Coordinates and thermal parameters are listed in Tables 1 and 2. A table of structure factors is obtainable.* Average bond lengths and angles are in Fig. 1.

Discussion. This structure was studied to determine the degree of regularity in the environment of the metal atom. Recent work by Bursey & Rogerson (1971) has focused attention on the energy relationship between Rh and the ring atoms. The structure is essentially that of $(C_5H_7O_2)_3Cr$ (Morosin, 1965). The thermal motion of C(*M*11) and C(*M*12) is very much less than that of corresponding atoms in the Cr analog. The mean of Rh–O intraring distances is significantly shorter than the mean Rh–O distance 2·02 Å observed in potassium tris(oxalato)rhodate(III) by Dalzell & Eriks (1971).

* This table has been deposited with the National Lending Library, England, as Supplementary Publication No. SUP 30057. Copies may be obtained through the Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

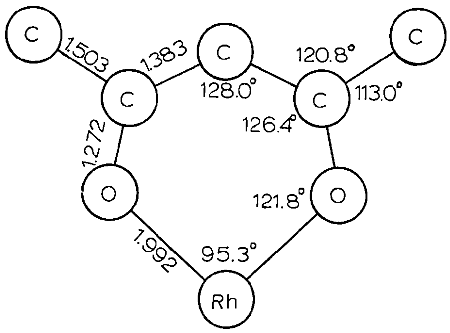

Fig. 1. Mean values of bond lengths and angles for the three rings in $(C_5H_7O_2)_3Rh$. E.s.d.'s are as follows: Rh–O, 0·003; C–O, 0·005; C–C, 0·008 Å; O–Rh–O, 0·1°; other angles, 0·5°.

Table 2. *Final fractional coordinates* ($\times 10^3$) *and assigned thermal parameters for the hydrogen atoms*

The parameter B in the expression $\exp[-B\sin^2\theta/\lambda^2]$ was not varied. Atom H(111) was not resolved in the difference maps.

	x	y	z	B	Bonded to
H(112)	−100 (4)	411 (6)	402 (3)	6·7	C(*M*11)
H(113)	−87 (4)	291 (7)	376 (4)	6·7	C(*M*11)
H(121)	14 (4)	72 (7)	648 (3)	7·4	C(*M*12)
H(122)	116 (4)	56 (7)	694 (3)	7·4	C(*M*12)
H(123)	50 (5)	206 (8)	670 (4)	7·4	C(*M*12)
H(13)	−38 (4)	223 (6)	524 (3)	7·3	C(13)
H(211)	380 (3)	797 (6)	614 (3)	5·8	C(*M*21)
H(212)	275 (3)	764 (6)	621 (3)	5·8	C(*M*21)
H(213)	291 (3)	832 (6)	551 (3)	5·8	C(*M*21)
H(221)	555 (3)	150 (6)	551 (3)	5·9	C(*M*22)
H(222)	589 (3)	311 (6)	590 (3)	5·9	C(*M*22)
H(223)	533 (3)	178 (6)	644 (3)	5·9	C(*M*22)
H(23)	468 (3)	522 (5)	605 (2)	4·4	C(23)
H(311)	374 (3)	466 (6)	253 (3)	5·8	C(*M*31)
H(312)	314 (3)	342 (6)	200 (3)	5·8	C(*M*31)
H(313)	416 (4)	322 (7)	257 (3)	5·8	C(*M*31)
H(321)	138 (3)	−245 (5)	332 (3)	4·9	C(*M*32)
H(322)	207 (4)	−231 (6)	291 (3)	4·9	C(*M*32)
H(323)	234 (3)	−298 (5)	371 (3)	4·9	C(*M*32)
H(33)	287 (3)	28 (5)	252 (2)	4·2	C(33)

We wish to acknowledge financial support for this work from Contract SD-100 with the Advanced Research Projects Agency, through the University program in materials research.

