

data\_Po5C\_120K\_Bodenmais

\_audit\_creation\_method        SHELXL-97  
\_chemical\_name\_systematic  
;  
Nonairondecasulfide  
;  
\_chemical\_name\_common        '5C pyrrhotite'  
\_chemical\_melting\_point       ?  
\_chemical\_formula\_moiety      'Fe9.02 S10'  
\_chemical\_formula\_sum        'Fe9.02 S10'  
\_chemical\_formula\_weight      824.30

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                6.8673(4)  
\_cell\_length\_b                28.6536(9)  
\_cell\_length\_c                6.8592(4)  
\_cell\_angle\_alpha              90.00  
\_cell\_angle\_beta               119.975(7)  
\_cell\_angle\_gamma              90.00  
\_cell\_volume                   1169.18(10)  
\_cell\_formula\_units\_Z         4  
\_cell\_measurement\_temperature 120.0  
\_cell\_measurement\_reflns\_used 12660  
\_cell\_measurement\_theta\_min   2.8378  
\_cell\_measurement\_theta\_max   30.4677

\_exptl\_crystal\_description    irregular-fragment  
\_exptl\_crystal\_colour        dark-gray  
\_exptl\_crystal\_size\_max       0.1393  
\_exptl\_crystal\_size\_mid       0.1031  
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\_exptl\_crystal\_density\_meas   .

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_exptl_absorpt_coefficient_mu   12.586
_exptl_absorpt_correction_type  'analytical'
_exptl_absorpt_correction_T_min 0.288
_exptl_absorpt_correction_T_max 0.525
_exptl_absorpt_process_details
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CrysAlisPro, Oxford Diffraction Ltd.,
Version 1.171.34.41 (release 13-09-2010 CrysAlis171 .NET)
(compiled Sep 13 2010,14:28:38)
Analytical numeric absorption correction using a multifaceted crystal
model based on expressions derived by R.C. Clark & J.S. Reid.
(Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897)
;

_exptl_special_details
;
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_diffn_ambient_temperature      120.0
_diffn_radiation_wavelength     0.71073
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_diffn_radiation_monochromator 'mirror'
_diffn_measurement_device_type 'SuperNova, Dual, Cu at zero, Atlas'
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_diffn_detector_area_resol_mean 10.3693
_diffn_standards_number        .
_diffn_standards_interval_count .
_diffn_standards_interval_time .
_diffn_standards_decay_%       .
_diffn_reflns_number           28580
_diffn_reflns_av_R_equivalents 0.0207
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_diffn_reflns_limit_h_min      -9
_diffn_reflns_limit_h_max      9
_diffn_reflns_limit_k_min      -40
_diffn_reflns_limit_k_max      40
_diffn_reflns_limit_l_min      -9
_diffn_reflns_limit_l_max      9
_diffn_reflns_theta_min        2.84
_diffn_reflns_theta_max        30.54
_diffn_measured_fraction_theta_max 0.999
_reflns_number_total           7121
_reflns_number_gt              5727
_reflns_threshold_expression    >2\sigma(I)

_computing_data_collection
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CrysAlisPro, Oxford Diffraction Ltd.,
Version 1.171.34.41 (release 13-09-2010 CrysAlis171 .NET)

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(compiled Sep 13 2010,14:28:38)

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_computing_cell_refinement  
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Version 1.171.34.41 (release 13-09-2010 CrysAlis171 .NET)  
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_computing_data_reduction  
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Version 1.171.34.41 (release 13-09-2010 CrysAlis171 .NET)  
(compiled Sep 13 2010,14:28:38)  
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_computing_structure_solution 'SHELXS-97 (Sheldrick, 1990)'  
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 2008)'  
_computing_molecular_graphics ?  
_computing_publication_material ?
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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  
 $F^2 > 2\sigma(F^2)$  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.
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_refine_ls_weighting_details  
'calc w=1/[\sigma^2(Fo^2)+(0.0138P)^2+0.4767P] 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 0.00045(2)  
_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'  
_refine_ls_abs_structure_Flack 0.47(4)  
_refine_ls_number_reflns 7121  
_refine_ls_number_parameters 368  
_refine_ls_number_restraints 1  
_refine_ls_R_factor_all 0.0354  
_refine_ls_R_factor_gt 0.0261  
_refine_ls_wR_factor_ref 0.0574  
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_refine_ls_shift/su_max 0.002
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\_refine\_ls\_shift/su\_mean 0.000  
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\_refine\_diff\_density\_rms 0.130

loop\_

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\_atom\_site\_fract\_z  
\_atom\_site\_U\_iso\_or\_equiv  
\_atom\_site\_adp\_type  
\_atom\_site\_occupancy  
\_atom\_site\_symmetry\_multiplicity  
\_atom\_site\_calc\_flag  
\_atom\_site\_refinement\_flags  
\_atom\_site\_disorder\_assembly  
\_atom\_site\_disorder\_group

