CrystEngComm

Supporting Information

Self-assembly of lacunary building blocks into high-nuclear $[Ln_{16}As_{16}W_{164}O_{576}(OH)_8(H_2O)_{42}]^{80-}$ ($Ln = Eu^{III}$, Gd^{III}, Tb^{III}, Dy^{III}, and Ho^{III}) polyoxotungstates

Firasat Hussain and Greta R. Patzke**

Table of Contents

Synthetic details S1:
Synthesis, FT-IR spectroscopy and elemental analysis of compounds Eu-1, Tb-1, Dy-1, and Ho-1.

Synthesis of polyanion **Eu-1**: A sample of $K_{14}[As_2W_{19}O_{67}(H_2O)]$ (0.526 g (0.10 mmol), synthesized according to Kortz *et al.*[24c]) was added under stirring to a solution of 0.086 g (0.20 mmol) $Eu(NO_3)_3{\cdot}6H_2O$ in 25 mL 1 M NaCl. This solution was heated to 50 ºC for 30 minutes and then filtered. Addition of 0.50 mL of 1.0 M CsCl solution to the colorless filtrate leads to instant precipitation which eventually vanishes after the solution was stirred for 10 min. at room temperature. Slow evaporation of this solution at room temperature affords single crystals for further analysis.
FT-IR of **Eu-1**: 1258 (w), 947 (s), 860 (s), 788 (s), 707 (s), 636 (sh), 476 (s) cm^{-1}. Yield: 19.3% (0.119 g), Elemental analysis (%); calcd. (found): Na 2.5 (2.8), K 0.93 (1.0), Cs 2.6 (3.1), As 2.3 (2.3), W 59.3 (58.2), Eu 4.8 (5.0).

Synthesis of polyanion **Tb-1**: Experimental procedure cf. above, $Tb(NO_3)_3{\cdot}6H_2O$ (0.087 g, 0.20 mmol) was used instead of $Gd(NO_3)_3{\cdot}6H_2O$. FT-IR of **Tb-1**: 1258 (w), 949 (s), 859 (s), 788 (s), 709 (s), 636 (sh), 470 (s) cm^{-1}. Yield: 26.6% (0.163 g), Elemental analysis (%); calcd. (found): Na 2.5 (2.6), Cs 3.4 (2.6), As 2.3 (2.3), W 59.9 (58.5), Tb 4.9 (5.0).

Synthesis of polyanion **Dy-1**: Experimental procedure cf. above, $Dy(NO_3)_3{\cdot}6H_2O$ (0.088 g, 0.20 mmol) was used instead of $Gd(NO_3)_3{\cdot}6H_2O$. FT-IR of **Dy-1**: 1258 (w), 949 (s), 860 (s), 787 (s), 706 (s), 636 (sh), 477 (s) cm^{-1}. Yield: 26.2% (0.161 g), Elemental analysis (%); calcd. (found): Na 2.3 (2.2), Cs 3.9 (3.9), As 2.3 (2.3), W 58.6 (57.3), Dy 5.1 (5.2).

Synthesis of polyanion **Ho-1**: Experimental procedure cf. above, $Ho(NO_3)_3{\cdot}6H_2O$ (0.088 g, 0.20 mmol) was used instead of $Gd(NO_3)_3{\cdot}6H_2O$. FT-IR of **Ho-1**: 1258 (w), 948 (s), 861 (s), 788 (s), 709 (s), 632 (sh), 479 (s) cm^{-1}. Yield: 23.8% (0.146 g), Elemental analysis (%); calcd. (found): Na 2.6 (2.8), Cs 2.4 (2.9), As 2.4 (2.4), W 59.1 (57.7), Ho 5.2 (5.2).

Elemental analyses of all the polyanions were performed by Mikroanalytisches Labor Pascher, Remagen, Germany.

