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Structure of a Bifunctional Organic Reagent: 2,2′-Bis(dimethylaminomethylene)-2,2′-sulfonyldiacetonitrile

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Abstract. The title compound (I*a*) was prepared as a potential cross-linking reagent for hemoglobin. $C_{10}H_{14}N_4O_2S$, $M_r = 254{\cdot}31$, monoclinic, $P2_1/n$, $a = 14{\cdot}335$ (6), $b = 7{\cdot}614$ (4), $c = 24{\cdot}36$ (1) Å, $\beta = 107{\cdot}54$ (3)°, $V = 2534$ (2) Å^3, $Z = 8$, $D_x = 1{\cdot}33$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 2{\cdot}41$ cm^{-1}, $F(000) = 1072$, $T = 295$ K. Final $R = 0{\cdot}051$ for 2350 observed reflections. There are two independent molecules with different conformations. The bond distances to the central S atom are: S—O = 1·43 (3) and S—C = 1·75 (4) Å. The observed bond lengths O_1—S—C_3—C_4 and O_2—S—C_1—C_2 are compatible with a resonance hybrid structure which has bond delocalization over all atoms between the terminal amino N atoms, giving the molecule an anionic character. The distance between the potential cross-linking sites (5·680 Å) is in the range required.

Introduction. One of our current projects involves chemical modification of cell-free hemoglobins for potential use as substitutes for blood in emergency transfusion. The need for such an alternative is becoming increasingly pressing in view of the scarcity of blood especially when rare types are needed, and the possible transmission of diseases such as AIDS or hepatitis associated with blood transfusion. Our aim is to exploit the abundantly available and the relatively inexpensive human and bovine hemoglobins as an alternative to blood for a cell-free oxygen carrier [for recent advances in this area, see Bolin, Beyer & Nemo (1983)]. To this end, however, two major problems inherent in cell-free hemoglobins need be overcome: first, the retention time of the cell-free hemoglobins is short such that most of the infused hemoglobin is quickly eliminated from the circulating blood and, second, the oxygen-binding affinity for cell-free hemoglobins is too high, thus preventing adequate release of oxygen to the tissues. We intend to overcome these problems by covalently cross linking the hemoglobin subunits–β_1 to β_2 (Fig. 1)–with an anionic organic reagent. In whole blood, these subunits are held together simply through ionic and van der Waals interactions. Covalent cross linking will prevent their dissociation and the consequent rapid elimination by kidneys. Introduction of anionic character in the cross link will reduce their oxygen affinity. The negative charges of 2,3-diphosphoglycerate (DPG) and other polyanionic phosphates which occupy the space between tetrameric structure of hemoglobin (Fig. 1) are known to play a major role in reducing the oxygen affinity of hemoglobins *in vivo*. To this end, the bis-enamine, 2,2′-bis(dimethylaminomethylene)-2,2′-sulfonyldiacetonitrile (I*a*) was deemed a good candidate for a cross-linking agent since it contains the two cross-linking sites (*A* and *A*′) which can exchange the attached dimethylamino functions for the lysine NH_2 present at position 82 in each of the β_1 and β_2 subunits of hemoglobin. These lysine NH_2 groups are in proximity to the DPG pocket and thus are the potential targets for cross linking. The reagent (I*a*) potentially contains considerable anionic character by virtue of major resonance contributions by structures such as (I*b*) as shown. This anionic character would be retained even after formation of the cross link as shown in (II). The reagent (I*a*) was synthesized (Hosmane & Bertha, 1986) commencing from 2,2′-sulfonyldiacetonitrile (McCormick & McElhinney, 1972). The latter compound was treated with excess trimethyl orthoformate, catalyzed by concentrated sulfuric acid to obtain 2,2′-(methoxymethylene)-2,2′-sulfonyldiacetonitrile which, upon treatment with two equivalents of dimethylamine, afforded the required (I*a*). The reagent (I*a*) is a stable colorless crystalline solid (m.p. 461 K) and was characterized by IR, ^{1}H NMR, mass spectrum and microanalytical data. The compound was recrystallized from acetonitrile for X-ray analysis.

