

data\_Po5C\_293K\_Sudbury

\_audit\_creation\_method SHELXL-97  
\_chemical\_name\_systematic  
;  
Nonairondecasulfide  
;  
\_chemical\_name\_common '5C pyrrhotite'  
\_chemical\_melting\_point ?  
\_chemical\_formula\_moiety 'Fe18.01 S20'  
\_chemical\_formula\_sum 'Fe18.01 S20'  
\_chemical\_formula\_weight 1647.06

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 6.893(3)  
\_cell\_length\_b 28.643(12)  
\_cell\_length\_c 6.899(3)  
\_cell\_angle\_alpha 90.00  
\_cell\_angle\_beta 120.048(6)  
\_cell\_angle\_gamma 90.00  
\_cell\_volume 1179.0(8)  
\_cell\_formula\_units\_Z 2  
\_cell\_measurement\_temperature 293(2)  
\_cell\_measurement\_reflns\_used 2326  
\_cell\_measurement\_theta\_min 2.845  
\_cell\_measurement\_theta\_max 26.343

\_exptl\_crystal\_description irregular-fragment  
\_exptl\_crystal\_colour dark-gray  
\_exptl\_crystal\_size\_max 0.14  
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\_exptl\_crystal\_density\_meas .

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_exptl_absorpt_correction_type  multi-scan
_exptl_absorpt_correction_T_min 0.389
_exptl_absorpt_correction_T_max 0.688
_exptl_absorpt_process_details  'SADABS (Bruker, 2001)'

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_diffn_ambient_temperature      293(2)
_diffn_radiation_wavelength     0.71073
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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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_diffn_reflns_number            6369
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_reflns_number_total            3843
_reflns_number_gt               2701
_reflns_threshold_expression     >2\sigma(I)

_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
;
Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 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/[s2(Fo2)+(0.0168P)2+9.5307P] where P=(Fo2+2Fc2)/3'
_atom_sites_solution_primary direct
_atom_sites_solution_secondary difmap
_refine_ls_extinction_method SHELXL
_refine_ls_extinction_coef 0.00019(5)
_refine_ls_extinction_expression
'Fc*2=kFc[1+0.001xFc2/l3/sin(2\q)]-1/4'
_refine_ls_abs_structure_details
'Flack H D (1983), Acta Cryst. A39, 876-881'
_refine_ls_abs_structure_Flack 0.41(12)
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_refine_ls_number_restraints 1
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_refine_ls_wR_factor_gt 0.1174
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_refine_ls_restrained_S_all 1.242
_refine_ls_shift/su_max 0.000
_refine_ls_shift/su_mean 0.000
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_refine_diff_density_min -0.994
_refine_diff_density_rms 0.194

loop_
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_atom_site_type_symbol
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_U_iso_or_equiv
_atom_site_adp_type
_atom_site_occupancy
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_atom_site_calc_flag
_atom_site_refinement_flags
_atom_site_disorder_assembly

