

A Reference List of Organic Structures whose Absolute Configurations have been determined by X-Ray Methods. Part 3.

By F. H. ALLEN, S. NEIDLE, and D. ROGERS*

(*Chemical Crystallography Laboratory, Imperial College, London, S.W.7*)

PARTS 1 and 2 of this list (F. H. Allen and D. Rogers, *Chem. Comm.*, 1966, 838; and F. H. Allen, S. Neidle, and D. Rogers, *Chem. Comm.*, 1968, 308) contained 94 entries. This supplement, believed to be complete to the end of 1968, contains 39 new entries.

1. Using the Anomalous Dispersion Method.

<i>Compound</i>	<i>Fluorescent atom</i>	<i>Radiation used</i>	<i>Reference</i>
(1) <i>Simple compounds and acids</i>			
1,1'-Binaphthyl as (+)-2,2'-dihydroxy-1,1'-binaphthyl-3,3'-dicarboxylic acid dimethyl ester/ bromobenzene adduct	Br	Cu	H. Akimoto, T. Shioiri, Y. Iitaka, and S. Yamada, <i>Tetrahedron Letters</i> , 1968, 97.

Compound	Fluorescent atom	Radiation used	Reference
(2) Terpenoids			
Alisol A as acetonide monobromoacetate	Br	Mo	T. Murata, K. Kamiya, M. Nishikawa, and M. Miyamoto, <i>Tetrahedron Letters</i> , 1968, 103.
Ceroplastol I as 4-bromobenzoate	Br	Cu	Y. Iitaka, I. Watanabe, I. T. Harrison, and S. Harrison, <i>J. Amer. Chem. Soc.</i> , 1968, 90 , 1092.
Chamaecyrenol as 4-bromo-3-nitrobenzoate	Br	Cu	K. Takase, S. Ibe, T. Asao, T. Nozoe, H. Shimanouchi, and Y. Sasada, <i>Chem. and Ind.</i> , 1968, 1638.
Eunicin as iodoacetate	I	Cu(?)	M. B. Hossain, A. F. Nicholas, and D. van der Helm, <i>Chem. Comm.</i> , 1968, 385.
Fenchane as bromo-2-nitro-2-fenchane	Br	Cu	C. Rerat, <i>Compt. rend.</i> , 1968, 266 , C, 612.
β -Gorgonene as AgNO ₃ complex	Ag	Cu	M. B. Hossain and D. van der Helm, <i>J. Amer. Chem. Soc.</i> , 1968, 90 , 6607.
Lumiphorbol as 4-[<i>p</i> -bromobenzoate]	Br	Cu	E. Hecker, E. Härle, H. U. Schairer, P. Jacobi, W. Hoppe, J. Gassmann, M. Röhrli, and H. Abel, <i>Angew. Chem. Internat. Edn.</i> , 1968, 11 , 890.
Neophorbol as 13,20-diacetate 3-[<i>p</i> -bromobenzoate]	Br	Cu	W. Hoppe, F. Brandl, I. Strell, M. Röhrli, J. Gassmann, E. Hecker, H. Bartsch, G. Kreibich, and Ch. von Szczepanski, <i>Angew. Chem. Internat. Edn.</i> , 1967, 6 , 809.
Ophicbolin as methoxybromide	Br	Cu	M. Morisaki, S. Nozoe, and Y. Iitaka, <i>Acta Cryst.</i> , 1968, B24 , 1293.
Platicodigenin as bromolactone	Br	Cu	T. Akiyama, Y. Iitaka, and O. Tanaka, <i>Tetrahedron Letters</i> , 1968, 5577.
(3) Sugar Derivatives			
Methyl 4,6-dichloro-4,6-dideoxy- α -D-glucopyranoside	Cl	Cu	R. Hoge and J. Trotter, <i>J. Chem. Soc. (A)</i> , 1968, 267.
Kanamycin as selenate	Se	Mo	G. Koyama, Y. Iitaka, K. Maeda, and H. Umezawa, <i>Tetrahedron Letters</i> , 1968, 1875.
Kasugamycin as hydrobromide	Br	Cu	T. Ikekawa, H. Umezawa, and Y. Iitaka, <i>J. Antibiotics, Ser. A</i> , 1966, 19 , 49.
Streptomycin as oxime selenate	Se	Cu	S. Neidle, D. Rogers, and M. B. Hursthouse, <i>Tetrahedron Letters</i> , 1968, 4725.
(4) Alkaloids			
Acutumine	Cl	Cu	N. Nishikawa, K. Kamiya, M. Tomita, Y. Okamoto, T. Kikuchi, K. Osaki, Y. Tomiie, I. Nitta, and K. Goto, <i>J. Chem. Soc. (B)</i> , 1968, 652.
Annopodine as hydrobromide	Br	Cu	W. A. Ayer, G. G. Iverach, J. K. Jenkins, and N. Masaki, <i>Tetrahedron Letters</i> , 1968, 4597.
(-)-Aspidospermine as <i>N</i> (b)-methiodide	I	Cu	B. M. Craven and D. E. Zacharias, <i>Experientia</i> , 1968, 24 , 770.
Camptothecin as iodoacetate	I	Cu	A. T. McPhail and G. A. Sim, <i>J. Chem. Soc. (B)</i> , 1968, 923.
Coclaurine as hydrobromide monohydrate	Br	Cu	J. Fridrichsons and A. McL. Mathieson, <i>Tetrahedron</i> , 1968, 24 , 5785.
4-Demethylhasubanonine as <i>p</i> -bromobenzene sulphonate	Br	Cu	S. M. Kupchan, M. I. Suffness, D. N. J. White, A. T. McPhail, and G. A. Sim, <i>J. Org. Chem.</i> , 1968, 33 , 4529.
(-)-Kopsanone	I	Cu	B. M. Craven, B. Gilbert, and L. A. Paes Leine, <i>Chem. Comm.</i> , 1968, 955.
Kreysiginine as methiodide and morphine as hycriodide	I	Cu	J. Fridrichsons, M. F. Mackay, and A. McL. Mathieson, <i>Tetrahedron Letters</i> , 1968, 2887.
Lythridine as methiodide	I	Cu	G. A. Jeffrey, B. Douglas, J. K. Kirkpatrick, and J. A. Weisbach, <i>Chem. and Ind.</i> , 1966, 1795.
Rauvoxinine as methiodide	I	Cu	C. Pascard-Billy, <i>Bull. Soc. chim. France</i> , 1968, 3289.
Schelhammerine as hydrobromide	Br	Co	S. R. Johns, C. Kowala, J. A. Lamberton, A. A. Sioumis, and J. A. Wunderlich, <i>Chem. Comm.</i> , 1968, 1102.
Verticinone as methobromide	Br	Cu	S. Ito, Y. Fukazawa, T. Okuda, and Y. Iitaka, <i>Tetrahedron Letters</i> , 1968, 5373.
(5) Steroids			
Fusidic acid as 3- <i>p</i> -bromobenzoate methyl ester	Br	Cu	A. Cooper and D. C. Hodgkin, <i>Tetrahedron</i> , 1968, 24 , 909.
12 α -Eromo-11 β -hydroxy-progesterone	Br	Cu	A. Cooper and D. A. Norton, <i>Acta Cryst.</i> , 1968, B24 , 811.
Testosterone as mercuric acetate	Hg	Cu	A. Cooper, E. M. Gopalakrishna, and D. A. Norton, <i>Acta Cryst.</i> , 1968, B24 , 935.
Withaferin A as <i>p</i> -bromobenzoate monoacetate	Br	Cu	A. T. McPhail and G. A. Sim, <i>J. Chem. Soc. (B)</i> , 1968, 962.