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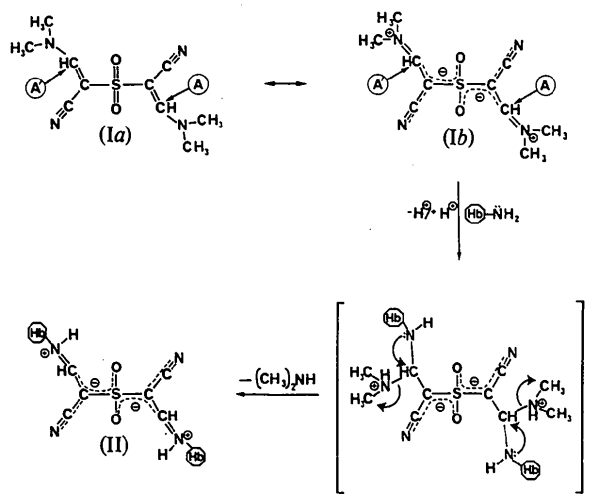

We were specifically interested in exploring the following two questions in (I*a*) through X-ray analysis: (1) Does the reagent, in fact, exist mainly as the mesomeric structure (I*b*) as anticipated? This is a crucial factor in reducing the oxygen affinity of the modified hemoglobins as delineated above. (2) Equally importantly what is the distance between the cross-linking sites *A* and *A'*? Provided the reagent is sufficiently electrophilic to react with the amine nucleophiles of hemoglobin (*i.e.* lysine NH_2 groups), the effectiveness of the cross-linking reagent is dependent upon the length of the cross-linking bridge. If this length is too short or too long, the cross link may not form at all. The estimated average minimum diagonal distance between β_1 and β_2 82 lysines or α_1 and α_2 91 lysines is in the range 5–7 Å depending upon the form, liganded or unliganded, of hemoglobin (Walder, Walder & Arnone, 1980, and references cited therein).

Experimental. Crystals of the title compound are colorless square plates; a single crystal (0·35 × 0·25 × 0·15 mm) was mounted on a goniometer head with an epoxy resin; unit-cell parameters by least-squares fit of 15 reflections in the range $10 < 2\theta < 25°$; space group $P2_1/n$ from systematic absences ($0k0$, k odd, $h0l$, $h+l$ odd); automatic Syntex $P2_1$ diffractometer, graphite-monochromated Mo $K\alpha$ radiation, $\theta/2\theta$ scan mode; 3330 independent reflections in the range $3 < 2\theta < 45°$, hkl range h 14→−15, k 0→8, l 0→25; 2350 observed reflections with $I > 3\sigma(I)$, $\sigma(I)$ from counting statistics; 3 standard reflections remeasured after every 100 reflections did not show any significant change in intensity during data collection; Lorentz–polarization correction, no absorption or extinction corrections, $R_{int} = 0{\cdot}005$. Direct methods, *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), refinement by full-matrix least squares using *SHELX*76 (Sheldrick, 1976), anisotropic; H atoms located in difference Fourier maps, except for H positions of methyls attached to N atoms which were calculated; H atoms included in the refinement with isotropic temperature factors; $w = 1/[\sigma^2(F) + 0{\cdot}011848F^2]$, $\sum w(|F_o| - |F_c|)^2$ minimized, $R = 0{\cdot}051$, $wR = 0{\cdot}059$; $(\Delta/\sigma)_{max} = 0{\cdot}29$, $\Delta\rho_{(max,min)} = 0{\cdot}33$, $-0{\cdot}19$ e Å^{-3} in final difference Fourier map. Atomic scattering factors for C, H, N, O, S, and the real and imaginary parts of the dispersion correction for S were taken from *International Tables for X-ray Crystallography* (1974).

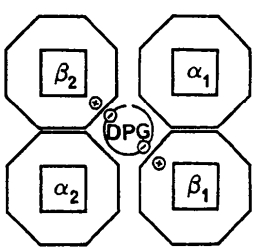

Fig. 1. Hemoglobin subunits and 2,3-diphosphoglycerate (DPG).

