

Supporting Information

Barium(II)-based molecular perovskite energetic compounds for next-generation pyrotechnic materials

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Experimental details:

Caution. Energetic materials are generally more sensitive to mechanical stimulation than other similar materials. Although it was safe in the syntheses in the course of this research, small-scale syntheses are strongly encouraged.

Materials and Methods: All chemicals were obtained from commercial sources and used without further purification. Decomposition temperatures were measured via DTA with an OZM Research DTA 552-Ex instrument at a rate of 5 and 10 °C·min⁻¹ and in a

range from RT to 400 °C under air condition. The PXRD patterns (Cu K α) for identifying the phase purity were collected by Bragg–Brentano geometry on a Bruker Advance D8 diffractometer. Detonation parameters were calculated using DFT calculation and the extended K–J equation. Friction sensitivity was tested on FSKM 10 BAM friction apparatus.

The estimation on detonation performance (S1)

In this study, we attempted to employ the empirical correction formula [S1] proposed by Louisa J. Hope-Weeks in 2011 publication in *JACS* on computational simulations of complex energetic materials to calculate the detonation parameters of the energetic perovskite. To estimate the detonation performances, using density functional theory (DFT) calculation and extended Kamlet-Jacob's (K-J) equation. DFT was employed to calculate the energy of detonation (ΔE_{det}), performing with the code DMol3 under 3D periodic boundary conditions accompanied with the Monkhorst-Pack multiple K-point sampling of the Brillouin zone and the Perdew-Becke-Ezerhoff (PBE) exchange correlation function. The heat of detonation (ΔH_{det}) was estimated from ΔE_{det} by a linear correlation equation.

$$\Delta H_{det} = 1.127\Delta E_{det} + 0.046, r = 0.968$$

Detonation velocity and pressure were estimated by a method using extended Kamlet-Jacob's equation for explosives.

$$D = 1.01 \Phi^{1/2} (1 + 1.30\rho)$$

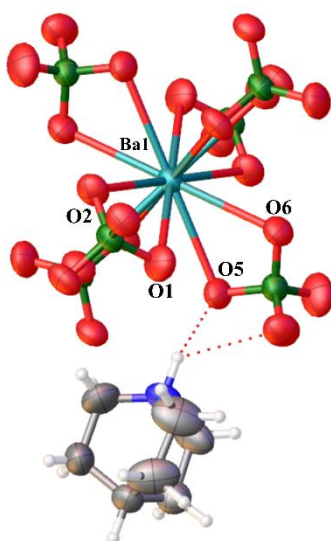
$$P=1.558 \Phi \rho^2$$

$$\Phi = 31.68 N(MQ)^{1/2}$$

Here, ρ represents the density of explosive ($\text{g}\cdot\text{cm}^{-3}$), N and M are the characteristic parameters of the detonation products, N is the moles of detonation gases per gram of explosive and M is the average molecular weight of these gases, Q is the heat of detonation (ΔH_{det} , $\text{kcal}\cdot\text{g}^{-1}$), D is the detonation velocity ($\text{km}\cdot\text{s}^{-1}$), and P is the detonation pressure (GPa).

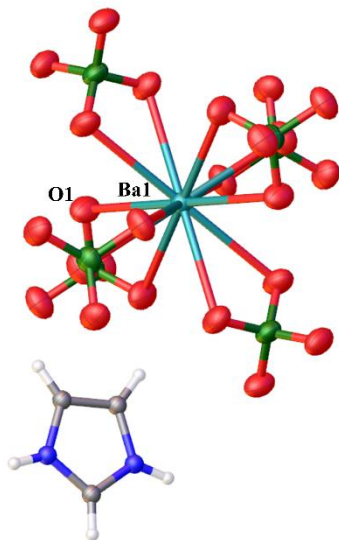
The distance of Ba–O bond in QBP, IBP and BaClO₄ (Table S1)

QBP	
Atom–Atom	Length [Å]
Ba1–O1	2.906
Ba1–O2	2.982
Ba1–O5	2.859
Ba1–O6	2.876
Av. Ba–O	2.906



