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Structure of (*R*,*S*)-4-Methoxydalbergione,* $C_{16}H_{14}O_3$

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Abstract. $M_r = 254{\cdot}29$, monoclinic, $P2_1/n$, $a = 6{\cdot}701\,(1)$, $b = 38{\cdot}826\,(1)$, $c = 5{\cdot}365\,(1)$ Å, $\beta = 109{\cdot}56\,(1)^\circ$, $V = 1315{\cdot}3\,(6)$ Å^3, $Z = 4$, $D_x = 1{\cdot}284$ Mg m^{-3}, Cu $K\alpha$ radiation, $\lambda = 1{\cdot}5418$ Å, $T = 296$ K, $F(000) = 536$, $\mu = 0{\cdot}728$ mm^{-1}, final $R = 0{\cdot}053$ for 1449 observed reflections. The quinone ring is almost planar with a maximum out-of-plane deviation of $-0{\cdot}031\,(3)$ Å for C(2). The average dimensions of the C_{sp^3}—C_{sp^2} distances and corresponding angles are 1·508 (4) Å and 112·5 (3)°; those for the quinone ring are C—C = 1·477 (4), C=C = 1·333 (4), C=O = 1·220 (4) Å, C—C—C = 118·2 (3), C=C—C = 120·9 (3) and O=C—C = 121·0 (3)°. The methylene distance is 1·279 (5) Å. The structure consists of discrete molecules; the shortest O···O and C···O contacts are 3·28 (1) and 3·41 (1) Å respectively.

Introduction. The group of dalbergiones as naturally occurring compounds in South American commercial timbers (*Dalbergia* sp.) has been discovered and their structures elucidated by spectroscopic methods. They represent a new class of 4-arylchroman-type quinones for which the name neoflavanoids has been suggested (Eyton, Ollis, Sutherland, Gottlieb, Taveira Magalhães & Jackman, 1965).

Cases of contact dermatitis due to Brazilian rosewood (*Dalbergia nigra* All.) have been reported since 1922 and to African blackwood (*Dalbergia melanoxylon* Guill. & Perr.) since 1924; important cases are summarized in the manual *Woods Injurious to Human Health* (Hausen, 1981). The sensitizing power of the dalbergiones from *Dalbergia* species has been established by Schulz, Garbe, Hausen & Simatupang (1979) and the following sequence of diminishing allergenic potency has been revealed: (*R*)-3,4-dimethoxydalbergione (*R*-3,4-DMD) > (*R*)-

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* IUPAC name: (*R*,*S*)-2-methoxy-5-(1-phenylallyl)-1,4-benzoquinone.

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and (*S*)-4-methoxydalbergione (*R,S*-4-MD) > (*S*)-4,4′-dimethoxydalbergione (*S*-4,4′-DMD) > (*S*)-4-hydroxy-4-methoxydalbergione. X-ray structure analysis has been performed for *R,S*-4-MD, *R*-3,4-DMD and *S*-4,4′-DMD in order to discover the relations between the conformations of their allergenic functional groups. With respect to their different sensitizing capacities the chemical correlations of *R,S*-4-MD, *R*-3,4-DMD and *S*-4,4′-DMD have been compared with other related naturally occurring allergenic benzoquinones (Schmalle, Jarchow, Hausen & Schulz, 1983*a,b*). Structural details of *R,S*-4-MD are presented in this paper as part I of a series on the X-ray structures of dalbergiones.