Discussion. The final atomic parameters of the non-H atoms are given in Table 1.* The identification of the atoms and the configuration of the title compound are shown in the *ORTEP* (Johnson, 1965) drawing of Fig. 2. Bond lengths, bond angles and selected torsion angles with their standard deviations are given in Table 2. Fig. 3 represents the stereoscopic unit-cell packing arrangement. Although the bond lengths and the bond angles of the two molecules do not differ significantly, a superposition of the two conformers reveals that one half of the dimer is similar, but the other end differs significantly in orientation. As is evident from the tables, the bonds N_1—C_2 and N_2—C_4 in fact show significant double-bond character [1·304 (5) Å], while the bond lengths O_1—S—C_3—C_4 and O_2—S—C_1—C_2 are compatible with the delocalized structure (I*b*) as shown. The diagonal distance *A*–*A'* was calculated from the two sets of fractional coordinates and the unit-cell measurements. The average value of 5·680 Å [$= \frac{1}{2}(5{\cdot}6495 + 5{\cdot}7110)$] was computed, thus indicating that the reagent (I*a*) also meets the requirement of chain length to qualify it for a potential cross linker. Therefore, provided that it meets the third requirement, *i.e.* the criterion of electrophilicity as described in the *Introduction*, the reagent (I*a*) is a potentially good candidate for a cross-linking agent for hemoglobins, and such an endeavor is currently in progress.

* Lists of structure factors and anisotropic temperature factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44015 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Fractional atomic coordinates with equivalent isotropic thermal parameters for non-*H *and isotropic for* H *atoms (e.s.d.'s in parentheses)*

