checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FeHMTSOCO4

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: FeHMTSOCO4

```
Bond precision:   Si- C = 0.0040 A         Wavelength=0.71075

Cell:          a=6.888(3)          b=9.109(4)         c=13.932(6)
               alpha=85.725(12)    beta=84.120(11)    gamma=81.210(11)
Temperature:   123 K

                Calculated                 Reported
Volume          857.8(6)                   857.7(7)
Space group     P -1                       P -1
Hall group      -P 1                       -P 1
Moiety formula  C10 H18 Fe O6 Si3          C10 H18 Fe O6 Si3
Sum formula     C10 H18 Fe O6 Si3          C10 H18 Fe O6 Si3
Mr              374.36                     374.35
Dx,g cm-3       1.449                      1.449
Z               2                          2
Mu (mm-1)       1.105                      1.104
F000            388.0                      388.0
F000'           389.32
h,k,lmax                                   8,11,18
Nref                                       3764
Tmin,Tmax       0.974,0.989                0.768,0.989
Tmin'           0.967

Correction method= # Reported T Limits: Tmin=0.768 Tmax=0.989
AbsCorr = MULTI-SCAN

Data completeness=                 Theta(max)= 27.539

R(reflections)= 0.0571( 3490)                wR2(reflections)=
                                             0.1538( 3764)
S = 1.101                  Npar= 187
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.123
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full value Low .      0.974 Why?
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor ....        2.1 Note
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      3.093 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          9 Note
                1  0  0,   0  1  0,   1  1  0,   0 -1  1,  -1  0  1,   0  0  1,
                1  0  1,   0  1  1,   0  0  2,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         71 Report
                2  2  0,   3  2  0,  -4 -3  1,  -2 -2  1,   2  2  1,   5  4  1,
                1 -2  2,   2 -1  2,  -1  2  2,   5 -6  3,  -1 -3  3,   0 -2  3,
                1 -1  3,   3 -1  3,   0  2  3,   2  4  3,   1 -1  4,   3  0  4,
               -3 -9  7,  -4 -8  7,  -3 -8  8,   2 -7  8,  -3 -8  9,  -2 -8  9,
               -4 -7  9,  -3 -7  9,  -5 -5  9,   7  1  9,   1  9  9,  -1 -8 10,
               -3 -7 10,  -2 -7 10,  -3 -6 10,  -2 -6 10,  -2 -7 11,  -1 -7 11,
               -3 -6 11,  -2 -6 11,  -1 -6 11,  -4 -5 11,  -3 -1 11,  -2 -6 12,
               -1 -6 12,  -3 -5 12,  -2 -5 12,  -1 -5 12,  -1 -6 13,   0 -6 13,
               -2 -5 13,  -1 -5 13,   0 -5 13,  -1 -4 13,   0 -4 13,  -1 -5 14,
                0 -5 14,   1 -5 14,  -2 -4 14,  -1 -4 14,   0 -4 14,   1 -4 14,
                0 -3 14,   0 -4 15,  -1 -3 15,   0 -3 15,   1 -3 15,   0 -2 15,
                1 -2 15,   0 -2 16,   1 -2 16,   1 -1 16,   2 -1 16,
PLAT977_ALERT_2_C Check Negative Difference Density on H2B       .      -0.34 eA-3
```

Alert level G

```
CHEMS02_ALERT_1_G  Please check that you have entered the correct
           _publ_requested_category classification of your compound;
           FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
           FO or CO or EO for organic.
           From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or A
           From the CIF: _chemical_formula_sum :C10 H18 Fe1 O6 Si3
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.123 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1      --C7       .        6.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1      --C8       .        5.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1      --C9       .        6.8 s.u.
PLAT396_ALERT_2_G Deviating Si-O-Si  Angle From 150 for O1       .      140.0 Degree
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         92 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          3 Note
                1  1  0,   1 -2  2,   0  2  3,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        1.8 Low
```

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0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

```
  6 ALERT type 2 Indicator that the structure model may be wrong or deficient
  8 ALERT type 3 Indicator that the structure quality may be low
  1 ALERT type 4 Improvement, methodology, query or suggestion
  0 ALERT type 5 Informative message, check
```

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Publication of your CIF in IUCr journals