Fe1 Fe 0.46648(19) 0.21539(5) 0.7509(3) 0.0084(2) Uani 1 1 d . . .  
Fe2 Fe 0.0001(5) -0.09022(8) 0.7288(5) 0.0099(5) Uani 0.500(3) 1 d P . .  
Fe3 Fe 0.5014(4) 0.11532(6) 0.7334(3) 0.0141(2) Uani 1 1 d . . .  
Fe4 Fe 0.0191(3) -0.08458(5) 0.2765(2) 0.0110(2) Uani 1 1 d . . .  
Fe5 Fe -0.0113(2) 0.01172(4) 0.76610(19) 0.0097(2) Uani 1 1 d . . .  
Fe6 Fe 0.5269(3) 0.31543(5) 0.7506(3) 0.0108(2) Uani 1 1 d . . .  
Fe7 Fe -0.03518(18) 0.01518(5) 0.2126(2) 0.0093(2) Uani 1 1 d . . .  
Fe8 Fe 0.9841(3) 0.31513(5) 0.7582(3) 0.0101(2) Uani 1 1 d . . .  
Fe9 Fe 0.0038(5) -0.17982(8) 0.7731(5) 0.0084(5) Uani 0.496(3) 1 d P . .  
Fe10 Fe -0.4702(2) 0.01493(4) 0.7818(2) 0.0075(2) Uani 1 1 d . . .  
Fe11 Fe 0.4744(3) -0.08539(5) 0.7246(3) 0.0095(2) Uani 1 1 d . . .  
Fe12 Fe 0.5083(2) 0.01958(5) 0.2333(2) 0.0086(3) Uani 0.877(3) 1 d P . .  
Fe13 Fe 0.0110(4) 0.11568(6) 0.2556(4) 0.0128(2) Uani 1 1 d . . .  
Fe14 Fe 0.4937(2) 0.21045(5) 0.2252(3) 0.0098(3) Uani 0.878(3) 1 d P . .  
Fe15 Fe 0.01268(19) 0.21833(4) 0.2772(3) 0.0090(2) Uani 1 1 d . . .  
Fe16 Fe 0.03225(17) 0.21504(4) 0.7466(3) 0.0080(2) Uani 1 1 d . . .  
Fe17 Fe 0.4970(3) -0.18685(5) 0.7388(4) 0.0129(3) Uani 1 1 d . . .  
Fe18 Fe -0.0118(4) 0.11425(5) 0.7441(3) 0.0119(2) Uani 1 1 d . . .  
Fe19 Fe 0.4964(11) 0.1149(2) 0.2644(8) 0.0159(10) Uani 0.283(2) 1 d P . .  
Fe20 Fe -0.5049(3) -0.08322(5) 0.2569(3) 0.0126(3) Uani 1 1 d . . .  
S1 S 0.3310(2) -0.02954(6) 0.4159(3) 0.0039(3) Uani 1 1 d . . .  
S2 S 0.3322(2) -0.03473(7) 0.9162(3) 0.0053(3) Uani 1 1 d . . .  
S3 S -0.1623(2) 0.16557(8) 0.4176(2) 0.0049(3) Uani 1 1 d . . .  
S4 S 0.1645(2) -0.13736(8) 0.5816(3) 0.0067(3) Uani 1 1 d . . .  
S5 S -0.1712(2) -0.04062(7) 0.9167(3) 0.0061(3) Uani 1 1 d . . .  
S6 S -0.1697(2) -0.03387(7) 0.4155(3) 0.0049(3) Uani 1 1 d . . .  
S7 S 0.6690(2) 0.26050(7) 0.5852(2) 0.0058(3) Uani 1 1 d . . .  
S8 S 0.3320(2) 0.16087(8) 0.9126(2) 0.0071(3) Uani 1 1 d . . .  
S9 S 0.1629(3) 0.06521(7) 0.0804(3) 0.0052(3) Uani 1 1 d . . .  
S10 S 0.1641(3) 0.06239(8) 0.5809(3) 0.0057(3) Uani 1 1 d . . .  
S11 S 0.3337(2) 0.16702(8) 0.4153(2) 0.0054(3) Uani 1 1 d . . .  
S12 S 0.6688(3) 0.26564(7) 0.0844(2) 0.0057(3) Uani 1 1 d . . .  
S13 S 0.1688(3) 0.26496(7) 0.0849(2) 0.0044(3) Uani 1 1 d . . .  
S14 S -0.3378(2) -0.13449(9) 0.0812(3) 0.0056(3) Uani 1 1 d . . .  
S15 S 0.1709(2) 0.27156(7) 0.5879(2) 0.0033(3) Uani 1 1 d . . .

