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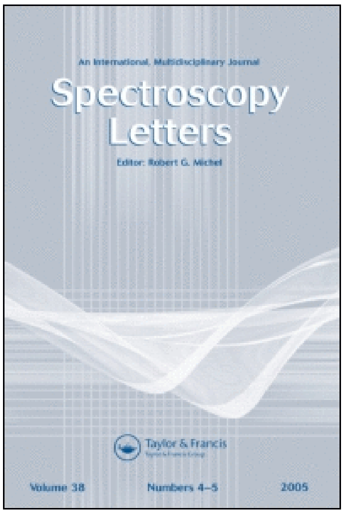

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MOLECULAR STRUCTURE OF HALF-CAGE: X-RAY DIFFRACTION AND SEMIEMPIRICAL CALCULATIONS OF EXO-(±)-1, 8, 9, 10, 11, 11-HEXACHLOROPENTACYCLO [6.2.1.1^{3,6}.0^{2,7}.0^{5,9}]DODECAN-4-ALCOHOL

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MOLECULAR STRUCTURE OF HALF-CAGE: X-RAY DIFFRACTION AND SEMIEMPIRICAL CALCULATIONS OF EXO-(±)-1,8,9,10,11,11-HEXACHLOROPENTACYCLO [6.2.1.1^{3,6}.0^{2,7}.0^{5,9}]DODECAN-4-ALCOHOL

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ABSTRACT

The crystal structure of *exo*-(±)-1,8,9,10,11,11-hexachloropentacyclo-[6.2.1.1^{3,6}.0^{2,7}.0^{5,9}]dodecan-4-alcohol (*half-cage* **1**) was determined by a single crystal X-ray diffraction at 293 K. The crystal parameters of this compound are as follows: triclinic, space group $P\bar{1}$, $a = 8.0709(9)$, $b = 8.3721(9)$, and $c = 11.4812$ (9) Å, $\alpha = 86.571(8)^\circ$, $\beta = 87.360(8)^\circ$, $\gamma = 62.815(10)^\circ$, $R =$ 3.28% and w$R_2 = 8.01\%$. MNDO-PM3, AM1, and MNDO semiempirical methods were performed to establish one comparison

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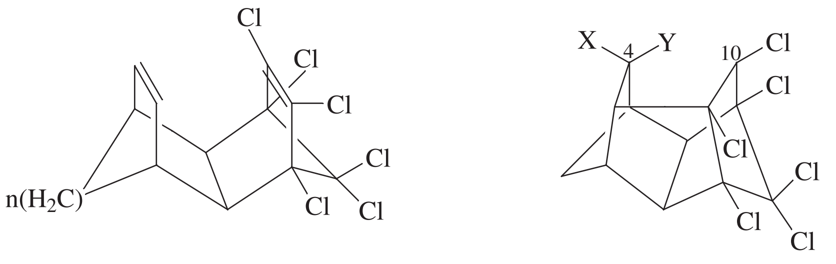
between X-ray and theoretical data in order to verify what theoretical method calculations best reflect the molecular structure.

Key Words: Half-cage; X-ray structure; Semiempirical calculations.

INTRODUCTION

The synthesis of hexachlorinated polycyclic systems, isodrin, endrin insecticides and their derivatives was reported thirty years ago (1). Lipmaa and Pehk (2), using the ^{13}C NMR technique, verified that it is very useful for the elucidation of polycyclic systems. The investigation of dechlorinated polycyclic systems with unique conformations has contributed to the understanding of several aspects of NMR spectroscopy like, steric compression, long-range and short-range interactions (3,4). Our work group has recently demonstrated that the pentacyclo $[6.2.1.1^{3,6}.0^{2,7}.0^{5,9}]$ dodecane derivatives, known as half-cage compounds, are interesting models for the development of methodologies for enantiomeric analysis in NMR spectroscopy, using a mixture of chiral and achiral shift reagents (5); the development of an approach to determine the optimal position of a lanthanide ion in complexes formed by shift reagents and substrate using the pseudocontact model (6).

The *endo-endo* configuration of **isodrin** (n = 1) was confirmed by X-ray diffraction as well as their homologous series (n = 2, and 3), comparative analysis of these structures has shown decreasing across-space between double-bond/double-bond repulsion which is correlated with the observed ease of ciclization in solution. (7) The structure of chlorinated pentacyclic *exo*-benzoate, *half-cage* **1** was determined by low temperature neutron diffraction, and a nonbonded short H–H



Isodrin (n=1)

half-cage **1**: X = OBz; Y=H
half-cage **2**: X = H; Y=OAc

Scheme 1.

