Cocrystal of 4-nitrophenol and 2,1,3-benzoselenadizole

Honghong Lan*, Shaobin Miao and Weizhou Wang

College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471934, China;
* Correspondence: lantianlh@126.com; Tel.: +86-379-68618321

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: miao20200914-2

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

Cell:             a=14.1004(10)     b=3.9390(2)         c=23.4020(15)
                  alpha=90          beta=105.790(7)     gamma=90
Temperature:      291 K

                  Calculated                  Reported
Volume            1250.74(14)                 1250.73(14)
Space group       P 21/c                      P 1 21/c 1
Hall group        -P 2ybc                     -P 2ybc
Moiety formula    C6 H5 N O3, C6 H4 N2 Se     C6 H4 N2 Se, C6 H5 N O3
Sum formula       C12 H9 N3 O3 Se             C12 H9 N3 O3 Se
Mr                322.18                      322.18
Dx,g cm-3         1.711                       1.711
Z                 4                           4
Mu (mm-1)         3.009                       3.009
F000              640.0                       640.0
F000'             639.89
h,k,lmax          18,5,31                     18,5,31
Nref              3144                        2829
Tmin,Tmax         0.476,0.548                 0.574,1.000
Tmin'             0.467

Correction method= # Reported T Limits: Tmin=0.574 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.900             Theta(max)= 28.410

R(reflections)= 0.0573( 2020)                    wR2(reflections)=
                                                 0.0805( 2829)

S = 1.126                   Npar= 173
```

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 A

```
PLAT430_ALERT_2_A Short Inter D...A Contact  Se1      ..N3       .       2.88 Ang.
                                             2-x,2-y,1-z  =      3_776 Check
```

🟠 Alert level B

```
PLAT430_ALERT_2_B Short Inter D...A Contact  N3       ..N3       .       2.84 Ang.
                                             2-x,2-y,1-z  =      3_776 Check
```

🟡 Alert level C

```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.  C1       -C6       .       1.37 Ang.
```

⚪ Alert level G

```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............      1 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =      3 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..........    4.8 Low
```

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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 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
```

checkCIF publication errors

🔴 Alert level A

```
PUBL004_ALERT_1_A  The contact author's name and address are missing,
          _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
          _publ_contact_author_phone are all missing.
          At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
          e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
```

```
PUBL012_ALERT_1_A   _publ_section_abstract is missing.
              Abstract of paper in English.
```