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Fe2 Fe 0.0018(10) -0.0884(3) 0.7298(10) 0.0115(15) Uani 0.475(9) 1 d P . .  
Fe3 Fe 0.5093(10) 0.11557(19) 0.7489(8) 0.0221(7) Uani 1 1 d . . .  
Fe4 Fe 0.0184(7) -0.08469(16) 0.2721(6) 0.0181(8) Uani 1 1 d . . .  
Fe5 Fe -0.0109(8) 0.01169(17) 0.7573(8) 0.0266(12) Uani 0.938(7) 1 d P . .  
Fe6 Fe 0.5254(8) 0.31573(16) 0.7502(7) 0.0244(10) Uani 1 1 d . . .  
Fe7 Fe -0.0324(7) 0.01501(14) 1.2168(7) 0.0177(7) Uani 1 1 d . . .  
Fe8 Fe 0.9876(8) 0.31558(16) 0.7637(7) 0.0229(9) Uani 1 1 d . . .  
Fe9 Fe 0.0026(9) -0.1806(2) 0.7670(9) 0.0137(13) Uani 0.598(9) 1 d P . .  
Fe10 Fe -0.4744(7) 0.01473(15) 0.7793(7) 0.0178(8) Uani 1 1 d . . .  
Fe11 Fe 0.4762(6) -0.08503(16) 0.7254(7) 0.0161(9) Uani 0.950(7) 1 d P . .  
Fe12 Fe 0.5072(6) 0.01925(15) 0.2395(6) 0.0187(9) Uani 1 1 d . . .  
Fe13 Fe 0.0019(9) 0.11622(18) 0.2397(9) 0.0212(7) Uani 1 1 d . . .  
Fe14 Fe 0.5016(7) 0.20994(17) 1.2358(10) 0.0199(13) Uani 0.803(9) 1 d P . .  
Fe15 Fe 0.0133(5) 0.21822(14) 0.2770(7) 0.0155(8) Uani 1 1 d . . .  
Fe16 Fe 1.0260(6) 0.21484(15) 0.7422(8) 0.0143(9) Uani 0.947(9) 1 d P . .  
Fe17 Fe 0.4998(6) -0.18628(15) 0.7463(8) 0.0184(9) Uani 1 1 d . . .  
Fe18 Fe -0.0115(7) 0.11475(17) 0.7447(7) 0.0154(6) Uani 1 1 d . . .  
Fe19 Fe 0.529(4) 0.1198(7) 1.271(4) 0.114(9) Uani 0.302(11) 1 d P . .  
Fe20 Fe -0.5093(7) -0.08260(15) 0.2597(6) 0.0183(9) Uani 1 1 d . . .  
S1 S 0.3305(6) -0.0302(2) 0.4160(7) 0.0091(10) Uani 1 1 d . . .  
S2 S 0.3305(6) -0.0347(2) 0.9154(7) 0.0109(10) Uani 1 1 d . . .  
S3 S -0.1612(6) 0.1651(2) 0.4158(7) 0.0106(10) Uani 1 1 d . . .  
S4 S 0.1649(6) -0.1376(2) 0.5813(7) 0.0107(11) Uani 1 1 d . . .  
S5 S -0.1694(7) -0.0402(2) 0.9151(7) 0.0119(12) Uani 1 1 d . . .  
S6 S -0.1693(7) -0.0344(2) 0.4143(7) 0.0101(9) Uani 1 1 d . . .  
S7 S 0.6696(7) 0.2612(2) 0.5851(8) 0.0139(12) Uani 1 1 d . . .  
S8 S 0.3326(7) 0.1613(2) 0.9145(8) 0.0136(11) Uani 1 1 d . . .  
S9 S 0.1613(7) 0.0650(2) 1.0768(8) 0.0127(10) Uani 1 1 d . . .  
S10 S 0.1664(7) 0.0630(3) 0.5802(8) 0.0145(11) Uani 1 1 d . . .  
S11 S 0.3356(7) 0.1656(2) 0.4171(8) 0.0125(10) Uani 1 1 d . . .  
S12 S 0.6676(7) 0.2650(2) 1.0847(8) 0.0110(11) Uani 1 1 d . . .  
S13 S 1.1717(7) 0.2640(2) 1.0857(8) 0.0100(11) Uani 1 1 d . . .  
S14 S -0.3386(6) -0.1342(2) 0.0809(8) 0.0124(10) Uani 1 1 d . . .  
S15 S 0.1703(7) 0.27064(19) 0.5877(8) 0.0087(11) Uani 1 1 d . . .  
S16 S 0.8364(6) 0.1686(2) 0.9152(7) 0.0081(9) Uani 1 1 d . . .  
S17 S 0.1650(6) -0.1324(2) 1.0829(8) 0.0124(10) Uani 1 1 d . . .  
S18 S -0.3403(6) -0.1347(2) 0.5805(8) 0.0115(10) Uani 1 1 d . . .  
S19 S 0.6684(7) 0.0689(2) 1.0816(8) 0.0136(11) Uani 1 1 d . . .  
S20 S 0.6663(7) 0.0642(2) 0.5838(8) 0.0123(10) Uani 1 1 d . . .

