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: LCP-Cmcm-ST-DEG

```
Bond precision:  P- O = 0.0067 A         Wavelength=0.70930

Cell:              a=5.4347(4)      b=8.1638(5)      c=6.2135(4)
                   alpha=90         beta=90          gamma=90
Temperature:       298 K
```

	Calculated	Reported
Volume	275.68(3)	275.68(3)
Space group	C m c m	C m c m
Hall group	-C 2c 2	-C -2x;-2yc
Moiety formula	Co2 O8 P2, 2(Li)	?
Sum formula	Co2 Li2 O8 P2	Co1 Li1 O4 P1
Mr	321.68	160.80
Dx,g cm-3	3.875	3.875
Z	2	4
Mu (mm-1)	6.528	6.358
F000	308.0	112.0
F000’	309.96	
h,k,lmax	7,11,8	
Nref	239	
Tmin,Tmax		
Tmin’		

```
Correction method= Not given

Data completeness= 0.000          Theta(max)=

R(reflections)= 0.0175( 0)        wR2(reflections)= wR= 0.0206( 0)

S = 1.570                 Npar= 75
```

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

```
ABSMU01_ALERT_1_C  The ratio of given/expected absorption coefficient lies
               outside the range 0.99 <> 1.01
            Calculated value of mu =     6.605
            Value of mu given      =     6.358
PLAT127_ALERT_1_C Implicit Hall Symbol  Inconsistent with Explicit    -C -2x;-2yc;-2
```

Alert level G

```
RADNT01_ALERT_1_G  Extra text has been found in the _diffrn_radiation_type field.
            Radiation given as Mo K\a1
            Radiation identified as Mo K\a
RADNW01_ALERT_1_G  The radiation wavelength given implies that Mo Kalpha1 has
            been used. Please check that this is correct.
            Wavelength given =    0.70930
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT092_ALERT_4_G Check: Wavelength given is not Cu,Ga,Mo,Ag,In Ka    0.70930 Ang.
PLAT793_ALERT_4_G The Model has Chirality at P1      (Centro SPGR)          S Verify
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT984_ALERT_1_G The  P-f'=     0.104 Deviates from the B&C-Value      0.102 Check
```

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

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

Datablock: LCP-Cmcm-ST-TEG

```
Bond precision:  P- O = 0.0103 A         Wavelength=0.70930

Cell:              a=5.4354(5)      b=8.1680(7)      c=6.2159(5)
                   alpha=90         beta=90          gamma=90
Temperature:       298 K
```

	Calculated	Reported
Volume	275.96(4)	275.97(4)
Space group	C m c m	C m c m
Hall group	-C 2c 2	-C -2x;-2yc
Moiety formula	Co2 O8 P2, 2(Li)	?
Sum formula	Co2 Li2 O8 P2	Co1 Li1 O4 P1
Mr	321.68	160.80
Dx,g cm-3	3.871	3.871
Z	2	4
Mu (mm-1)	6.521	6.565
F000	308.0	112.0
F000’	309.96	
h,k,lmax	7,11,8	
Nref	239	
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.000 Theta(max)=

R(reflections)= 0.0243(0) wR2(reflections)= wR= 0.0278(0)

S = 2.160 Npar= 75

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

PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -C -2x;-2yc;-2

Alert level G

RADNT01_ALERT_1_G Extra text has been found in the _diffrn_radiation_type field.
Radiation given as Mo K\a1
Radiation identified as Mo K\a

RADNW01_ALERT_1_G The radiation wavelength given implies that Mo Kalpha1 has
been used. Please check that this is correct.
Wavelength given = 0.70930

PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT092_ALERT_4_G Check: Wavelength given is not Cu,Ga,Mo,Ag,In Ka 0.70930 Ang.
PLAT793_ALERT_4_G The Model has Chirality at P1 (Centro SPGR) S Verify
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT984_ALERT_1_G The P-f’= 0.104 Deviates from the B&C-Value 0.102 Check

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

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

Datablock: LCP-Cmcm_ST-TTEG

Bond precision: P- O = 0.0080 A Wavelength=0.70930

Cell: a=5.4341(4) b=8.1676(5) c=6.2176(4)
alpha=90 beta=90 gamma=90
Temperature: 298 K