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   0 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
```
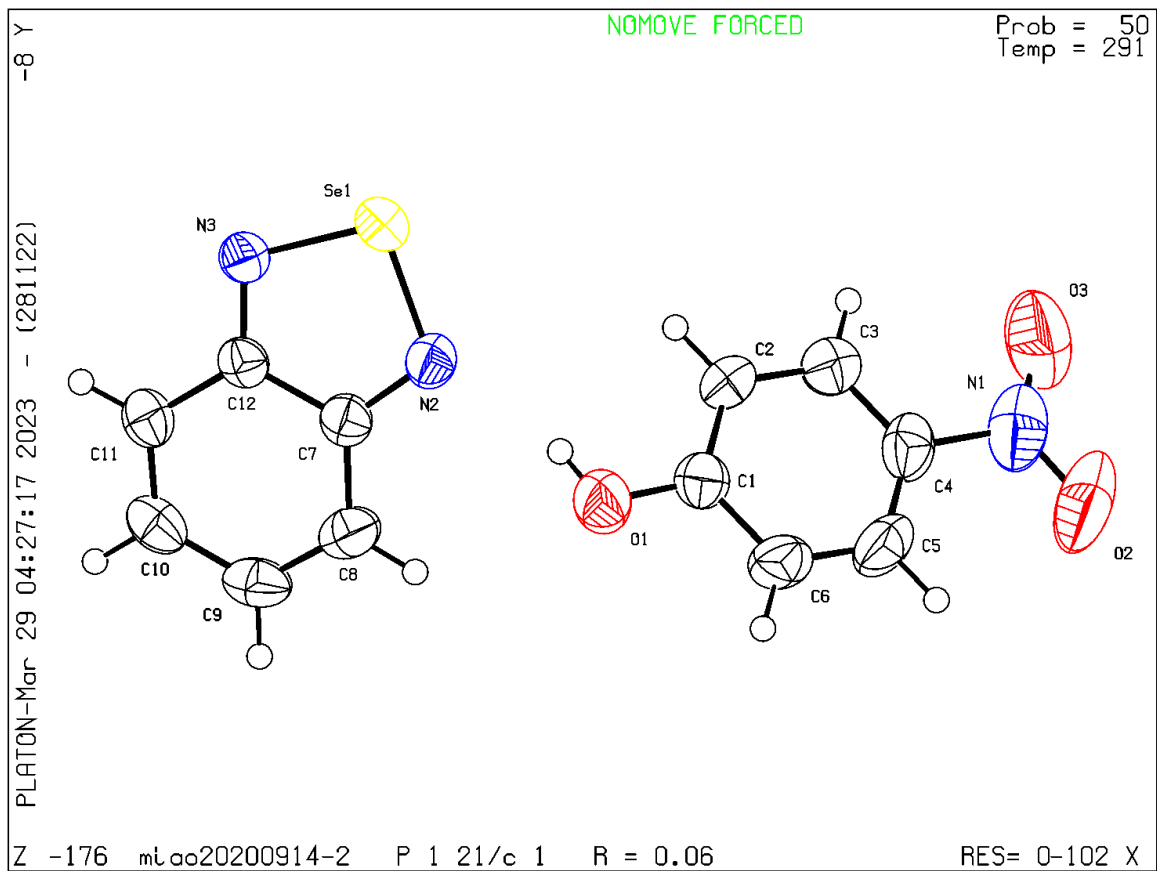
```
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PLAT430_miao20200914-2
;