S16 S 0.8355(2) 0.16862(8) 0.9169(2) 0.0049(3) Uani 1 1 d . . .  
S17 S 0.1646(2) -0.13160(8) 0.0833(3) 0.0056(3) Uani 1 1 d . . .  
S18 S -0.3416(2) -0.13465(8) 0.5790(3) 0.0058(3) Uani 1 1 d . . .  
S19 S 0.6674(3) 0.07015(8) 0.0801(3) 0.0046(3) Uani 1 1 d . . .  
S20 S 0.6658(3) 0.06412(8) 0.5814(3) 0.0052(3) Uani 1 1 d . . .

loop\_

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Fe1 0.0079(4) 0.0063(5) 0.0130(4) -0.0001(4) 0.0066(3) 0.0007(4)  
Fe2 0.0157(9) 0.0047(9) 0.0087(10) 0.0001(7) 0.0056(7) 0.0024(7)  
Fe3 0.0306(4) 0.0047(4) 0.0126(5) 0.0021(5) 0.0150(4) 0.0038(3)  
Fe4 0.0186(4) 0.0057(5) 0.0103(4) -0.0009(5) 0.0083(4) -0.0004(4)  
Fe5 0.0130(4) 0.0065(6) 0.0078(4) -0.0003(4) 0.0039(3) -0.0013(4)  
Fe6 0.0111(4) 0.0061(5) 0.0139(4) -0.0002(4) 0.0052(4) 0.0007(4)  
Fe7 0.0094(4) 0.0069(5) 0.0079(4) -0.0002(4) 0.0016(3) -0.0011(4)  
Fe8 0.0179(4) 0.0035(5) 0.0115(5) 0.0003(5) 0.0094(4) 0.0004(4)  
Fe9 0.0094(8) 0.0043(8) 0.0110(10) -0.0037(7) 0.0048(7) -0.0033(6)  
Fe10 0.0103(4) 0.0025(5) 0.0086(4) 0.0006(4) 0.0038(3) 0.0005(4)  
Fe11 0.0115(4) 0.0026(5) 0.0148(4) -0.0001(4) 0.0068(4) -0.0010(4)  
Fe12 0.0068(4) 0.0069(6) 0.0089(5) 0.0008(5) 0.0015(4) -0.0002(4)  
Fe13 0.0139(4) 0.0061(5) 0.0228(5) -0.0016(4) 0.0124(4) -0.0004(3)  
Fe14 0.0131(5) 0.0072(6) 0.0137(6) -0.0006(5) 0.0101(4) -0.0005(5)  
Fe15 0.0073(3) 0.0064(5) 0.0129(5) -0.0006(4) 0.0048(3) -0.0002(4)  
Fe16 0.0107(4) 0.0030(5) 0.0113(4) -0.0001(4) 0.0064(3) 0.0003(4)  
Fe17 0.0159(5) 0.0050(5) 0.0229(5) 0.0006(4) 0.0136(4) 0.0015(4)  
Fe18 0.0145(4) 0.0045(4) 0.0102(4) 0.0001(4) 0.0012(4) -0.0014(3)  
Fe19 0.0102(13) 0.0326(19) 0.0056(14) -0.0001(16) 0.0044(11) 0.0011(12)  
Fe20 0.0121(4) 0.0055(5) 0.0137(5) -0.0011(5) 0.0016(4) -0.0025(4)  
S1 0.0037(5) 0.0026(8) 0.0055(6) 0.0001(5) 0.0022(5) -0.0002(5)  
S2 0.0045(5) 0.0089(9) 0.0029(6) -0.0002(5) 0.0021(5) 0.0001(5)  
S3 0.0048(6) 0.0060(7) 0.0046(5) 0.0013(5) 0.0029(5) -0.0001(5)  
S4 0.0045(5) 0.0110(9) 0.0040(6) -0.0002(5) 0.0017(5) -0.0009(5)  
S5 0.0048(6) 0.0106(9) 0.0030(6) 0.0004(5) 0.0021(5) -0.0002(5)  
S6 0.0039(5) 0.0068(8) 0.0039(6) -0.0001(5) 0.0019(5) 0.0003(5)  
S7 0.0040(6) 0.0091(9) 0.0036(5) 0.0006(5) 0.0014(5) 0.0008(5)  
S8 0.0047(5) 0.0138(9) 0.0031(5) 0.0005(5) 0.0022(5) 0.0002(5)  
S9 0.0055(7) 0.0048(8) 0.0054(6) -0.0001(5) 0.0027(6) 0.0015(5)  
S10 0.0050(6) 0.0102(9) 0.0018(6) 0.0002(5) 0.0016(5) 0.0000(5)  
S11 0.0048(6) 0.0076(9) 0.0040(5) 0.0010(5) 0.0023(5) 0.0009(5)  
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S13 0.0037(6) 0.0059(9) 0.0035(5) -0.0001(5) 0.0017(5) -0.0002(5)  
S14 0.0042(5) 0.0071(7) 0.0054(6) 0.0007(5) 0.0023(5) 0.0010(5)  
S15 0.0043(6) 0.0009(7) 0.0046(5) 0.0003(5) 0.0021(5) 0.0007(4)  
S16 0.0047(6) 0.0074(8) 0.0035(5) -0.0009(5) 0.0026(5) -0.0015(5)  
S17 0.0040(5) 0.0074(8) 0.0056(6) 0.0008(5) 0.0024(5) 0.0004(5)  
S18 0.0039(5) 0.0112(7) 0.0024(6) -0.0004(5) 0.0015(5) 0.0013(6)  
S19 0.0040(6) 0.0055(8) 0.0040(6) -0.0004(5) 0.0018(5) 0.0005(5)  
S20 0.0046(6) 0.0071(8) 0.0036(6) -0.0001(5) 0.0019(5) 0.0002(5)

