Supplementary Data
for

$K_2HCr_2AsO_{10}$: Redetermination of phase II and the predicted structure of phase I

T. J. R. Weakley,[a] E. R. Ylvisaker,[b] R. J. Yager,[b] P. Wu,[b] P. Photinos[b] & S. C. Abrahams[b]

[a] Department of Chemistry, University of Oregon, Eugene, OR 97403, USA

[b] Physics Department, Southern Oregon University, Ashland, OR 97520, USA.

Abstract

Our prediction that $K_2HCr_2AsO_{10}$ phase II is ferroelectric, based on analysis of Averbuch-Pouchot *et al.*'s (1978) atomic coordinates, led to its independent redetermination with two separate crystals. The resulting improved accuracy allows the inference that the H atom is located in the 2.555(5) Å bonds formed between terminal oxygen atoms O5 and O6 of the shared AsO_3OH tetrahedra in adjacent $HCr_2AsO_{10}^{2-}$ ions. The largest atomic displacement, 0.586 Å, between phase II and the predicted paraelectric phase I is by these two oxygen atoms. The H atoms form helices with radius ~0.60 Å about the 3_1 or 3_2 axes. Normal probability analysis reveals systematic error in seven or more of the earlier atomic coordinates.

Table S1. Recent literature distances (Å) in arsenates, with terminal and bridging distances except for isolated anions†

Compound	Reference	$\langle d_{\text{As-O}} \rangle_{\text{term}}$	$\langle d_{\text{As-O}} \rangle_{\text{bridg}}$
$C_2H_{10}N_2^{2+}\cdot HAsO_4^{2-}$	Averbuch-Puchot *et al*., (1987)	1.669(11)	1.734(3)
LiH_2AsO_4	Fanchon *et al*., (1987)	1.686(3)	-
$(NH_3)_2C_3H_6$ $[HAsO_4]H_2O$	Lee & Harrison (2003a)	1.666(1)	1.730(1)
$[C_5H_{10}N_2]^+[H_2AsO_4]^-$	Lee & Harrison (2003b)	1.68(4)	-
$CeAsO_4$	Brahim *et al*., (2002)	1.690(7)	-
$Mn_2^{II}\ Mn^{III}\ AsO_4(OH)_4$	Kolitsch (2001)	-	1.690(4)
$Na_3Cr_2(AsO_4)_3$	Bouzemi *et al*., (2002)	1.698 (2)	1.698 (2)
$Ag_{1.49}Mn^{II}_{1.49}Mn^{III}_{1.51}(AsO_4)_4$	Brahim & Amor (2003)	-	1.688(7)

† Uncertainties in averaged distances calculated by Bessel's method.

Figure captions

Figure S1. $K_2HCr_2AsO_{10}$ structure in phase II with all atoms labelled and O6–H···O5 bonds dashed, in red.

Figure S2. Predicted structure of $K_2HCr_2AsO_{10}$ in phase I viewed along a_2 axis with c axis horizontal; the O6–H···O5 bonds are dashed, in red.

Figure S3. Predicted structure of $K_2HCr_2AsO_{10}$ in phase I along the c axis with a_2 axis horizontal.

Figure S4. Normal probability Q_{exp}-Q_{norm} plot for the atomic coordinates determined with Crystal 1 of $K_2HCr_2AsO_{10}$ *vs.* those reported by Averbuch *et al.* (1978).

Figure S5. Normal probability Q_{exp}-Q_{norm} plot for the atomic coordinates determined with Crystal 2 of $K_2HCr_2AsO_{10}$ *vs.* those reported by Averbuch *et al.* (1978).