PROBLEM: Short Inter D...A Contact  Se1      ..N3       .        2.88 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```
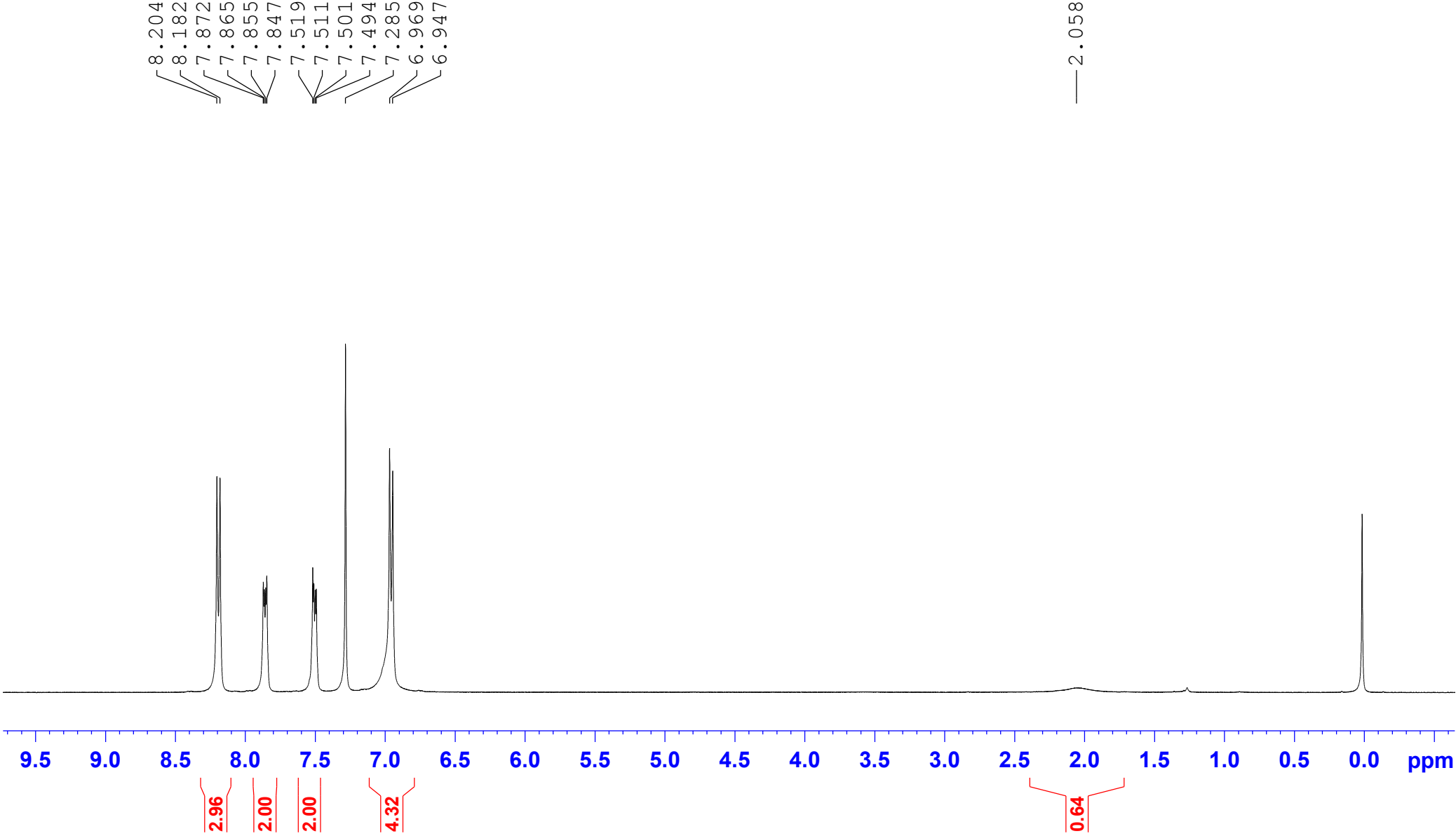
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.
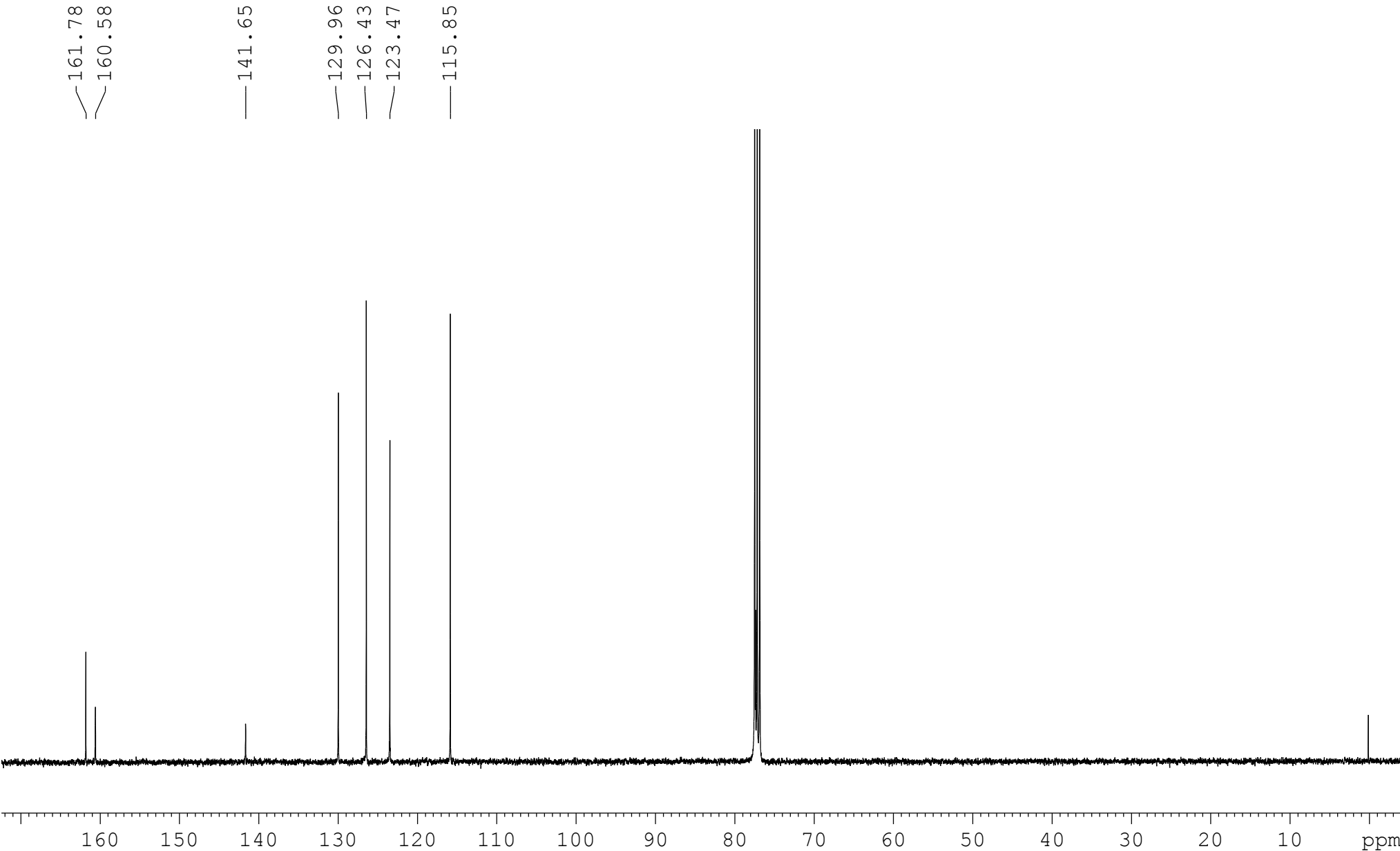

