**INTRODUCTION**

The imide moiety is an integral structural part of various important bioactive molecules such as fumar amidmycin, granulatimide, isogranulatimide and rebeccamycin. These molecules are reported to exhibit antitumor, antiinflammatory and antimicrobial activities. A mixture of exo-7-oxa-bicyclo[2,2,1]hept-5-ene-2,3-dicarboxylic anhydride and its N-substituent compounds have recently become an intense research topic in heterocyclic chemistry because of their antitumor, antivirus, analgesic, sedative and fungicidal activities. In this paper, N-propyl-7-oxa-bicyclo[2,2,1]hept-5-ene-2,3-dicarboximide and its molecular structure was investigated by elemental analysis, FT-IR, $^1$H NMR and X-ray crystallographic techniques.

**EXPERIMENTAL**

All the reagents were of AR grade and used without further purification. IR spectra (4000–400 cm$^{-1}$) as KBr pellets, were recorded on a Nicolet FT-IR 510P spectrometer. $^1$H NMR spectra were measured with a Bruker ALP 80 nuclear magnetic resonance spectrometer (CD$_3$OD as solvent, TMS as internal standard).

**RESULTS and DISCUSSION**

The compound N-propyl-7-oxa-bicyclo[2,2,1]hept-5-ene-2,3-dicarboximide (C$_7$H$_{11}$NO$_2$, M$_r$ = 207.22) was synthesized and characterized by elemental analysis, $^1$H NMR spectra, IR spectra and single crystal X-ray diffraction. The compound belongs to monoclinic, space group P2$_1$/c, with a = 9.7040(10), b = 8.9501(8), c = 15.4719(16) Å, $\beta = 128.845$ (2)$^\circ$, V = 1046.58(18) Å$^3$, Z = 4, D$_c$ = 1.315 g/cm$^3$, $\lambda$$= 0.71073$ Å, $\mu$(MoK$\alpha$) = 0.096 mm$^{-1}$, F(000) = 736. The final refinement gave R = 0.0434, wR(F$^2$) = 0.0998 for 5.254 observed reflections with I > 2$\sigma$(I). The structure of this compound comprises a racemic mixture of chiral molecules containing four stereogenic centers. X-ray diffraction analysis reveals that the cyclohexene ring tends towards a boat conformation, the tetrahydrofuran ring and the dihydrofuran ring adopt envelope conformation. The plan C3/C4/C5/C8 and the plan C5/C6/C7/C8 form dihedral angles of 69.1 (2)$^\circ$ and 64.2 (2)$^\circ$, respectively with the pyrrole ring. The crystal structure is stabilized by C-H...O hydrogen bonds.

**Key Words:** N-propyl-7-oxa-bicyclo[2,2,1]hept-5-ene-2,3-dicarboximide, Synthesis, Structure characterization.
5.254 with 1.853 independent ones (Rint = 0.0434), of which 138 were observed with I > 2σ(I). Intensities were corrected for Lorentz and polarization effects and empirical absorption and all data were corrected using SADABB program.

The structure was solved by direct methods using SHELXS-97 program. All the non-hydrogen atoms were refined on F^2 anisotropically by full-matrix least squares method. All hydrogen atoms were placed in the geometrically calculated positions. The contributions of these hydrogen atoms were included in the structure factor calculations. The atomic scattering factors and anomalous dispersion corrections were taken from international table for X-ray crystallography. The final least-square cycle gave R = 0.0672 and Rint = 0.1169 (w = 1/σ^2(Fo) + 0.0386P^2 + 0.3785P), where, P = (Fo^2 + 2Fc^2)/3. S = 1.066, (Δρ)_{min} = -0.164 and (Δρ)_{max} = 0.177 e/Å^3. CIF file containing complete information on the studied structure was deposited with CCDC, deposition number 825618 and is freely available upon request from the following web site: www.ccdc.cam.ac.uk/data_request/cif.

RESULTS AND DISCUSSION

Furan reacts in a Diels-Alder reaction with maleic anhydride in tetrahydrofuran at room temperature to give exo-7-oxa-bicyclo[2,2,1]hept-5-ene-2,3-dicarboxylic anhydride, as shown in Scheme-I. The condensation reaction between exo-7-oxa-bicyclo[2,2,1]hept-5-ene-2,3-dicarboxylic anhydride and 1-propanamine proceeded smoothly in methanol at room temperature for 5 h and refluxed temperature for 1 h, respectively, leading to the title compound in high yield, as shown in Scheme-II. The elemental analysis, IR spectra and ^1H NMR data clearly indicated the condensation reaction of exo-7-oxabicyclo[2,2,1]hept-5-ene-2,3-dicarboxylic anhydride with 1-propanamine in a ratio of 1:1.

Scheme-I: Synthesis of exo-7-oxa-bicyclo[2,2,1]hept-5-ene-2,3-dicarboxylic anhydride

Scheme-II: Synthesis of the N-propyl-7-oxa-bicyclo[2,2,1]hept-5-ene-2,3-dicarboximide

The selected bond distances and bond angles are listed in Table-1. A displacement ellipsoid plot with atomic numbering scheme is shown in Fig. 1 and a perspective view of the crystal packing in the unit cell is shown in Fig. 2. Hydrogen bond schemes (Å) are listed in Table-2.

The title compound comprises a racemic mixture of chiral molecules containing four stereogenic centres. As seen from

<table>
<thead>
<tr>
<th>Table-1</th>
<th>Selected Bond Lengths (Å) and Bond Angles (°)</th>
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<tbody>
<tr>
<td>Bond</td>
<td>Length (Å)</td>
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<tr>
<td>O(1)-C(1)</td>
<td>1.210(2)</td>
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<tr>
<td>O(2)-C(2)</td>
<td>1.203(2)</td>
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<td>O(3)-C(3)</td>
<td>1.431(3)</td>
</tr>
<tr>
<td>O(3)-C(8)</td>
<td>1.436(3)</td>
</tr>
<tr>
<td>N(1)-C(1)</td>
<td>1.371(3)</td>
</tr>
<tr>
<td>N(1)-C(2)</td>
<td>1.378(3)</td>
</tr>
<tr>
<td>N(1)-C(9)</td>
<td>1.463(3)</td>
</tr>
<tr>
<td>C(6)-C(7)</td>
<td>1.305(3)</td>
</tr>
</tbody>
</table>

Table-2 | Hydrogen Bond Schemes (Å) |
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<tr>
<td>D-H...A</td>
<td>D-H</td>
</tr>
<tr>
<td>C6-H6...O2</td>
<td>0.93</td>
</tr>
<tr>
<td>C7-H7...O1</td>
<td>0.93</td>
</tr>
<tr>
<td>C14-H14...N2</td>
<td>0.98</td>
</tr>
</tbody>
</table>

Symmetry codes: i) x, 1/2-y, 1/2+z; ii) 1-x, 1/2-y, 1/2+z

Fig. 1. Molecular structure with atomic numbering scheme

Fig. 2. View of crystal packing down the a-axis
exo-4-[(4-bromophenyl)amino]-10-oxa-4-azatricyclo(5,2,1,0^2,6^2)dec-8-ene-3,5-dine and 4-(2-aminophenyl)-10-oxa-4-azatricyclo(5,2,1,0^2,6^2)dec-8-ene-3,5-dine. The crystal structure is stabilized by C-H...O intermolecular hydrogen bonds (Fig. 2 and Table-2).

ACKNOWLEDGEMENTS

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REFERENCES