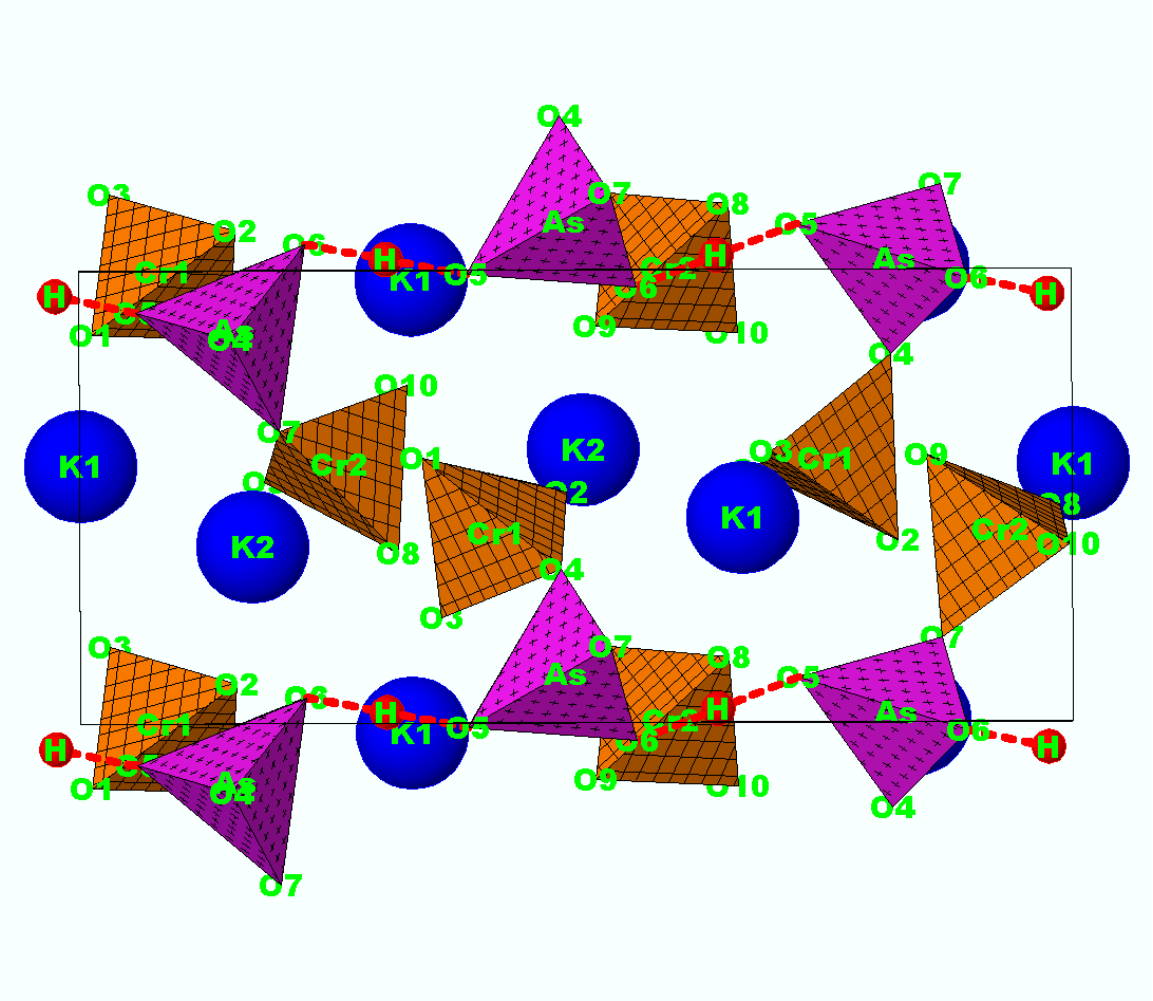

Figure S1

$K_2HCr_2AsO_{10}$ structure in phase II with all atoms labelled and O6–H···O5 bonds dashed, in red.