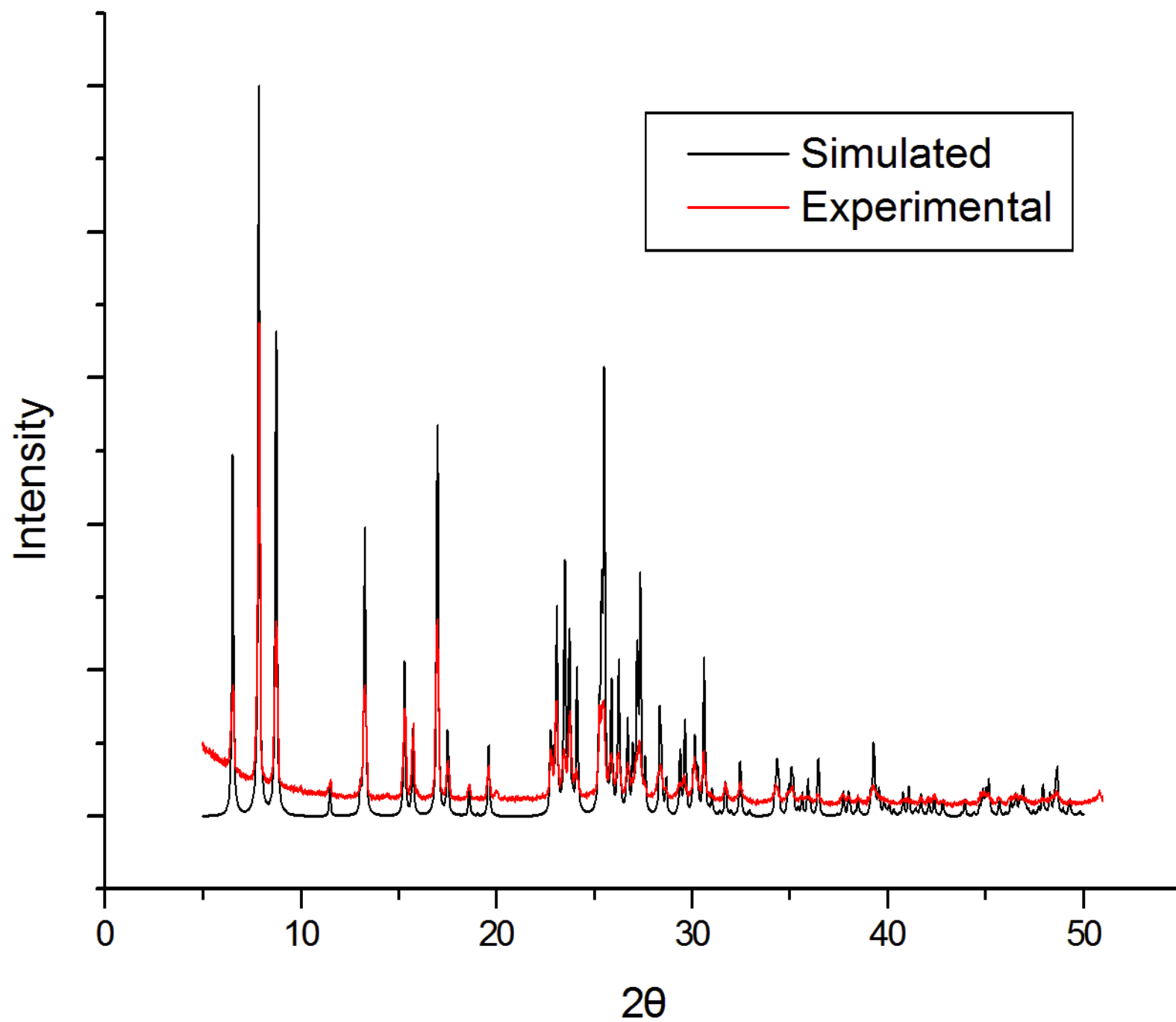**PLATON version of 28/11/2022; check.def file version of 09/08/2022**

