

## Professor Colin R. Pulham Professor of High-Pressure Chemistry

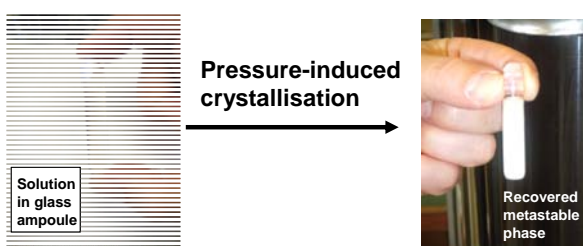
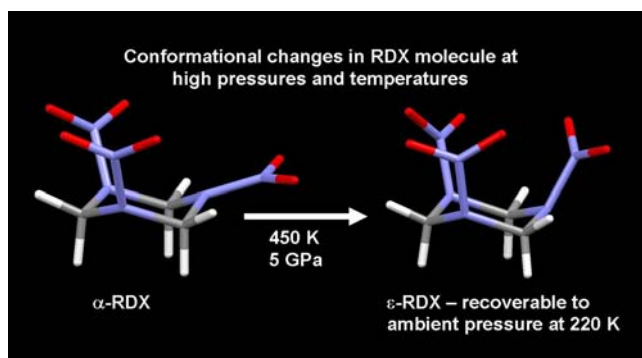
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Research Interests: Studies of pharmaceuticals, explosives, and propellants at high pressure. Polymorphism, crystal engineering.



Our research interests include the study of the effects of high pressure on the crystal structures of pharmaceutical compounds and energetic materials (explosives and propellants). By compressing single crystals or powders to pressures as high as 10 GPa contained in diamond-anvil cells or larger volume cells, we are able to use spectroscopic and diffraction (X-ray and neutron) methods to monitor and measure structural changes in the materials. For energetic materials, this information is crucial for the modelling of the characteristics and performance of these compounds under detonation conditions, especially as extreme conditions can lead to the formation of different polymorphs.



Useful information can be obtained about the polymorphic behaviour of pharmaceutical compounds, particularly when they undergo processing such as tableting and grinding. It is also possible to grow crystals of these compounds from solution at high pressure and this method has proved to be particularly effective for the formation of new polymorphs and solvates, some of which can be recovered back to ambient pressure.

We are also exploring the crystallisation of salt hydrates under a range of conditions, with a particular focus on hydrates which exist under only a limited stability range, but which nevertheless can play an important role in crystallisation processes associated with terrestrial weathering, heat-storage materials, and the environments of extra-terrestrial icy moons.

### SELECTED RECENT PUBLICATIONS

1. Pressure-cooking of explosives - the crystal structure of  $\epsilon$ -RDX as determined by X-ray and neutron diffraction. D. I. A. Millar, I. D. H. Oswald, C. Barry, D. J. Francis, W. G. Marshall, C. R. Pulham and A. S. Cumming, *Chem. Commun.*, 2010, **46**, 5662-5664.
2. Putting the squeeze on energetic materials - structural characterisation of a high-pressure phase of CL-20. D. I. A. Millar, H. E. Maynard-Casely, A. K. Kleppe, W. G. Marshall, C. R. Pulham and A. S. Cumming, *CrystEngComm.*, 2010, **12**, 2524-2527.
3. Co-crystallisation at high pressure - an additional tool for the preparation and study of co-crystals. I. D.H. Oswald and C. R. Pulham, *CrystEngComm.*, 2008, **10**, 1114-1116.
4. Putting pressure on elusive polymorphs and solvates. I. D. H. Oswald, I. Chataigner, S. Elphick, F. P. A. Fabbiani, A. R. Lennie, J. Maddaluno, W. G. Marshall, C. R. Pulham, T. J. Prior, R. I. Smith, *CrystEngComm*, 2009, **11**, 359-366.
5. High-pressure structural studies of the pharmaceutical, chlorothiazide. I. D. H. Oswald, A. R. Lennie, C. R. Pulham and K. Shankland, *CrystEngComm*, 2010, **12**, 2533-2540.
6. In-situ characterization of elusive salt hydrates - the crystal structures of the heptahydrate and octahydrate of sodium sulfate. I. D. H. Oswald, A. Hamilton, C. Hall, W. G. Marshall, T. J. Prior and C. R. Pulham, *J. Am. Chem. Soc.*, 2008, **130**, 17795-17800.