Experimental. Natural *R,S*-4-MD from *Dalbergia nigra* All., separated by thin-layer-chromatography, yellow needle-shaped single crystals grown by slow evaporation of a methanol solution. Space-group determination from Weissenberg photographs. Crystal 0·18 × 0·18 × 0·46 mm. Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Cu *Kα* radiation. Cell dimensions from least-squares refinement of 25 reflections in the interval $13° < \theta < 32°$. Max. $\sin\theta/\lambda = 0\cdot531$ Å^{-1}, θ–2θ scan method, variable scan rate 0·22° to 20·0° min^{-1}, $0 \leq h \leq 7$, $-41 \leq k \leq 41$, $-5 \leq l \leq 5$. 3595 reflections measured. Two standard reflections checked every hour, no loss of intensity. Orientation controlled every 300 reflections using four standard reflections. Data reduction with the program of the CAD-4 structure determination package. Lorentz–polarization correction, no absorption correction. $R_{\rm int} = 0\cdot019$, 1659 unique reflections, 1449 with $I > 3\sigma(I)$, 210 unobserved. Structure solved by direct methods with *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980). Anisotropic full-matrix least-squares refinement based on F_{hkl}. All H-atom positions from difference Fourier synthesis, refined with fixed isotropic temperature parameters ($B = 2\cdot4$ Å^2). Number of reflections in final refinement cycle, $m = 1449$; parameters refined, $n = 214$; unit weight, $R = 0\cdot053$. $(\Delta/\sigma)_{\rm max} = 0\cdot24$ in final refinement cycle. Max. and min. heights in final difference Fourier synthesis 0·17 and −0·27 e Å^{-3}. Additional computer programs: *SHELX* (Sheldrick, 1976), *XANADU* (Roberts & Sheldrick, 1975), *ORTEP* (Johnson, 1971), *ORFFE* (Busing, Martin, Levy, Brown, Johnson & Thiessen, 1971).

Table 1. *Final atomic coordinates and* $B_{\rm eq}$ *values for R,S-4-MD with e.s.d.'s in parentheses*

$B_{\rm eq}$ values are given in the form $4[(b_{11}/a^{*2})\,(b_{22}/b^{*2})\,(b_{33}/c^{*2})]^{1/3}$. The H atoms are identified by the number of the attached C atom. $B_{\rm iso} = 2\cdot4$ Å^2 for all H.

	x	*y*	*z*	$B_{\rm eq}$(Å^2)
O(1)	1·1406 (4)	0·0988 (1)	0·1264 (5)	4·9 (1)
O(2)	1·0267 (3)	0·0275 (1)	0·7797 (4)	3·6 (1)
O(3)	0·6345 (4)	0·0492 (1)	0·6123 (5)	4·9 (1)
C(1)	0·8070 (4)	0·1023 (1)	0·1835 (6)	2·8 (1)
C(2)	1·0285 (5)	0·0888 (1)	0·2511 (6)	3·1 (2)
C(3)	1·1046 (5)	0·0636 (1)	0·4609 (6)	3·0 (2)
C(4)	0·9787 (4)	0·0508 (1)	0·5849 (6)	2·8 (2)
C(5)	0·7521 (5)	0·0619 (1)	0·5074 (6)	3·1 (2)
C(6)	0·6812 (5)	0·0886 (1)	0·3038 (6)	3·0 (2)
C(7)	0·7459 (5)	0·1315 (1)	−0·0137 (6)	3·2 (2)
C(8)	0·8279 (5)	0·1650 (1)	0·1261 (6)	3·3 (2)
C(9)	0·9933 (7)	0·1821 (1)	0·0852 (9)	5·1 (3)
C(10)	1·0658 (9)	0·2126 (2)	0·218 (2)	7·4 (4)
C(11)	0·977 (1)	0·2263 (1)	0·386 (1)	6·9 (4)
C(12)	0·819 (1)	0·2091 (1)	0·429 (1)	6·7 (3)
C(13)	0·7428 (8)	0·1788 (1)	0·3033 (8)	5·1 (3)
C(14)	0·5147 (5)	0·1312 (1)	−0·1765 (7)	4·0 (1)
C(15)	0·3909 (7)	0·1569 (1)	−0·2604 (9)	5·2 (3)
C(16)	1·2459 (6)	0·0172 (1)	0·8865 (9)	4·1 (2)
H(3)	1·241 (5)	0·057 (1)	0·502 (5)	
H(6)	0·549 (5)	0·096 (1)	0·268 (5)	
H(7)	0·820 (4)	0·127 (1)	−0·133 (5)	
H(9)	1·049 (5)	0·173 (1)	−0·021 (6)	
H(10)	1·167 (5)	0·220 (1)	0·176 (6)	
H(11)	1·029 (4)	0·246 (1)	0·471 (5)	
H(12)	0·756 (4)	0·216 (1)	0·543 (6)	
H(13)	0·636 (5)	0·168 (1)	0·330 (6)	
H(14)	0·459 (4)	0·109 (1)	−0·231 (5)	
H(151)	0·245 (5)	0·153 (1)	−0·375 (5)	
H(152)	0·439 (5)	0·178 (1)	−0·206 (6)	
H(161)	1·249 (4)	0·001 (1)	1·007 (6)	
H(162)	1·327 (4)	0·037 (1)	0·958 (5)	
H(163)	1·289 (4)	0·007 (1)	0·736 (6)	