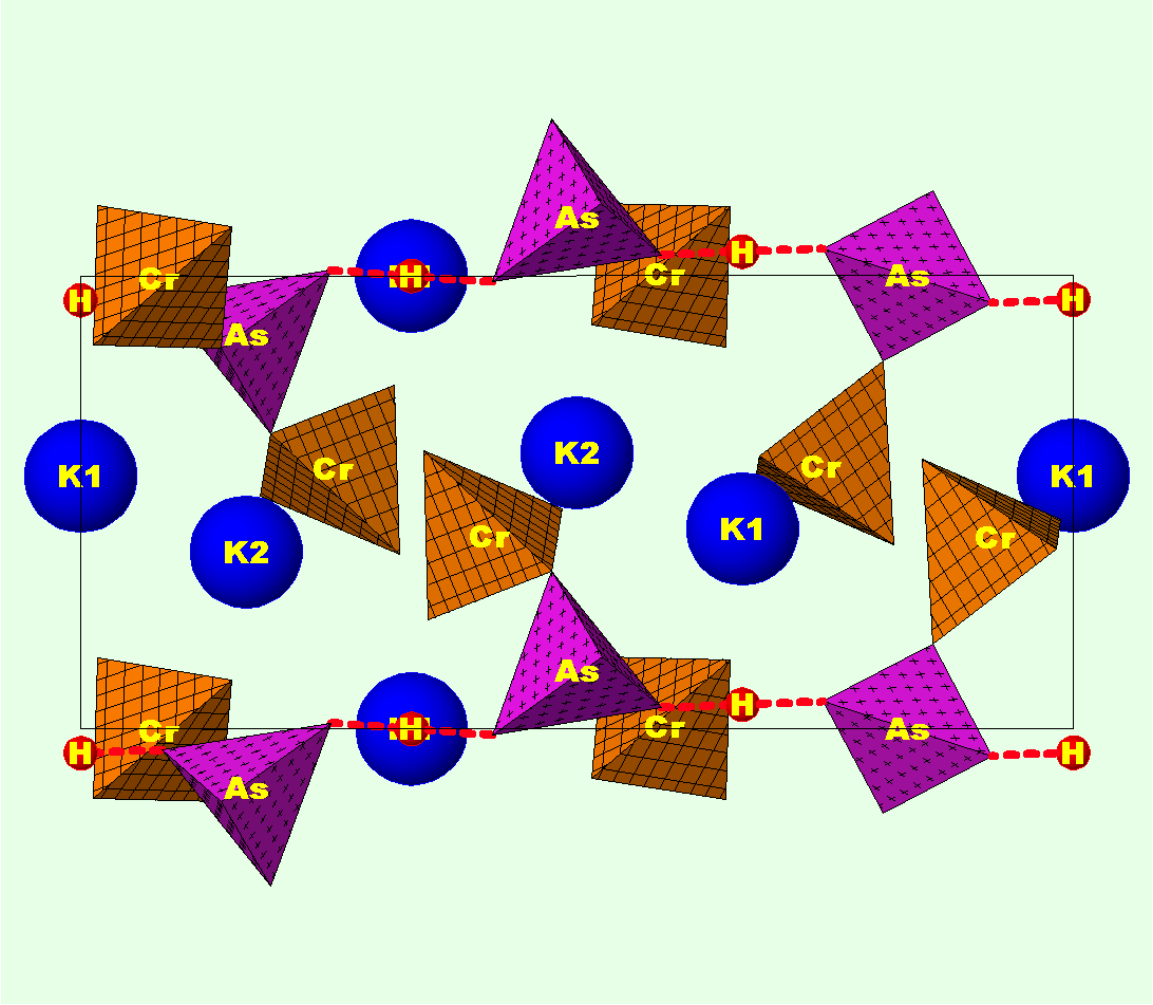

Figure S2.

Predicted structure of $K_2HCr_2AsO_{10}$ in phase I viewed along a_2 axis with c axis horizontal; the O6–H···O5 bonds are dashed, in red.

