Supplementary Information

A New Energetic Complex: Synthesis, Structure, and Combustion Catalysis Performance

Chengfang Qiao, Zhengyu Fu, Runrun Wang, Yulin Gao, Fengying Chen, Xia Gao, Chunsheng Zhou, and Zhengqiang Xia

*a Shaanxi Key Laboratory of Comprehensive Utilization of Tailings Resources, College of Chemical Engineering and Modern Materials, Shangluo University, 726000 Shangluo, PR China

b Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, College of Chemistry and Materials Science, Northwest University, Xi’an 710127, PR China

*e-mail: slzhoucs@126.com; northwindy@126.com
checkCIF/PLATON report

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: I

Bond precision: C-C = 0.0300 A  Wavelength=0.71073

Cell: a=13.516(3)  b=9.901(2)  c=25.699(4)
     alpha=90  beta=110.138(9)  gamma=90

Temperature: 296 K

Volume 3228.8(11)  Reported 3228.8(11)
Space group P 21/c  Reported P2(1)/c
Hall group -P 2ybc  Reported ?

MoIety formula C8 H14 N8 O5 Pb, C8 H10 N8 Pb3 O3 Pb, 5(H2 O)
Sum formula C16 H34 N16 O13 Pb2  Reported C16 H34 N16 O13 Pb2
Mr 1072.99  Reported 1072.97
Dx, g cm-3 2.207  2.207
Z 4  4
Mu (mm-1) 10.498  10.498
P000 2040.0  2040.0
P000’ 2014.80
h,k,lmax 16,11,30  16,11,30
Nref 5738  5698
Tmin,Tmax 0.044,0.350  0.044,0.350
Tmin’ 0.022

Correction method= EMPIRICAL

Data completeness= 0.993  Theta(max)= 25.100

R(reflections)= 0.1108( 3858)  wr2(reflections)= 0.2187( 5698)

S = 3.228  Npar= 424

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 B
DIFMX01_ALERT_2_B  The maximum difference density is > 0.1*ZMAX*1.00
     refine_diff_density_max given = 11.674
     Test value = 8.200
Alert level C

ABSTY02_ALERT_1_C An _exptl_absorp_correction_type has been given without a literature citation. This should be contained in the _exptl_absorp_process_details field.

Absorption correction given as empirical

DIFM02_ALERT_1_C The maximum difference density is > 0.1*MAX*0.75
The relevant atom site should be identified.

GOODF01_ALERT_2_C The least squares goodness of fit parameter lies outside the range 0.50 <= 2.00
Goodness of fit given = 3.226

RPAC03_ALERT_3_C The value of the R factor is > 0.10
R factor given 0.111

Alert level G

PLAT001_ALERT_2_C Number of Uiso or Uij Restricted Atom Sites ....... 28
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints ........ 216

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

**Alert level G**
- PUBL013_ALERT_1_0 The `_publ_section_comment` (discussion of study) is missing. This is required for a full paper submission (but is optional for an electronic paper).
- PUBL017_ALERT_1_0 The `_publ_section_references` section is missing or empty.

- ALERT level A = Date missing that is essential or data in wrong format
- 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 Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.

If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

# 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
;
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 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 24/03/2011; check.def file version of 16/03/2011

Datablock I-ellipsoid plot

Z 109 1 P211/c R = 0.11 RES = 0 -96 X