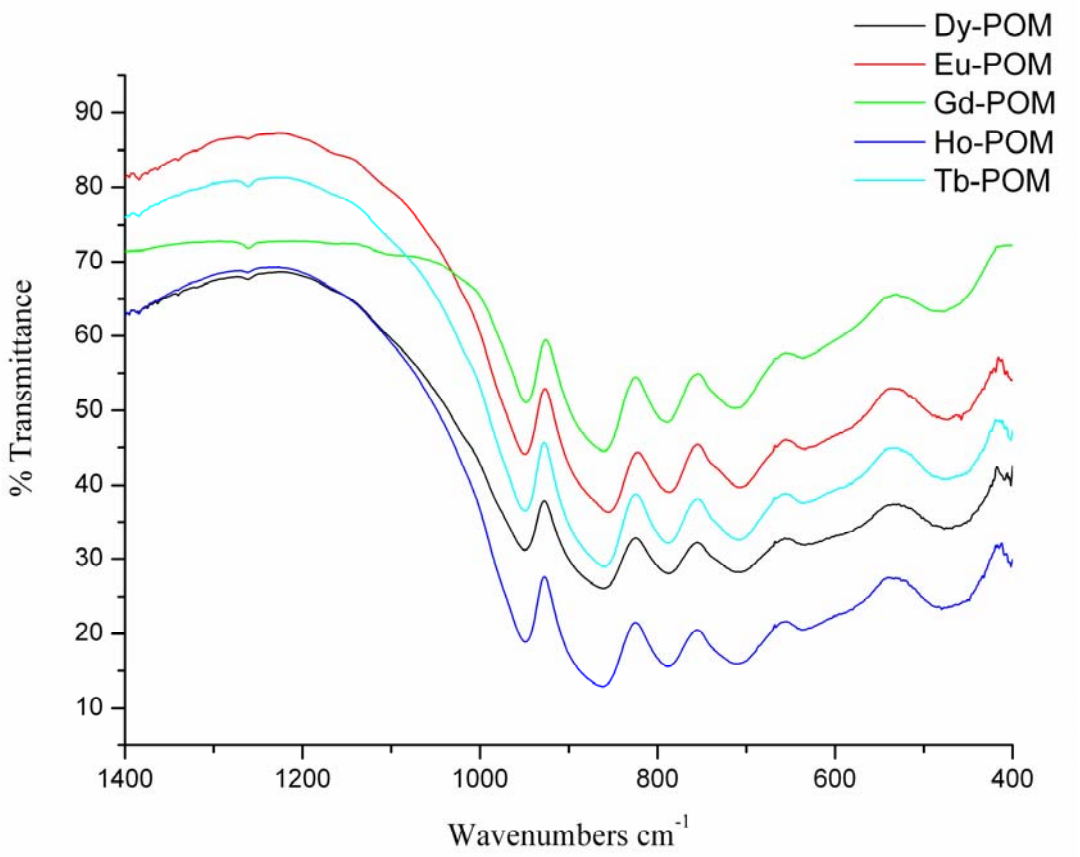

Figure S2. FT-IR spectra of compounds **Eu-1 – Ho-1** (recorded in KBr, only the polyoxometalate *"fingerprint region"* is displayed).

