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# Crystal and Electronic Structure of a Hexacarbonyldiiron Cluster Tethered To Naphthalene-2-Thiolate Ligands

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STRUCTURAL  
CHEMISTRY

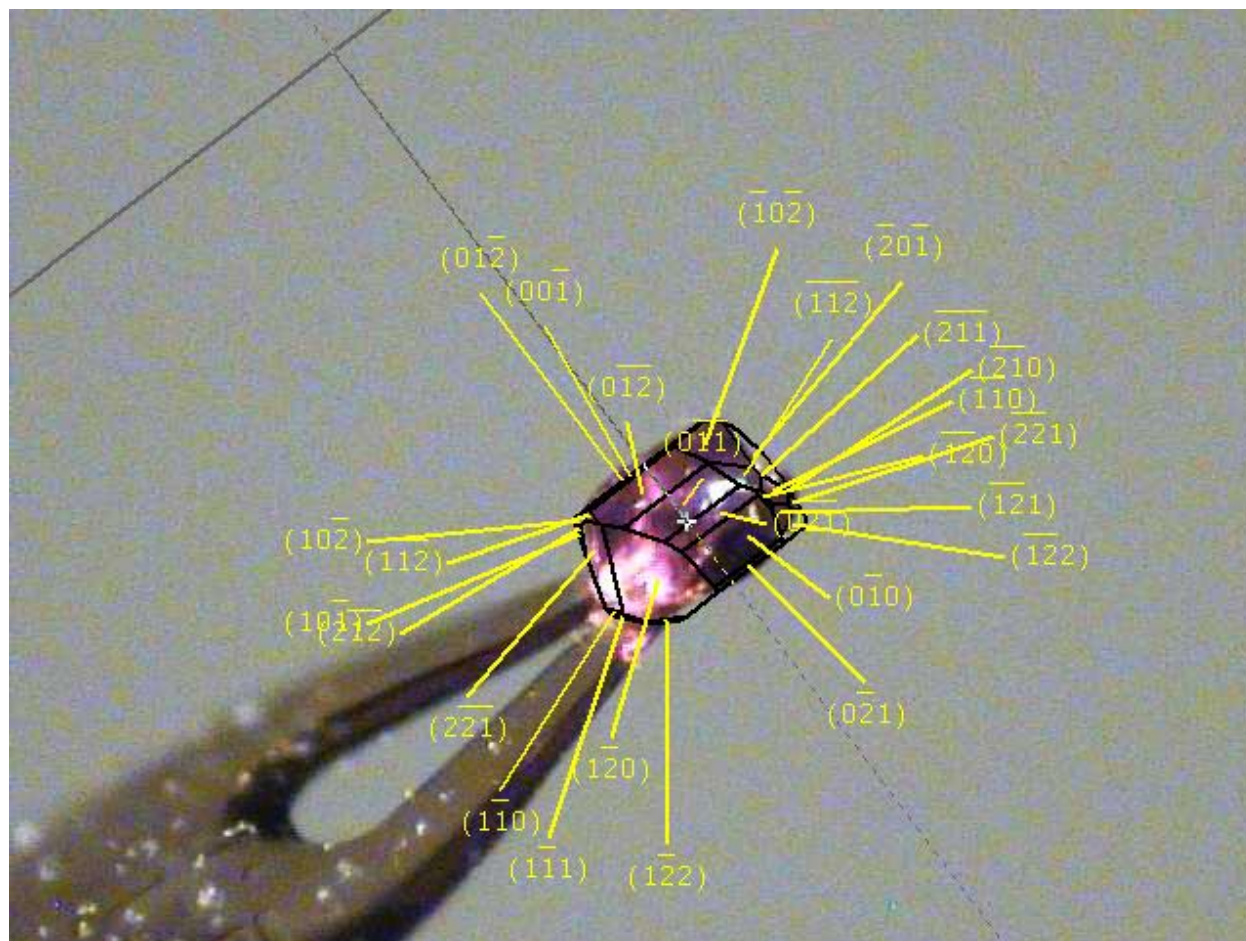
**Volume 74 (2018)**

**Supporting information for article:**

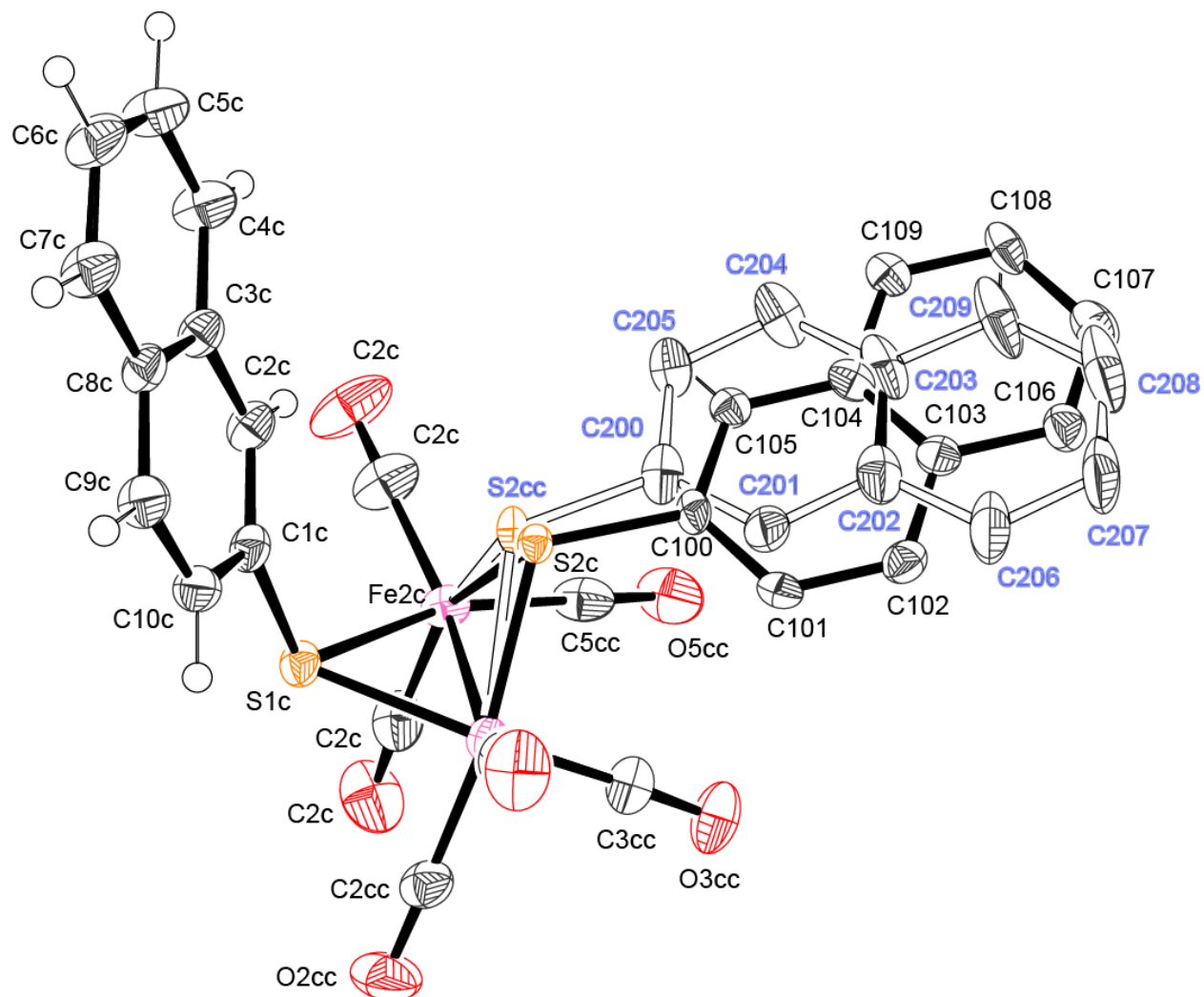
**Crystal and electronic structure of a hexacarbonyldiiron cluster  
tethered to naphthalene-2-thiolate ligands**

