

s13.m35.p4 **X-ray Diffraction Study of Novel Luminescent Iridium Complexes.** K. F. Bowes, J. M. Cole, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, UK. E-mail: kfb25@cam.ac.uk

Keywords: Luminescent; Iridium; Z'

Much interest in the luminescent properties of iridium complexes has recently been generated. Bis-cyclometalated compounds have shown potential as efficient phosphors in organic light emitting diodes (OLEDs) [1], whilst terpyridine derivatives are being investigated as ligands for iridium complexes that can act as luminescent sensors for biologically important ions and molecules [2]. Iridium complexes have also shown highly efficient electrochemiluminescence [3]. In this poster we present the crystal structures of seven new luminescent iridium complexes. The compounds all have two bidentate phenyl-benzothiazole derivative ligands. The distorted octahedral coordination is completed by an acac ligand in six of the compounds, and by a 2-pyridinecarboxylic acid ligand in the other compound. The compounds display a range of Z' values, and differ considerably in their supramolecular packing, bearing in mind the similarities of their structures.

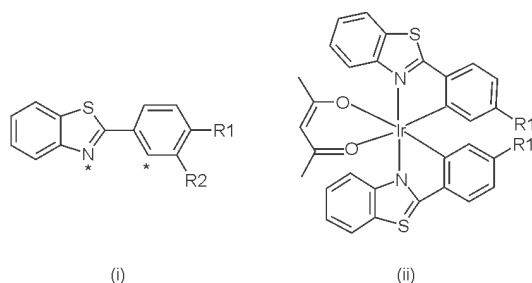


Figure 1. (i) Phenyl-benzothiazole ligand (asterisks illustrating points of binding to metal) and (ii) generic iridium complex structure (R2 is omitted for clarity).

- [1] S. Lamansky, P. Djurovich, D. Murphy, F. Abdel-Razzaq, H-E Lee, C. Adachi, P. Burrows, S.R. Forrest and M. E. Thompson, *J. Am. Chem. Soc.*, 2001, **123**, 4304 - 4312
- [2] W. Goodall and J. A. G. Williams, *J. Chem. Soc., Dalton Trans.*, 2000, 2893-2895, M. Licini and J. A. G. Williams, *Chem. Commun.*, 1999, 1943-1944, J-P. Collin, I. M. Dixon, J-P. Sauvage, J. A. G. Williams, F. Barigelletti and L. Flamigni, *J. Am. Chem. Soc.*, 1999, **121**, 5009-5016
- [3] A. Kapturkiewicz and G. Angulo, *J. Chem. Soc., Dalton Trans.*, 2003, 3907-3913, R. R. Das, C-L Lee and J-J Kim, *Mat. Res. Soc. Symp. Proc.*, 2002, **708**, BB3.39.

s13.m35.p5 **Crystal Structure of the Superionic Phase of CsH_2PO_4 and CsD_2PO_4 .** Wiesława Bronowska,^a Adam Pietraszko, ^b ^aInstitute of Physics, Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland, ^bInstitute for Low Temperature and Structure Research, Wrocław, Poland. E-mail: bron@rainbow.if.pwr.wroc.pl

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Superionic conductors are not only scientific curiosities, since these materials have a number technological applications ranging from hydrogen fuel cells, electrochemical sensors, mobile phones and laptop computers, miniature solid-state batteries for heart pacemakers to high energy storage devices for next-generation electric vehicles. Among solid acids demonstrating high protonic conductivity, cesium dihydrogen phosphate, CsH_2PO_4 (CDP) has received significant attention owing to their simple crystal structure and well defined location of protons in hydrogen bonds. At room temperature CDP and its deuterated isomorph CsD_2PO_4 (DCDP) is monoclinic and belong to the $P2_1/m$ space symmetry group). Under normal air conditions the superionic transition ($T_s = 504$ K for CDP and $T_s = 501$ K for DCDP [1]) occurs very close to the region where the crystal decomposes by dehydration [2] and these two simultaneous effects considerably perplex the interpretation of the phase relation. There are two competing views as to whether the superionic transition in CDP corresponds to a polymorphic transition or to decomposition. Following Lee [3] Ortiz *et al.* [4] and recently Park *et al.* [5] attribute the increase in conductivity at high temperature region of CDP (as well as in other KDP-family compounds) to dehydration process starting on the sample surfaces and partial polymerization. On the other hand our previous powder X-ray investigations of CDP under humidified conditions [6, 7] support Baranov's *et al* [1] suggestion, that superprotonic phase of CDP is cubic and reversible with hysteresis on cooling. Recently Boysen *et al.* [8] and Otomo *et al.* [9] reconfirmed the reversibility of the superionic phase transition in these crystals. In order to demonstrate the structural changes occurring in the CDP and DCDP crystals related to the reported superionic phase transition the *single crystal* measurements were carried out on the four circle X-ray KM4-CCD diffractometer. Detailed structural analyses were performed. The crystal structures of the superionic phase of CDP and DCDP were solved and refined using SHELXS-97 and SHELXL-97 programs. The results unequivocally established a cubic symmetry (Pm-3m) of the superionic phase for both CDP and DCDP. The cubic phase is stable on cooling over the ap. 40 deg temperature regime. The reversible nature of the superionic transformation in CDP and DCDP is strong evidence for a polymorphic character of this transition.

- [1] A. I. Baranov, *et al.*, *Ferroelectrics* **100**, 135, 1989.
- [2] W. Bronowska *et al.*, *Solid State Commun.* **76**, 293, 1990.
- [3] K.-S. Lee, *J. Phys. Chem. Solids* **57**, 333, 1996.
- [4] E. Ortiz *et al.*, *J. Chem. Phys.* **110**, 4847, 1999.
- [5] J.-H. Park, *Phys. Rev. B* **69**, 054104, 2004.
- [6] A. Preisinger *et al.*, *Mat. Sc. Forum* **166-169**, 511, 1994.
- [7] W. Bronowska, *J. Chem. Phys.* **114**, 611, 2001.
- [8] D. A. Boysen *et al.*, *Chem. Mater.* **15**, 727, 2003.
- [9] J. Otomo *et al.*, *Solid State Ionics* **156**, 357, 2003.