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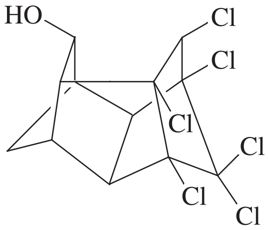

half-cage **3**

Scheme 2.

distance of 1.617 (3) Å was measured between H-10 and H-4 (8). Recently, haxachlorinated pentacyclic isomer *endo* and *exo* acetate or alcohol was obtained from isodrin under proper conditions and separated in highly pure form (9). The X-ray structure of the hexachlorinated pentacyclic *endo*-acetate, *half-cage* **2** showed that it is still more sterically congested than the previously reported to *half-cage* **1** (10).

This paper, presents the X-ray structure of *half-cage* **3** and a comparative study among X-ray structure and semiempirical calculations in order to verify what theoretical method calculations that best reflect the molecular structure.

RESULTS AND DISCUSSION

The bond lengths and bond angles for *half-cage* **3** obtained from X-ray diffraction and MNDO-PM3, AM1, and MNDO calculations are presented in Tables 1 and 2, respectively.

On Table 1, it is possible to observe that MNDO method presents long bond lengths in relation to MNDO-PM3 and AM1 methods, with one unique exception for O(1)-C(4) bond which the order of increase of bond length is MNDO, MNDO-PM3 and AM1. On the other hand, it is not possible to establish what method has longer bond lengths between MNDO-PM3 and AM1 calculations.

The comparison between X-ray and semiempirical methods shows a good correlation over the data for all methods. However, for long bond lengths (Cl–C) the MNDO method has more accuracy than MNDO-PM3 and AM1, excepting Cl(6)–C(11) and Cl(4)–C(10) which MNDO-PM3 presented better approximation. On the other hand, for short bond length (O(1)–C(4)) the AM1 method showed more appropriate value.

For intermediary bond lengths (C–C), AM1, and mainly, MNDO-PM3 methods presented more approximation with X-ray data. Only to C(5)–C(9) bond the MNDO method showed a better response which X-ray data presents a long bond length (1.604 (3) Å).

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Table 1. Selected Bond Lengths Determined by X-Ray Diffraction and Calculated by MNDO-PM3, AM1, and MNDO for *Half-Cage* **3**

	Bond Lenght (Å)			
Atoms	X-Ray	MNDO-PM3	AM1	MNDO
C1(6)–C(11)	1.777(3)	1.774	1.769	1.802
C1(1)–C(1)	1.758(3)	1.726	1.725	1.777
C1(4)–C(10)	1.783(3)	1.769	1.750	1.797
C1(3)–C(9)	1.766(2)	1.744	1.740	1.785
C1(2)–C(8)	1.758(3)	1.717	1.718	1.772
C1(5)–C(11)	1.772(3)	1.737	1.737	1.781
O(1)–C(4)	1.422(3)	1.413	1.424	1.397
C(1)–C(2)	1.578(4)	1.578	1.571	1.602
C(1)–C(10)	1.527(4)	1.537	1.544	1.566
C(1)–C(11)	1.561(4)	1.554	1.581	1.585
C(2)–C(7)	1.579(4)	1.593	1.590	1.601
C(2)–C(3)	1.578(4)	1.567	1.558	1.589
C(3)–C(4)	1.548(4)	1.561	1.563	1.586
C(3)–C(12)	1.539(4)	1.551	1.560	1.565
C(4)–C(5)	1.538(4)	1.560	1.554	1.586
C(5)–C(6)	1.560(4)	1.571	1.571	1.585
C(5)–C(9)	1.605(3)	1.564	1.563	1.596
C(6)–C(7)	1.505(4)	1.524	1.526	1.543
C(6)–C(12)	1.542(4)	1.543	1.548	1.558
C(7)–C(8)	1.498(4)	1.526	1.532	1.549
C(8)–C(9)	1.587(3)	1.580	1.599	1.611
C(9)–C(10)	1.567(3)	1.548	1.558	1.597
C(11)–C(8)	1.540(4)	1.545	1.567	1.576

From these observations above it is possible to suggest that the best semiempirical methods for bond length depends on the size of bond present on the molecular structure.

Differently of bond lengths, the bond angles calculated by semiempirical methods (Table 4) did not present anomalous behavior between themselves. In general, the difference of bond angle between X-ray and semiempirical methods were below 2.5 degrees. Only the angle which involves the oxygen atom presented differences above 3.0 degrees (3.28° (MNDO-PM3), 3.50° (MNDO) for C(3)–C(4)–O(1), and 4.03° (AM1) for C(5)–C(4)–O(1)). In fact, it is not possible to establish what method is more accurate, as all methods give good approximations of the bond angles determined by X-ray.