$$U_{eq} = \tfrac{1}{3}\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}†(Å²)
S	0·4932 (1)	0·9487 (1)	0·37757 (4)	0·0456 (2)
O(1)	0·5138 (2)	1·0723 (3)	0·4241 (1)	0·0560 (7)
O(2)	0·5217 (2)	0·9858 (4)	0·3275 (1)	0·0683 (8)
N(1)	0·6185 (2)	0·5956 (4)	0·4961 (1)	0·0465 (7)
N(2)	0·2277 (2)	0·8814 (4)	0·2673 (1)	0·0488 (8)
N(3)	0·5451 (3)	0·5265 (6)	0·3276 (2)	0·0823 (11)
N(4)	0·2953 (3)	0·9264 (6)	0·4376 (2)	0·0778 (12)
C(1)	0·5468 (2)	0·7498 (5)	0·4061 (1)	0·0415 (8)
C(2)	0·5753 (2)	0·7287 (5)	0·4648 (1)	0·0420 (8)
C(3)	0·3667 (3)	0·9172 (5)	0·3539 (2)	0·0455 (9)
C(4)	0·3209 (3)	0·8994 (5)	0·2959 (1)	0·0427 (8)
C(5)	0·5483 (3)	0·6224 (6)	0·3635 (2)	0·0502 (9)
C(6)	0·6361 (3)	0·5961 (7)	0·5588 (2)	0·0588 (11)
C(7)	0·6549 (4)	0·4415 (6)	0·4723 (2)	0·0667 (12)
C(8)	0·3241 (3)	0·9206 (5)	0·3990 (2)	0·0507 (9)
C(9)	0·1502 (3)	0·8756 (8)	0·2951 (2)	0·0786 (16)
C(10)	0·1955 (3)	0·8827 (7)	0·2041 (2)	0·0609 (12)
H(1)	0·560 (2)	0·817 (4)	0·486 (1)	0·030 (8)
H(2)	0·360 (2)	0·903 (4)	0·271 (1)	0·040 (9)
H(3)	0·6723 (3)	0·476 (1)	0·5770 (2)	0·170 (78)
H(4)	0·5671 (3)	0·606 (1)	0·5680 (2)	0·148 (45)
H(5)	0·6828 (3)	0·707 (1)	0·5776 (2)	0·112 (59)
H(6)	0·6885 (4)	0·350 (1)	0·5065 (2)	0·110 (17)
H(7)	0·7091 (4)	0·483 (1)	0·4523 (2)	0·167 (37)
H(8)	0·5948 (4)	0·379 (1)	0·4406 (2)	0·104 (17)
H(9)	0·0802 (3)	0·860 (1)	0·2627 (2)	0·179 (28)
H(10)	0·1505 (3)	0·996 (1)	0·3184 (2)	0·182 (32)
H(11)	0·1627 (3)	0·766 (1)	0·3246 (2)	0·141 (24)
H(12)	0·1170 (3)	0·866 (1)	0·1885 (2)	0·177 (41)
H(13)	0·2303 (3)	0·776 (1)	0·1884 (2)	0·161 (68)
H(14)	0·2153 (3)	1·006 (1)	0·1894 (2)	0·196 (75)
S(')	0·4403 (1)	0·8939 (1)	0·13343 (4)	0·0416 (2)
O(1')	0·4184 (2)	0·8638 (4)	0·1864 (1)	0·0598 (6)
O(2')	0·3736 (2)	1·0009 (3)	0·0907 (1)	0·0552 (7)
(N1')	0·6786 (2)	1·1288 (4)	0·2321 (1)	0·0417 (7)
N(2')	0·3765 (2)	0·5293 (4)	0·0121 (1)	0·0457 (7)
N(3')	0·6219 (3)	1·0243 (6)	0·0655 (2)	0·0833 (11)
N(4')	0·5645 (3)	0·4793 (5)	0·1692 (2)	0·0691 (10)
C(1')	0·5569 (3)	0·9871 (5)	0·1518 (2)	0·0426 (8)
C(2')	0·5966 (2)	1·0450 (4)	0·2075 (2)	0·0393 (8)
C(3')	0·4477 (2)	0·6927 (4)	0·1012 (1)	0·0382 (7)
C(4')	0·3916 (3)	0·6686 (5)	0·0445 (2)	0·0425 (8)
C(5')	0·5941 (3)	1·0101 (5)	0·1045 (2)	0·0495 (9)
C(6')	0·6980 (3)	1·1949 (6)	0·2912 (2)	0·0592 (10)
C(7')	0·7484 (3)	1·1860 (6)	0·2024 (2)	0·0573 (10)
C(8')	0·5107 (3)	0·5709 (5)	0·1376 (2)	0·0457 (8)
C(9')	0·3057 (3)	0·5348 (7)	−0·0458 (2)	0·0653 (12)
C(10')	0·4155 (3)	0·3572 (5)	0·0326 (2)	0·0651 (12)
H(1')	0·559 (2)	1·011 (1)	0·232 (1)	0·042 (48)
H(2')	0·358 (2)	0·768 (5)	0·027 (1)	0·051 (10)
H(3')	0·7681 (3)	1·260 (1)	0·3044 (2)	0·204 (32)
H(4')	0·6982 (3)	1·087 (1)	0·3202 (2)	0·202 (35)
H(5')	0·6411 (3)	1·287 (1)	0·2933 (2)	0·205 (72)
H(6')	0·8093 (3)	1·252 (1)	0·2334 (2)	0·145 (22)
H(7')	0·7132 (3)	1·276 (1)	0·1683 (2)	0·157 (24)
H(8')	0·7756 (3)	1·073 (1)	0·1842 (2)	0·237 (25)
H(9')	0·3031 (3)	0·408 (1)	−0·0661 (2)	0·200 (21)
H(10')	0·3282 (3)	0·633 (1)	−0·0712 (2)	0·268 (48)
H(11')	0·234 (2)	0·567 (4)	−0·043 (1)	0·268 (9)
H(12')	0·3933 (3)	0·263 (1)	−0·0023 (2)	0·193 (20)
H(13')	0·3881 (3)	0·317 (1)	0·0672 (2)	0·212 (35)
H(14')	0·4943 (3)	0·363 (1)	0·0481 (2)	0·098 (16)

† The standard deviations of U_{eq} were calculated according to Schomaker & Marsh (1983).

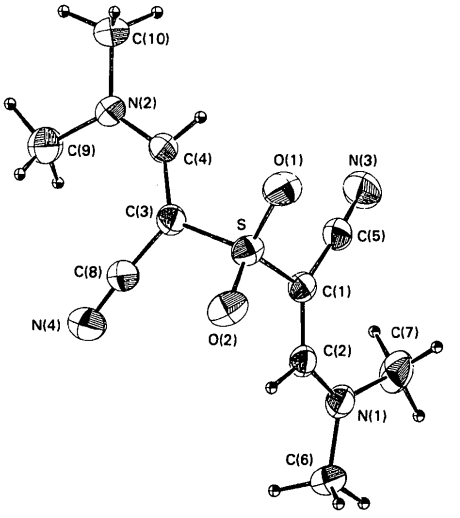

Fig. 2. *ORTEP* drawing of molecule 1. Thermal ellipsoids scaled to enclose 40% probability. H atoms are represented as spheres of arbitrary radii.