Table 2. *Bond lengths* (Å) *and angles* (°) *of R,S-4-MD to complete Fig.* 1

E.s.d.'s are given in parentheses.

C(7)–C(14)	1·502 (4)	C(1)–C(7)–C(14)	112·7 (3)
C(7)–C(8)	1·510 (4)	C(1)–C(7)–C(8)	109·3 (2)
C(8)–C(9)	1·371 (5)	C(8)–C(7)–C(14)	115·4 (3)
C(9)–C(10)	1·384 (8)	C(7)–C(8)–C(9)	121·1 (3)
C(10)–C(11)	1·343 (9)	C(7)–C(8)–C(13)	121·0 (3)
C(11)–C(12)	1·340 (9)	C(9)–C(8)–C(13)	117·9 (4)
C(12)–C(13)	1·367 (7)	C(8)–C(9)–C(10)	119·7 (5)
C(8)–C(13)	1·371 (5)	C(9)–C(10)–C(11)	121·8 (6)
		C(10)–C(11)–C(12)	118·2 (5)
		C(11)–C(12)–C(13)	122·0 (6)
		C(12)–C(13)–C(8)	120·4 (5)
		C(7)–C(14)–C(15)	128·3 (4)

Discussion. Final atomic parameters are listed in Table 1.* The atom-numbering scheme and some bond distances and angles are shown in the *ORTEP* drawing of Fig. 1. Other bond lengths and angles are given in Table 2. The *ab* projection of the unit cell is shown in Fig. 2. The quinone ring is approximately planar with torsion angles C(1)–C(2)–C(3)–C(4) 3·7 (4), C(2)–C(3)–C(4)–C(5) 0·8 (4) and C(3)–C(4)–C(5)–C(6) −3·7 (4)°. Different C_{sp^2}–C_{sp^2} single-bond lengths and valence angles in quinone rings of *p*-benzoquinones with different ligands were observed for *R,S*-4-MD as well as for *R*-3,4-DMD, *S*-4,4′-DMD and primin (Schmalle, Jarchow, Hausen & Schulz, 1984). The maximum out-of-plane deviation of the quinone ring C(1) to C(6) is −0·031 (3) Å for C(2). Atoms O(1), O(2), O(3), C(7) and C(16) deviate −0·130 (5), 0·050 (4), −0·071 (5), 0·148 (3) and 0·214 (7) Å from this plane. The angle

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* Lists of structure factors, anisotropic thermal parameters of the C and O atoms and, for *R,S*-4-MD, *R*-3,4-DMD and *S*-4,4′-DMD, selected torsion angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39298 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

between the planes of the quinone ring and of the phenyl ring is 100·2 (3)°. Atom C(7) is chiral with configuration *S* in the enantiomer used for the refinement. The configuration *R* in Fig. 1 has been chosen in order to compare the structure with *R*-3,4-DMD, which is the strongest allergen out of the dalbergiones. The *R* and *S* enantiomers of 4-MD reveal the same, albeit weaker, sensitizing potency (Schulz *et al.*, 1979).