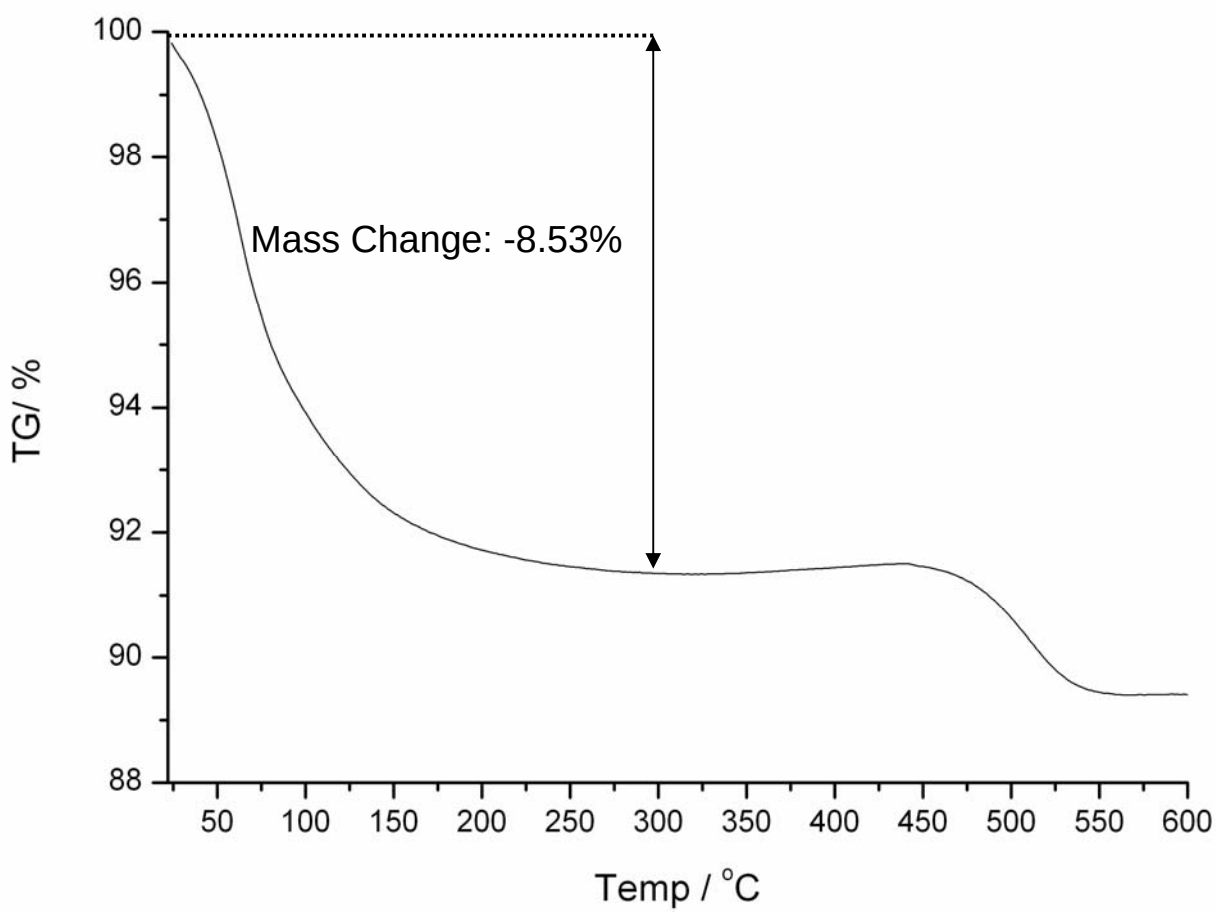

Figure S3. Representative thermogravimetric analysis of **Gd-1** displaying the mass loss corresponding to crystal water molecules (**Eu-1** = 9.63 %; **Tb-1** = 8.62 %; **Dy-1** = 8.57 %; **Ho-1** = 8.26 %).

TG measurements were performed on a Netzsch STA 449 C between 25 and 600 °C with a heating rate of 5 K/min in nitrogen atmosphere. The first weight loss corresponds to the crystal water content of the compound. We found that the percentage loss indicates the presence of approx. ~ 220 crystal water molecules in the gadolinium complex and subsequent values in the range of 240 – 210 crystal water molecules were obtained for all other complexes.

checkCIF/PLATON report

No syntax errors found. **CIF dictionary** **Interpreting this report**

Datablock: fh54

```
Bond precision:  Na- O = 0.0700 A        Wavelength=0.71073

Cell:          a=21.1358(3)      b=23.2411(3)      c=45.1923(6)
               alpha=81.399(1)   beta=83.095(1)    gamma=82.393(1)
Temperature:   183 K
```

	Calculated	Reported
Volume	21642.0(5)	21642.0(5)
Space group	P -1	P -1
Hall group	-P 1	?
Moiety formula	As16 Gd16 O624 W164, 2(Cs4.70 K2 Na20 O17), 26(O0.50), 2(Cs0.40	?
Sum formula	As16 Cs11.20 Gd16 K4 Na40 O777 W164	As16 Cs11.20 Gd16 K4 Na40 O777 W164
Mr	48861.06	48862.71
Dx,g cm-3	3.749	3.749
Z	1	1
Mu (mm-1)	24.108	24.108
F000	21036.0	21036.0
F000'	20929.17	
h,k,lmax	25,28,55	25,28,55
Nref	82205	81725
Tmin,Tmax	0.088,0.485	0.558,1.000
Tmin'	0.056	

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Correction method= MULTI-SCAN

Data completeness= 0.994          Theta(max)= 25.680

R(reflections)= 0.0896( 42782)    wR2(reflections)= 0.1871( 81725)

