A Reference List of Organic Structures whose Absolute Configurations have been determined by X-ray Methods. Part 2

By F. H. ALLEN, S. NEIDLE, and D. ROGERS*
(*Chemical Crystallography Laboratory, Imperial College, London, S.W.*7)

Part 1 of this list (F. H. Allen and D. Rogers, *Chem. Comm.*, 1966, 838) contained 54 entries. This supplement, believed to be complete to the end of 1967, contains 40 new entries.

1. Using the Anomalous Dispersion Method

Compound	*Fluorescent atom*	*Radiation used*	*Reference*
(1) *Amino-acids*			
(+)-2-Benzylglutamic acid as hydrobromide dihydrate	Br	Cu	T. Ashida, Y. Sasada, and M. Kakudo, *Bull. Chem. Soc. Japan*, 1967, **40**, 476.
(+)-2-Methyl-2-isopropylglutaric acid (+)-2-Methyl-2-isopropylsuccinic acid as Rb salt	Rb	Cu	M. R. Cox, H. P. Koch, W. B. Whalley, M. B. Hursthouse, and D. Rogers, *Chem. Comm.*, 1967, 212.
Cucurbitine as perchlorate (erroneously included under alkaloids in the first list)	Cl	Cu	Fan Hai-Fu and Lin Cheng-Chiung, *Acta Phys. Sinica*, 1965, **21**, 253.
(2) *Terpenoids*			
Ginkgolide A as mono-*p*-bromobenzoate	Br	Cu	N. Sakabe, S. Takada, and K. Okabe, *Chem. Comm.*, 1967, 259.
Caryophyllene iodonitrosite	I	Mo	D. M. Hawley, J. S. Roberts, G. Ferguson, and A. L. Porte, *Chem. Comm.*, 1967, 942.
Pseudoclovene A as mono-*p*-bromobenzene sulphonate ester	Br	Cu	G. Ferguson, D. M. Hawley, T. F. W. McKillop, J. Martin, W. Parker, and P. Doyle, *Chem. Comm.*, 1967, 1123.
Laurinterol as acetate (also establishes aplysin)	Br	Mo	A. F. Cameron, G. Ferguson, and J. M. Robertson, *Chem. Comm.*, 1967, 271.
Desmotroposantonin as 2-bromo-(−)-β-compound	Br	Cu	A. T. McPhail, B. Rimmer, J. M. Robertson, and G. A. Sims, *J. Chem. Soc.* (*B*), 1967, 101.
Beyerol as monoethylidene iodoacetate derivative	I	Cu	A. M. O'Connell and E. N. Maslen, *Acta Cryst.*, 1966, **21**, 744.
Caesalpin as *p*-bromobenzoate	Br	Mo	A. Balmain, K. Bjamer, J. D. Connolly, and G. Ferguson, *Tetrahedron Letters*, 1967, 5027.
Gibberellic acid as methyl bromogibberellate	Br	Cu	F. McCapra, A. T. McPhail, A. I. Scott, G. A. Sim, and D. W. Young, *J. Chem. Soc.* (*C*), 1966, 1577.