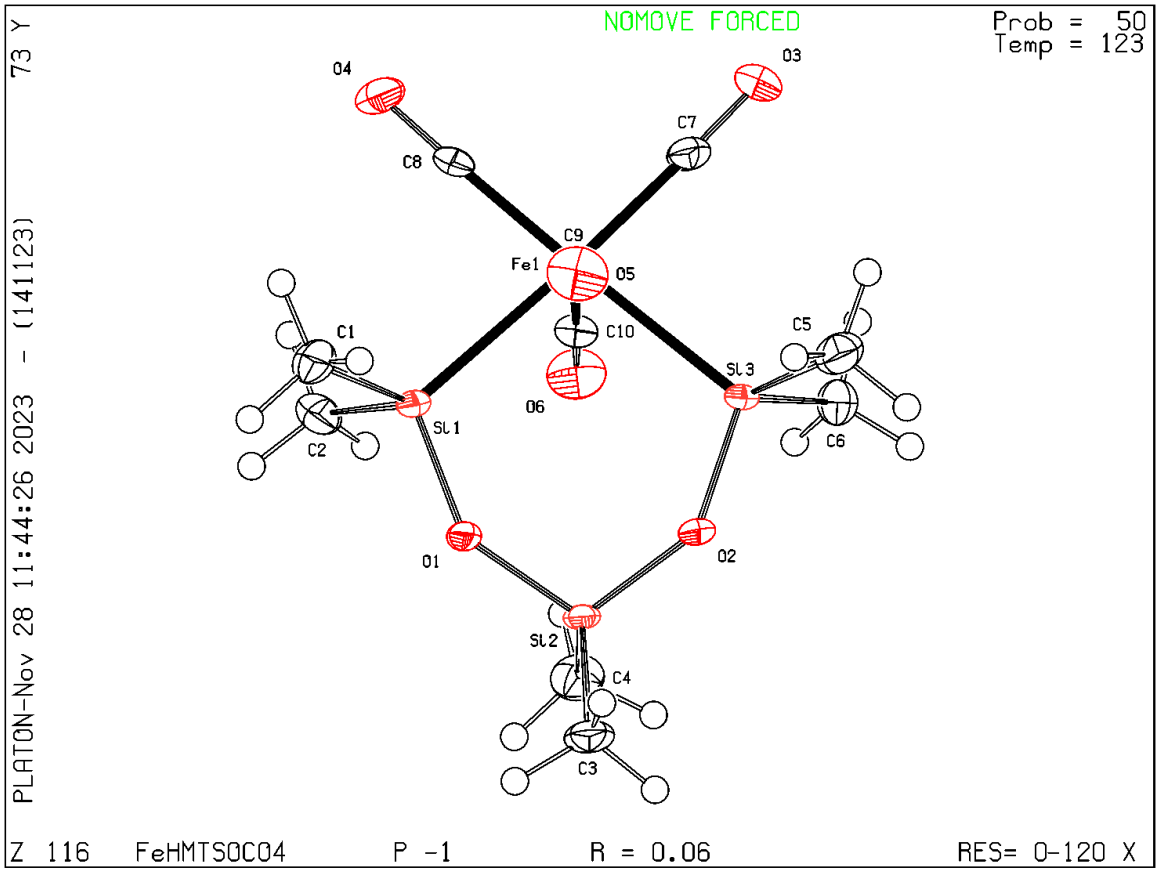
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 14/11/2023; check.def file version of 14/09/2023

Datablock FeHMTSOCO4 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FeC3Ph2CO4

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: FeC3Ph2CO4

```
Bond precision:   C-C = 0.0023 A          Wavelength=0.71075

Cell:             a=10.7449(5)     b=17.8737(5)         c=8.8682(4)
                  alpha=90         beta=111.834(5)      gamma=90
Temperature:      123 K

                 Calculated                Reported
Volume           1580.97(12)               1580.97(12)
Space group      P 21/c                    P 1 21/c 1
Hall group       -P 2ybc                   -P 2ybc
Moiety formula   C19 H10 Fe O4             C19 H10 Fe O4
Sum formula      C19 H10 Fe O4             C19 H10 Fe O4
Mr               358.12                    358.13
Dx,g cm-3        1.505                     1.505
Z                4                         4
Mu (mm-1)        0.973                     0.972
F000             728.0                     728.0
F000'            729.70
h,k,lmax                                   14,25,12
Nref                                       4356
Tmin,Tmax        0.981,0.990               0.881,0.990
Tmin'            0.981

Correction method= # Reported T Limits: Tmin=0.881 Tmax=0.990
AbsCorr = MULTI-SCAN

Data completeness=                 Theta(max)= 31.119

R(reflections)= 0.0308( 3602)                wR2(reflections)=
                                             0.0810( 4356)
S = 1.034                  Npar= 217
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         36 Report
                   1   0   2, -12   0   4,    2   2   4, -12   1   5, -12   0   6, -11   0   6,
                 -12   1   6, -11   1   6, -12   2   6, -12   3   6, -12   1   7, -11   1   7,
                 -12   2   7, -11   2   7, -12   3   7, -11   3   7, -11   0   8, -10   0   8,
                  -9   0   8, -11   1   8, -10   1   8, -11   2   8, -10   2   8, -11   3   8,
                 -11   4   8, -10   1   9,  -9   1   9, -10   2   9,  -9   2   9, -10   3   9,
                 -10   4   9,  -8   0 10,  -7   0 10,  -8   1 10,  -7   1 10,  -8   2 10,
```