Table 2. *Bond lengths* (Å), *bond angles* (°) *and selected torsion angles* (°)

	Molecule 1	Molecule 2		Molecule 1	Molecule 2
S–O(1)	1·433 (3)	1·436 (3)	O(1)–S–O(2)	120·1 (2)	117·6 (2)
S–O(2)	1·427 (3)	1·435 (3)	O(1)–S–C(1)	107·1 (2)	106·6 (2)
S–C(1)	1·745 (3)	1·746 (4)	O(1)–S–C(3)	107·3 (2)	109·0 (2)
S–C(3)	1·746 (4)	1·739 (4)	O(2)–S–C(1)	107·9 (2)	109·4 (2)
N(1)–C(2)	1·307 (4)	1·313 (5)	O(2)–S–C(3)	106·3 (2)	106·8 (2)
N(1)–C(6)	1·471 (6)	1·470 (5)	C(1)–S–C(3)	107·5 (2)	106·9 (2)
N(1)–C(7)	1·472 (6)	1·466 (5)	C(2)–N(1)–C(6)	120·4 (3)	119·5 (3)
N(2)–C(4)	1·315 (5)	1·301 (5)	C(2)–N(1)–C(7)	123·4 (3)	124·7 (3)
N(2)–C(9)	1·466 (6)	1·468 (6)	C(6)–N(1)–C(7)	116·1 (3)	115·2 (3)
N(2)–C(10)	1·468 (6)	1·453 (5)	C(4)–N(2)–C(9)	123·3 (3)	120·0 (3)
N(3)–C(5)	1·130 (6)	1·141 (6)	C(4)–N(2)–C(10)	120·2 (3)	123·4 (3)
N(4)–C(8)	1·136 (6)	1·147 (6)	C(9)–N(2)–C(10)	116·2 (3)	116·0 (3)
C(1)–C(2)	1·373 (4)	1·376 (6)	S–C(1)–C(2)	118·2 (2)	117·6 (3)
C(1)–C(5)	1·425 (6)	1·419 (6)	S–C(1)–C(5)	113·7 (3)	114·0 (2)
C(3)–C(4)	1·374 (6)	1·385 (5)	C(2)–C(1)–C(5)	127·8 (3)	128·1 (3)
C(3)–C(8)	1·409 (6)	1·407 (5)	N(1)–C(2)–C(1)	129·7 (3)	130·8 (4)
			S–C(3)–C(4)	118·7 (3)	118·1 (2)
			S–C(3)–C(8)	113·0 (3)	114·2 (2)
			C(4)–C(3)–C(8)	128·2 (4)	127·7 (3)
			N(2)–C(4)–C(3)	130·5 (4)	130·8 (3)
			N(3)–C(5)–C(1)	176·0 (5)	177·7 (5)
			N(4)–C(8)–C(3)	175·7 (5)	176·2 (5)

	Molecule 1	Molecule 2
S–C(1)–C(2)–N(1)	−178·2 (3)	−175·2 (3)
S–C(1)–C(5)–N(3)	−23 (7)	−22 (12)
S–C(3)–C(4)–N(2)	−177·1 (3)	−173·1 (4)
S–C(3)–C(8)–N(4)	7 (7)	−19 (7)
O(1)–S–C(1)–C(2)	15·5 (3)	−12·2 (4)
O(1)–S–C(1)–C(5)	−169·1 (3)	174·3 (3)
O(1)–S–C(3)–C(4)	141·5 (3)	127·2 (3)
O(1)–S–C(3)–C(8)	−36·1 (4)	−51·8 (3)
O(2)–S–C(1)–C(2)	146·2 (3)	116·0 (3)
O(2)–S–C(1)–C(5)	−38·4 (3)	−57·5 (4)
O(2)–S–C(3)–C(4)	11·8 (4)	−0·9 (3)
O(2)–S–C(3)–C(8)	−165·8 (3)	−179·9 (3)
N(1)–C(2)–C(1)–C(5)	7·1 (6)	−2·8 (8)
N(2)–C(4)–C(3)–C(8)	0·1 (7)	5·7 (8)
N(3)–C(5)–C(1)–C(2)	152 (6)	164 (12)
N(4)–C(8)–C(3)–C(4)	−170 (6)	162 (7)
C(1)–S–C(3)–C(4)	−103·5 (3)	−118·0 (3)
C(1)–S–C(3)–C(8)	78·0 (3)	63·0 (3)
C(1)–C(2)–N(1)–C(6)	−175·5 (4)	172·5 (4)
C(1)–C(2)–N(1)–C(7)	6·5 (6)	1·9 (6)
C(2)–C(1)–S–C(3)	−99·5 (3)	−128·6 (3)
C(3)–S–C(1)–C(5)	75·8 (3)	57·9 (4)
C(3)–C(4)–N(2)–C(9)	−0·5 (6)	174·4 (4)
C(3)–C(4)–N(2)–C(10)	173·7 (4)	3·6 (7)