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\_atom\_site\_aniso\_U\_11  
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Fe1 0.0167(12) 0.0086(16) 0.0181(16) 0.0006(11) 0.0079(11) 0.0024(12)  
Fe2 0.008(2) 0.023(4) 0.004(2) -0.001(2) 0.0033(19) 0.007(2)  
Fe3 0.0375(15) 0.0091(14) 0.0225(14) 0.0048(13) 0.0171(12) 0.0062(12)  
Fe4 0.0241(14) 0.0151(17) 0.0131(14) -0.0040(13) 0.0078(11) 0.0019(13)

Fe5 0.0317(18) 0.017(2) 0.0233(18) -0.0023(16) 0.0080(14) 0.0065(16)  
 Fe6 0.0296(18) 0.0120(18) 0.0290(17) -0.0020(14) 0.0127(14) -0.0070(13)  
 Fe7 0.0249(16) 0.0092(17) 0.0154(15) 0.0030(14) 0.0075(11) 0.0012(14)  
 Fe8 0.0377(18) 0.0137(18) 0.0274(17) -0.0005(14) 0.0239(14) -0.0024(13)  
 Fe9 0.016(2) 0.016(3) 0.005(2) -0.0008(17) 0.0026(16) -0.0021(18)  
 Fe10 0.0209(15) 0.0084(17) 0.0228(17) -0.0033(14) 0.0100(11) -0.0007(14)  
 Fe11 0.0136(14) 0.0129(18) 0.0225(16) -0.0015(13) 0.0095(12) -0.0039(12)  
 Fe12 0.0128(13) 0.0149(18) 0.0211(16) -0.0011(14) 0.0031(11) -0.0032(13)  
 Fe13 0.0246(11) 0.0092(14) 0.0357(18) 0.0018(13) 0.0195(13) -0.0011(11)  
 Fe14 0.0164(19) 0.014(2) 0.034(3) 0.0058(17) 0.0162(18) 0.0065(14)  
 Fe15 0.0186(13) 0.0129(17) 0.0153(16) -0.0069(12) 0.0086(12) -0.0042(12)  
 Fe16 0.0191(14) 0.0128(19) 0.0167(16) -0.0003(12) 0.0133(13) -0.0050(12)  
 Fe17 0.0215(14) 0.0138(19) 0.0214(15) 0.0064(13) 0.0120(13) -0.0009(12)  
 Fe18 0.0143(10) 0.0107(14) 0.0122(12) 0.0036(12) -0.0003(9) 0.0019(11)  
 Fe19 0.151(16) 0.052(11) 0.148(15) -0.002(9) 0.081(12) -0.057(9)  
 Fe20 0.0214(16) 0.0102(18) 0.0204(18) -0.0001(13) 0.0082(14) 0.0001(12)  
 S1 0.0120(16) 0.007(2) 0.009(2) -0.0009(16) 0.0057(15) -0.0044(14)  
 S2 0.0092(16) 0.014(3) 0.009(2) -0.0028(18) 0.0045(16) -0.0056(15)  
 S3 0.0091(17) 0.013(3) 0.009(2) 0.0029(17) 0.0044(16) 0.0004(15)  
 S4 0.0097(17) 0.015(3) 0.008(2) 0.0017(16) 0.0049(16) 0.0046(15)  
 S5 0.0099(17) 0.015(3) 0.012(2) -0.0020(17) 0.0060(16) 0.0044(15)  
 S6 0.0115(17) 0.010(3) 0.008(2) 0.0053(17) 0.0045(16) 0.0017(15)  
 S7 0.0095(18) 0.023(3) 0.009(2) 0.0044(17) 0.0048(16) 0.0017(16)  
 S8 0.0105(17) 0.020(3) 0.010(2) 0.0025(17) 0.0052(16) -0.0042(15)  
 S9 0.0120(19) 0.017(3) 0.008(2) 0.0103(18) 0.0048(16) 0.0099(15)  
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 S14 0.0101(18) 0.015(3) 0.013(2) -0.0029(17) 0.0061(16) -0.0001(15)  
 S15 0.0124(17) 0.004(2) 0.009(2) 0.0015(15) 0.0047(15) 0.0010(14)  
 S16 0.0114(16) 0.006(2) 0.0069(19) 0.0007(16) 0.0048(15) -0.0016(14)  
 S17 0.0108(18) 0.014(3) 0.011(2) -0.0030(16) 0.0044(16) 0.0060(15)  
 S18 0.0107(18) 0.017(3) 0.009(2) 0.0033(17) 0.0061(16) 0.0002(16)  
 S19 0.0112(18) 0.021(3) 0.007(2) 0.0015(17) 0.0033(16) -0.0029(15)  
 S20 0.0101(18) 0.019(3) 0.008(2) -0.0082(17) 0.0052(16) -0.0025(15)