	Calculated	Reported
Volume	275.96(3)	275.96(3)
Space group	C m c m	C m c m
Hall group	-C 2c 2	-C -2x;-2yc
Moiety formula	Co2 O8 P2, 2(Li)	?
Sum formula	Co2 Li2 O8 P2	Co1 Li1 O4 P1
Mr	321.68	160.80
Dx,g cm-3	3.871	3.871
Z	2	4
Mu (mm-1)	6.521	6.565
F000	308.0	112.0
F000’	309.96	
h,k,lmax	7,11,8	
Nref	239	
Tmin,Tmax		
Tmin’		

Correction method= Not given

Data completeness= 0.000 Theta(max)=

R(reflections)= 0.0268(0) wR2(reflections)= wR= 0.0311(0)

S = 1.570 Npar= 75

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
PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -C -2x;-2yc;-2

Alert level G

```
RADNT01_ALERT_1_G  Extra text has been found in the _diffrn_radiation_type field.
           Radiation given as Mo K\a1
           Radiation identified as Mo K\a
RADNW01_ALERT_1_G  The radiation wavelength given implies that Mo Kalpha1 has
           been used. Please check that this is correct.
           Wavelength given =    0.70930
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ...       0.50 Check
PLAT092_ALERT_4_G Check: Wavelength given is not Cu,Ga,Mo,Ag,In Ka    0.70930 Ang.
PLAT793_ALERT_4_G The Model has Chirality at P1      (Centro SPGR)          S Verify
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters          1 Info
PLAT984_ALERT_1_G The  P-f'=     0.104 Deviates from the B&C-Value      0.102 Check
```

```
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   1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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   5 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   0 ALERT type 2 Indicator that the structure model may be wrong or deficient
   0 ALERT type 3 Indicator that the structure quality may be low
   3 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

Datablock: LCP-Cmcm-PO

