) 0.0160(10) -0.0013(9) 0.0065(9) -0.0008(10)  
 Fe17 0.0215(13) 0.0075(12) 0.0277(13) 0.0052(11) 0.0148(11) 0.0033(10)  
 Fe18 0.0186(10) 0.0087(11) 0.0167(10) 0.0045(10) 0.0022(8) -0.0009(8)  
 Fe19 0.031(4) 0.066(7) 0.040(5) 0.013(5) 0.018(4) 0.008(4)  
 Fe20 0.0168(12) 0.0136(16) 0.0186(13) -0.0022(11) 0.0056(10) -0.0006(11)  
 S1 0.0079(13) 0.0078(18) 0.0086(16) -0.0012(12) 0.0042(12) -0.0032(12)  
 S2 0.0088(14) 0.0088(19) 0.0054(17) 0.0010(11) 0.0028(13) 0.0003(12)  
 S3 0.0063(14) 0.012(2) 0.0052(14) 0.0025(12) 0.0006(12) -0.0020(11)  
 S4 0.0084(14) 0.0062(17) 0.0104(17) -0.0014(12) 0.0036(13) -0.0011(13)  
 S5 0.0096(15) 0.008(2) 0.0102(18) 0.0001(12) 0.0065(14) -0.0004(11)  
 S6 0.0076(14) 0.010(2) 0.0104(17) 0.0012(12) 0.0059(13) 0.0012(12)  
 S7 0.0085(14) 0.015(2) 0.0075(14) 0.0018(13) 0.0042(12) 0.0001(14)  
 S8 0.0086(15) 0.011(2) 0.0115(15) -0.0007(12) 0.0047(13) -0.0017(11)  
 S9 0.0080(16) 0.0113(18) 0.0108(17) -0.0002(12) 0.0051(14) 0.0030(11)  
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 S16 0.0059(13) 0.0091(19) 0.0080(14) -0.0031(11) 0.0042(11) -0.0036(11)  
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 S18 0.0075(14) 0.0122(19) 0.0071(16) 0.0009(11) 0.0049(12) 0.0033(12)  
 S19 0.0070(16) 0.016(2) 0.0076(17) -0.0016(12) 0.0027(13) -0.0007(11)  
 S20 0.0073(16) 0.0116(18) 0.0044(15) 0.0006(12) 0.0004(12) 0.0011(11)

\_geom\_special\_details

;

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

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loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_2

\_geom\_bond\_publ\_flag

Fe1 S8 2.358(4) . ?

Fe1 S15 2.401(4) . ?  
Fe1 S11 2.445(5) . ?  
Fe1 S12 2.485(5) 1\_556 ?  
Fe1 S7 2.557(5) . ?  
Fe1 S16 2.576(4) . ?  
Fe1 Fe6 2.900(4) . ?  
Fe1 Fe3 2.904(5) . ?  
Fe2 S4 2.313(7) . ?  
Fe2 S18 2.397(7) . ?  
Fe2 S17 2.430(8) 1\_556 ?  
Fe2 S6 2.486(8) . ?  
Fe2 S5 2.567(7) . ?  
Fe2 S2 2.572(8) . ?  
Fe2 Fe9 2.603(8) . ?  
Fe2 Fe5 2.933(6) . ?  
Fe3 S20 2.389(5) . ?  
Fe3 S11 2.420(5) . ?  
Fe3 S19 2.424(5) 1\_556 ?  
Fe3 S8 2.454(5) . ?  
Fe3 S10 2.503(5) . ?  
Fe3 S16 2.531(5) . ?  
Fe3 Fe10 2.877(5) 1\_655 ?  
Fe4 S4 2.369(5) . ?  
Fe4 S17 2.433(5) . ?  
Fe4 S6 2.459(5) . ?  
Fe4 S1 2.466(5) . ?  
Fe4 S5 2.500(5) 1\_554 ?  
Fe4 S14 2.540(5) . ?  
Fe4 Fe8 2.869(4) 2\_646 ?  
Fe4 Fe7 2.907(4) . ?  
Fe5 S5 2.379(4) . ?  
Fe5 S2 2.440(4) . ?  
Fe5 S9 2.453(5) . ?  
Fe5 S6 2.457(5) . ?  
Fe5 S20 2.463(4) 1\_455 ?  
Fe5 S10 2.608(5) . ?  
Fe5 Fe18 2.948(4) . ?  
Fe6 S17 2.388(4) 2\_656 ?  
Fe6 S7 2.405(5) . ?  
Fe6 S18 2.433(5) 2\_556 ?  
Fe6 S12 2.467(5) 1\_556 ?  
Fe6 S15 2.471(5) . ?  
Fe6 S14 2.574(5) 2\_556 ?  
Fe6 Fe20 2.902(4) 2\_556 ?  
Fe7 S19 2.379(5) 1\_455 ?  
Fe7 S5 2.388(4) 1\_554 ?  
Fe7 S9 2.447(5) 1\_554 ?  
Fe7 S6 2.470(4) . ?  
Fe7 S1 2.531(4) . ?  
Fe7 S10 2.581(5) . ?  
Fe7 Fe13 2.907(5) . ?  
Fe8 S17 2.390(5) 2\_656 ?  
Fe8 S13 2.429(5) 1\_556 ?  
Fe8 S7 2.440(5) . ?