Alert level G

```
CHEMS02_ALERT_1_G  Please check that you have entered the correct
            _publ_requested_category classification of your compound;
            FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
            FO or CO or EO for organic.
            From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or A
            From the CIF: _chemical_formula_sum :C19 H10 Fe1 O4
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O1       --C16      .        7.8 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    O2       --C17      .        5.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1      --C1       .        7.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1      --C16      .       12.8 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1      --C17      .       10.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1      --C18      .       10.4 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Fe1      --C19      .        8.5 s.u.
PLAT794_ALERT_5_G Tentative Bond Valency for Fe1       (II)      .       1.99 Info
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        665 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF ....          1 Note
                   1   0   2,
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File          1 Note
                   2   2   4,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........        3.4 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.        12 Info
```

---

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0 **ALERT level B** = A potentially serious problem, consider carefully
1 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
15 **ALERT level G** = General information/check it is not something unexpected

2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
9 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

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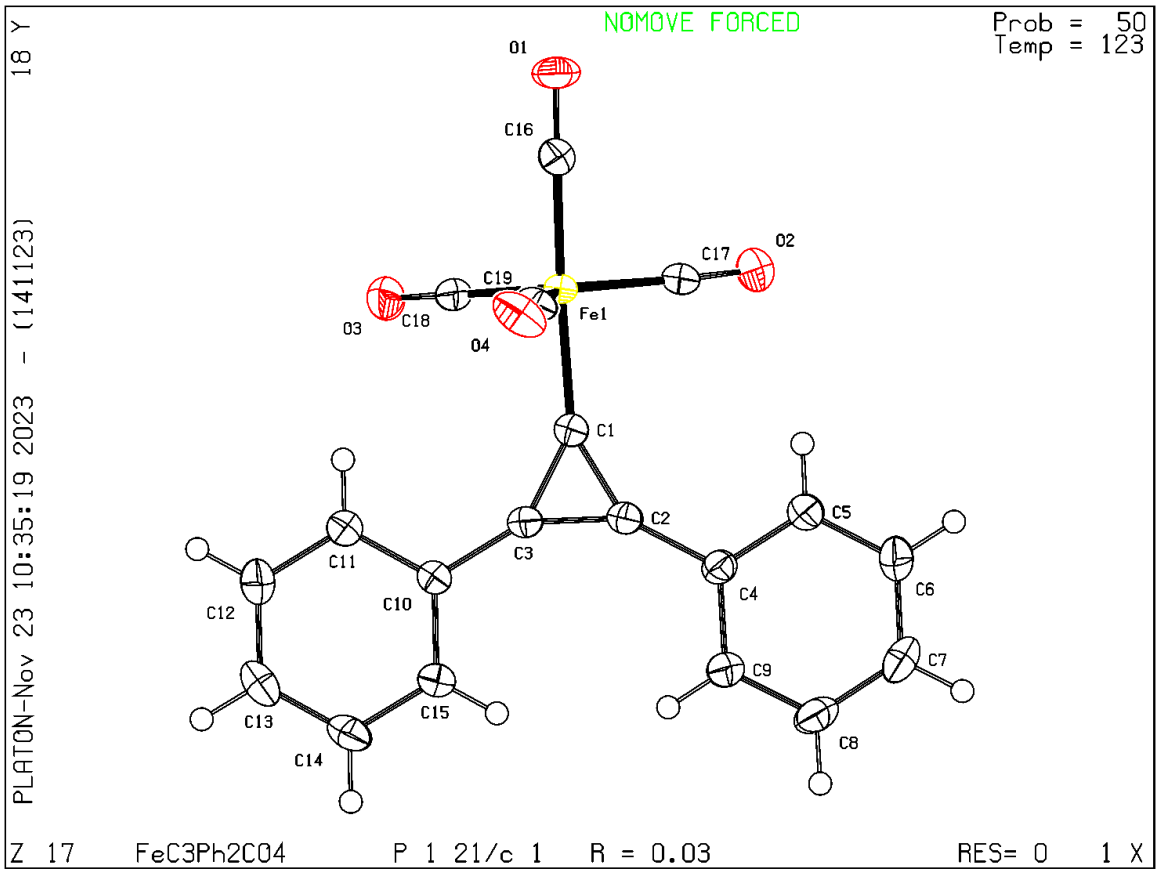
PLATON version of 14/11/2023; check.def file version of 14/09/2023