Conformational mobility of single-bonded ligands of the hapten (allergen), the flexibility and softness of the receptor protein (surface antigen of the Langerhans cells) and charge distributions are some of the important parameters which have to be taken into account when structure–function relationship is discussed. Furthermore, the size and shape of the allergenic molecule are essential because the variable part of the surface marker (receptor) presents a cleft into which the sensitizer fits like a key into a keyhole. The strongest hapten of a series of chemically related compounds can be described as a master-key in the system of different receptors.

Experimentally, cross-reactions were obtained between different quinones, especially between primin and dalbergiones (Hausen, 1981). In a patient, sensitized with *R*,*S*-4-MD, it has been observed that eliciting of epicutaneous reactions was slightly stronger with the *R* form (Hausen, 1982). Hypothetically, anchorage of strong contact allergens (*e.g.* primin) in the lipid layer of the cell membrane of immuno-competent cells is assumed to occur with the aliphatic side chain. This function is probably adopted in dalbergiones by their phenyl ring. In *R*,*S*-4-MD C(3) and C(6) of the quinonoid ring are available for nucleophilic attack of $-SH$ and $-NH_3$ groups of specific surface markers (receptors) of epidermal Langerhans cells.

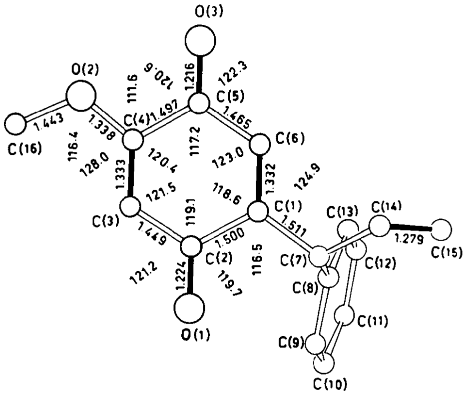

Fig. 1. *ORTEP* drawing of *R*,*S*-4-MD with selected bond distances (Å) and angles (°). The e.s.d.'s range from 0·003 to 0·005 Å for distances and are 0·3° for angles. Blackened bond lines indicate C=C and C=O double bonds.

In the Newman projection C(1)→C(7) only slight differences in the torsion angles (deposited) are observed when the title compound is compared with *R*-3,4-DMD and *S*-4,4′-DMD. On the other hand, rotation of the phenyl ring around the C(7)→C(8) bond axis is clearly recognized by the torsion angles in *R*-4-MD, *R*-3,4-DMD and *S*-4,4′-DMD: C(1)—C(7)—C(8)—C(9) −108·8 (4), −131·8 (1·4) and 119·4 (6)°.

The methylene groups of the dalbergiones do not interact with any C=O carbonyl group, indicating that there are no intramolecular hydrogen bonds in the molecules. The methylene distances are significantly shorter than the mean value of 1·337 (6) Å cited in *International Tables for X-ray Crystallography* (1968): *R*,*S*-4-MD = 1·279 (5), *R*-3,4-DMD = 1·306 (13) and *S*-4,4′-DMD = 1·240 (9) Å. Therefore, the methylene CH_2 group may be considered as a further position for the hapten–protein coupling.

The mean C—H bond distance of the title compound for all H atoms involved is 0·91 (3) Å. Intermolecular distances were calculated up to 3·6 Å with *ORFFE* (Busing *et al.*, 1971). The shortest O···H interactions between neighbouring molecules are found in the **a** direction. Distances for this interaction are $O(3)\cdots C(3^i)$ 3·41 (1), C(3)—H(3) 0·90 (3) and $H(3)\cdots O(3^i)$ 2·52 (3) Å, the intermolecular angle C—H···O being 170 (4)°. This may be a weak C—H···O interaction but, otherwise, the structure consists of discrete molecules.

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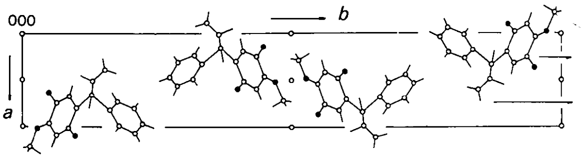

Fig. 2. The *ab* projection of the structure of *R*,*S*-4-MD. Filled circles of the molecular models show O atoms and open circles C atoms.