Fe8 S4 2.454(5) 2\_656 ?  
Fe8 S15 2.463(5) 1\_655 ?  
Fe8 S14 2.558(4) 2\_656 ?  
Fe8 Fe4 2.869(4) 2\_656 ?  
Fe8 Fe16 2.895(4) 1\_655 ?  
Fe9 S17 2.315(7) 1\_556 ?  
Fe9 S4 2.439(7) . ?  
Fe9 S13 2.458(7) 2\_646 ?  
Fe9 S18 2.459(7) . ?  
Fe9 S12 2.497(7) 2\_646 ?  
Fe9 S15 2.550(7) 2\_546 ?  
Fe9 Fe15 2.933(6) 2\_546 ?  
Fe10 S19 2.388(5) 1\_456 ?  
Fe10 S5 2.393(4) . ?  
Fe10 S2 2.442(5) 1\_455 ?  
Fe10 S20 2.462(5) 1\_455 ?  
Fe10 S1 2.514(5) 1\_455 ?  
Fe10 S10 2.575(4) 1\_455 ?  
Fe10 Fe3 2.877(5) 1\_455 ?  
Fe10 Fe11 2.890(4) 1\_455 ?  
Fe11 S4 2.395(4) . ?  
Fe11 S18 2.428(5) 1\_655 ?  
Fe11 S1 2.453(5) . ?  
Fe11 S5 2.471(5) 1\_655 ?  
Fe11 S2 2.477(5) . ?  
Fe11 S14 2.530(5) 1\_656 ?  
Fe11 Fe10 2.890(4) 1\_655 ?  
Fe11 Fe17 2.918(4) . ?  
Fe12 S19 2.364(5) . ?  
Fe12 S20 2.434(5) . ?  
Fe12 S9 2.447(5) 1\_554 ?  
Fe12 S2 2.450(5) 1\_554 ?  
Fe12 S6 2.471(5) 1\_655 ?  
Fe12 S1 2.549(5) . ?  
Fe12 Fe19 2.71(2) . ?  
Fe12 Fe20 2.965(4) 1\_655 ?  
Fe13 S11 2.419(5) . ?  
Fe13 S9 2.429(5) 1\_554 ?  
Fe13 S19 2.444(5) 1\_455 ?  
Fe13 S3 2.448(5) . ?  
Fe13 S10 2.474(6) . ?  
Fe13 S16 2.524(5) 1\_454 ?  
Fe13 Fe15 2.925(4) . ?  
Fe14 S8 2.363(5) 1\_554 ?  
Fe14 S3 2.400(4) 1\_655 ?  
Fe14 S11 2.428(5) . ?  
Fe14 S12 2.486(5) . ?  
Fe14 S13 2.517(5) 1\_455 ?  
Fe14 S7 2.578(5) . ?  
Fe14 Fe19 2.76(2) . ?  
Fe14 Fe17 2.965(4) 2\_656 ?  
Fe15 S15 2.405(4) . ?  
Fe15 S3 2.410(4) . ?  
Fe15 S11 2.433(4) . ?

