A comparison of $Mn^{2+}\cdots H$ distances from this study with those found by n.m.r. studies in the absence and presence of the enzyme aconitase (Villafranca *et al.*, 1972) indicates that the model involving a ternary enzyme–manganous citrate complex with the citrate ion directly chelated to the metal ion is probably correct.

We thank Miss Barbara Gallen, Miss Judy Giannini and Mr Bruce Haggerty for technical assistance and Dr Helen M. Berman for helpful discussions.

This research was supported by grants CA-10925, CA-06927 and RR-05539 from the National Institutes of Health, U.S. Public Health Service, and by an appropriation from the Commonwealth of Pennsylvania.

References

CROMER, D. T. & LIBERMAN, D. (1970). *J. Chem. Phys.* **53**, 1891–1898.

GANTZEL, P. K., SPARKS, R. A., LONG, R. E. & TRUEBLOOD, K. N. (1969). *UCLALS*4 Program in Fortran IV.

GLUSKER, J. P. & CARRELL, H. L. (1973). *J. Mol. Struct.* **15**, 151–159.

GRZYBOWSKI, A. K., TATE, S. S. & DATTA, S. P. (1970). *J. Chem. Soc.* (*A*), 241–245.

International Tables for X-ray Crystallography (1962). Vol. III, pp. 201–207. Birmingham: Kynoch Press.

JOHNSON, C. K. (1963). 1620 Programs from I.C.R. I.C.R. No. 10. *Absorption Factors for a crystal Ground as an Ellipsoid of Revolution.*

JOHNSON, C. K. (1965). *Acta Cryst.* **18**, 1004–1018.

STEWART, R. F., DAVIDSON, E. R. & SIMPSON, W. T. (1965). *J. Chem. Phys.* **42**, 3175–3187.

STEWART, J. M., KUNDELL, F. A. & BALDWIN, J. C. (1970). *The X-ray System, Version of* 1970. Chemistry Department, Univ. of Maryland 20740, U.S.A.

VILLAFRANCA, J. J. & MILDVAN, A. S. (1971). *J. Biol. Chem.* **246**, 5791–5798.

VILLAFRANCA, J. J. & MILDVAN, A. S. (1972). *J. Biol. Chem.* **247**, 3454–3463.

SHORT COMMUNICATION

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

Acta Cryst. (1973). B**29**, 640

The crystallography of nitramine–solvent complexes. II.* Classification and crystallographic data of some complexes of 1,7-diacetoxy-2,4,6-trinitro-2,4,6-triazaheptane (BSX).

By R. E. COBBLEDICK and R. W. H. SMALL, *Chemistry Department, The University, Lancaster, England*

(*Received* 18 *November* 1972; *accepted* 20 *November* 1972)

Crystallographic data of some further complexes of the title compound with organic solvents are given. The complexes are classified into types depending on the internal symmetry within the crystals.

The crystalline complexes of BSX, formed with various solvents by simple recrystallisation, can be divided into four main groups; within each group the cell dimensions are similar and the internal symmetry the same. Table 1 shows the four types of complex formed with a number of organic solvents. Those marked (2:1) have that molecular ratio of BSX to solvent and the remainder have a 1:1 ratio. These ratios were obtained from crystal density and unit-cell dimension measurements and confirmed by thermogravimetric analysis or in some cases from n.m.r. spectra of solutions.

Unit-cell dimensions and space groups were determined for most of the complexes from oscillation and Weissenberg photographs using Cu $K\alpha$ radiation ($\lambda = 1{\cdot}5418$ Å). Crystal data for the complexes are shown in Table 2. Crystals grown from benzene and monofluorobenzene (type *D*) were too small to determine unit-cell dimensions.

Table 1. *BSX complexes*

Type *A*. Monoclinic	
Acetonitrile	*N*-Methyl-2-pyrrolidinone
Acetone	Nitrobenzene (2:1)
Nitromethane	Acetophenone (2:1)
Pyridine	Acetylacetone (2:1)
N,*N*-Dimethylformamide	Cyclohexanone (2:1)
N,*N*-Dimethylacetamide	Pentafluorobenzene (2:1)
Dichloromethane	1,1,2,2-Tetrachloroethane (2:1)
Dibromomethane	
Type *B*. Monoclinic	
4-Hydroxybutanoic acid lactone	3-Bromopyridine (2:1)
1,4-Thioxane (2:1)	3-Methylpyridine (2:1)
Type *C*. Monoclinic	
1,4-Dioxane	
Type *D*. Triclinic	
Benzene	Monofluorobenzene

* Part I: Claringbull & Small, *Acta Cryst.* B**27**, 863–864.

