Bence-Jones Protein Pav: the first ISIR structure

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This amazing story begins with a need. In the early 1980's macromolecular crystals structures were determined by the technique of Multiple Isomorphous Replacement. The technique required the collection of a minimum of three data sets: a native data set plus two or more data sets collected on crystals of isomorphous heavy atom derivatives.

The 45 kD Bence-Jones Protein Pav had been crystallized and 4.5Å data sets were collected on crystals of the native protein and an isomorphous $K_2Pt(CNS)_4$ derivative. Unfortunately, obtaining a second isomorphous derivative needed for phasing proved to be problematic. This need for a means of solving a protein structure based only on one derivative is what prompted B.C. Wang to develop what we now know as solvent flattening.

The presentation will describe the non-routine (even by 1980's standards) structure determination of Pav by Wang's ISIR technique including the (1) generation of a 2.8 Å native data set based on film and diffractometer data, (2) phase extension from 4.5 to 2.8Å (3) the use of a wire model and a 2D Richards Box to carryout the initial real space alignment of the model with the ED map and (4) the resulting 2.8Å refined structure.