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Structure of (*R*)-3,4-Dimethoxydalbergione,* $C_{17}H_{16}O_4$

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Abstract. $M_r = 284{\cdot}31$, orthorhombic, $P2_12_12_1$, $a = 7{\cdot}462\,(1)$, $b = 7{\cdot}961\,(1)$, $c = 25{\cdot}254\,(2)$ Å, $V = 1500{\cdot}2\,(5)$ Å^3, $Z = 4$, $D_x = 1{\cdot}259$ Mg m^{-3}, Cu $K\alpha$ radiation, $\lambda = 1{\cdot}5418$ Å, $T = 296$ K, $F(000) = 600$, $\mu = 0{\cdot}745$ mm^{-1}, final $R = 0{\cdot}095$ for 885 observed reflections. The quinone ring is almost planar with a maximum out-of-plane deviation of $-0{\cdot}02\,(1)$ Å for C(3). The average values of the C—C distances and corresponding angles of the chiral atom C(7) are $1{\cdot}51\,(2)$ Å and $112{\cdot}1\,(1{\cdot}3)°$. The mean dimensions of the quinone ring are C—C = $1{\cdot}485\,(11)$, C=C = $1{\cdot}346\,(16)$, C=O = $1{\cdot}206\,(14)$ Å and C—C—C = 118 (1), C=C—C = 121 (1), O=C—C = 121 (1)°. The methylene distance is $1{\cdot}306\,(13)$ Å. The structure consists of discrete molecules.

Introduction. The structure determination of the title compound (*R*-3,4-DMD) was undertaken in order to compare its conformation with those of related dalbergiones causing contact dermatitis (Schmalle, Jarchow, Hausen & Schulz, 1984*b*). *R*-3,4-DMD possesses the highest sensitizing power of all dalbergiones; its chemical structure and absolute configuration have been established by Eyton, Ollis, Fineberg, Gottlieb, Salignac de Souza Guimarães & Taveira Magalhães (1965). The results of an X-ray analysis are given in this paper as part II of a series on dalbergiones.

Experimental. For additional details see part I (Schmalle *et al.*, 1984*b*). *R*-3,4-DMD from the heartwood of Brazilian Pao ferro (*Machaerium scleroxylum* Tul.). Very soft red needle- and plate-shaped crystals, m.p. 314–316 K. Crystal $0{\cdot}49 \times 0{\cdot}37 \times 0{\cdot}09$ mm. Unit cell: 13 reflections in the interval $4° < \theta < 36°$. $(\sin\theta/\lambda)_{\max} = 0{\cdot}531$ Å^{-1}, $-7 \le h \le 0$, $-8 \le k \le 0$, $-26 \le l \le 17$. 1893 reflections measured, $R_{\rm int} = 0{\cdot}076$, 1148 unique reflections, 886 with $I \ge 3\sigma(I)$, 262 unobserved. The crystal changed its quality during the measurement; because of the resulting poor data set the molecule was refined as a fixed model. H-atom positions calculated and their distances fixed at 1·08 Å within an error of 0·015 Å in the full-matrix least-squares refinement. Number of reflections in final refinement cycle, $m = 885$ (002 omitted, because secondary extinction was suspected); parameters refined, $n = 225$; unit weight, $R = 0{\cdot}095$. $(\Delta/\sigma)_{\max} = 1{\cdot}67$ (H-atom positional parameter) in final refinement cycle. Max. and min. heights in final difference Fourier synthesis 0·26 and $-0{\cdot}29$ e Å^{-3}.

Discussion. The atomic parameters of the C and O atoms are listed in Table 1.† The atom-numbering

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* IUPAC name: (*R*)-2,3-dimethoxy-5-(1-phenylallyl)-1,4-benzoquinone.

† Lists of structure factors, anisotropic thermal parameters of the C and O atoms, positional H-atom parameters and some selected torsion angles of the dalbergiones have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39300 (10 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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