S = 1.002                  Npar= 2609
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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

```
PLAT202_ALERT_3_A Isotropic non-H Atoms in Anion/Solvent .........        58
PLAT220_ALERT_2_A Large Non-Solvent    O     Ueq(max)/Ueq(min) ...     10.00 Ratio
PLAT220_ALERT_2_A Large Non-Solvent    W     Ueq(max)/Ueq(min) ...     10.00 Ratio
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PLAT220_ALERT_2_A Large Non-Solvent   Na     Ueq(max)/Ueq(min) ...      10.00 Rati
PLAT220_ALERT_2_A Large Non-Solvent    O     Ueq(max)/Ueq(min) ...      10.00 Rati
PLAT241_ALERT_2_A Check High      Ueq as Compared to Neighbors for        W82
PLAT306_ALERT_2_A Isolated Oxygen Atom (H-atoms Missing ?) .......       O377
PLAT306_ALERT_2_A Isolated Oxygen Atom (H-atoms Missing ?) .......       O378
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PLAT306_ALERT_2_A Isolated Oxygen Atom (H-atoms Missing ?) .......       O375
PLAT306_ALERT_2_A Isolated Oxygen Atom (H-atoms Missing ?) .......       O376
PLAT602_ALERT_2_A VERY LARGE Solvent Accessible VOID(S) in Structure       !
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Alert level B

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PLAT241_ALERT_2_B Check High      Ueq as Compared to Neighbors for       O222
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for       O265
PLAT242_ALERT_2_B Check Low       Ueq as Compared to Neighbors for       O268
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    NA1    --  NA24    ..       4.09 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    NA1    --  CS2     ..       4.93 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    NA4    --  CS1     ..       4.97 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    NA6    --  NA22    ..       4.04 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    NA9    --  K4      ..       4.48 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    NA10   --  CS1     ..       4.38 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    NA10   --  K4      ..       4.51 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    CS1    --  W35     ..       4.03 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    CS1    --  W55     ..       4.08 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    CS5    --  W22     ..       4.17 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    CS5    --  W1      ..       4.17 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    CS5    --  W23     ..       4.18 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    CS4    --  W13     ..       4.05 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    CS6    --  W63     ..       4.29 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    GD6    --  K3      ..       4.12 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    GD7    --  K3      ..       4.43 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    W4     --  K4      ..       4.03 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    W13    --  CS4     ..       4.05 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    W14    --  CS4     ..       4.14 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    W22    --  CS5     ..       4.17 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    W22    --  CS4     ..       4.43 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    W23    --  CS5     ..       4.18 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    W26    --  CS7     ..       4.47 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    W28    --  CS5     ..       4.29 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    W29    --  CS5     ..       4.40 Ang.
PLAT774_ALERT_1_B Suspect X-Y Bond in CIF:    W65    --  K3      ..       4.03 Ang.
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Alert level C

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DIFMN02_ALERT_2_C  The minimum difference density is < -0.1*ZMAX*0.75
           _refine_diff_density_min given =     -7.204
           Test value =     -5.550
DIFMN03_ALERT_1_C  The minimum difference density is < -0.1*ZMAX*0.75
           The relevant atom site should be identified.
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.147
PLAT020_ALERT_3_C The value of Rint is greater than 0.12 .........       0.15
PLAT098_ALERT_2_C Large Reported Min.  (Negative) Residual Density      -7.20 eA-3
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        O62
PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for        O91
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PLAT241_ALERT_2_C Check High      Ueq as Compared to Neighbors for       O142
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       O271
PLAT242_ALERT_2_C Check Low       Ueq as Compared to Neighbors for       O272
PLAT077_ALERT_4_C Unitcell contains non-integer number of atoms ..          ?
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O50    --  CS7     ..       3.63 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O71    --  CS7     ..       3.73 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O72    --  CS2     ..       3.74 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O76    --  CS2     ..       3.51 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O91    --  CS2     ..       3.63 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O110   --  CS4     ..       3.72 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O111   --  CS2     ..       3.71 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O161   --  CS3     ..       3.60 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O179   --  CS2     ..       3.58 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O309   --  CS6     ..       3.62 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O359   --  CS2     ..       3.68 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   O378   --  CS2     ..       3.73 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NA3    --  NA5     ..       3.98 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NA5    --  NA3     ..       3.98 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   NA6    --  NA23    ..       3.91 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   K3     --  W64     ..       3.72 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   K3     --  W61     ..       3.80 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   K4     --  W5      ..       3.78 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   K4     --  W3      ..       3.87 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   K4     --  W54     ..       3.89 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   K4     --  W2      ..       3.92 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   CS1    --  W54     ..       3.95 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   CS4    --  O110    ..       3.72 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   GD5    --  W41     ..       3.60 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   W2     --  K4      ..       3.92 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   W3     --  K4      ..       3.87 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   W4     --  NA20    ..       3.55 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   W5     --  K4      ..       3.78 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   W32    --  CS7     ..       3.98 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   W33    --  CS7     ..       3.88 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   W61    --  K3      ..       3.80 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   W62    --  K3      ..       3.92 Ang.
PLAT774_ALERT_1_C Suspect X-Y Bond in CIF:   W64    --  K3      ..       3.72 Ang.
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Alert level G

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PLAT301_ALERT_3_G Note: Main Residue  Disorder .....................      0.00 Perc.
PLAT154_ALERT_1_G The su's on the Cell Angles are Equal  (x 10000)        100 Deg.
PLAT302_ALERT_4_G Note: Anion/Solvent Disorder .....................      7.00 Perc.
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  80 ALERT level A = In general: serious problem
  29 ALERT level B = Potentially serious problem
  44 ALERT level C = Check and explain
   3 ALERT level G = General alerts; check

  61 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
  89 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
   2 ALERT type 4 Improvement, methodology, query or suggestion
   0 ALERT type 5 Informative message, check
```

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*, 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 29/06/2010; check.def file version of 26/06/2010

Datablock fh54 - ellipsoid plot