**Charles Mebi, Nikolay Gerasimchuk and Jordan Labrecque**

**S1.** Indexed crystal faces of **1** by using the videomicroscope for the numerical absorption correction.



**S2.** Resolved disorder in the structure of **1** (unit C). Thermal ellipsoids are drawn at their 50% probability level; H-atoms on disordered naphthyl- fragment are not shown for clarity.



## S3. checkCIF/PLATON (basic structural check)

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*Structure factors have been supplied for datablock(s) 1*

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](#)

Please wait while processing ...

[Interpreting this report](#)

[Structure factor report](#)

### Datablock: 1

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Bond precision: C-C = 0.0042 Å Wavelength=0.71073

Cell: a=10.1425(5) b=16.1771(7) c=24.5865(11)  
alpha=106.980(1) beta=99.453(1) gamma=96.998(1)

Temperature: 100 K

|                        | Calculated        | Reported          |
|------------------------|-------------------|-------------------|
| Volume                 | 3743.7(3)         | 3743.7(3)         |
| Space group            | P -1              | P -1              |
| Hall group             | -P 1              | -P 1              |
| Moiety formula         | C26 H14 Fe2 O6 S2 | C26 H14 Fe2 O6 S2 |
| Sum formula            | C26 H14 Fe2 O6 S2 | C26 H14 Fe2 O6 S2 |
| Mr                     | 598.19            | 598.19            |
| Dx, g cm <sup>-3</sup> | 1.592             | 1.592             |
| Z                      | 6                 | 6                 |
| Mu (mm <sup>-1</sup> ) | 1.370             | 1.370             |
| F000                   | 1812.0            | 1812.0            |
| F000'                  | 1818.32           |                   |
| h, k, lmax             | 13, 21, 32        | 13, 21, 32        |
| Nref                   | 18948             | 18799             |
| Tmin, Tmax             | 0.717, 0.753      | 0.656, 0.750      |
| Tmin'                  | 0.674             |                   |

Correction method= # Reported T Limits: Tmin=0.656  
Tmax=0.750 AbsCorr = NUMERICAL

Data completeness= 0.992 Theta(max)= 28.483

R(reflections)= 0.0429( 14329) wR2(reflections)= 0.1140( 18799)

S = 1.072 Npar= 1056

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.

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### Alert level C

[PLAT213 ALERT 2 C](#) Atom O6AA

has ADP max/min Ratio .....

3.1 prolat

[PLAT213 ALERT 2 C](#) Atom O06A has ADP max/min Ratio ..... 3.1 prolat  
[PLAT220 ALERT 2 C](#) Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.3 Ratio  
[PLAT230 ALERT 2 C](#) Hirshfeld Test Diff for C13A -- C14A .. 7.0 s.u.  
[PLAT911 ALERT 3 C](#) Missing # FCF Refl Between THmin & STh/L= 0.600 16 Report

## ●Alert level G

[PLAT002 ALERT 2 G](#) Number of Distance or Angle Restraints on AtSite 12 Note  
[PLAT154 ALERT 1 G](#) The s.u.'s on the Cell Angles are Equal ..(Note) 0.001 Degree  
[PLAT171 ALERT 4 G](#) The CIF-Embedded .res File Contains EADP Records 2 Report  
[PLAT172 ALERT 4 G](#) The CIF-Embedded .res File Contains DFIX Records 10 Report  
[PLAT230 ALERT 2 G](#) Hirshfeld Test Diff for O6BB -- C6BB .. 5.5 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe1C -- C1CC .. 6.4 s.u.