```
Bond precision:  P- O = 0.0040 A         Wavelength=0.70930

Cell:              a=5.4433(3)      b=8.1694(4)      c=6.2129(3)
                   alpha=90         beta=90          gamma=90
Temperature:       298 K
```

	Calculated	Reported
Volume	276.28(2)	276.28(2)
Space group	C m c m	C m c m
Hall group	-C 2c 2	-C -2x;-2yc
Moiety formula	Co2 O8 P2, 2(Li)	?
Sum formula	Co2 Li2 O8 P2	Co1 Li1 O4 P1
Mr	321.68	160.80
Dx,g cm-3	3.867	3.866
Z	2	4
Mu (mm-1)	6.513	6.557
F000	308.0	308.0
F000'	309.96	
h,k,lmax	7,11,8	
Nref	240	
Tmin,Tmax		
Tmin'		

Correction method= Not given

Data completeness= 0.000 Theta(max)=

R(reflections)= 0.0128(0) wR2(reflections)= wR= 0.0153(0)

S = 1.080 Npar= 55

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

PLAT127_ALERT_1_C Implicit Hall Symbol Inconsistent with Explicit -C -2x;-2yc;-2

Alert level G

RADNT01_ALERT_1_G Extra text has been found in the _diffrn_radiation_type field.
Radiation given as Mo K\a1
Radiation identified as Mo K\a
RADNW01_ALERT_1_G The radiation wavelength given implies that Mo Kalpha1 has
been used. Please check that this is correct.
Wavelength given = 0.70930
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension 3 Info