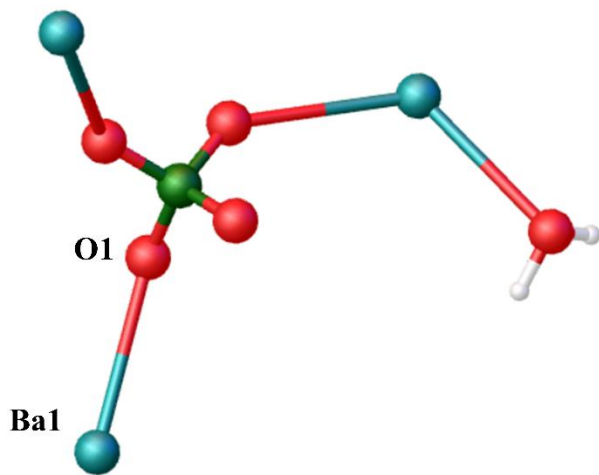
IBP

Atom–Atom	Length [Å]
Ba1–O1	2.898



BaClO₄

Atom–Atom	Length [Å]
Ba1–O1	3.062



Hygroscopicity measurements (S3)

The hygroscopicity was determined by the weight gain method [S2]. About 2 g of ground test samples were initially dried to a constant weight (with a fluctuation less than 0.2 mg) and then placed in chambers at room temperature and a relative humidity of 86%, and 100%, respectively. The moisture absorption rate was calculated by the following equation.

$$\omega = \frac{m_1}{m_0} \times 100\%$$

where m_0 denotes the initial mass, and m_1 denotes the mass after moisture absorption.

Computational details (S4)

Considering the periodic structures, geometry optimizations were conducted in CASTEP using the Perdew—Burke-Ernzerhof (PBE) functional with Grimme's D3 dispersion correction in the Becke-Johnson formalism and hence noted as DFT-B3(BJ) [S3]. The ultrasoft pseudopotential was used. For all the electron self-consistent calculations, the cutoff and relative cutoff were set as 489.80 eV, respectively. The k-point was set as $1 \times 1 \times 1$. At the beginning, both the cell and the atom positions were optimized, during which the convergence criteria were set as the maximum energy change of 5×10^{-5} eV, maximum geometry changes of $< 5 \times 10^{-3}$ Å, maximum force of < 0.1 eV/Å, RMS force of $< 3 \times 10^{-4}$ Ha/Bohr. Then we reduce the angle of the unit cell and model it every 1 degree to simulate the situation where the unit cell is subjected to shear force. For all models, we fix the unit cell angle and optimize the atom positions. After the calculation converges, we read out the internal pressure of the unit cell and make a stress-strain curve.

Constant-volume combustion (S5)

A constant-volume combustion cell was used to study the temporal pressures of different energetic materials. In this study, 60 mg of the loose sample was placed inside a 50 mL combustion cell and was ignited with a nichrome coil on top of the loose powder. An attached piezoresistive pressure sensor together with an in-line

charge amplifier and signal conditioner were used to record the pressure history.

High-speed camera (S6)

The combustion experiment system consists of an ignition system, a signal acquisition system, and high-speed photography. Following the setup in Figure S1, the experimental platform is constructed by connecting the bridge wire to the electrodes of the power supply and fixing the bridge wire to the experimental table. The experimental image acquisition parameters are set by connecting the high-speed camera to the computer. During the experiment, the pre-weighed substances are stacked in a conical shape on the bridge wire. Upon pressing the synchronization trigger, the experimental images captured by the high-speed photography system are processed using specialized software. The total duration of the recording is 4 seconds. A direct current power supply with a voltage of 100 V is used. The bridge wire is made of iron-chromium alloy with a resistance of 2.7 Ω . The amount of substance used is 60 mg, and the high-speed frame rate is set at 1000 frames per second.

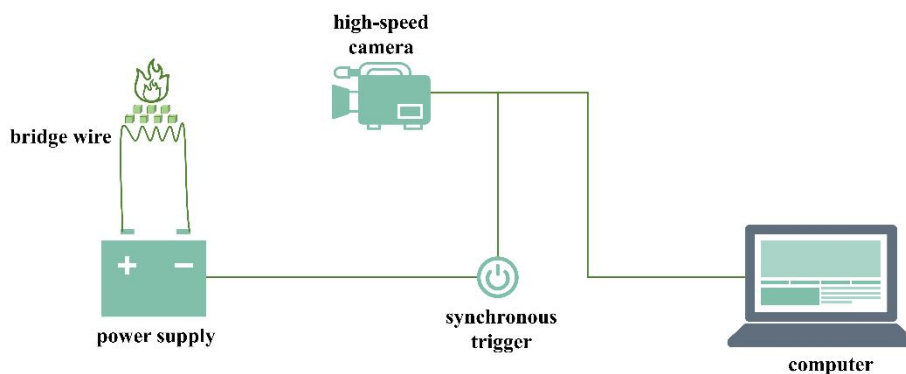


Figure S1. Diagram of the combustion process testing system.