Table 2. *Crystal data*

(*a*) Crystallographic data for the type *A* crystals

Solvent	*a* (Å)	*b* (Å)	*c* (Å)	*β* (°)	*V* (Å^3)	Stoichiometry BSX: solvent	Observed density (g cm^{-3})	Calculated density (g cm^{-3})	Space group
Acetylacetone	14·04	20·38	6·39	96·1	1818·0	2:1	1·44	1·48	All $P2_1/n$
Cyclohexanone	14·31	20·02	6·41	96·7	1823·9	2:1	1·44	1·47	
Pyridine	14·82	20·02	6·41	95·9	1891·7	1:1	1·52	1·52	
N,*N*-Dimethylformamide	15·36	19·79	6·41	97·2	1933·1	1:1	1·47	1·47	
Nitrobenzene	14·34	20·09	6·43	95·5	1843·9	2:1	1·50	1·50	
Pentafluorobenzene	14·20	19·96	6·44	97·1	1811·2	2:1	1·59	1·61	
N-Methyl-2-pyrrolidinone	15·23	20·45	6·47	96·7	2001·4	1:1	1·50	1·50	
Dibromomethane	14·75	20·02	6·50	97·3	1903·9	1:1	1·84	1·84	
Dichloromethane	14·46	19·97	6·51	93·1	1877·0	1:1	1·56	1·55	
1,1,2,2-Tetrachloroethane	14·35	19·96	6·55	96·5	1864·1	2:1	1·55	1·56	
N,*N*-Dimethylacetamide	14·78	20·68	6·56	96·2	1993·4	1:1	1·47	1·47	
(*b*) Crystallographic data for the type *B* crystals									
1,4-Thioxane	13·95	6·56	20·14	106·2	1769·9	2:1	1·54	1·55	All $P2_1/c$
4-Hydroxybutanoic acid lactone	14·97	6·59	20·80	106·8	1964·5	1:1	1·49	1·49	
3-Methylpyridine	13·17	6·65	20·32	91·7	1778·9	2:1	1·50	1·50	
3-Bromopyridine	13·03	6·72	20·30	92·0	1775·3	2:1	1·61	1·62	
(*c*) Crystallographic data for the type *C* crystals									
1,4-Dioxane	22·13	13·83	6·50	96·7	1975·8	1:1	1·49	1·49	$P2_1/n$

The crystal structures of pure BSX and of the 1:1 complexes with *N*,*N*-dimethylformamide (type *A*), 4-hydroxybutanoic acid lactone (type *B*) and 1,4-dioxane (type *C*) have been determined, and will be described in subsequent papers.

The authors wish to thank Dr T. N. Huckerby for the n.m.r. spectra, Dr D. Stubley for the thermogravimetric analysis, and the Procurement Executive, Ministry of Defence, for a grant in support of this work.

Reference

CLARINGBULL, G. F. & SMALL, R. W. H. (1971). *Acta Cryst.* B**27**, 863–864.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. The notes (in duplicate) should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).

Dr Walter C. Hamilton 1931–1973

Dr Walter C. Hamilton, a Co-editor of *Acta Crystallographica* since 1969, died on Tuesday 23 January 1973. A full obituary notice will be published later in Section A of this journal.

Molecular Structures and Dimensions

Interatomic Distances 1960–65, *Organic and Organometallic Crystal Structures* will be published for the International Union of Crystallography and the Crystallographic Data Centre, Cambridge by Oosthoek Publishing Company in March 1973 at a price of Netherlands guilders 175 (equivalent to U.S. $57·00 or £23·70 at present rates of exchange). Copies for the personal use of scientists may be obtained at a reduced price of Netherlands guilders 125 (U.S. $40·50 or £16·90).

This book, Volume A1 in the *Molecular Structures and Dimensions series*, is a continuation of *Tables of Interatomic Distances and Configuration in Molecules and Ions* which covered the iterature up to the end of 1959. It has been prepared by the Crystallographic Data Centre, Cambridge and contains numerical data, including bond lengths, bond angles and torsion angles, for about 1300 structures analysed by X-ray and neutron diffraction. The entries are illustrated by specially prepared stereoscopic diagrams and by chemical formulae. All bond lengths were checked by computer and errors detected were traced and corrected as far as possible. Torsion angles of greatest conformational interest were selected and these were calculated from published coordinates. Only rarely have they been listed in the original publication. There are extensive summary tables of bond lengths, arranged by element-pairs, and a variety of indexes.

Volume 4 in the *Molecular Structure and Dimensions* series, *Bibliography* 1971–1972, *Organic and Organometallic*