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

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STRUCTURAL
CHEMISTRY

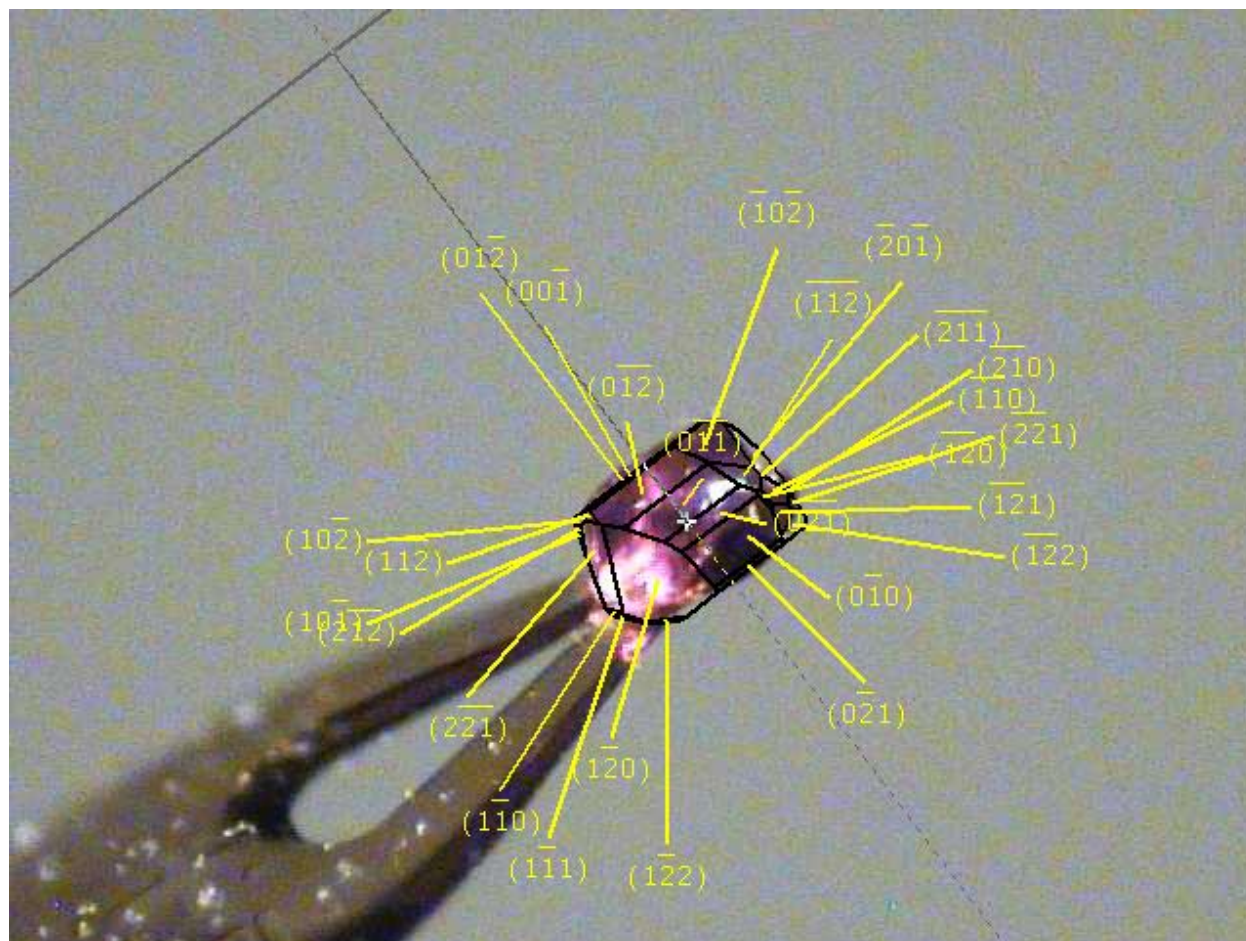
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Supporting information for article:

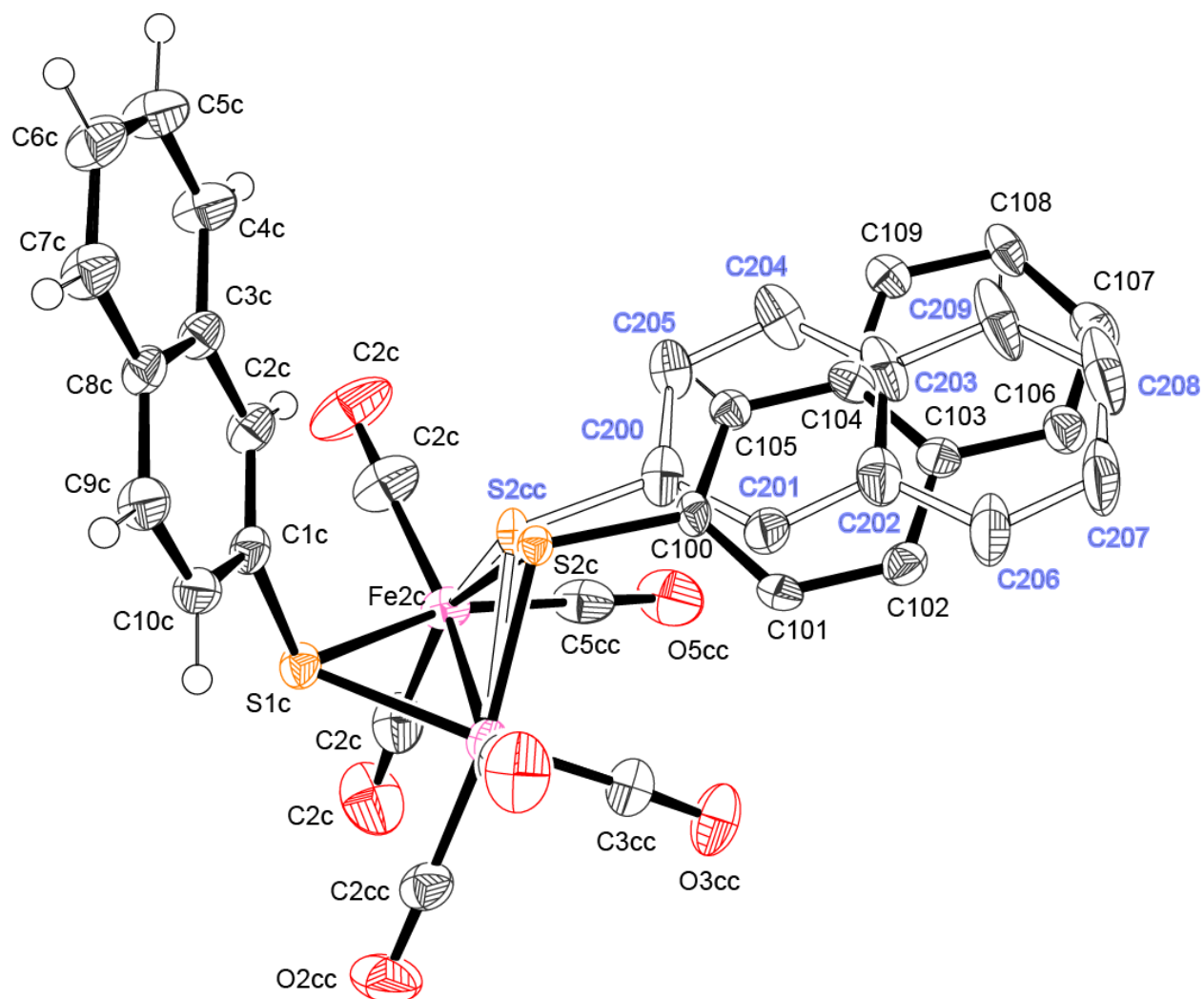
**Crystal and electronic structure of a hexacarbonyldiiron cluster
tethered to naphthalene-2-thiolate ligands**

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)

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.

Please wait while processing

[Structure factor report](#)

[CIF dictionary](#)

[Interpreting this report](#)

Datablock: 1

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 ⁻³	1.592	1.592
Z	6	6
Mu (mm ⁻¹)	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.