Emission spectrum (S7)

The flame emission spectral analysis of 50 mg compound QBP was performed using a visible spectrometer (HP320, DUOTONE CLOUD).

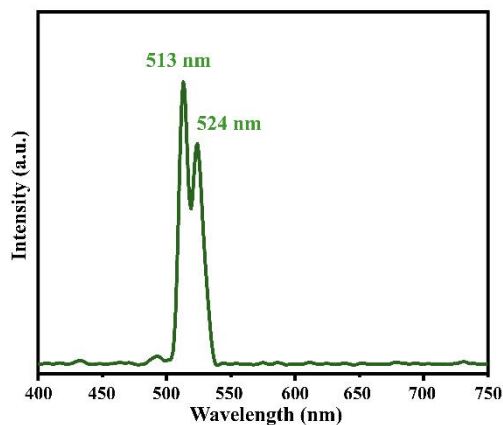


Figure S2. Emission spectrum of QBP.

Table S2 Normalized line and band intensities for BaCl and BaOH

BaCl		BaOH	
wavelength / nm	relative intensity	wavelength / nm	relative intensity
507	8	488	72
514	100	502	30
517	21	513	100
521	14	524	86
524	99	745	47
532	34	/	/

W. Meyerriecks, K. L. Kosanke, Color values and spectra of the principal emitters in colored flames, *J. Pyrotech.* 2003, **18**, 710-731.

The green light emission observed during the combustion of QBP is likely attributed to the combined contribution of BaCl and BaOH, as both substances exhibit strong emission peaks at 514, 524 nm (for BaCl), and 513, 524 nm (for BaOH), respectively.

Reference

[S1] Bushuyev, O. S., *et al.* J. Am. Chem. Soc. 2012, 1422.

[S2] GRIMME S., *et al.* J. Chem. Phys., 2010, 132.

[S3] Jun W., *et al.* Mater. Chem. Front. 2023, 7, 2251.

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) ibp

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: ibp

Bond precision: Ba- O = 0.0030 Å Wavelength=1.34138

Cell: a=14.0014 (9) b=14.0014 (9) c=14.0014 (9)
 alpha=90 beta=90 gamma=90

Temperature: 298 K

	Calculated	Reported
Volume	2744.8 (5)	2744.8 (5)
Space group	F m -3 c	F m -3 c
Hall group	-F 4c 2 3	-F 4c 2 3
Moiety formula	Ba0.08 Cl0.25 O, 0.003 (C72 H120 N48)	Ba Cl3 O12, C3 H5 N2
Sum formula	C0.25 H0.42 Ba0.08 Cl0.25 N0.17 O	C3 H5 Ba Cl3 N2 O12
Mr	42.07	504.78
Dx, g cm-3	2.443	2.443
Z	96	8
Mu (mm-1)	19.526	19.216
F000	1920.2	1920.0
F000'	1931.08	
h, k, lmax	17, 17, 17	17, 17, 15
Nref	148	145
Tmin, Tmax	0.288, 0.316	0.482, 0.752
Tmin'	0.187	

Correction method= # Reported T Limits: Tmin=0.482 Tmax=0.752
AbsCorr = MULTI-SCAN

Data completeness= 0.980 Theta (max)= 58.969

R(reflections)= 0.0197(126)

wR2(reflections)=
0.0451(145)

S = 1.137

Npar= 32

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

PLAT088_ALERT_3_A Poor Data / Parameter Ratio 4.53 Note

Author Response: The high rotational freedom of the imidazolium cation leads to 24-fold disorder, which increases the complexity of the crystal structure. This disorder likely contributes to the poor data-to-parameter ratio.