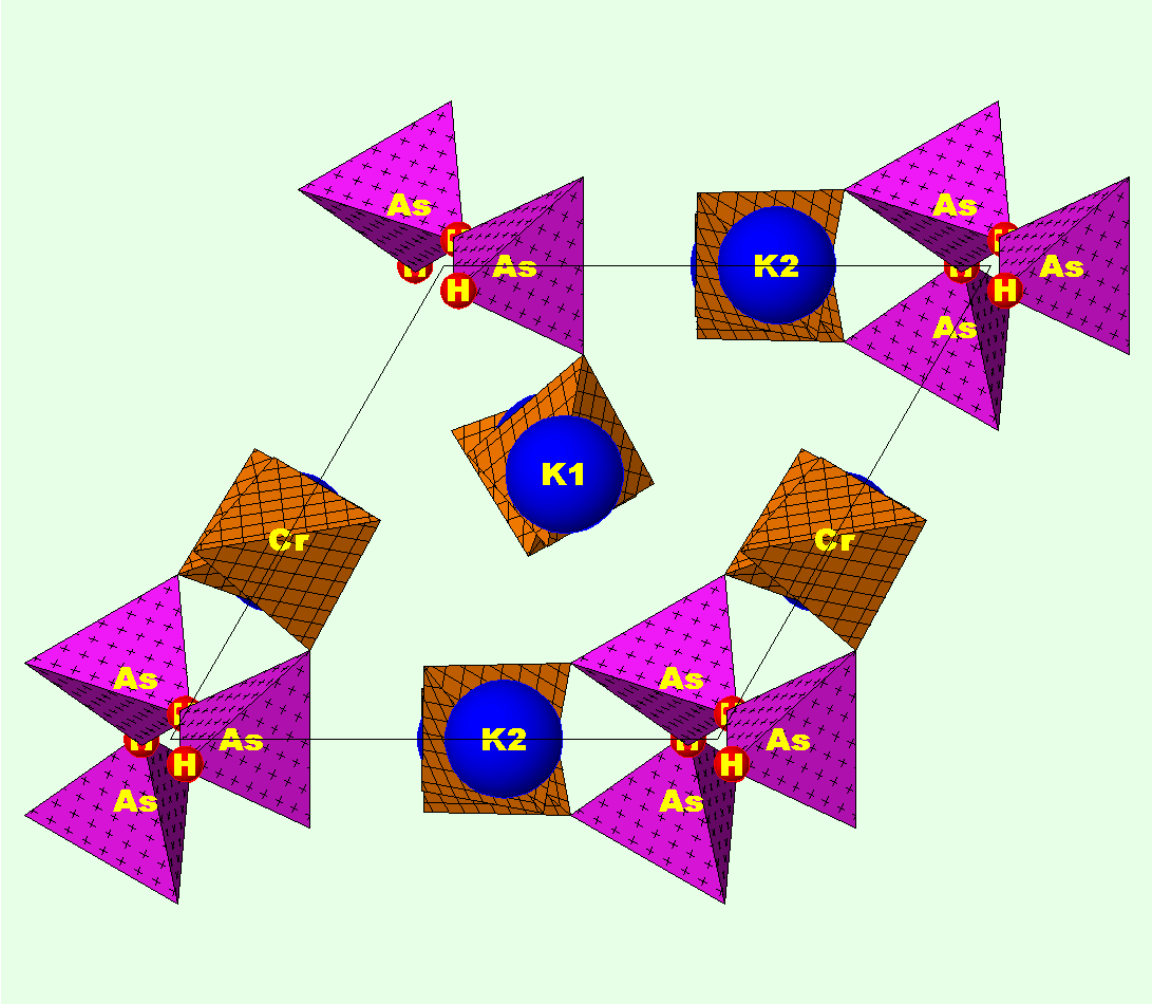

Figure S3.

Predicted structure of $K_2HCr_2AsO_{10}$ phase I along the *c* axis

with a_2 axis horizontal.