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

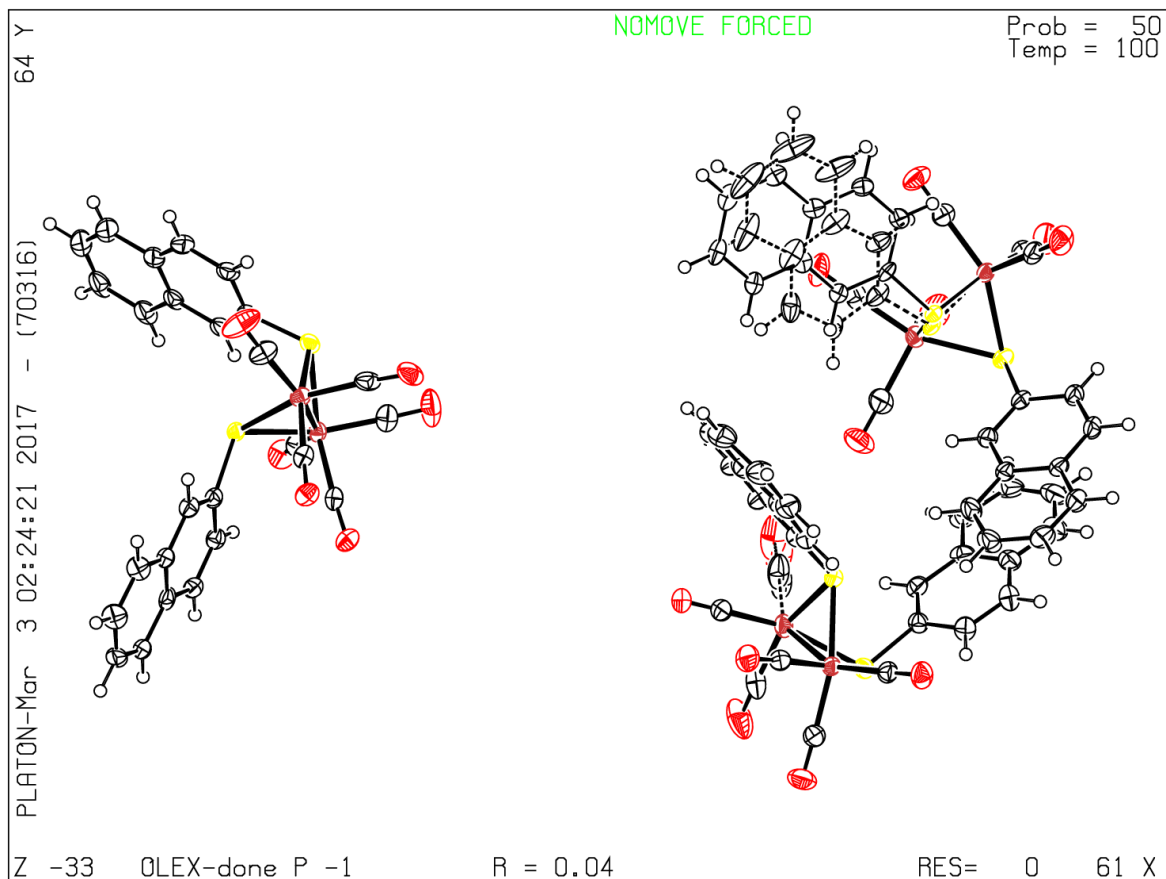
Less ...

[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

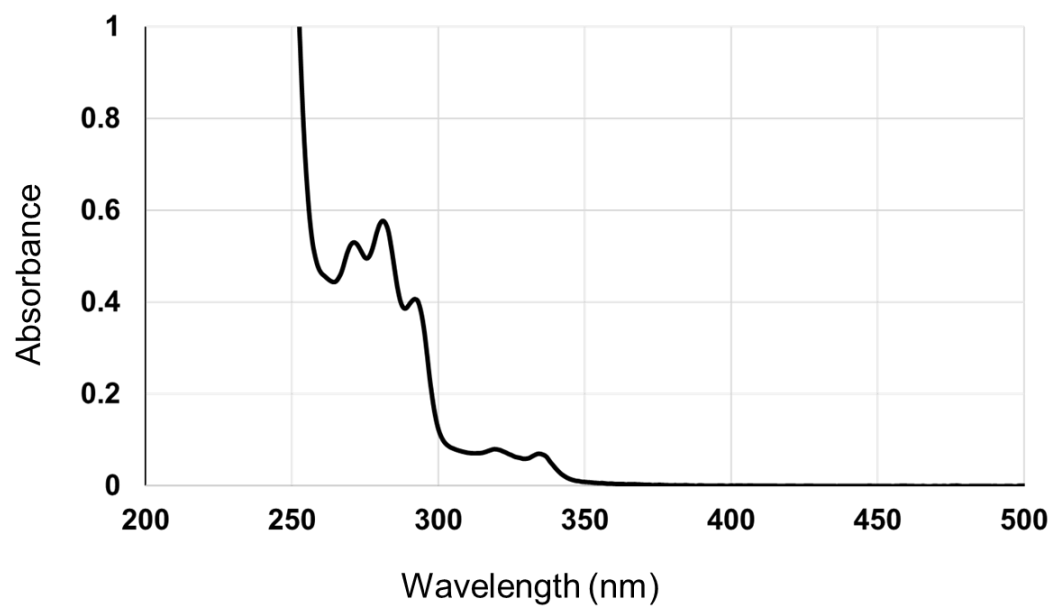
0 **ALERT level A** = Most likely a serious problem - resolve or explain
 0 **ALERT level B** = A potentially serious problem, consider carefully
 5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
 31 **ALERT level G** = General information/check it is not something unexpected

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 \(publCIF\) 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.