Alert level C

PLAT041_ALERT_1_C Calc. and Reported SumFormula Strings Differ Please Check
Calc: C0.25 H0.42 Ba0.08 Cl0.25 N0.17 O
Rep.: C3 H5 Ba Cl3 N2 O12
PLAT042_ALERT_1_C Calc. and Reported MoietyFormula Strings Differ Please Check
Calc: Ba0.08 Cl0.25 O, 0.003(C72 H120 N48)
Rep.: Ba Cl3 O12, C3 H5 N2
PLAT051_ALERT_1_C Mu(calc) and Mu(cif) Ratio Differs from 1.0 by . 1.62 %
PLAT243_ALERT_4_C High 'Solvent' Ueq as Compared to Neighbors of 01 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 3 Report
0 2 2, 2 2 2, 8 8 10,
PLAT927_ALERT_1_C Reported and Calculated wR2 Differ by -0.0020 Check

Alert level G

ABSMU01_ALERT_1_G Calculation of _exptl_absorpt_correction_mu
not performed for this radiation type.
CELLZ01_ALERT_1_G Difference between formula and atom_site contents detected.
CELLZ01_ALERT_1_G ALERT: check formula stoichiometry or atom site occupancies.
From the CIF: _cell_formula_units_Z 8
From the CIF: _chemical_formula_sum C3 H5 Ba Cl3 N2 O12
TEST: Compare cell contents of formula and atom_site data

atom	Z*formula	cif sites	diff
C	24.00	24.02	-0.02
H	40.00	40.03	-0.03
Ba	8.00	8.00	0.00
Cl	24.00	24.00	0.00
N	16.00	16.01	-0.01
O	96.00	96.00	0.00

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 5 Note
PLAT003_ALERT_2_G Number of Uiso or U(i,j) Restrained non-H-Atoms 5 Report
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms 2 Report
H1 H2

PLAT019_ALERT_1_G	_diffn_measured_fraction_theta_full/*_max < 1.0	0.996	Report
PLAT045_ALERT_1_G	Calculated and Reported Z Differ by a Factor ...	12	Check
PLAT068_ALERT_1_G	Reported F000 Differs from Calcd (or Missing)...		Please Check
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	9.71	Why ?
PLAT171_ALERT_4_G	The CIF-Embedded .res File Contains EADP Records	1	Report
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	2	Report
PLAT173_ALERT_4_G	The CIF-Embedded .res File Contains DANG Records	2	Report
PLAT174_ALERT_4_G	The CIF-Embedded .res File Contains FLAT Records	1	Report
PLAT176_ALERT_4_G	The CIF-Embedded .res File Contains SADI Records	4	Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1	Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1	Report
PLAT187_ALERT_4_G	The CIF-Embedded .res File Contains RIGU Records	1	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT191_ALERT_3_G	A Non-default SADI Restraint Value has been used	0.0400	Report
PLAT300_ALERT_4_G	Atom Site Occupancy of N1 Constrained at	0.0417	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of N2 Constrained at	0.0417	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C1 Constrained at	0.0417	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C2 Constrained at	0.0417	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of C3 Constrained at	0.0417	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1 Constrained at	0.0417	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H1A Constrained at	0.0417	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2 Constrained at	0.0417	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H2A Constrained at	0.0417	Check
PLAT300_ALERT_4_G	Atom Site Occupancy of H3 Constrained at	0.0417	Check
PLAT301_ALERT_3_G	Main Residue Disorder(Resd 2)	100%	Note
PLAT722_ALERT_1_G	Angle Calc 126.00, Rep 124.80 Dev...	1.20	Degree
	C1 -N1 -H1 1_555 1_555 1_555 #	83	Check
PLAT789_ALERT_4_G	Atoms with Negative _atom_site_disorder_group #	10	Check
PLAT811_ALERT_5_G	No ADDSYM Analysis: Too Many Excluded Atoms ...	!	Info
PLAT822_ALERT_4_G	CIF-embedded .res Contains Negative PART Numbers	1	Check
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	104	Note
PLAT883_ALERT_1_G	Absent Datum for _atom_sites_solution_primary ..		Please Do !
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3	Note
	0 2 2, 2 2 2, 8 8 10,		
PLAT952_ALERT_5_G	Calculated (ThMax) and CIF-Reported Lmax Differ.	2	Units
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .	2	Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	3.283	Note
	Predicted wr2: Based on SigI**2 1.37 or SHELX Weight	3.96	
PLAT984_ALERT_1_G	The C-f' = 0.0148 Deviates from the B&C-Value	0.0137	Check
PLAT984_ALERT_1_G	The Ba-f' = -0.1863 Deviates from the B&C-Value	-0.3132	Check
PLAT984_ALERT_1_G	The Cl-f' = 0.3294 Deviates from the B&C-Value	0.3281	Check
PLAT984_ALERT_1_G	The N-f' = 0.0253 Deviates from the B&C-Value	0.0241	Check
PLAT984_ALERT_1_G	The O-f' = 0.0412 Deviates from the B&C-Value	0.0389	Check
PLAT985_ALERT_1_G	The Ba-f" = 7.2115 Deviates from the B&C-Value	6.7527	Check
PLAT985_ALERT_1_G	The Cl-f" = 0.5404 Deviates from the B&C-Value	0.5435	Check