\_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 S15 2.393(6) . ?

Fe1 S8 2.393(7) . ?  
Fe1 S11 2.450(7) . ?  
Fe1 S12 2.465(7) . ?  
Fe1 S7 2.530(7) . ?  
Fe1 S16 2.562(6) . ?  
Fe1 Fe3 2.874(6) . ?  
Fe1 Fe6 2.895(5) . ?  
Fe2 S4 2.336(9) . ?  
Fe2 S6 2.439(9) . ?  
Fe2 S18 2.440(9) . ?  
Fe2 S17 2.460(9) . ?  
Fe2 S2 2.496(9) . ?  
Fe2 S5 2.538(8) . ?  
Fe2 Fe9 2.653(10) . ?  
Fe2 Fe5 2.876(9) . ?  
Fe3 S19 2.395(7) . ?  
Fe3 S20 2.421(7) . ?  
Fe3 S8 2.428(7) . ?  
Fe3 S11 2.446(7) . ?  
Fe3 S16 2.473(7) . ?  
Fe3 S10 2.540(8) . ?  
Fe3 Fe10 2.894(6) 1\_655 ?  
Fe4 S4 2.390(7) . ?  
Fe4 S1 2.432(7) . ?  
Fe4 S17 2.433(7) 1\_554 ?  
Fe4 S6 2.446(7) . ?  
Fe4 S5 2.485(6) 1\_554 ?  
Fe4 S14 2.560(7) . ?  
Fe4 Fe8 2.866(5) 2\_646 ?  
Fe4 Fe7 2.879(5) 1\_554 ?  
Fe5 S5 2.404(8) . ?  
Fe5 S2 2.434(7) . ?  
Fe5 S6 2.438(7) . ?  
Fe5 S9 2.445(8) . ?  
Fe5 S20 2.446(7) 1\_455 ?  
Fe5 S10 2.577(9) . ?  
Fe5 Fe18 2.953(6) . ?  
Fe6 S17 2.371(7) 2\_657 ?  
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Fe6 S12 2.476(7) . ?  
Fe6 S15 2.484(6) . ?  
Fe6 S14 2.564(7) 2\_556 ?  
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Fe7 S19 2.362(7) 1\_455 ?  
Fe7 S5 2.399(7) . ?  
Fe7 S6 2.458(7) 1\_556 ?  
Fe7 S9 2.460(8) . ?  
Fe7 S1 2.525(6) 1\_556 ?  
Fe7 S10 2.572(7) 1\_556 ?  
Fe7 Fe4 2.879(5) 1\_556 ?  
Fe7 Fe13 2.906(6) 1\_556 ?  
Fe8 S17 2.357(8) 2\_657 ?  
Fe8 S13 2.431(7) . ?