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1-Morpholinomethyl-3-methyl-3-phenylpyrrolidin-2,5-dione

BY GY. ARGAY*

Eduard-Zintl-Institut, Technische Hochschule Darmstadt, Germany (BRD)

AND J. SERES

Chinoin Factory for Pharmaceutical and Chemical Products, Budapest, Hungary

(*Received* 30 *January* 1973; *accepted* 1 *February* 1973)

Abstract. The structure determination is reported of an efficacious antiepileptic drug [registered under the names 'Perlepsyn' (in Hungary) and 'Morpholep' (Seres, Tardos & Leszkovszki, 1962, Hungarian patent No. 151425)] which crystallizes from ethanol in prismatic needles. Its space group is monoclinic $P2_1/c$ (No. 14), $a=11{\cdot}659$ (10), $b=5{\cdot}795$ (10), $c=22{\cdot}861$ (10) Å, $\beta=100{\cdot}75$ (5)°, (from oscillation and Weissenberg photographs and refined on a diffractometer), $Z=4$, $D_c=1{\cdot}269$, $D_x=1{\cdot}258$ g cm^{-3} (by flotation). The

* Permanent address: Central Research Institute for Chemistry of the Hungarian Academy of Sciences, 1525-Budapest, PF. 17, Hungary.

succinimide ring is even less planar than in other succinimide derivatives investigated.

Introduction. 2474 independent reflexions were collected from layers $h0l$ to $h5l$ on a Stoe–Güttinger automatic Weissenberg goniometer, using monochromated Cu $K\alpha$ ($\lambda = 1{\cdot}5418$ Å) radiation, of which only 1653 F_o were found to be greater than $3{\cdot}0 \times \sigma(F_o)$. This phenomenon can be explained by the rather small size of the crystal used for the measurements. No absorption correction was necessary. 283 reflexions with $E > 1{\cdot}5$ were used in a sign determination process using the program written by Long (1965). The origin was fixed by the reflexions $74\bar{9}$, 315 and $41\bar{1}$ with E values 3·03, 2·45 and 2·74, respectively. A set with a consistency index of 0·85 (for other combinations it was less than 0·63) gave an E map which revealed the positions of all 21 non-hydrogen atoms unambiguously. The coordinates of all non-hydrogen atoms with a $\bar{B}$ value of 4·0 Å^2 resulted in a residual of 0·35 for all reflexions.

Full-matrix least-squares refinement of the fractional atomic coordinates with anisotropic vibrational parameters for the heavy atoms and isotropic ones for hydrogen was carried out by the program *ORFLS* written by Busing, Martin & Levy (1962). In order to shorten the computing time, the part of *ORFLS* for the matrix set-up was rewritten in assembler language (TAS) by Dr E. Carstensen-Oeser and a modification to calculate more than one cycle of refinement with the same matrix was inserted since it is known (Stout & Jensen, 1968) that the formation of the matrix of re-

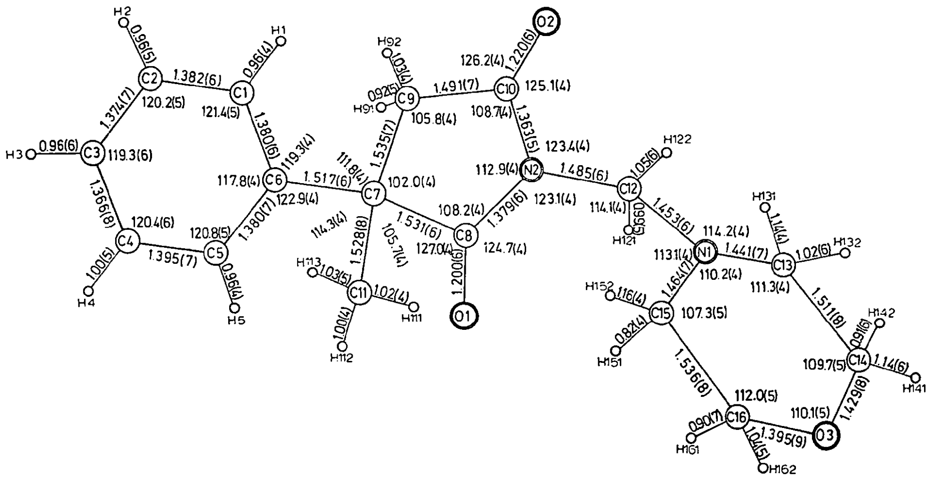

Fig. 1. Bond distances and angles with their e.s.d.'s.