-
- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
6 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
49 **ALERT level G** = General information/check it is not something unexpected
- 20 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
4 ALERT type 2 Indicator that the structure model may be wrong or deficient
6 ALERT type 3 Indicator that the structure quality may be low
21 ALERT type 4 Improvement, methodology, query or suggestion
5 ALERT type 5 Informative message, check

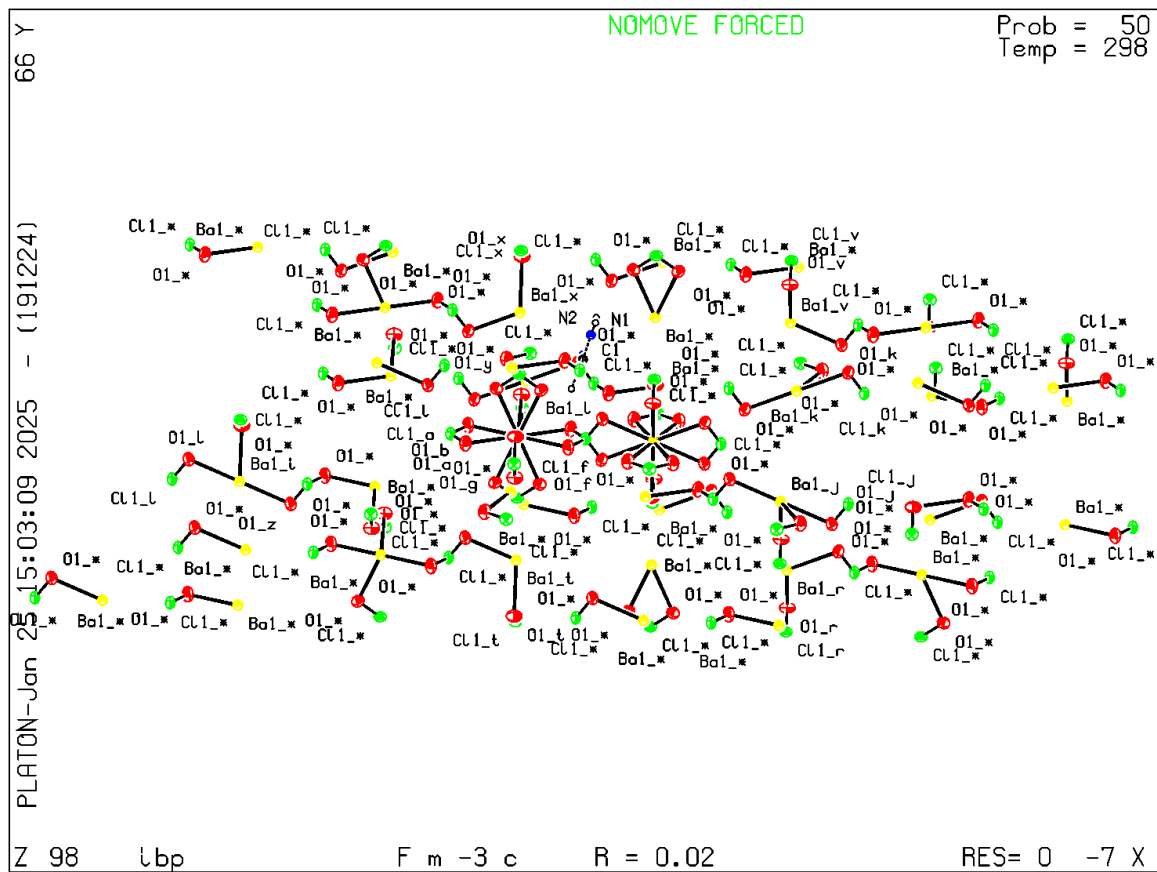
It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious 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.