Fe8 S7 2.459(8) . ?  
Fe8 S4 2.462(7) 2\_656 ?  
Fe8 S15 2.500(6) 1\_655 ?  
Fe8 S14 2.545(7) 2\_656 ?  
Fe8 Fe4 2.866(5) 2\_656 ?  
Fe8 Fe16 2.908(5) . ?  
Fe9 S17 2.337(8) . ?  
Fe9 S4 2.417(8) . ?  
Fe9 S18 2.433(8) . ?  
Fe9 S13 2.495(8) 2\_647 ?  
Fe9 S12 2.513(8) 2\_647 ?  
Fe9 S15 2.538(8) 2\_546 ?  
Fe9 Fe15 2.911(6) 2\_546 ?  
Fe10 S19 2.381(7) 1\_455 ?  
Fe10 S5 2.409(7) . ?  
Fe10 S2 2.441(7) 1\_455 ?  
Fe10 S20 2.465(8) 1\_455 ?  
Fe10 S1 2.523(6) 1\_455 ?  
Fe10 S10 2.554(7) 1\_455 ?  
Fe10 Fe11 2.880(5) 1\_455 ?  
Fe10 Fe3 2.894(6) 1\_455 ?  
Fe11 S4 2.393(7) . ?  
Fe11 S1 2.427(7) . ?  
Fe11 S18 2.428(7) 1\_655 ?  
Fe11 S2 2.475(7) . ?  
Fe11 S5 2.476(6) 1\_655 ?  
Fe11 S14 2.548(7) 1\_656 ?  
Fe11 Fe10 2.880(5) 1\_655 ?  
Fe11 Fe17 2.904(5) . ?  
Fe12 S19 2.378(7) 1\_554 ?  
Fe12 S20 2.428(7) . ?  
Fe12 S9 2.446(7) 1\_554 ?  
Fe12 S6 2.469(7) 1\_655 ?  
Fe12 S2 2.478(7) 1\_554 ?  
Fe12 S1 2.540(6) . ?  
Fe12 Fe19 2.89(2) 1\_554 ?  
Fe12 Fe20 2.926(5) 1\_655 ?  
Fe13 S19 2.409(7) 1\_454 ?  
Fe13 S9 2.421(8) 1\_554 ?  
Fe13 S11 2.444(7) . ?  
Fe13 S16 2.450(7) 1\_454 ?  
Fe13 S3 2.464(7) . ?  
Fe13 S10 2.541(8) . ?  
Fe13 Fe7 2.907(6) 1\_554 ?  
Fe13 Fe15 2.931(5) . ?  
Fe14 S8 2.372(8) . ?  
Fe14 S3 2.388(7) 1\_656 ?  
Fe14 S11 2.433(7) 1\_556 ?  
Fe14 S12 2.466(8) . ?  
Fe14 S13 2.506(7) 1\_455 ?  
Fe14 S7 2.551(8) 1\_556 ?  
Fe14 Fe19 2.59(2) . ?  
Fe14 Fe17 2.976(5) 2\_657 ?  
Fe15 S15 2.387(7) . ?

Fe15 S3 2.415(7) . ?  
Fe15 S11 2.447(7) . ?  
Fe15 S12 2.464(6) 1\_454 ?  
Fe15 S13 2.468(7) 1\_454 ?  
Fe15 S16 2.586(6) 1\_454 ?  
Fe15 Fe9 2.911(6) 2\_556 ?  
Fe16 S8 2.391(7) 1\_655 ?  
Fe16 S15 2.397(7) 1\_655 ?  
Fe16 S3 2.419(7) 1\_655 ?  
Fe16 S13 2.494(7) . ?  
Fe16 S7 2.511(6) . ?  
Fe16 S16 2.540(6) . ?  
Fe16 Fe18 2.879(6) 1\_655 ?  
Fe17 S13 2.424(7) 2\_747 ?  
Fe17 S4 2.436(6) . ?  
Fe17 S18 2.442(7) 1\_655 ?  
Fe17 S12 2.446(7) 2\_647 ?  
Fe17 S7 2.486(7) 2\_646 ?  
Fe17 S14 2.494(7) 1\_656 ?  
Fe17 Fe14 2.975(5) 2\_647 ?  
Fe18 S20 2.406(7) 1\_455 ?  
Fe18 S3 2.439(7) . ?  
Fe18 S9 2.443(7) . ?  
Fe18 S8 2.448(6) . ?  
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 Fe9 S13 Fe14 138.4(2) 2\_657 1\_655 ?  
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 Fe17 S14 Fe11 70.32(17) 1\_454 1\_454 ?  
 Fe8 S14 Fe11 129.1(2) 2\_646 1\_454 ?