m-01-cdcl3-H

m-01-cdcl3-C13

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: miao20200914-2

```
Bond precision:    C-C = 0.0061 A              Wavelength=0.71073

Cell:              a=14.1004(10)      b=3.9390(2)         c=23.4020(15)
                   alpha=90           beta=105.790(7)     gamma=90
Temperature:       291 K

                   Calculated                  Reported
Volume             1250.74(14)                 1250.73(14)
Space group        P 21/c                      P 1 21/c 1
Hall group         -P 2ybc                     -P 2ybc
Moiety formula     C6 H5 N O3, C6 H4 N2 Se     C6 H4 N2 Se, C6 H5 N O3
Sum formula        C12 H9 N3 O3 Se             C12 H9 N3 O3 Se
Mr                 322.18                      322.18
Dx,g cm-3          1.711                       1.711
Z                  4                           4
Mu (mm-1)          3.009                       3.009
F000               640.0                       640.0
F000'              639.89
h,k,lmax           16,4,28                     16,4,28
Nref               2264                        2258
Tmin,Tmax          0.476,0.548                 0.574,1.000
Tmin'              0.467

Correction method= # Reported T Limits: Tmin=0.574 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.997            Theta(max)= 25.250

R(reflections)= 0.0493( 1838)                   wR2(reflections)=
                                                0.0700( 2258)
S = 1.154                     Npar= 172
```

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 A
```
PLAT430_ALERT_2_A Short Inter D...A Contact  Se1      ..N3        .        2.88 Ang.
                                             2-x,2-y,1-z  =      3_776 Check
```

Alert level B
```
PLAT430_ALERT_2_B Short Inter D...A Contact  N3       ..N3        .        2.85 Ang.
                                             2-x,2-y,1-z  =      3_776 Check
```

Alert level C
```
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings  Differ    Please Check
PLAT334_ALERT_2_C Small <C-C> Benzene Dist.   C1       -C6        .       1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on  C-C Bonds ..............   0.00608 Ang.
```

Alert level G
```
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............       1 Report
PLAT180_ALERT_4_G Check Cell Rounding: # of Values Ending with 0 =       3 Note
PLAT967_ALERT_5_G Note: Two-Theta Cutoff Value in Embedded .res ..    50.5 Degree
```

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

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   3 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 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
```

checkCIF publication errors

Alert level A
```
PUBL004_ALERT_1_A  The contact author's name and address are missing,
          _publ_contact_author_name and _publ_contact_author_address.
PUBL005_ALERT_1_A  _publ_contact_author_email, _publ_contact_author_fax and
          _publ_contact_author_phone are all missing.
          At least one of these should be present.
PUBL006_ALERT_1_A  _publ_requested_journal is missing
          e.g. 'Acta Crystallographica Section C'
PUBL008_ALERT_1_A  _publ_section_title is missing. Title of paper.
PUBL009_ALERT_1_A  _publ_author_name is missing. List of author(s) name(s).
PUBL010_ALERT_1_A  _publ_author_address is missing. Author(s) address(es).
```

```
PUBL012_ALERT_1_A  _publ_section_abstract is missing.
             Abstract of paper in English.
```

```
   7 ALERT level A = Data missing that is essential or data in wrong format
   0 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should 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 nature of your study may justify the reported deviations from journal submission requirements and the more serious of these should 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.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in a journal, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. This will allow your explanation to be considered as part of the review process.