Compound	*Fluorescent atom*	*Radiation used*	*Reference*
(2) *Terpenoids—continued*			
Taxa-4(16),11-diene-5α,9α,10β,13α-tetraol as dihydro-anhydroisopropylidine derivative	Br	Cu	K. Bjamer, G. Ferguson, and J. M. Robertson, *J. Chem. Soc.* (*B*), 1967, 1272.
(+)-Camphor—see Retusamine below			
(3) *Sugar Derivatives*			
Aristeromycin as hydrobromide	Br	Cu(?)	T. Kishi, M. Muroi, T. Kusaka, M. Nishikawa, K. Kamiya, and K. Mizuno, *Chem. Comm.*, 1967, 852.
Showdomycin as isopropylidine-*N*-methylbisdeoxycycloshowdomycin hydrobromide	Br	Mo(?)	Y. Tsukuda, Y. Nakagawa, H. Kano, T. Sato, M. Shiro, and H. Koyama, *Chem. Comm.*, 1967, 975.
Formycin as monohydrobromide monohydrate	Br	Cu	G. Koyama, K. Maeda, H. Umezawa, and Y. Iitaka, *Tetrahedron Letters*, 1966, 597.
α-D-Glucosamine as hydrochloride	Cl	Cu	G. N. Ramachandran, R. Chandrasekaran and K. S. Chandrasekaran, *Biochim. Biophys. Acta.*, 1967, **148**, 317.
Ethyl 1-thio-α-D-glucofuranoside	S	Cu	R. Parthasarathy and R. E. Davis, *Acta. Cryst.*, 1967, **23**, 1049.
(4) *Alkaloids*			
Tuberostemonine as methobromide dihydrate	Br	Cu	H. Harada, H. Irie, N. Masaki, K. Osaki, and S. Uyeo, *Chem. Comm.*, 1967, 460.
Quinidine as (−)-1,1′-dimethylferrocene-3-carboxylic acid	Fe	Cu	O. L. Carter, A. T. McPhail, and G. A. Sim, *J. Chem. Soc.* (*A*), 1967, 365.
Buxenine-G as dihydroiodide	I	Cu(?)	R. T. Puckett, G. A. Sim, E. Abushanab, and S. M. Kupchan, *Tetrahedron Letters*, 1966, 3815.
Corymine as hydrobromide monohydrate	Br	Cu	C. W. L. Bevan, M. B. Patel, A. H. Rees, D. R. Harris, M. L. Marshak, and H. H. Mills, *Chem. and Ind.*, 1965, 603.
Gliotoxin (also establishes sporidesmin)	S	Cu	J. Fridrichsons and A. McL. Mathieson, *Acta Cryst.*, 1967, **23**, 439.
19-Propylthevinol as hydrobromide (also establishes morphine series)	Br	Cu	J. H. Van den Hende and N. R. Nelson, *J. Amer. Chem. Soc.*, 1967, **89**, 2901.
Mitomycin A as *N*-*p*-bromobenzenesulphonyl compound	Br,S	Cu	A. Tulinsky and J. H. Van den Hende, *J. Amer. Chem. Soc.*, 1967, **89**, 2905.
Haplophytine as dihydrobromide	Br	Cu	I. D. Rae, M. Rosenberger, A. G. Szabo, C. R. Willis, P. Yates, D. E. Zacharias, G. A. Jeffrey, B. Douglas, J. L. Kirkpatrick, and J. A. Weisbach, *J. Amer. Chem. Soc.*, 1967, **89**, 3061.
Retusamine as α′-bromo-D-camphor-*trans*-π-sulphonate monohydrate [also establishes absolute configuration of (+)-camphor]	Br	Cu	J. A. Wunderlich, *Acta Cryst.*, 1967, **23**, 846.
(5) *Steroids*			
Cholestane as 2α,3β-dibromo-5α-compound	Br	Cu	E. Van Heijkoop, H. J. Geise, and C. Romers, *Rec. Trav. chim.*, 1965, **83**, 1626.
17aβ-*p*-Bromobenzenesulphonyloxy-17α-methyl-19-nor-9β,10α-D-homoandrost-4-en-3-one	Br,S	Cu	R. T. Puckett, G. A. Sim, A. D. Cross, and J. B. Siddall, *J. Chem. Soc.* (*B*), 1967, 783.
17β-Bromoacetoxy-9β,10α-androst-4-en-3-one	Br	Cu	W. E. Oberhänsli and J. M. Robertson, *Helv. Chim. Acta*, 1967, **50**, 53.
(6) *Miscellaneous large molecules and mould metabolites* (*antibiotics*)			
Erythromycin A as hydriodide dihydrate	I	Cu	D. R. Harris, S. G. McGeachin, and H. H. Mills, *Tetrahedron Letters*, 1965, 679.
Siccanin as *p*-bromobenzene sulphonate	Br	Cu	K. Hirai, S. Nozoe, K. Tsuda, Y. Iitaka, K. Ishibashi, and M. Shirasaka, *Tetrahedron Letters*, 1967, 2177.
Ryridomycin as dihydrobromide	Br	Cu	G. Koyama, Y. Iitaka, K. Maeda, and H. Umezawa, *Tetrahedron Letters*, 1967, 3587.

2. By Internal Comparison with a Reference Centre

Compound	*Internal comparison centre*	*Reference*
(+)-*S*-Methyl-L-cysteine *S*-oxide	L$_S$-Amino-acid	R. Hine and D. Rogers, *Chem. and Ind.*, 1956, 1428; R. Hine, *Acta Cryst.*, 1962, **15**, 635.
(−)-Menthyl (−)-*p*-iodobenzenesulphinate	(−)-Menthyl group	E. B. Fleischer, M. Axelrod, M. Green, and K. Mislow, *J. Amer. Chem. Soc.*, 1964, **86**, 3395.
(−)-Iberin as a thiourea (also establishes all naturally derived sulphoxide mustard oils)	(+)-*R*-Phenylethylamine	K. K. Cheung, A. Kjaer, and G. A. Sim, *Chem. Comm.*, 1965, 100.
Cycloalliin hydrochloride monohydrate	L-Amino acid (from a natural source)	K. J. Palmer and K. S. Leed, *Acta Cryst.*, 1966, 20, 790.
Monotropein as Rb salt	D-Glucose unit	N. Masaki, M. Hirabayashi, K. Fuji, K. Osaki, and H. Inouye, *Tetrahedron Letters*, 1967, 2367.

3. By External Correlation with a Related Compound

1,2-*O*-Aminoisopropylidene-α-D-glucopyranose hydriodide	Derived from D-glucose	J. Trotter and J. K. Fawcett, *Acta Cryst.*, 1966, **21**, 366.
Triol Q as *p*-iodobenzoate	Correlation with rosenonolactone	G. Ferguson, J. W. B. Fulke, and R. McCrindle, *Chem. Comm.*, 1966, 691.
Bromoambrosin	Correlation with analogous compound, parthenin	M. T. Emerson, W. Herz, C. N. Caughlan, and R. W. Witters, *Tetrahedron Letters*, 1966, 6151.

(*Received, January* 17*th*, 1968; *Com.* 064.)