

Professor Colin R. Pulham Professor of High-Pressure Chemistry

e-mail: C.R.Pulham@ed.ac.uk

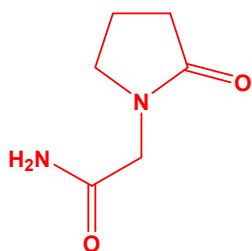
tel: 0131 650 4756

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

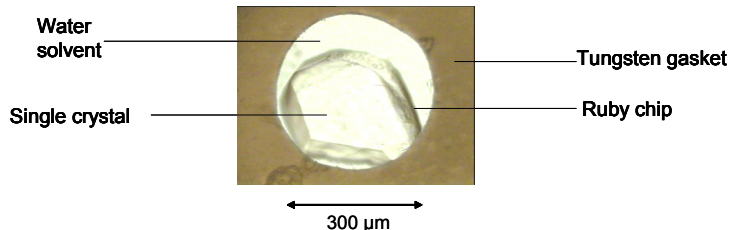


Our research interests include the study of the effects of high pressure on the crystal structures of pharmaceutical compounds and energetic materials (explosives and propellants). By compressing single crystals or powders to pressures as high as 10 GPa contained in diamond-anvil cells or larger volume 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 and/or deflagration conditions. Useful information can be obtained about the polymorphic behaviour of pharmaceutical compounds, particularly when they undergo processing such as tableting and grinding.

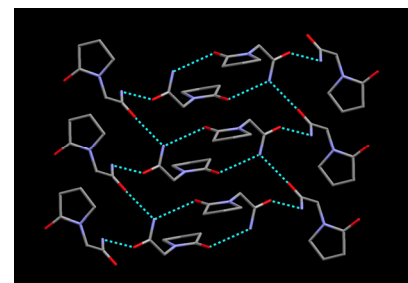
It is also possible to grow crystals of these compounds from solution at high pressure and this method has proved to be particularly effective for the formation of new polymorphs and solvates, some of which can be recovered back to ambient pressure.



Piracetam

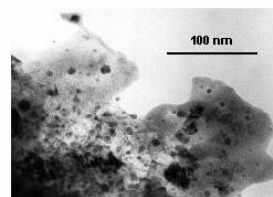


Optical image of crystal of piracetam grown at 0.4 GPa



Crystal structure of new polymorph of piracetam

We are also exploring (with Dr A.R. Mount) the growth of technologically important metal nitrides (e.g. TiN) as either thin films or particles using electrochemical methods that involve liquid ammonia and metal amides. Such processes operate at or near ambient temperature and therefore offer advantages over more conventional high-temperature routes.



TEM image of TiN nanoparticles

SELECTED RECENT PUBLICATIONS

1. High-pressure studies of pharmaceuticals: an exploration of the behavior of piracetam. F.P. A. Fabbiani, D.R. Allan, W. I. F. David, A. J. Davidson, A. R. Lennie, S. Parsons, C.R. Pulham, and J. E. Warren. *Crystal Growth & Design*, 2007, **7**, 1115-1124.
2. Explosives under pressure - the crystal structure of γ -RDX as determined by high-pressure X-ray and neutron diffraction. A. J. Davidson, I. D. H. Oswald, D. J. Francis, A. R. Lennie, W. G. Marshall, D. I. A. Millar, C. R. Pulham, J. E. Warren and A. S. Cumming. *CrystEngComm.*, 2008, **10**, 162-165.
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. A high-pressure form of sulfuric acid monohydrate as determined by X-ray and neutron diffraction. F. P. A. Fabbiani, D. R. Allan, A. Dawson, D. J. Francis, W. G. Marshall, and C. R. Pulham, *Inorg. Chim. Acta*, 2008, **361** 487-494.
5. High-pressure studies of pharmaceutical compounds and energetic materials. F.P.A. Fabbiani and C.R. Pulham, *Chem. Soc. Rev.*, 2006, **35**, 932-942.