Fe17 S14 Fe20 133.77(19) 1\_454 . ?  
 Fe8 S14 Fe20 133.9(2) 2\_646 . ?  
 Fe11 S14 Fe20 90.9(3) 1\_454 . ?  
 Fe17 S14 Fe4 132.6(2) 1\_454 . ?  
 Fe8 S14 Fe4 68.30(14) 2\_646 . ?  
 Fe11 S14 Fe4 94.5(3) 1\_454 . ?  
 Fe20 S14 Fe4 89.3(3) . . ?  
 Fe17 S14 Fe6 89.6(3) 1\_454 2\_546 ?  
 Fe8 S14 Fe6 94.6(3) 2\_646 2\_546 ?  
 Fe11 S14 Fe6 128.53(19) 1\_454 2\_546 ?  
 Fe20 S14 Fe6 69.34(17) . 2\_546 ?  
 Fe4 S14 Fe6 130.4(2) . 2\_546 ?  
 Fe15 S15 Fe1 84.2(3) . . ?  
 Fe15 S15 Fe16 83.0(3) . 1\_455 ?  
 Fe1 S15 Fe16 79.0(2) . 1\_455 ?  
 Fe15 S15 Fe6 129.3(2) . . ?  
 Fe1 S15 Fe6 72.80(18) . . ?  
 Fe16 S15 Fe6 132.9(2) 1\_455 . ?  
 Fe15 S15 Fe8 130.4(2) . 1\_455 ?  
 Fe1 S15 Fe8 130.2(2) . 1\_455 ?  
 Fe16 S15 Fe8 72.83(18) 1\_455 1\_455 ?  
 Fe6 S15 Fe8 97.8(3) . 1\_455 ?  
 Fe15 S15 Fe9 72.41(19) . 2\_556 ?  
 Fe1 S15 Fe9 133.7(3) . 2\_556 ?  
 Fe16 S15 Fe9 134.2(3) 1\_455 2\_556 ?  
 Fe6 S15 Fe9 91.7(3) . 2\_556 ?  
 Fe8 S15 Fe9 94.4(3) 1\_455 2\_556 ?  
 Fe13 S16 Fe18 86.5(3) 1\_656 1\_655 ?  
 Fe13 S16 Fe3 87.0(3) 1\_656 . ?  
 Fe18 S16 Fe3 84.3(3) 1\_655 . ?  
 Fe13 S16 Fe16 129.4(2) 1\_656 . ?  
 Fe18 S16 Fe16 70.17(18) 1\_655 . ?  
 Fe3 S16 Fe16 131.8(2) . . ?  
 Fe13 S16 Fe1 129.4(2) 1\_656 . ?  
 Fe18 S16 Fe1 132.1(2) 1\_655 . ?  
 Fe3 S16 Fe1 69.58(16) . . ?  
 Fe16 S16 Fe1 97.9(3) . . ?  
 Fe13 S16 Fe15 71.10(17) 1\_656 1\_656 ?  
 Fe18 S16 Fe15 134.08(19) 1\_655 1\_656 ?  
 Fe3 S16 Fe15 131.7(2) . 1\_656 ?  
 Fe16 S16 Fe15 93.5(2) . 1\_656 ?  
 Fe1 S16 Fe15 91.6(3) . 1\_656 ?  
 Fe9 S17 Fe8 86.2(3) . 2\_647 ?  
 Fe9 S17 Fe6 88.7(3) . 2\_647 ?  
 Fe8 S17 Fe6 83.2(3) 2\_647 2\_647 ?  
 Fe9 S17 Fe20 135.3(3) . 1\_656 ?  
 Fe8 S17 Fe20 131.2(2) 2\_647 1\_656 ?  
 Fe6 S17 Fe20 75.03(16) 2\_647 1\_656 ?  
 Fe9 S17 Fe4 134.3(2) . 1\_556 ?  
 Fe8 S17 Fe4 73.48(19) 2\_647 1\_556 ?  
 Fe6 S17 Fe4 127.3(2) 2\_647 1\_556 ?  
 Fe20 S17 Fe4 85.9(3) 1\_656 1\_556 ?  
 Fe9 S17 Fe2 67.1(3) . . ?  
 Fe8 S17 Fe2 133.1(3) 2\_647 . ?