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 0.50 Check
PLAT092_ALERT_4_G Check: Wavelength given is not Cu,Ga,Mo,Ag,In Ka 0.70930 Ang.
PLAT793_ALERT_4_G The Model has Chirality at P1 (Centro SPGR) S Verify
PLAT802_ALERT_4_G CIF Input Record(s) with more than 80 Characters 1 Info
PLAT984_ALERT_1_G The P-f'= 0.104 Deviates from the B&C-Value 0.102 Check

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0 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 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

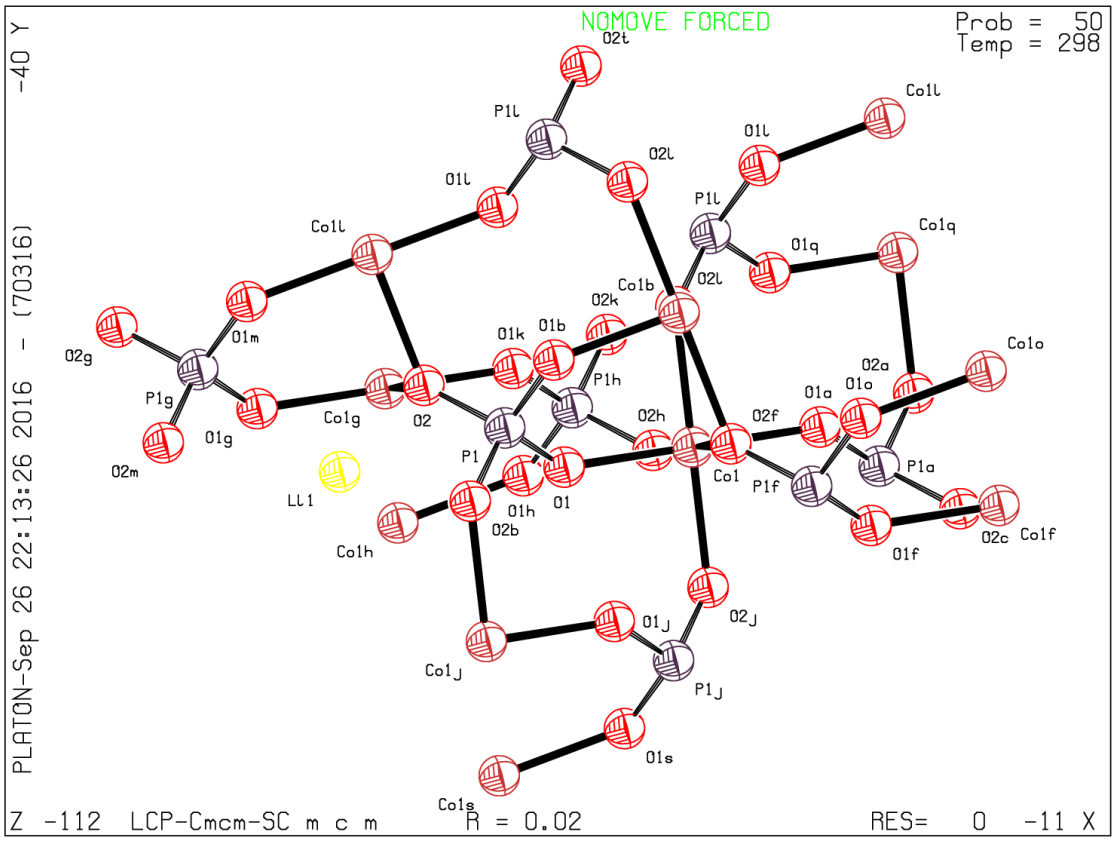
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica, Journal of Applied Crystallography, Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section 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

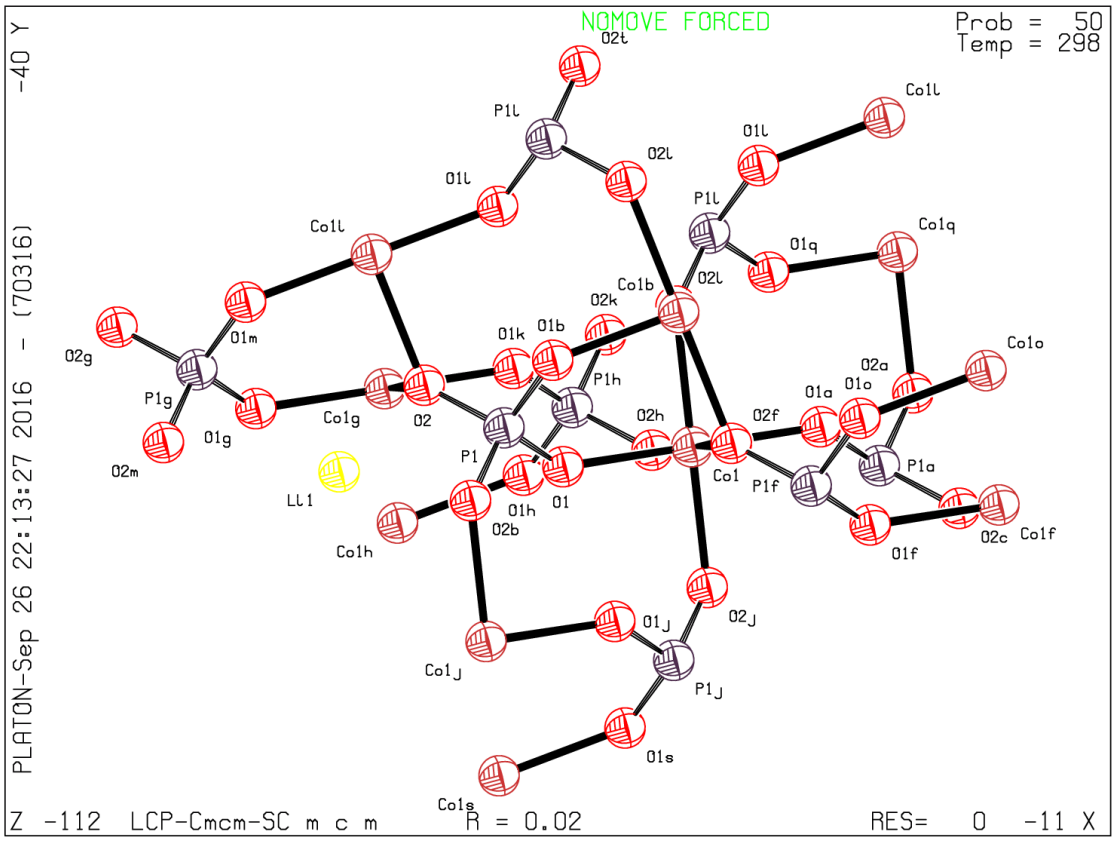
Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 11/08/2016; check.def file version of 04/08/2016

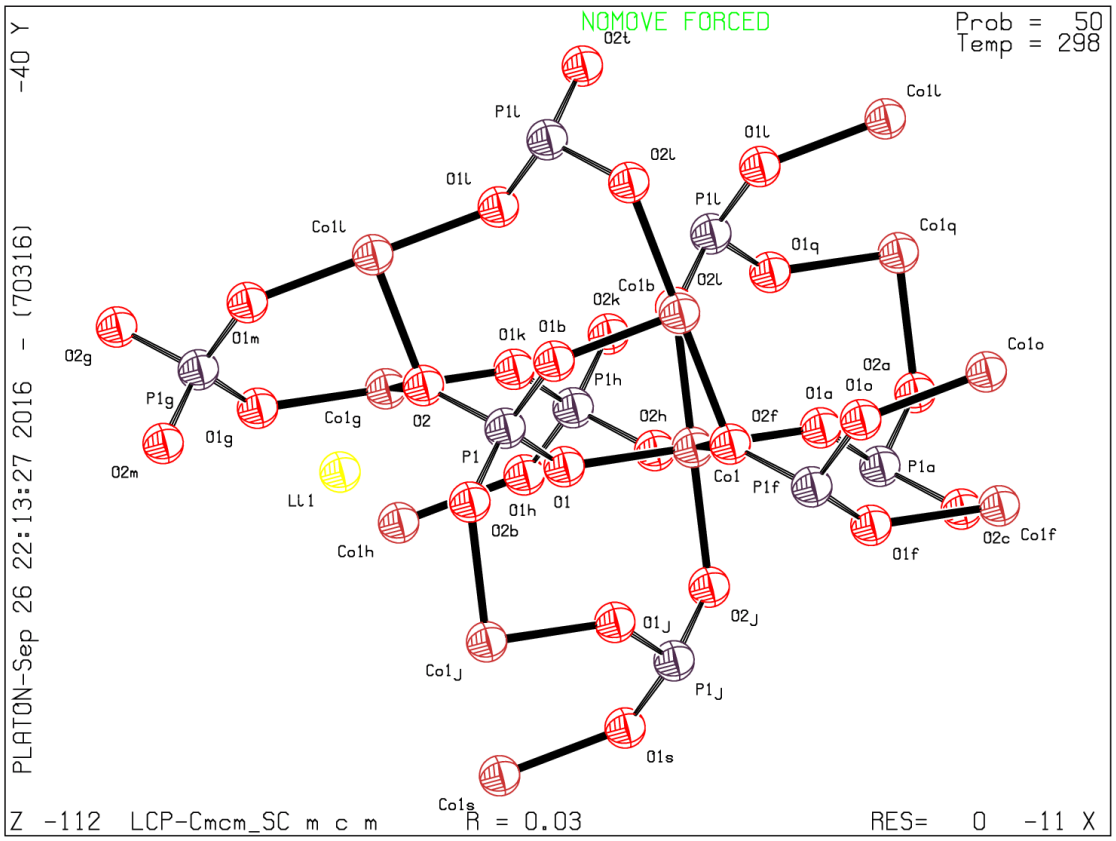
Datablock LCP-Cmcm-ST-DEG - ellipsoid plot



Datablock LCP-Cmcm-ST-TEG - ellipsoid plot



Datablock LCP-Cmcm_ST-TTEG - ellipsoid plot



Datablock LCP-Cmcm-PO - ellipsoid plot