The crystallographic data and the atomic coordinates including the equivalent isotropic displacement parameters for non-hydrogen atoms of *half-cage* **3** are

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Table 2. Selected Bond Angles Determined by X-Ray Diffraction and Calculated by MNDO-PM3-, AM1, and MNDO for *Half-Cage* **3**

		Bond Angles (Degrees)		
Atoms	X-Ray	MNDO-PM3	AM1	MNDO
C(10)–C(1)–Cl(1)	114.54 (19)	114.19	114.54	113.66
C(10)–C(1)–C(11)	103.1 (2)	100.63	100.82	101.34
C(2)–C(3)–C(12)	98.6 (2)	100.79	100.82	101.04
C(3)–C(4)–O(1)	111.7 (2)	114.78	112.20	115.00
C(5)–C(4)–O(1)	111.2 (2)	108.57	106.57	109.79
C(4)–C(5)–C(9)	112.0 (2)	111.42	111.88	113.08
C(7)–C(6)–C(12)	98.7 (2)	99.18	99.27	99.46
C(6)–C(7)–C(8)	109.8 (2)	107.85	107.68	108.86
C(7)–C(8)–Cl(2)	114.43 (19)	116.85	115.97	114.80
C(7)–C(8)–C(11)	102.2 (2)	99.92	99.95	100.44
C(10)–C(9)–Cl(3)	112.71 (17)	112.41	113.45	113.17
C(5)–C(9)–C(10)	110.5 (2)	112.16	110.83	111.95
C(1)–C(10)–Cl(4)	117.13 (19)	114.75	116.58	117.15
C(1)–C(10)–C(9)	99.4 (2)	100.14	100.85	99.69
C(1)–C(11)–C(8)	93.3 (2)	93.55	93.08	91.94
C(8)–C(11)–Cl(6)	113.3 (2)	113.17	112.94	114.82
C(8)–C(11)–Cl(5)	114.03 (19)	115.16	114.57	116.00

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given in Tables 3 and 4, respectively. An *ZORTEP* (11) drawing of the molecular structure of *half-cage* **3** is shown on Figure 1.

CONCLUSIONS

A comparison between X-ray data with the results obtained from the MNDO-PM3, AM1 and MNDO semi-empirical methods has demonstrated equivalent results for calculating the optimized geometry of *half-cage* polycyclic compounds.

EXPERIMENTAL

Compound

The *half-cage* **3** was synthesized as in the referance (9). Single crystals suitable for crystallographic analysis were obtained by slow evaporation of a solution of *half-cage* **3** in chloroform.

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Table 3. Crystallographic Data for *Half-Cage* **3,** with e.s.d.'s in Parentheses

Formula	$C_{12}H_{10}Cl_6O$
Formula weight	382.90
Temperature (K)	293(2)
Radiation	Mo Kα
Wavelength (Å)	0.71073
Monochromator	Graphite
Crystal System	Triclinic
Space group	$P\bar{1}$
a (Å)	8.0709(9)
b (Å)	8.3721(9)
c (Å)	11.4812(9)
α(°)	86.571(8)
β(°)	87.360(8)
γ(°)	62.815(10)
V(Å^3)	688.70(12)
Z	2
D_{calc} (g cm^{-3})	1.846
Absorption coefficient (mm^{-1})	1.233
F(000)	384
Crystal size (mm)	0.50 × 0.30 × 0.13
Theta range for data collection (°)	2.74 to 25.47
Index ranges	$-9 \leq h \leq 8, -10 \leq k \leq 0, -13 \leq 1 \leq 13$
Reflections collected / unique	2740/2552 [$R_{\text{int}} = 0.0171$]
Criterion for observation	[$I > 2\sigma(I)$]
Absorption correction	Psi-scan
Max. and min. transmission (%)	98.12 and 86.50
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2552 / 0 / 209
Goodness-of-fit on F^2	1.028
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0328$, $wR_2 = 0.0801$
Extinction coefficient	0.0057(16)
Largest difference peak / hole (e.Å^{-3})	0.697 and −0.519

X-Ray Diffraction

A transparent, colorless crystal with a prismatic shape of *half-cage* **3** was mounted on a glass fiber and used for intensity data collection. For data collection the unit cell dimensions and the orientation matrix were obtained from a least square fit of 25 reflections in the range $8.61 \leq \theta \geq 13.67°$ (12). The automatic intensity search and indexing method indicated a cell belonging to the triclinic crystal system with a P lattice. X-ray intensity data were collected on an Enraf-Nonius