<i>Compound</i>	<i>Fluorescent atom</i>	<i>Radiation used</i>	<i>Reference</i>
(6) Mould Metabolites			
Acetylaranotin as bisdethiodi(methylthio) derivative	S	Cu	J. W. Moncrief, <i>J. Amer. Chem. Soc.</i> , 1968, 90 , 6517 (and see the two ensuing papers).
Bostrycin as <i>p</i> -bromobenzoate	Br	Cu	A. Takenake, A. Furusaki, T. Wanatabé, T. Noda, T. Take, T. Wanatabe, and J. Abe, <i>Tetrahedron Letters</i> , 1968, 6091.
Crotopoxide as iodohydrin	I	Cu	S. M. Kupchan, R. J. Hemingway, P. Coggon, A. T. McPhail, and G. A. Sim, <i>J. Amer. Chem. Soc.</i> , 1968, 90 , 2982.
Monobromoduclauxin	Br	Cu	Y. Ogihara, Y. Iitaka, and S. Shibata, <i>Acta Cryst.</i> , 1968, B24 , 1037.
Pederin as di- <i>p</i> -bromobenzoate]	Br	Cu	A. Furusaki, T. Wanatabé, T. Matsumoto, and M. Yanagiya, <i>Tetrahedron Letters</i> , 1968, 6301.
(+)-Rugulosin as (+)-dibromo-dehydro-tetrahydrorugulosin	Br	Cu	N. Kobayashi, Y. Iitaka, U. Sankawa, Y. Ogihara, and S. Shibata, <i>Tetrahedron Letters</i> , 1968, 6135.
Viomycin as dihydrobromide	Br	Cu	B. W. Bycroft, D. Cameron, L. R. Croft, A. W. Johnson, T. Webb, and P. Coggon, <i>Tetrahedron Letters</i> , 1968, 2925.
2. By Internal Comparison with a Reference Centre			
Caldariomycin as bis[(+)-3-bromocamphor-9-sulphonate]	(+)-Bromocamphor		S. M. Johnson, I. C. Paul, K. L. Rinehart, jun., and R. Srinivasan, <i>J. Amer. Chem. Soc.</i> , 1968, 90 , 136.
3. By External Correlation with a Related Compound			
Labdanolic acid		Sclareol	K. Bjåmer, G. Ferguson, and R. D. Melville, <i>Acta Cryst.</i> , 1968, B24 , 855.

(Received, March 7th, 1969, Com. 325.)