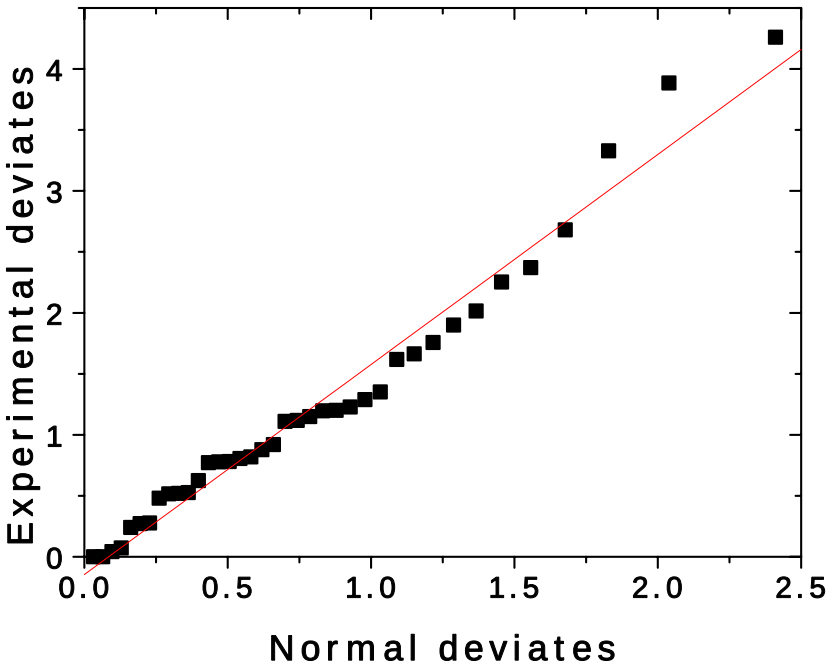

Figure S4

Normal probability Q_{exp}-Q_{norm} plot for the atomic coordinates determined with $K_2HCr_2AsO_{10}$ Crystal 1 *vs.* those of Averbuch-Puchot *et al.* (1978)

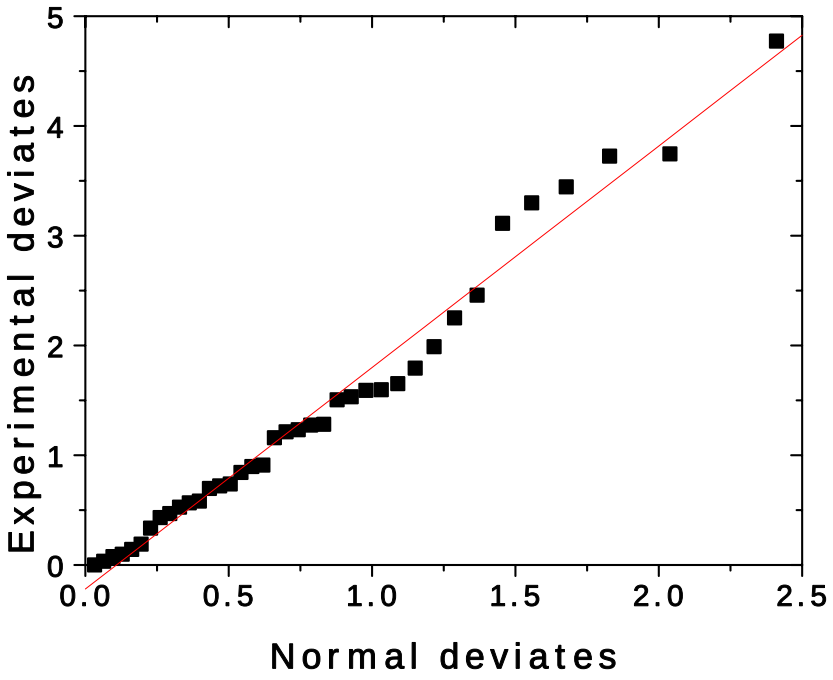

Figure S5

Normal probability Q_{exp}-Q_{norm} plot for the atomic coordinates determined with $K_2HCr_2AsO_{10}$ Crystal 2 *vs.* those of Averbuch-Puchot *et al.* (1978)

Supplementary data for this paper are available from the IUCr electronic archives (Reference:). Services for accessing these data are described at the back of the journal.