\_geom\_special\_details

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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 2.355(2) . ?

Fe1 S15 2.3858(19) . ?

Fe1 S11 2.440(2) . ?

Fe1 S12 2.462(2) 1\_556 ?

Fe1 S7 2.544(2) . ?

Fe1 S16 2.575(2) . ?

Fe1 Fe3 2.8851(19) . ?

Fe1 Fe6 2.8965(18) . ?

Fe1 Fe16 2.9674(11) . ?

Fe2 S4 2.293(3) . ?

Fe2 S18 2.403(3) . ?

Fe2 S17 2.419(3) 1\_556 ?

Fe2 S6 2.466(3) . ?

Fe2 S2 2.540(3) . ?

Fe2 S5 2.565(3) . ?

Fe2 Fe9 2.584(3) . ?

Fe2 Fe5 2.937(3) . ?

Fe3 S20 2.385(2) . ?

Fe3 S11 2.402(2) . ?

Fe3 S19 2.433(2) 1\_556 ?

Fe3 S8 2.449(2) . ?

Fe3 S16 2.509(2) . ?

Fe3 S10 2.518(2) . ?

Fe3 Fe10 2.8911(19) 1\_655 ?

Fe4 S4 2.361(2) . ?

Fe4 S17 2.428(2) . ?

Fe4 S6 2.436(2) . ?

Fe4 S1 2.438(2) . ?

Fe4 S5 2.483(2) 1\_554 ?

Fe4 S14 2.562(2) . ?

Fe4 Fe8 2.8826(14) 2\_646 ?

Fe4 Fe7 2.8876(19) . ?

Fe5 S5 2.378(2) . ?

Fe5 S9 2.419(2) 1\_556 ?

Fe5 S20 2.443(2) 1\_455 ?

Fe5 S2 2.444(2) . ?

Fe5 S6 2.462(2) . ?