Table 1. *Final atomic coordinates and vibration parameters*

(*a*) Atomic coordinates and anisotropic vibration parameters for Perlepsyn. The b_{ij} are defined by $T = \exp\left[-10^{-4}(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + 2b_{12}hk + 2b_{13}hl + 2b_{23}kl)\right]$. The e.s.d.'s are in parentheses and refer to the least significant digits.

	x/a	y/b	z/c	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
C(1)	0·2287 (4)	0·5087 (8)	0·2995 (2)	64 (4)	200 (63)	22 (1)	3 (7)	11 (2)	12 (4)
C(2)	0·1278 (5)	0·6344 (8)	0·2806 (2)	76 (5)	267 (62)	28 (1)	6 (8)	2 (2)	33 (5)
C(3)	0·0348 (5)	0·6120 (9)	0·3093 (3)	59 (5)	274 (61)	35 (2)	28 (9)	−2 (2)	−9 (5)
C(4)	0·0434 (5)	0·4657 (9)	0·3567 (3)	70 (5)	309 (62)	32 (2)	15 (8)	17 (2)	−17 (5)
C(5)	0·1459 (4)	0·3413 (8)	0·3762 (2)	80 (5)	263 (61)	22 (1)	15 (8)	13 (2)	6 (4)
C(6)	0·2403 (3)	0·3637 (6)	0·3481 (2)	55 (4)	127 (60)	18 (1)	−3 (6)	9 (2)	−1 (3)
C(7)	0·3528 (4)	0·2293 (6)	0·3668 (2)	70 (4)	61 (61)	18 (1)	13 (6)	10 (2)	3 (3)
C(8)	0·4601 (4)	0·3861 (7)	0·3736 (2)	73 (4)	93 (60)	15 (1)	23 (7)	−1 (2)	2 (3)
C(9)	0·3744 (4)	0·0613 (9)	0·3181 (3)	67 (5)	189 (61)	29 (1)	8 (8)	10 (2)	−23 (5)
C(10)	0·4985 (4)	0·0959 (7)	0·3124 (2)	68 (4)	186 (61)	14 (1)	35 (7)	1 (2)	−10 (3)
C(11)	0·3624 (6)	0·1033 (11)	0·4262 (3)	113 (7)	357 (56)	30 (2)	75 (11)	21 (3)	49 (6)
C(12)	0·6606 (4)	0·3764 (9)	0·3476 (2)	63 (5)	192 (61)	20 (1)	−7 (7)	6 (2)	24 (4)
C(13)	0·7690 (4)	0·0352 (9)	0·3875 (2)	68 (5)	257 (62)	21 (1)	40 (8)	3 (2)	12 (4)
C(14)	0·8726 (5)	−0·0485 (12)	0·4324 (3)	73 (5)	404 (61)	29 (2)	41 (10)	4 (2)	26 (5)
C(15)	0·7337 (5)	0·3324 (10)	0·4539 (2)	81 (5)	288 (59)	19 (1)	−15 (9)	2 (2)	−12 (4)
C(16)	0·8410 (5)	0·2414 (12)	0·4972 (3)	94 (6)	469 (67)	20 (2)	−58 (11)	−6 (3)	17 (6)
N(1)	0·7509 (3)	0·2793 (6)	0·3935 (2)	51 (3)	255 (61)	18 (1)	5 (5)	0 (1)	16 (3)
N(2)	0·5424 (3)	0·2795 (5)	0·3467 (1)	52 (3)	163 (60)	14 (1)	7 (5)	5 (1)	−7 (3)
O(1)	0·4747 (3)	0·5654 (5)	0·4002 (1)	89 (3)	212 (60)	30 (1)	28 (5)	−1 (1)	−41 (3)
O(2)	0·5531 (3)	−0·0204 (5)	0·2825 (1)	91 (3)	357 (60)	23 (1)	35 (5)	11 (1)	−44 (3)
O(3)	0·8555 (3)	0·0041 (7)	0·4912 (2)	75 (3)	443 (61)	26 (1)	3 (6)	−3 (1)	46 (3)

Table 1 (*cont.*)