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PUBL004_GLOBAL
;
PROBLEM: The contact author's name and address are missing,
RESPONSE: ...
;
_vrf_PUBL005_GLOBAL
;
PROBLEM: _publ_contact_author_email, _publ_contact_author_fax and
RESPONSE: ...
;
_vrf_PUBL006_GLOBAL
;
PROBLEM: _publ_requested_journal is missing
RESPONSE: ...
;
_vrf_PUBL008_GLOBAL
;
PROBLEM: _publ_section_title is missing. Title of paper.
RESPONSE: ...
;
```
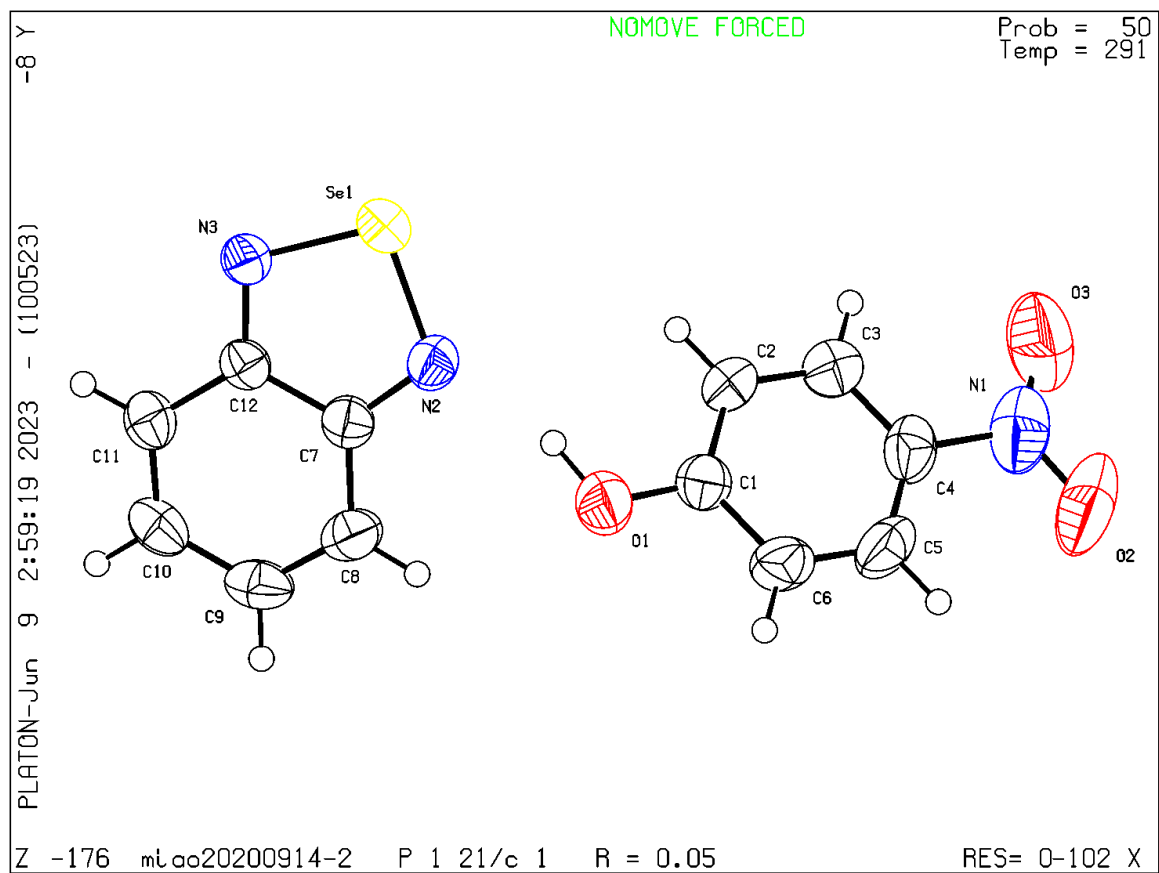
```
_vrf_PUBL009_GLOBAL
;
PROBLEM: _publ_author_name is missing. List of author(s) name(s).
RESPONSE: ...
;