Datablock FeC3Ph2CO4 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ys240827_auto

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ys240827_auto

```
Bond precision:   C-C = 0.0020 A          Wavelength=0.71073

Cell:              a=13.0378(6)      b=8.6924(4)      c=14.5590(7)
                   alpha=90          beta=90          gamma=90
Temperature:       123 K

                 Calculated                  Reported
Volume           1649.97(13)                 1649.97(13)
Space group      P b c n                     P b c n
Hall group       -P 2n 2ab                   -P 2n 2ab
Moiety formula   C9 H10 N2 O                 C9 H10 N2 O
Sum formula      C9 H10 N2 O                 C9 H10 N2 O
Mr               162.19                      162.19
Dx,g cm-3        1.306                       1.306
Z                8                           8
Mu (mm-1)        0.088                       0.088
F000             688.0                       688.0
F000'            688.27
h,k,lmax         18,12,21                    18,11,18
Nref             2609                        2102
Tmin,Tmax        0.987,0.996                 0.476,1.000
Tmin'            0.985

Correction method= # Reported T Limits: Tmin=0.476 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.806            Theta(max)= 30.885

                                                    wR2(reflections)=
R(reflections)= 0.0510( 1428)                       0.1354( 2102)
S = 1.074                  Npar= 111
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 6.068 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.151 Check

Alert level G

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 427 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.8 Low
PLAT952_ALERT_5_G Calculated (ThMax) and CIF-Reported Lmax Differ. 3 Units
PLAT958_ALERT_1_G Calculated (ThMax) and Actual (FCF) Lmax Differ. 3 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 3.316 Note
Predicted wR2: Based on SigI**2 4.08 or SHELX Weight 12.61
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 4 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
1 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check

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Publication of your CIF in IUCr journals

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Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/08/2024; check.def file version of 21/08/2024

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ys250320_auto

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: ys250320_auto

```
Bond precision:   O- C = 0.0060 A          Wavelength=0.71073

Cell:             a=17.2330(5)     b=18.2213(3)         c=15.0470(5)
                  alpha=90         beta=114.343(4)      gamma=90
Temperature:      123 K

                 Calculated                 Reported
Volume           4304.8(2)                  4304.8(2)
Space group      P 21/c                     P 1 21/c 1
Hall group       -P 2ybc                    -P 2ybc
Moiety formula   C13 H25 Fe N O7 Si3        C13 H25 Fe N O7 Si3
Sum formula      C13 H25 Fe N O7 Si3        C13 H25 Fe N O7 Si3
Mr               447.46                     447.46
Dx,g cm-3        1.381                      1.381
Z                8                          8
Mu (mm-1)        0.898                      0.898
F000             1872.0                     1872.0
F000'            1877.43
h,k,lmax         24,26,21                   21,25,20
Nref             13602                      11403
Tmin,Tmax        0.949,0.974                0.556,1.000
Tmin'            0.834

Correction method= # Reported T Limits: Tmin=0.556 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.838           Theta(max)= 30.903

R(reflections)= 0.0625( 8724)                wR2(reflections)=
                                             0.1680( 11403)
S = 1.160                  Npar= 467
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....       2.83 Report
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      8.180 Check
PLAT910_ALERT_3_C Missing # of FCF Reflection(s) Below Theta(Min).          6 Note
                  1   0   0,    1   1   0,    0   2   0,    1   2   0,  -1   1   1,    0   1   1,
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         10 Report
                 -6   2   1,   -6   4   1,   -1   4   1,    2   5   1,  -3   8   1,   -9 10   1,
                 -6  10   1,   -5  11   1,    0  13   1,   -1   4   3,
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers ..          1 Check
                  4   4   1,
```

Alert level G