(*b*) Coordinates and isotropic vibration parameters of the hydrogen atoms

	x/a	y/b	z/c	B
H(1)	0·293 (3)	0·502 (6)	0·279 (2)	0·3 (9)
H(2)	0·124 (4)	0·727 (7)	0·246 (2)	2·1 (11)
H(3)	−0·035 (5)	0·703 (10)	0·298 (2)	3·9 (16)
H(4)	−0·023 (4)	0·461 (8)	0·379 (2)	2·7 (12)
H(5)	0·152 (3)	0·249 (7)	0·411 (2)	1·0 (10)
H(91)	0·364 (4)	−0·034 (8)	0·332 (2)	3·4 (13)
H(92)	0·323 (4)	0·113 (6)	0·278 (2)	2·0 (10)
H(111)	0·437 (4)	0·011 (7)	0·439 (2)	1·8 (11)
H(112)	0·361 (3)	0·222 (7)	0·458 (2)	1·6 (10)
H(113)	0·295 (4)	−0·014 (7)	0·421 (2)	3·8 (12)
H(121)	0·656 (4)	0·542 (8)	0·358 (2)	2·8 (12)
H(122)	0·681 (5)	0·367 (8)	0·305 (3)	5·1 (15)
H(131)	0·695 (4)	−0·081 (7)	0·395 (2)	1·5 (9)
H(132)	0·783 (5)	−0·020 (10)	0·347 (3)	6·0 (17)
H(141)	0·945 (5)	0·031 (9)	0·429 (2)	4·9 (15)
H(142)	0·894 (5)	−0·198 (11)	0·430 (3)	7·2 (20)
H(151)	0·724 (4)	0·468 (7)	0·461 (2)	1·5 (12)
H(152)	0·657 (4)	0·220 (7)	0·463 (2)	1·7 (9)
H(161)	0·832 (5)	0·239 (12)	0·535 (3)	4·7 (21)
H(162)	0·910 (4)	0·349 (7)	0·492 (2)	3·4 (11)

finement requires the most time. The hydrogen positions were generated by the *BONDLA* program of *X-RAY*-63 (1964). The agreement index R for the final positional and vibrational parameters [Table 1(*a*) and (*b*)] was 0·062 for the 1653 observed reflexions. Inclusion of the reflexions affected by extinction and the 821 unobserved reflexions gave an R value of 0·112. A table of structure factors is available.*

At this stage the average shift of the coordinates was about $0{\cdot}1 \times \sigma$. All calculations were performed on a TR-440 computer in the German Computer Centre at Darmstadt, using atomic scattering factors taken from *International Tables for X-ray Crystallography* (1962).

* This table has been deposited with the National Lending Library, England, as Supplementary Publication No. SUP 30070. Copies may be obtained through the Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Discussion. The crystal structure of the compound and of some other succinimides (PH–PD[*o*], Argay & Kálmán, 1973; and PHA–PD, Argay & Carstensen-Oeser, 1973) were determined in order to facilitate their chemical and pharmaceutical studies (Seres, 1970). The bond lengths and angles (Fig. 1) in the succinimide ring show good agreement, within experimental error, with those found in the same group of PH–PD–[*o*] and PHA–PD molecules. The succinimide group is, however, less planar here than in succinimide (Mason, 1961) and in the succinimide derivatives mentioned. This is presumably due to the steric effect of the substituents. A similarly distorted succinimide ring was observed by Baudour & Messager (1971) in α-*p*-chlorophenyl-α-methyl-α′-cyanosuccinimide. The phenyl ring is planar within experimental error, and is not distorted as it is in PH–PD[*o*], where the distortion of the phenyl ring was explained by the insufficient number of reflexions in the refinement. (Argay & Kálmán, 1973). The conformation of the *N*-morpholinomethyl group resembles that of *N*-methylmorpholine in benzene (Aroney, Chen, Le Fèvre & Saxby, 1964). They showed, on the basis of dipole moment, electric birefringence, i.r. and n.m.r. measurements of morpholine and *N*-methylmorpholine in various (non-polar) media, that the morpholine ring, like that of cyclohexane, is in the chair configuration with the methyl group linked equatorially (Fig. 2). The geometrical model of *N*-methylmorpholine in the liquid phase, computed by the method of Corey & Sneen (1955), is confirmed by the bond lengths and angles found in crystalline Perlepsyn. The bonds to the nitrogen atom are disposed pyramidally with three nearly identical N(sp^3)–C(sp^3) lengths. Their mean value of 1·453 Å (without thermal correction) is near to the value expected for an N–C single bond (Pauling, 1960). The N(2)–C(12) bond, which is slightly longer

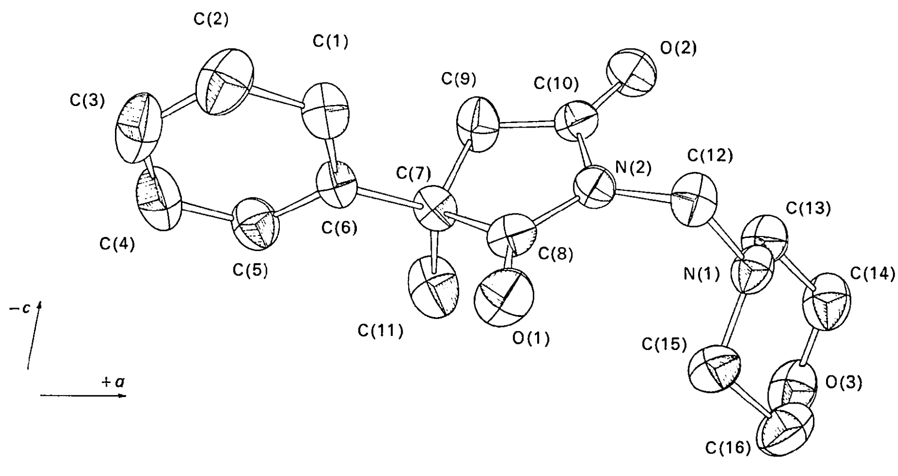

Fig. 2. *ORTEP* diagram.