### And 16 other PLAT232 Alerts

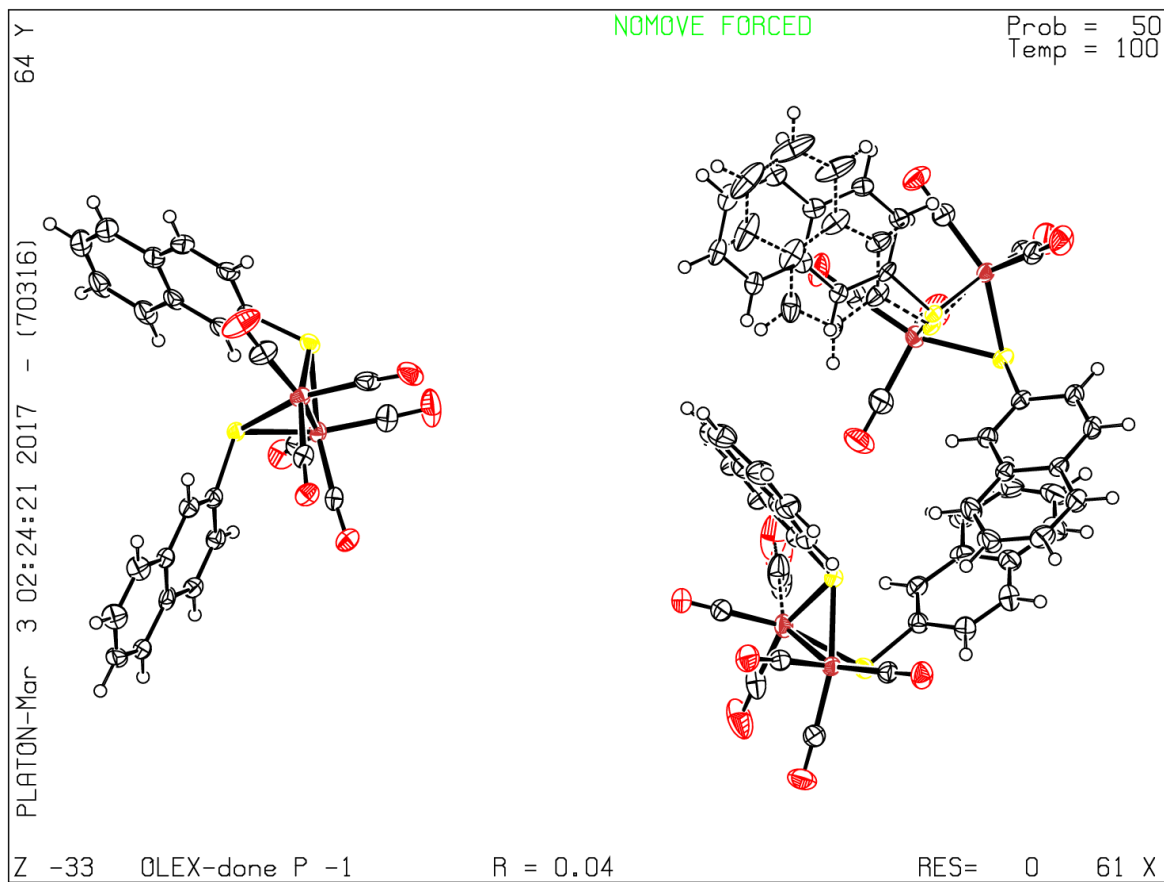
Less ...