Fe6 S17 Fe2 131.0(3) 2\_647 . ?  
 Fe20 S17 Fe2 92.6(3) 1\_656 . ?  
 Fe4 S17 Fe2 97.8(3) 1\_556 . ?  
 Fe11 S18 Fe20 84.5(3) 1\_455 . ?  
 Fe11 S18 Fe9 131.8(2) 1\_455 . ?  
 Fe20 S18 Fe9 135.2(3) . . ?  
 Fe11 S18 Fe6 126.21(19) 1\_455 2\_546 ?  
 Fe20 S18 Fe6 73.58(18) . 2\_546 ?  
 Fe9 S18 Fe6 95.5(3) . 2\_546 ?  
 Fe11 S18 Fe2 95.7(3) 1\_455 . ?  
 Fe20 S18 Fe2 88.4(3) . . ?  
 Fe9 S18 Fe2 66.0(2) . . ?  
 Fe6 S18 Fe2 130.9(3) 2\_546 . ?  
 Fe11 S18 Fe17 73.21(18) 1\_455 1\_455 ?  
 Fe20 S18 Fe17 132.5(2) . 1\_455 ?  
 Fe9 S18 Fe17 88.5(3) . 1\_455 ?  
 Fe6 S18 Fe17 86.5(3) 2\_546 1\_455 ?  
 Fe2 S18 Fe17 134.3(3) . 1\_455 ?  
 Fe7 S19 Fe12 86.8(3) 1\_655 1\_556 ?  
 Fe7 S19 Fe10 79.4(3) 1\_655 1\_655 ?  
 Fe12 S19 Fe10 85.9(3) 1\_556 1\_655 ?  
 Fe7 S19 Fe3 129.3(3) 1\_655 . ?  
 Fe12 S19 Fe3 132.7(2) 1\_556 . ?  
 Fe10 S19 Fe3 74.58(19) 1\_655 . ?  
 Fe7 S19 Fe13 75.06(19) 1\_655 1\_656 ?  
 Fe12 S19 Fe13 133.5(2) 1\_556 1\_656 ?  
 Fe10 S19 Fe13 130.2(2) 1\_655 1\_656 ?  
 Fe3 S19 Fe13 89.7(3) . 1\_656 ?  
 Fe7 S19 Fe19 132.5(6) 1\_655 . ?  
 Fe12 S19 Fe19 73.3(4) 1\_556 . ?  
 Fe10 S19 Fe19 138.9(6) 1\_655 . ?  
 Fe3 S19 Fe19 93.8(6) . . ?  
 Fe13 S19 Fe19 88.0(5) 1\_656 . ?  
 Fe18 S20 Fe3 86.8(3) 1\_655 . ?  
 Fe18 S20 Fe12 129.1(2) 1\_655 . ?  
 Fe3 S20 Fe12 133.9(3) . . ?  
 Fe18 S20 Fe5 74.98(19) 1\_655 1\_655 ?  
 Fe3 S20 Fe5 130.9(2) . 1\_655 ?  
 Fe12 S20 Fe5 90.4(3) . 1\_655 ?  
 Fe18 S20 Fe19 82.9(5) 1\_655 1\_554 ?  
 Fe3 S20 Fe19 87.3(6) . 1\_554 ?  
 Fe12 S20 Fe19 72.4(5) . 1\_554 ?  
 Fe5 S20 Fe19 133.2(6) 1\_655 1\_554 ?  
 Fe18 S20 Fe10 128.2(2) 1\_655 1\_655 ?  
 Fe3 S20 Fe10 72.6(2) . 1\_655 ?  
 Fe12 S20 Fe10 97.0(3) . 1\_655 ?  
 Fe5 S20 Fe10 83.7(3) 1\_655 1\_655 ?  
 Fe19 S20 Fe10 140.2(5) 1\_554 1\_655 ?