

### List of crystal structures

| Compound | CSD Refcode | Collection source | Temperature | Reference                                                                                                                                          |
|----------|-------------|-------------------|-------------|----------------------------------------------------------------------------------------------------------------------------------------------------|
| 2,6-PDCA | AFEBUI      | X-ray             | 300 K       | V. C. Téllez, B. S. Gaytán, S. Bernès and E. G. Vergara, <i>Acta Crystallogr., Sect. C: Cryst. Struct. Commun.</i> , 2002, <b>C58</b> , o228-o230. |
| 2,3-PDCA | QUICNA01    | Neutron           | 283-303 K   | A. Kvik, T. F. Koetzle, R. Thomas and F. Takusagawa, <i>J. Chem. Phys.</i> , 1974, <b>60</b> , 3866-3874.                                          |
| 3,5-PDCA | DINICA12    | Neutron           | 296 K       | J. A. Cowan, J. A. K. Howard, G. J. McIntyre, S. M. F. Lo and I. D. Williams, <i>Acta Crystallogr., Sect. B</i> , 2005, <b>61</b> , 724-730.       |
| 3,5-PDCA | DINICA11    | Neutron           | 15 K        | J. A. Cowan, J. A. K. Howard, G. J. McIntyre, S. M. F. Lo and I. D. Williams, <i>Acta Crystallogr., Sect. B</i> , 2005, <b>61</b> , 724-730.       |