```
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      13.80 Why ?
PLAT432_ALERT_2_G Short Inter X...Y Contact  O12      ..C20      .       2.98 Ang.
                                          x,1/2-y,-1/2+z  =      4_565 Check
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600       1750 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         10 Note
                 -9  10   1,   -6   2   1,   -6   4   1,   -6  10   1,   -5  11   1,   -3   8   1,
                 -1   4   1,   -1   4   3,    0  13   1,    2   5   1,
PLAT950_ALERT_5_G Calculated (ThMax) and CIF-Reported Hmax Differ           3 Units
PLAT956_ALERT_1_G Calculated (ThMax) and Actual (FCF) Hmax Differ           3 Units
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ............     4.870 Note
             Predicted wR2: Based on SigI**2  3.45 or SHELX Weight 14.48
```

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Publication of your CIF in other journals

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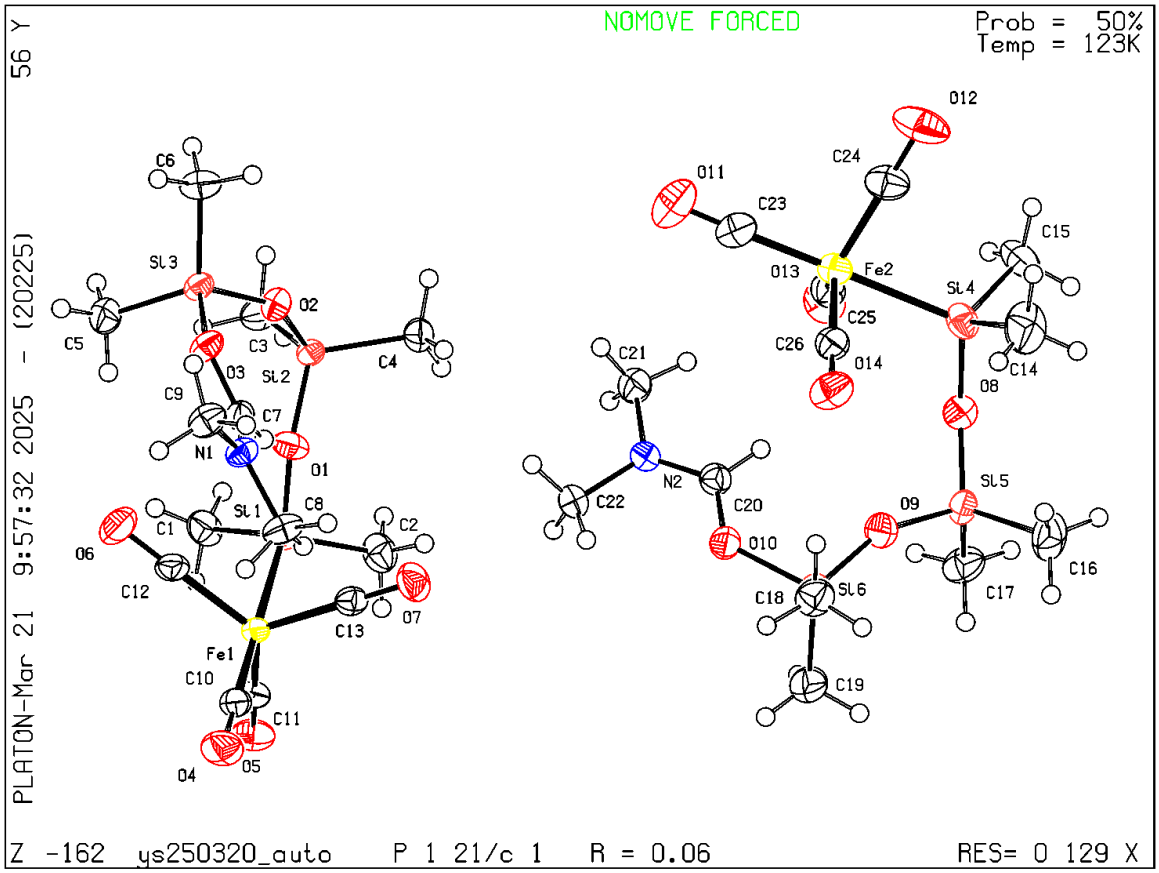
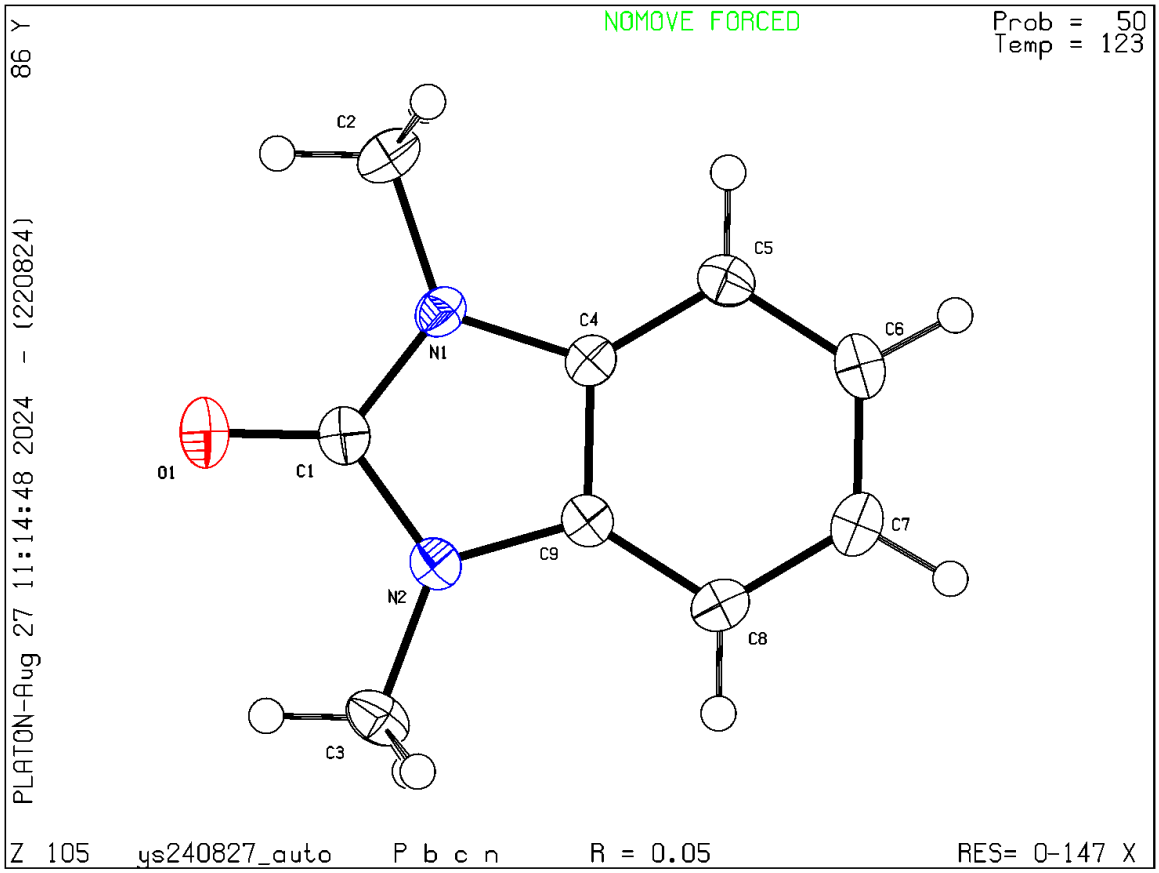
PLATON version of 02/02/2025; check.def file version of 02/02/2025

Datablock ys250320_auto - ellipsoid plot



Datablock ys240827_auto - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) FeHMTSO-O-MeBZIMCO4

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: FeHMTSO-O-MeBZIMCO4