than the mean of the N(1)–C distances, can be regarded as a weakened N–C single bond. The weakening is due to the effect of the two strong N(sp^2/sp^3)–C(sp^2) multiple bonds in the succinimide group.

The authors thank Professor E. R. Wölfel (Darmstadt) for providing one of them (Gy. A.) with technical and computing facilities and recommending him for a Fellowship granted by the DAAD. Thanks are due to Dr A. Kálmán (Budapest) for stimulating discussions, to Dr E. Carstensen-Oeser (Darmstadt) for help in the computing and to Dr Z. Mészáros, Research Manager of the Chinoin Factory for Pharmaceutical and Chemical Products (Budapest), for his interest.

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N-Méthyl Dipropylacétamide

PAR ANDRÉ GRAND ET CLAUDINE COHEN-ADDAD

Université Scientifique et Médicale de Grenoble, Laboratoire de Spectrométrie Physique, B.P. 53, *Centre de Tri*, 38041 *Grenoble Cedex, France*

(*Reçu le* 15 *décembre* 1972, *accepté le* 16 *janvier* 1973)

Abstract. *N*-Methyldipropylacetamide, $C_9H_{19}NO$, which belongs to a series of pharmaceutical compounds derived from dipropylacetic acid, crystallizes in the orthorhombic space group $Pna2_1$, $a=15{\cdot}498$ (3), $b=14{\cdot}163$ (2), $c=4{\cdot}8505$ (5) Å, $Z=4$. The dipropyl part is planar and fully extended to a total length of 7·568 Å. The molecules are linked by a hydrogen bond N–H···O of length 2·817 Å, which lies approximately along the **c** direction.

Introduction. Ce travail fait partie d'une étude structurale systématique des dérivés de l'acide dipropylacétique présentant des activités pharmacologiques variées (Cohen-Addad, Lajzérowicz, Benoit-Guyod & Boucherle, 1972; Cohen-Addad, 1973).

Ces dérivés sont synthétisés au laboratoire de Chimie et Toxicologie de l'Université de Grenoble par J. L. Benoit-Guyod.

Le *N*-méthyl dipropylacétamide est un anticonvulsi-

Tableau 1. *Coordonnées cristallographiques des atomes lourds et composantes de vibration thermique le long des trois axes principaux en* (Å)

	x	*y*	*z*	**a**	**b**	**c**
C(0)	0,1160 (5)	0,3006 (4)	0,1511 (24)	0,248 (5)	0,343 (7)	0,387 (8)
C(1)	0,1607 (3)	0,2130 (4)	0,0646 (16)	0,258 (4)	0,290 (6)	0,328 (6)
C(2)	0,1161 (3)	0,1233 (3)	0,1686 (14)	0,245 (4)	0,274 (6)	0,288 (6)
C(3)	0,1601 (2)	0·0334 (3)	0·0747 (9)	0·213 (4)	0·234 (4)	0·256 (4)
C(4)	0·1123 (3)	−0,0546 (2)	0,1715 (14)	0,235 (4)	0,261 (4)	0,285 (5)
C(5)	0,1523 (4)	−0,1476 (4)	0,0654 (16)	0,256 (6)	0,316 (6)	0,328 (8)
C(6)	0,1044 (6)	−0,2335 (4)	0,1554 (2)	0,275 (6)	0,355 (8)	0,386 (9)
C(7)	0,2521 (2)	0,0315 (3)	0,1770 (10)	0,192 (5)	0,249 (4)	0,252 (5)
O	0,2689 (2)	0,0316 (3)	0,4271	0,185 (4)	0,283 (3)	0,347 (3)
N	0,3140 (2)	0,0312 (2)	−0,0100 (9)	0,202 (4)	0,228 (3)	0,290 (3)
C(8)	0,4044 (2)	0,0296 (4)	0,0632 (13)	0,230 (4)	0,290 (6)	0,319 (5)