References

Abrahams, S. C. (2003). *Acta Cryst.* B**59**, 541–556.

Abrahams, S. C. & Keve, E. T. (1971). *Acta Cryst.* A**27**, 157–165.

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G., & Camalli, M. (1994). *J. Appl. Cryst.* 27, 435.

Averbuch-Pouchot, M. T., Durif, A. & Guitel, J. C. (1978). *Acta Cryst.* B**34**, 3725–3727.

Bouzemi, B., Boughzala, H. & Jouini, T. (2002). *Acta Cryst.* E58, i117-i118.

Brahim, A. & Amor, H. (2002). *Acta Cryst.* E59, i77-i79.

Brahim, A., Mongi, F. M. & Amor, H. (2002). *Acta Cryst.* E58, i98-i99.

de Meulenaer, J. & Tompa, H. (1965). *Acta Cryst.* **19**, 1014–1018.

Dowty, E. (2003). Atoms, Version 6.1. Shape Software, Kingsport, TN 37663. http://www.shapesoftware.com

Enraf–Nonius (1993). CAD-4/PC diffractometer software *v.* p. 1.2. Enraf–Nonius, Delft, The Netherlands.

Fanchon, E., Vicat, J., Qui, D. T. & Boudjada, A. (1987). *Acta Cryst.* C**43**, 1022–1025.

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Kolitsch, U. (2001). *Acta Cryst.* E57, i115-i118.

Lee, C. & Harrison, W. T. A. (2003a). *Acta Cryst.* E59, m739-m741.

Lee, C. & Harrison, W. T. A. (2003*b*). *Acta Cryst.* E59, m959-m960.

Molecular Structure Corp. (1997). TeXsan structure analysis software, *v.* p. 1.8. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.

OriginLab. Corp. (1994). 1 Roundhouse Plaza, Northampton, MA 01060.

Ross, C. R. (2003). NORMPA. Unpublished. Department of Structural Biology, St Jude Children's Research Hospital, Memphis, TN 38105–2794, USA.

Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.

Tolédano, J.-C., Glazer, A. M., Hahn, Th., Parthé, E., Roth, R. S. , Berry, R. S.,Metselaar, R. & Abrahams, S. C. (1998). *Acta Cryst.* A**54**, 1028–1033.

Tolédano, J.-C., Berry, R. S., Brown, P. J., Glazer, A. M., Metselaar, R., Pandey, D., Perez-Mato, J. M., Roth, R. S. & Abrahams, S. C. (2001). *Acta Cryst.* A**57**, 614–626.

Weakley, T. J. R., Ylvisaker, E. R., Yager, R. J., Stephens, J. E., Wiegel, R. D.,Mengis, M., Bauer, M. R., Wu, P. , Photinos P. & Abrahams, S. C. (2004). Submitted for publication.

Ylvisaker, E. R., Jones, B. M., Yager, R. J., Murata, C. R., Anderson, C., Photinos, P., Wu, P. & Abrahams, S. C. (2001). Unpublished report, Southern Oregon University, Ashland, USA.

Zachariasen, W. H. (1967). *Acta Cryst.* **23**, 558–564.

Fig. 1. Structure of $K_2HCr_2AsO_{10}$ phase II viewed along the a_2 axis with the c axis horizontal, K atoms in blue, CrO_4 tetrahedra in brown, As tetrahedra in purple and H in red.

Fig. 2. Structure of $K_2HCr_2AsO_{10}$ phase II viewed along the c axis with atom and tetrahedra colors