```
Bond precision:   C-C = 0.0135 A          Wavelength=0.71075

Cell:           a=8.8395(6)        b=8.8699(6)       c=16.5142(11)
                alpha=84.980(5)    beta=85.263(5)    gamma=83.593(5)
Temperature:    123 K

                Calculated                Reported
Volume          1278.31(15)               1278.31(15)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C19 H28 Fe N2 O7 Si3      C19 H28 Fe N2 O7 Si3
Sum formula     C19 H28 Fe N2 O7 Si3      C19 H28 Fe N2 O7 Si3
Mr              536.55                    536.54
Dx,g cm-3       1.394                     1.394
Z               2                         2
Mu (mm-1)       0.770                     0.769
F000            560.0                     560.0
F000'           561.39
h,k,lmax                                  12,12,23
Nref                                      7217
Tmin,Tmax       0.991,0.992               0.666,0.992
Tmin'           0.989

Correction method= # Reported T Limits: Tmin=0.666 Tmax=0.992
AbsCorr = MULTI-SCAN

Data completeness=                 Theta(max)= 31.120

R(reflections)= 0.1292( 3473)                wR2(reflections)=
                                             0.3439( 7217)
S = 1.054                  Npar= 297
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..        48% Check
PLAT082_ALERT_2_C High R1 Value ..................................       0.13 Report
PLAT084_ALERT_3_C High wR2 Value (i.e. > 0.25) ...................       0.34 Report
PLAT234_ALERT_4_C Large Hirshfeld Difference Si1      --C2       .       0.16 Ang.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O2 Check
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of         O3 Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of        Si3 Check
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ...............     0.0135 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     29.473 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      4.596 Check
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......      2.286 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600         84 Report
                  2  0  0,  -6  1  0,  -3  1  0,   3  2  0,   0  3  0,   0  6  0,
                  2  6  0,   1  7  0,   2 -4  1,  -1 -3  1,   0 -3  1,   1 -3  1,
                  2 -3  1,  -1 -2  1,   0 -2  1,   1  0  1,  -2  1  1,   2  1  1,
                 -4  4  1,   3 -4  2,   4 -4  2,   3 -3  2,   4 -3  2,   6 -2  2,
                  0 -1  2,   4 -1  2,   3  0  2,   6  0  2,  -1  2  2,  -5  3  2,
                  4 -4  3,   4 -3  3,  -1 -2  3,   0 -2  3,   2 -2  3,   3 -2  3,
                  1 -1  3,   2 -1  3,   5 -1  3,  -4  0  3,  -1  0  3,   5  0  3,
                  0  1  3,   7  1  3,  -4  3  3,  -3  6  3,  -5 -1  4,   4 -1  4,
                  0  1  4,   1  2  4,   4  2  4,  -4  3  4,  -2  3  4,   1  3  4,
                 -4  5  4,   4 -4  5,  -1  0  5,  -6  1  5,  -2  1  5,   0  4  5,
                 -2 -6  6,  -2 -1  6,   0 -1  6,   0  1  6,  -1  2  6,   1  2  6,
                 -1  3  6,  -4  4  6,  -2  4  6,   0  4  6,  -1  5  6,   7 -6  7,
                  3 -4  7,  -1 -2  7,   2 -1  7,   0  1  7,   1  5  7,   0 -5  8,
                  1 -2  8,  -4  2  8,   8 -4  9,   0 -3  9,   5 -1  9,  -2  1 11,
PLAT977_ALERT_2_C Check Negative Difference Density on H2B       .      -0.39 eA-3
PLAT977_ALERT_2_C Check Negative Difference Density on H6A       .      -0.51 eA-3
```

Alert level G