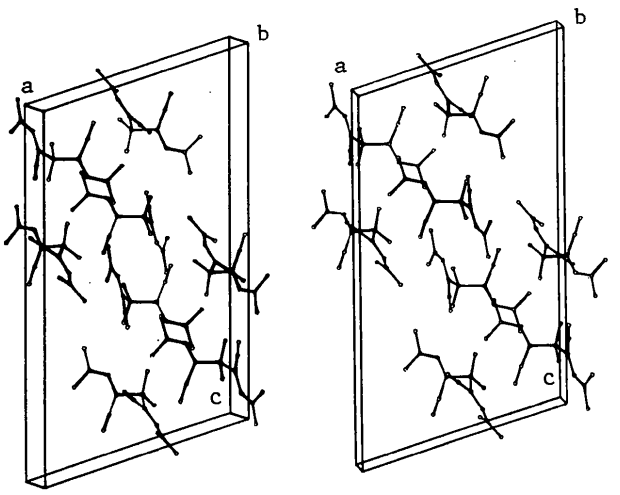

Fig. 3. Stereoscopic drawing of the molecular packing in the unit cell.

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X-ray Structure and Molecular-Packing Analysis of Artemetin

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Abstract. 5-Hydroxy-3,3′,4′,6,7-pentamethoxyflavone (flavone is 2-phenyl-4*H*-1-benzopyran-4-one), $C_{20}H_{20}O_8$, $M_r = 388{\cdot}4$, monoclinic, $P2_1/n$, $a = 7{\cdot}518$ (4), $b = 13{\cdot}625$ (3), $c = 17{\cdot}766$ (5) Å, $\beta = 98{\cdot}52$ (3)°, $V = 1803$ (1) Å^3, $Z = 4$, $D_x = 1{\cdot}430$ Mg m^{-3}, λ(Mo $K\alpha$) $= 0{\cdot}7107$ Å, $\mu = 0{\cdot}104$ mm^{-1}, $F(000) = 816$, room temperature, final $wR = 0{\cdot}063$ for 1480 observed reflexions. The benzopyran ring and the attached phenyl ring are quasi-planar. Dihedral angles between least-squares planes through each of the two rings are lower than 2°. An intramolecular O—H···O hydrogen bond exists involving hydroxyl and carbonyl groups of the phenyl and pyrone rings. Molecular-packing analysis in the atom–atom approach yields an equilibrium configuration in very good agreement with the experimental one.

Introduction. The genus *Artemisia,* which comprises several morphologically different sections, has received considerable attention from the point of view of sesquiterpene lactone content but flavonoid compounds are another important class of secondary metabolites frequently isolated from *Artemisia.*

Some sesquiterpene lactones of the guaiane type were isolated (González, Bermejo, de la Rosa & Martínez-Massanet, 1976) from *A. lanata* Willd, a perennial plant found in the calcareous hills in the south-east and east of the Iberian Peninsula. The crystal structure of one of these compounds was recently reported (Estrada, Conde, Márquez & Jiménez-Garay, 1986). Continuing the phytochemical investigation of the above species, the presence of several flavonoids was revealed (Esteban, González Collado, Macías, Martínez-Massanet & Rodríguez Luis, 1986). Artemetin (I) is one of the three flavonoids isolated from the ethanolic extract of the aerial part of the plant and the X-ray structure determination was suggested to characterize unambiguously its chemical details and path reactions.

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