_vrf_PUBL010_GLOBAL
;
PROBLEM: _publ_author_address is missing. Author(s) address(es).
RESPONSE: ...
;
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PLAT430_miao20200914-2
;
PROBLEM: Short Inter D...A Contact  Se1      ..N3       .         2.88 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```
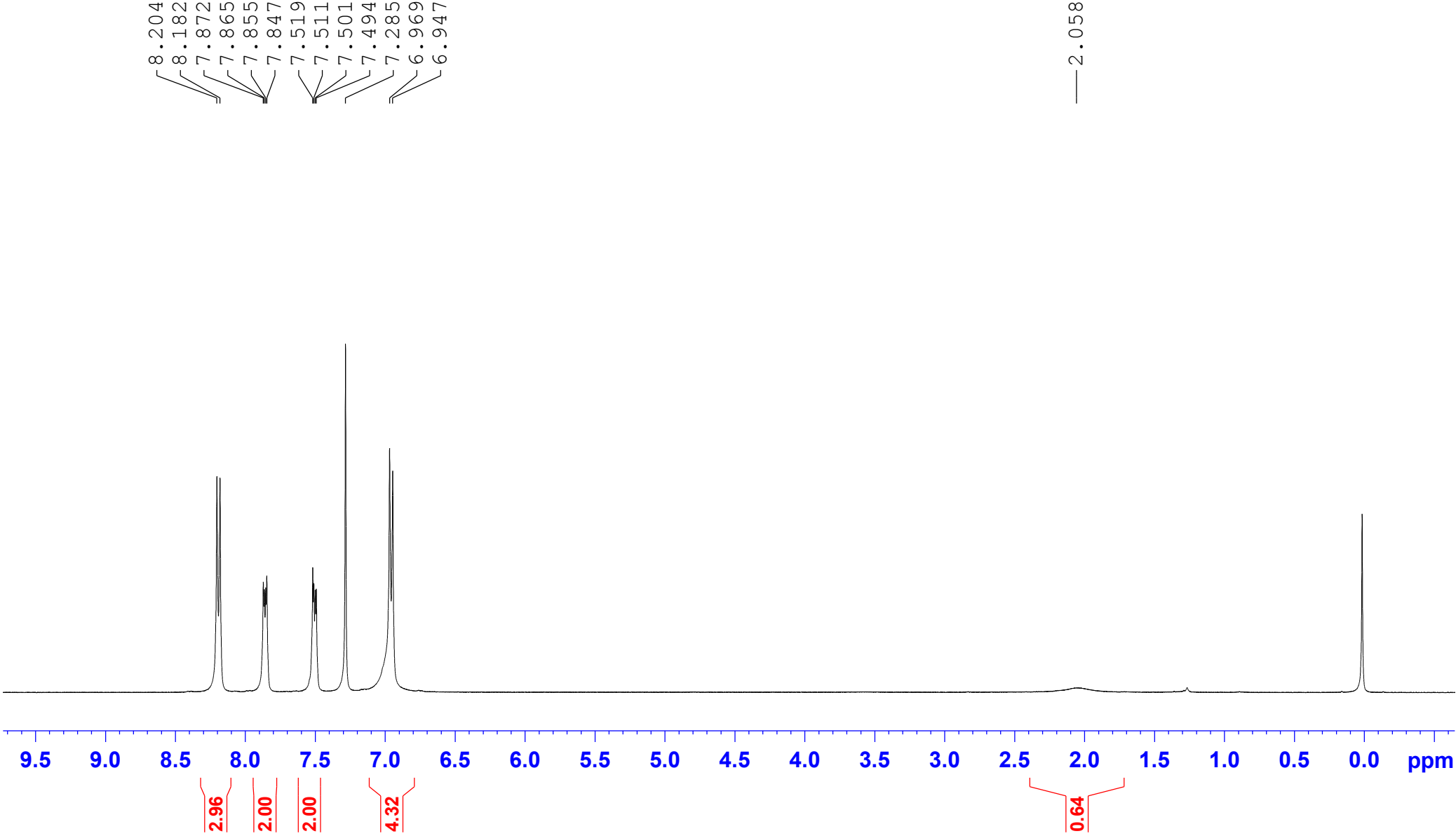
If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If you wish to submit your CIF for publication in IUCrData you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 10/05/2023; check.def file version of 10/05/2023

m-01-cdcl3-H

m-01-cdcl3-C13