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Table 4. Atomic Coordinates (10^4) and Equivalent Isotropic Displacement Parameters ($\text{Å}^2.10^3$) for *Half-Cage* **3**, with e.s.d.'s in Parentheses

	x	y	z	$U_{(eq)}$
Cl(1)	3718(1)	11866(1)	7089(1)	55(1)
Cl(2)	2121(1)	6375(1)	8768(1)	43(1)
Cl(3)	2747(1)	6163(1)	6047(1)	39(1)
Cl(4)	2170(1)	9990(1)	5214(1)	47(1)
Cl(5)	114(1)	10532(1)	7579(1)	45(1)
Cl(6)	2248(1)	10335(1)	9525(1)	60(1)
O(1)	9317(3)	4663(3)	6084(2)	50(1)
C(1)	3967(4)	9675(3)	7333(2)	32(1)
C(2)	5773(4)	8361(4)	8019(2)	33(1)
C(3)	7708(4)	7126(4)	7421(3)	33(1)
C(4)	7568(4)	6120(4)	6372(2)	33(1)
C(5)	6202(4)	5445(3)	6897(2)	29(1)
C(6)	6670(4)	5203(4)	8219(2)	32(1)
C(7)	5201(4)	6959(4)	8659(2)	31(1)
C(8)	3380(4)	7441(4)	8102(2)	29(1)
C(9)	4073(3)	6952(3)	6795(2)	26(1)
C(10)	3969(4)	8745(4)	6229(2)	31(1)
C(11)	2413(4)	9508(4)	8112(2)	35(1)
C(12)	8386(4)	5533(4)	8322(3)	39(1)

U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

CAD4 diffractometer (12) employing the $\omega-2\theta$ scan method with a scan speed of 30 sec/reflection. Every 120 min, the intensity and orientation of three standard reflections ($3\,0\,\bar{3}$, $\bar{4}\,\bar{4}\,\bar{4}$, $0\,\bar{4}\,4$) were measured; the observed intensity decay was less than 0.3% over the data collection. From the Bravais lattice and observed reflections, the space group was chosen to be $P\bar{1}$. Lorentz and polarization correction were made on the intensity data (13); due to the observed linear absorption coefficient of 1.233 mm^{-1} a semi-empirical absorption correction based on psi-scans was performed. The structure was solved using the direct methods employing the *SHELXS97* (14) program and all non-hydrogen atoms were located by subsequent Fourier difference synthesis. For structure refinement the *SHELXL97* (15) program was employed and the full-matrix least-squares minimized on $\sum w(F_o^2 - F_c^2)^2$ where w is a weighting scheme indicated below. All non-hydrogen atoms were refined using anisotropic thermal parameters. All hydrogen atom sites were found experimentally in the Fourier map and refined using isotropic thermal parameters,

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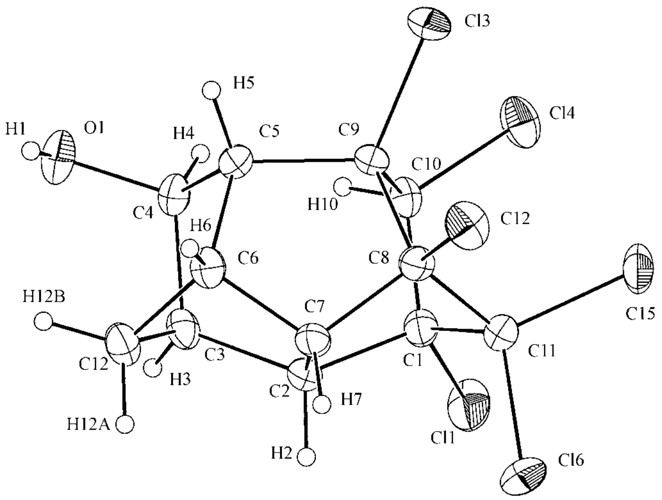

Figure 1. *ZORTEP* (11) plot with atom-labeling scheme of the structure of *half-cage* **3**; displacement ellipsoids at the 30% probability level.

except that of H1 obtained geometrically and its displacement parameters refined isotropically on a groupwise basis. For the final refinement of the structure, an isotropic extinction correction was included. The final refinements including 209 parameters converge to $R = 3.28$ and $R_w = 8.02\%$ with the weighting scheme, $w = 1/[\backslash s^2(Fo^2) + (0.0340P)^2 + 0.7741P]$ where $P = (Fo^2 + 2Fc^2)/3$.

Theoretical Data

The calculations of MNDO-PM3, AM1, and MNDO semiempirical method were performed using the UNICHEM 4.1-MNDO94 program[16], package on GRAY-YMP computer system.

Supplementary Material

Crystallographic data (excluding structure factors) for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-149227. Copies of available material can be obtained, free of charge, on application to the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44-(0)1223-336033 or Email: deposit@ccdc.cam.ac.uk).

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