```
CHEMS02_ALERT_1_G  Please check that you have entered the correct
            _publ_requested_category classification of your compound;
            FI or CI or EI for inorganic; FM or CM or EM for metal-organic;
            FO or CO or EO for organic.
            From the CIF: _publ_requested_category   CHOOSE FI FM FO CI CM CO or A
            From the CIF: _chemical_formula_sum :C19 H28 Fe1 N2 O7 Si3
PLAT072_ALERT_2_G SHELXL First  Parameter in WGHT  Unusually Large       0.11 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large      12.10 Why ?
PLAT154_ALERT_1_G The s.u.'s on the Cell Angles are Equal ..(Note)      0.005 Degree
PLAT395_ALERT_2_G Deviating  X-O-Y   Angle From 120 for O3       .      151.2 Degree
PLAT882_ALERT_1_G No Datum for _diffrn_reflns_av_unetI/netI ......     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          1 Note
                  0  0  1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        914 Note
PLAT930_ALERT_2_G FCF-based   Twin Law ( 1-1 0)         Est.d BASF       0.15 Check
PLAT931_ALERT_5_G CIFcalcFCF  Twin Law ( 1-1 0)         Est.d BASF       0.15 Check
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File         82 Note
                  1  0  1,   2 -3  1,  -2  1  5,   0 -1  2,  -1  0  5,  -1 -2  3,
                  0 -2  3,  -1  2  2,  -1  0  3,   3 -3  2,  -1 -2  7,   2 -1  3,
```

```
                 0 -2  1,    0  6  0,    1  2  4,    0 -1  6,   -1  2  6,    0  3  0,
                -1  5  6,    4 -3  3,    3 -2  3,    4 -3  2,    0  4  6,   -2  1  1,
                 1 -3  1,   -2 -1  6,    2 -4  1,   -3  6  3,    0 -3  1,    2  0  0,
                -4  3  4,   -1 -2  1,    2 -1  7,    3  2  0,    0  1  7,    1  7  0,
                 6  0  2,    4 -4  2,    5 -1  9,   -2  3  4,    0  1  3,    0  1  6,
                 3 -4  2,    3  0  2,    4 -4  3,    1  2  6,    4 -4  5,    7  1  3,
                 5  0  3,   -4  5  4,
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        2.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          0 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
  14 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  12 ALERT type 2 Indicator that the structure model may be wrong or deficient
   9 ALERT type 3 Indicator that the structure quality may be low
   2 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