[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe1C -- C2CC .. 6.3 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe1C -- C3CC .. 7.4 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe2C -- C4CC .. 6.1 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe2C -- C5CC .. 7.6 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe2C -- C6CC .. 5.4 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe1A -- C1AA .. 5.7 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe1A -- C2AA .. 5.1 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe1A -- C3AA .. 7.3 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe2A -- C4AA .. 6.5 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe2A -- C5AA .. 6.5 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe1B -- C1BB .. 6.5 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe1B -- C2BB .. 7.4 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe1B -- C3BB .. 7.3 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe2B -- C4BB .. 7.4 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe2B -- C5BB .. 5.1 s.u.  
[PLAT232 ALERT 2 G](#) Hirshfeld Test Diff (M-X) Fe2B -- C6BB .. 7.6 s.u.  
[PLAT301 ALERT 3 G](#) Main Residue Disorder .....(Resd 1).. 31 % Note  
[PLAT301 ALERT 3 G](#) Main Residue Disorder .....(Resd 2).. 6 % Note  
[PLAT432 ALERT 2 G](#) Short Inter X...Y Contact O3BB .. C1CC .. 3.00 Ang.  
[PLAT432 ALERT 2 G](#) Short Inter X...Y Contact O5CC .. C205 .. 2.99 Ang.  
[PLAT720 ALERT 4 G](#) Number of Unusual/Non-Standard Labels ..... 39 Note  
[PLAT860 ALERT 3 G](#) Number of Least-Squares Restraints ..... 10 Note  
[PLAT912 ALERT 4 G](#) Missing # of FCF Reflections Above STh/L= 0.600 133 Note  
[PLAT933 ALERT 2 G](#) Number of OMIT Records in Embedded .res File ... 12 Note  
[PLAT978 ALERT 2 G](#) Number C-C Bonds with Positive Residual Density. 3 Note

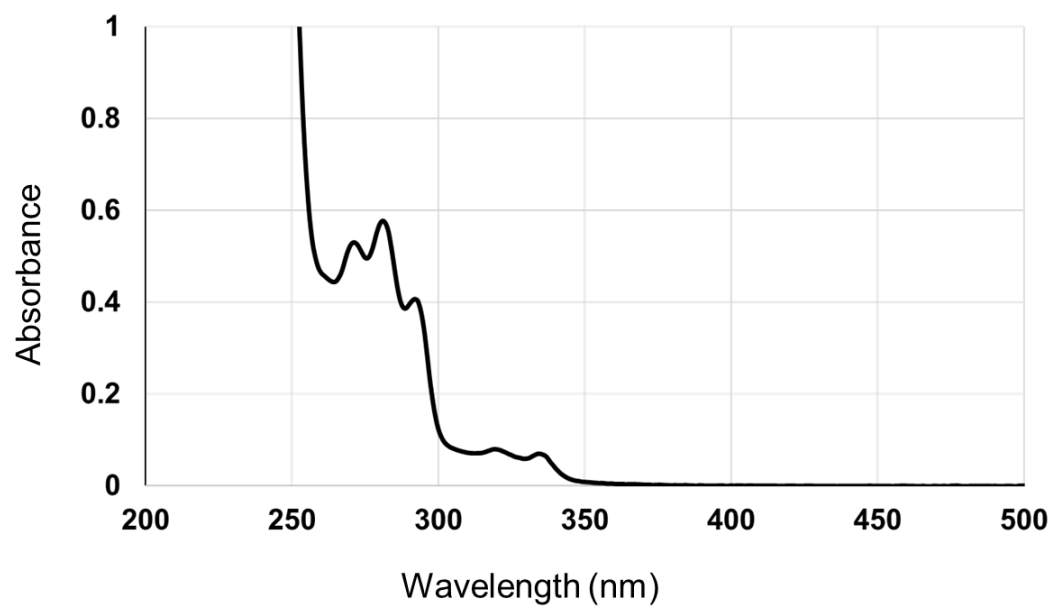
0 **ALERT level A** = Most likely a serious problem - resolve or explain  
 0 **ALERT level B** = A potentially serious problem, consider carefully  
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 31 **ALERT level G** = General information/check it is not something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

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

PLATON version of 26/02/2017; check.def file version of 21/02/2017

**Datablock 1** - ellipsoid plot[Download CIF editor \(pubCIF\) from the IUCr](#)[Download CIF editor \(enCIFer\) from the CCDC](#)[Test a new CIF entry](#)

**S4:** UV-visible spectrum of 2-naphthalenethiol



UV-visible spectrum of 2-naphthalenethiol (0.1 mM) measured in acetonitrile.