Fe15 S13 2.468(4) 1\_455 ?  
Fe15 S12 2.476(4) 1\_455 ?  
Fe15 S16 2.570(4) 1\_454 ?  
Fe15 Fe9 2.933(6) 2\_556 ?  
Fe16 S8 2.379(4) . ?  
Fe16 S3 2.425(4) . ?  
Fe16 S15 2.428(4) . ?  
Fe16 S13 2.483(4) 1\_456 ?  
Fe16 S16 2.530(4) 1\_455 ?  
Fe16 S7 2.534(4) 1\_455 ?  
Fe16 Fe8 2.895(4) 1\_455 ?  
Fe16 Fe18 2.900(4) . ?  
Fe17 S13 2.431(5) 2\_746 ?  
Fe17 S7 2.438(5) 2\_646 ?  
Fe17 S4 2.447(5) . ?  
Fe17 S18 2.450(5) 1\_655 ?  
Fe17 S12 2.457(5) 2\_646 ?  
Fe17 S14 2.542(5) 1\_656 ?  
Fe17 Fe14 2.965(4) 2\_646 ?  
Fe18 S20 2.411(5) 1\_455 ?  
Fe18 S3 2.446(5) . ?  
Fe18 S9 2.448(5) . ?  
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Fe11 S14 Fe4 95.2(2) 1\_454 . ?  
Fe20 S14 Fe17 133.65(14) . 1\_454 ?

Fe11 S14 Fe17 70.25(13) 1\_454 1\_454 ?  
 Fe4 S14 Fe17 132.81(18) . 1\_454 ?  
 Fe20 S14 Fe8 133.66(18) . 2\_646 ?  
 Fe11 S14 Fe8 129.95(17) 1\_454 2\_646 ?  
 Fe4 S14 Fe8 68.48(11) . 2\_646 ?  
 Fe17 S14 Fe8 86.7(2) 1\_454 2\_646 ?  
 Fe20 S14 Fe6 69.75(14) . 2\_546 ?  
 Fe11 S14 Fe6 128.37(14) 1\_454 2\_546 ?  
 Fe4 S14 Fe6 130.07(17) . 2\_546 ?  
 Fe17 S14 Fe6 89.32(17) 1\_454 2\_546 ?  
 Fe8 S14 Fe6 93.6(2) 2\_646 2\_546 ?  
 Fe1 S15 Fe15 83.18(18) . . ?  
 Fe1 S15 Fe16 77.67(14) . . ?  
 Fe15 S15 Fe16 82.65(17) . . ?  
 Fe1 S15 Fe8 129.96(15) . 1\_455 ?  
 Fe15 S15 Fe8 130.11(17) . 1\_455 ?  
 Fe16 S15 Fe8 72.59(13) . 1\_455 ?  
 Fe1 S15 Fe6 73.04(14) . . ?  
 Fe15 S15 Fe6 129.20(18) . . ?  
 Fe16 S15 Fe6 131.98(15) . . ?  
 Fe8 S15 Fe6 98.68(18) 1\_455 . ?  
 Fe1 S15 Fe9 133.7(2) . 2\_556 ?  
 Fe15 S15 Fe9 72.52(17) . 2\_556 ?  
 Fe16 S15 Fe9 134.6(2) . 2\_556 ?  
 Fe8 S15 Fe9 95.1(2) 1\_455 2\_556 ?  
 Fe6 S15 Fe9 92.4(2) . 2\_556 ?  
 Fe18 S16 Fe13 86.9(2) 1\_655 1\_656 ?  
 Fe18 S16 Fe16 70.16(12) 1\_655 1\_655 ?  
 Fe13 S16 Fe16 128.62(16) 1\_656 1\_655 ?  
 Fe18 S16 Fe3 83.3(2) 1\_655 . ?  
 Fe13 S16 Fe3 88.5(2) 1\_656 . ?  
 Fe16 S16 Fe3 130.88(16) 1\_655 . ?  
 Fe18 S16 Fe15 133.61(16) 1\_655 1\_656 ?  
 Fe13 S16 Fe15 70.09(13) 1\_656 1\_656 ?  
 Fe16 S16 Fe15 93.14(17) 1\_655 1\_656 ?  
 Fe3 S16 Fe15 133.29(15) . 1\_656 ?  
 Fe18 S16 Fe1 131.82(18) 1\_655 . ?  
 Fe13 S16 Fe1 129.21(16) 1\_656 . ?  
 Fe16 S16 Fe1 98.56(17) 1\_655 . ?  
 Fe3 S16 Fe1 69.30(13) . . ?  
 Fe15 S16 Fe1 92.39(17) 1\_656 . ?  
 Fe9 S17 Fe6 88.3(3) 1\_554 2\_646 ?  
 Fe9 S17 Fe8 85.6(2) 1\_554 2\_646 ?  
 Fe6 S17 Fe8 82.7(2) 2\_646 2\_646 ?  
 Fe9 S17 Fe20 134.4(2) 1\_554 1\_655 ?  
 Fe6 S17 Fe20 74.29(12) 2\_646 1\_655 ?  
 Fe8 S17 Fe20 131.50(19) 2\_646 1\_655 ?  
 Fe9 S17 Fe2 66.5(2) 1\_554 1\_554 ?  
 Fe6 S17 Fe2 131.0(2) 2\_646 1\_554 ?  
 Fe8 S17 Fe2 132.4(2) 2\_646 1\_554 ?  
 Fe20 S17 Fe2 93.7(3) 1\_655 1\_554 ?  
 Fe9 S17 Fe4 133.9(2) 1\_554 . ?  
 Fe6 S17 Fe4 127.12(19) 2\_646 . ?  
 Fe8 S17 Fe4 72.99(14) 2\_646 . ?