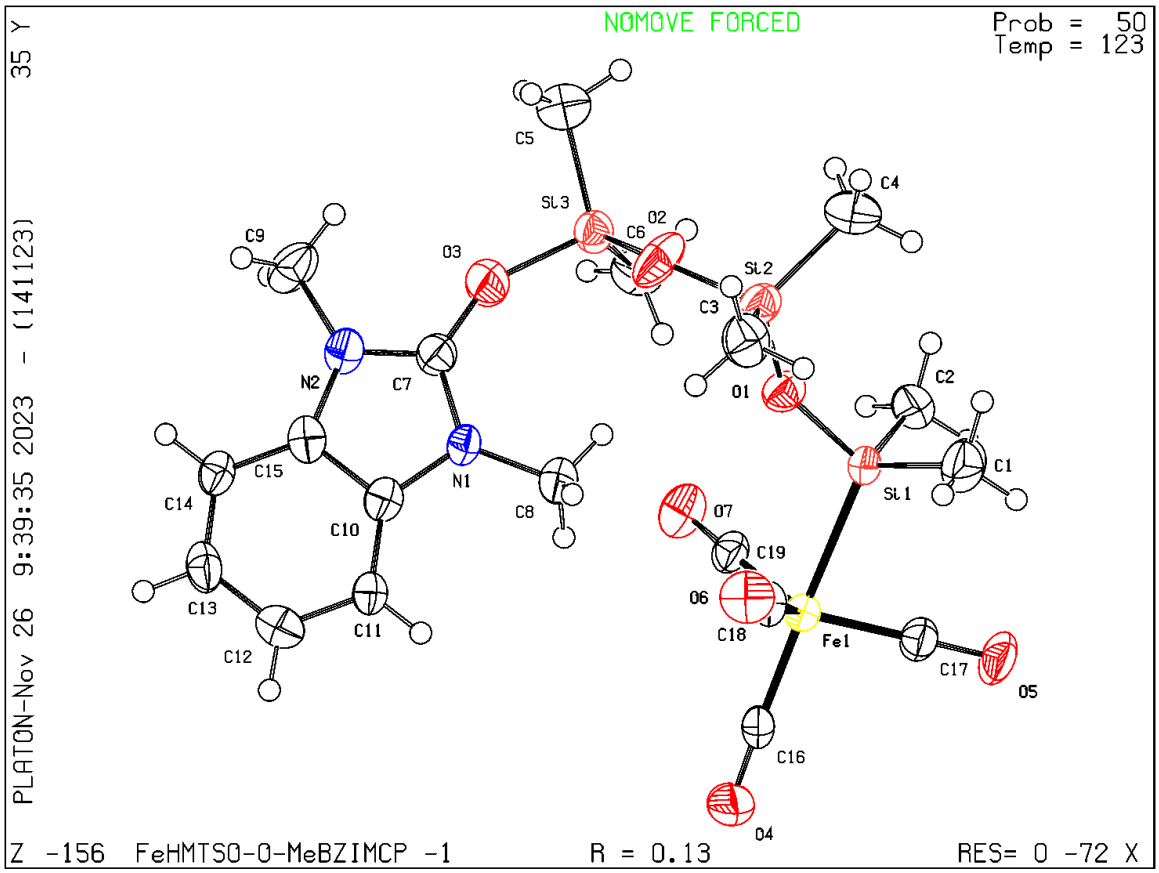
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 14/11/2023; check.def file version of 14/09/2023

Datablock FeHMTSO-O-MeBZIMCO4 - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ys240507_auto

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: ys240507_auto

```
Bond precision:   C-C = 0.0032 A           Wavelength=0.71073

Cell:              a=8.2066(3)      b=28.6912(9)         c=9.4600(3)
                   alpha=90         beta=94.376(3)       gamma=90
Temperature:       123 K

                 Calculated                  Reported
Volume           2220.93(13)                 2220.93(13)
Space group      P 21/n                      P 1 21/n 1
Hall group       -P 2yn                      -P 2yn
Moiety formula   C22 H16 Fe2 O6 S2           C22 H16 Fe2 O6 S2
Sum formula      C22 H16 Fe2 O6 S2           C22 H16 Fe2 O6 S2
Mr               552.17                      552.17
Dx,g cm-3        1.651                       1.651
Z                4                           4
Mu (mm-1)        1.531                       1.531
F000             1120.0                      1120.0
F000'            1124.17
h,k,lmax         11,41,13                    10,41,13
Nref             7049                        5975
Tmin,Tmax        0.921,0.970                 0.795,1.000
Tmin'            0.916

Correction method= # Reported T Limits: Tmin=0.795 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.848            Theta(max)= 30.957

R(reflections)= 0.0347( 4615)                    wR2(reflections)=
                                                 0.0821( 5975)
S = 1.045                  Npar= 291
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ..... 2.591 Check
PLAT934_ALERT_3_C Number of (Iobs-Icalc)/Sigma(W) > 10 Outliers .. 1 Check
-4 1 3,

Alert level G

PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe1 --C18 . 7.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe1 --C19 . 6.9 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe1 --C20 . 7.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe2 --S2 . 5.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe2 --C21 . 5.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Fe2 --C22 . 6.9 s.u.
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min). 2 Note
0 2 0, 0 1 1,
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 945 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.8 Low
PLAT969_ALERT_5_G The 'Henn et al.' R-Factor-gap value ..... 2.56 Note
Predicted wR2: Based on SigI**2 3.21 or SHELX Weight 8.05
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 5 Info

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Publication of your CIF in other journals

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PLATON version of 06/01/2024; check.def file version of 05/01/2024

Datablock ys240507_auto - ellipsoid plot