Structure factors have been supplied for datablock(s) qbp

No syntax errors found. CIF dictionary Interpreting this report

Bond precision:	C-C = 0.0087 Å	Wavelength=1.34138	
Cell:	a=12.9696(13) alpha=90	b=10.3066(8) beta=106.744(5)	c=10.146(1) gamma=90
Temperature:	298 K		
	Calculated	Reported	
Volume	1298.7(2)	1298.7(2)	
Space group	P 21/c	P 1 21/c 1	
Hall group	-P 2ybc	-P 2ybc	
Moiety formula	Ba Cl4 O16, 2(C7 H14 N)	Ba Cl4 O16, 2(C7 H14 N)	
Sum formula	C14 H28 Ba Cl4 N2 O16	C14 H28 Ba Cl4 N2 O16	
Mr	759.51	759.52	
Dx, g cm-3	1.942	1.942	
Z	2	2	
Mu (mm-1)	11.176	11.002	
F000	756.0	756.0	
F000'	759.88		
h,k,lmax	16,13,13	16,13,13	
Nref	2879	2852	
Tmin,Tmax	0.400,0.719	0.405,0.752	
Tmin'	0.167		

Data completeness= 0.991 Theta(max)= 59.440

```
R(reflections)= 0.0396( 2321)      wR2(reflections)=
S = 1.128                        0.1243( 2852)
Npar= 169
```

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

PLAT051_ALERT_1_C	Mu(calc) and Mu(cif) Ratio Differs from 1.0 by .	1.58 %
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	01 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	02 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	05 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	06 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	Ba1 Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C1 Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C2 Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C5 Check
PLAT243_ALERT_4_C	High 'Solvent' Ueq as Compared to Neighbors of	C7 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	N1 Check
PLAT244_ALERT_4_C	Low 'Solvent' Ueq as Compared to Neighbors of	C3 Check
PLAT342_ALERT_3_C	Low Bond Precision on C-C Bonds	0.00867 Ang.
PLAT906_ALERT_3_C	Large K Value in the Analysis of Variance	3.846 Check
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	9 Report
	0 2 0, 3 0 0, 13 1 1, -1 0 2, -1 2 2, 0 2 2,	
	-8 9 3, -4 10 7, 6 3 9,	
PLAT913_ALERT_3_C	Missing # of Very Strong Reflections in FCF	5 Note
	0 2 0, 1 0 0, 3 0 0, -1 2 2, 0 2 2,	
PLAT927_ALERT_1_C	Reported and Calculated wR2 Differ by	-0.0019 Check

Alert level G

ABSMU01_ALERT_1_G	Calculation of _exptl_absorpt_correction_mu	
	not performed for this radiation type.	
PLAT004_ALERT_5_G	Polymeric Structure Found with Maximum Dimension	2 Info
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms	1 Report
	H1	
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C11 Check
PLAT242_ALERT_2_G	Low 'MainMol' Ueq as Compared to Neighbors of	C12 Check
PLAT883_ALERT_1_G	No Info/Value for _atom_sites_solution_primary .	Please Do !
PLAT910_ALERT_3_G	Missing # of FCF Reflection(s) Below Theta(Min).	1 Note
	1 0 0,	
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	17 Note
PLAT941_ALERT_3_G	Average HKL Measurement Multiplicity	4.2 Low
PLAT955_ALERT_1_G	Reported (CIF) and Actual (FCF) Lmax Differ by .	1 Units
PLAT969_ALERT_5_G	The 'Henn et al.' R-Factor-gap value	2.571 Note
	Predicted wR2: Based on SigI**2 4.84 or SHELX Weight 11.02	
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	0 Info
PLAT984_ALERT_1_G	The C-f' = 0.0148 Deviates from the B&C-Value	0.0137 Check
PLAT984_ALERT_1_G	The Ba-f' = -0.1863 Deviates from the B&C-Value	-0.3132 Check
PLAT984_ALERT_1_G	The Cl-f' = 0.3294 Deviates from the B&C-Value	0.3281 Check
PLAT984_ALERT_1_G	The N-f' = 0.0253 Deviates from the B&C-Value	0.0241 Check
PLAT984_ALERT_1_G	The O-f' = 0.0412 Deviates from the B&C-Value	0.0389 Check
PLAT985_ALERT_1_G	The Ba-f'' = 7.2115 Deviates from the B&C-Value	6.7527 Check
PLAT985_ALERT_1_G	The Cl-f'' = 0.5404 Deviates from the B&C-Value	0.5435 Check

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7 ALERT type 4 Improvement, methodology, query or suggestion
3 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.

Datablock qbp - ellipsoid plot