Fe20 S17 Fe4 87.8(2) 1\_655 . ?  
 Fe2 S17 Fe4 98.8(2) 1\_554 . ?  
 Fe2 S18 Fe20 89.4(3) . . ?  
 Fe2 S18 Fe11 96.3(2) . 1\_455 ?  
 Fe20 S18 Fe11 86.6(2) . 1\_455 ?  
 Fe2 S18 Fe6 131.2(2) . 2\_546 ?  
 Fe20 S18 Fe6 73.55(14) . 2\_546 ?  
 Fe11 S18 Fe6 126.81(14) 1\_455 2\_546 ?  
 Fe2 S18 Fe17 133.9(3) . 1\_455 ?  
 Fe20 S18 Fe17 133.07(15) . 1\_455 ?  
 Fe11 S18 Fe17 73.47(13) 1\_455 1\_455 ?  
 Fe6 S18 Fe17 85.08(19) 2\_546 1\_455 ?  
 Fe2 S18 Fe9 64.8(2) . . ?  
 Fe20 S18 Fe9 135.0(2) . . ?  
 Fe11 S18 Fe9 130.1(2) 1\_455 . ?  
 Fe6 S18 Fe9 95.7(2) 2\_546 . ?  
 Fe17 S18 Fe9 87.4(2) 1\_455 . ?  
 Fe12 S19 Fe7 87.1(2) . 1\_655 ?  
 Fe12 S19 Fe10 85.8(2) . 1\_654 ?  
 Fe7 S19 Fe10 78.93(17) 1\_655 1\_654 ?  
 Fe12 S19 Fe19 69.2(4) . . ?  
 Fe7 S19 Fe19 134.7(4) 1\_655 . ?  
 Fe10 S19 Fe19 133.7(4) 1\_654 . ?  
 Fe12 S19 Fe3 131.8(2) . 1\_554 ?  
 Fe7 S19 Fe3 128.62(19) 1\_655 1\_554 ?  
 Fe10 S19 Fe3 73.42(15) 1\_654 1\_554 ?  
 Fe19 S19 Fe3 94.5(5) . 1\_554 ?  
 Fe12 S19 Fe13 131.61(19) . 1\_655 ?  
 Fe7 S19 Fe13 74.11(15) 1\_655 1\_655 ?  
 Fe10 S19 Fe13 131.1(2) 1\_654 1\_655 ?  
 Fe19 S19 Fe13 93.2(5) . 1\_655 ?  
 Fe3 S19 Fe13 92.8(3) 1\_554 1\_655 ?  
 Fe3 S20 Fe18 88.6(3) . 1\_655 ?  
 Fe3 S20 Fe12 132.58(19) . . ?  
 Fe18 S20 Fe12 128.7(2) 1\_655 . ?  
 Fe3 S20 Fe19 87.8(4) . . ?  
 Fe18 S20 Fe19 89.5(5) 1\_655 . ?  
 Fe12 S20 Fe19 67.6(4) . . ?  
 Fe3 S20 Fe10 72.73(15) . 1\_655 ?  
 Fe18 S20 Fe10 127.93(16) 1\_655 1\_655 ?  
 Fe12 S20 Fe10 97.0(2) . 1\_655 ?  
 Fe19 S20 Fe10 135.8(4) . 1\_655 ?  
 Fe3 S20 Fe5 130.58(18) . 1\_655 ?  
 Fe18 S20 Fe5 74.42(14) 1\_655 1\_655 ?  
 Fe12 S20 Fe5 91.40(18) . 1\_655 ?  
 Fe19 S20 Fe5 136.6(4) . 1\_655 ?  
 Fe10 S20 Fe5 81.9(2) 1\_655 1\_655 ?