Fe5 S10 2.589(2) . ?  
Fe5 Fe18 2.9416(19) . ?  
Fe6 S17 2.383(2) 2\_656 ?  
Fe6 S7 2.413(2) . ?  
Fe6 S18 2.429(2) 2\_556 ?  
Fe6 S12 2.449(2) 1\_556 ?  
Fe6 S15 2.465(2) . ?  
Fe6 S14 2.564(2) 2\_556 ?  
Fe6 Fe20 2.9071(17) 2\_556 ?  
Fe7 S19 2.371(2) 1\_455 ?  
Fe7 S5 2.378(2) 1\_554 ?  
Fe7 S9 2.441(2) . ?  
Fe7 S6 2.460(2) . ?  
Fe7 S1 2.531(2) . ?  
Fe7 S10 2.575(2) . ?  
Fe7 Fe13 2.896(2) . ?  
Fe7 Fe10 2.9723(13) 1\_554 ?  
Fe8 S17 2.380(2) 2\_656 ?  
Fe8 S13 2.420(2) 1\_656 ?  
Fe8 S4 2.439(2) 2\_656 ?  
Fe8 S7 2.444(2) . ?  
Fe8 S15 2.463(2) 1\_655 ?  
Fe8 S14 2.554(2) 2\_656 ?  
Fe8 Fe4 2.8827(14) 2\_656 ?  
Fe8 Fe16 2.8925(19) 1\_655 ?  
Fe9 S17 2.304(3) 1\_556 ?  
Fe9 S4 2.424(3) . ?  
Fe9 S18 2.433(3) . ?  
Fe9 S13 2.451(3) 2\_546 ?  
Fe9 S12 2.501(3) 2\_646 ?  
Fe9 S15 2.558(3) 2\_546 ?  
Fe9 Fe15 2.934(3) 2\_546 ?  
Fe10 S19 2.377(2) 1\_456 ?  
Fe10 S5 2.389(2) . ?  
Fe10 S2 2.443(2) 1\_455 ?  
Fe10 S20 2.456(2) 1\_455 ?  
Fe10 S1 2.522(2) 1\_455 ?  
Fe10 S10 2.569(2) 1\_455 ?  
Fe10 Fe3 2.8909(19) 1\_455 ?  
Fe10 Fe11 2.9004(17) 1\_455 ?  
Fe10 Fe7 2.9723(13) 1\_556 ?  
Fe11 S4 2.371(2) . ?  
Fe11 S18 2.418(2) 1\_655 ?  
Fe11 S1 2.435(2) . ?  
Fe11 S2 2.464(2) . ?  
Fe11 S5 2.470(2) 1\_655 ?  
Fe11 S14 2.544(2) 1\_656 ?  
Fe11 Fe10 2.9003(17) 1\_655 ?  
Fe11 Fe17 2.9105(16) . ?  
Fe12 S19 2.355(2) . ?  
Fe12 S20 2.433(2) . ?  
Fe12 S9 2.439(2) . ?  
Fe12 S2 2.447(2) 1\_554 ?  
Fe12 S6 2.457(2) 1\_655 ?

Fe12 S1 2.560(2) . ?  
Fe12 Fe19 2.743(7) . ?  
Fe12 Fe20 2.9537(19) 1\_655 ?  
Fe13 S11 2.419(2) . ?  
Fe13 S9 2.424(2) . ?  
Fe13 S19 2.425(2) 1\_455 ?  
Fe13 S3 2.452(2) . ?  
Fe13 S10 2.464(3) . ?  
Fe13 S16 2.521(2) 1\_454 ?  
Fe13 Fe15 2.9446(19) . ?  
Fe14 S8 2.339(2) 1\_554 ?  
Fe14 S3 2.421(2) 1\_655 ?  
Fe14 S11 2.426(2) . ?  
Fe14 S12 2.458(2) . ?  
Fe14 S13 2.490(2) . ?  
Fe14 S7 2.575(2) . ?  
Fe14 Fe19 2.751(7) . ?  
Fe14 Fe17 2.9509(19) 2\_656 ?  
Fe15 S15 2.395(2) . ?  
Fe15 S3 2.411(2) . ?  
Fe15 S11 2.415(2) . ?  
Fe15 S12 2.458(2) 1\_455 ?  
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 Fe6 S12 Fe14 134.28(8) 1\_554 . ?  
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 Fe6 S12 Fe15 130.58(9) 1\_554 1\_655 ?  
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 Fe17 S12 Fe9 90.51(10) 2\_656 2\_656 ?  
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 Fe8 S13 Fe17 92.94(12) 1\_454 2\_656 ?  
 Fe8 S13 Fe9 81.42(10) 1\_454 2\_556 ?  
 Fe17 S13 Fe9 87.66(10) 2\_656 2\_556 ?  
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 Fe17 S14 Fe4 133.22(9) 1\_454 . ?  
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