Synthesis of High Energy Density Materials Based on Strained Ring Chemistry

William P. Dailey

University of Pennsylvania
Department of Chemistry
Philadelphia PA 19104-6323

September 1998
Final Report

19990112 075

APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED.

AIR FORCE RESEARCH LABORATORY
AIR FORCE MATERIEL COMMAND
EDWARDS AIR FORCE BASE CA 93524-7048
NOTICE

When U.S. Government drawings, specifications, or other data are used for any purpose other than a definitely related Government procurement operation, the fact that the Government may have formulated, furnished, or in any way supplied the said drawings, specifications, or other data, is not to be regarded by implication or otherwise, or in any way licensing the holder or any other person or corporation, or conveying any rights or permission to manufacture, use or sell any patented invention that may be related thereto.

FOREWORD

This Final Technical Report was prepared by the Department of Chemistry at the University of Pennsylvania, Philadelphia, PA, under Contract F04611-94-K-0056, for the Air Force Research Laboratory (formerly OL-AC Phillips Laboratory), Edwards AFB, CA. The project manager for AFRL/PRSP was Capt Jessica Harper.

Due to a severe cut in the funding that was originally anticipated for this program, it was necessary to abruptly stop work under the contract. No final technical report was required of the contractor due to the lack of funds to pay for the effort. Despite this, the contract's principal investigator provided the following report on his own initiative, wanting to bring closure to the project. Results from the research carried out before the contract schedule modification are described in this report.

This report has been reviewed and is approved for release and distribution in accordance with the distribution statement on the cover and on the SF Form 298.

JESSICA HARPER, CAPT, USAF  
Project Manager

PATRICK G. CARRICK  
Chief, Propellants Branch

PHILIP A. KESSEL  
Technical Advisor  
Propulsion Sciences & Advanced Concepts Division

RANNEY G. ADAMS III  
Public Affairs Director
Synthesis of High Energy Density Materials Based on Strained Ring Chemistry

4. TITLE AND SUBTITLE

5. FUNDING NUMBERS

C: F04611-94-K-0056
PE: 62601F
PR: 3058
TA: RFEU

6. AUTHOR(S)

William P. Dailey

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

University of Pennsylvania
Department of Chemistry
Philadelphia PA 19104-6323

8. PERFORMING ORGANIZATION REPORT NUMBER

AFRL-PR-ED-TR-1998-0008

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/PRSP
10 East Saturn Blvd.
Edwards AFB CA 93524-7680

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

(Air Force Research Laboratory was formerly OL-AC Phillips Laboratory)

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

A

13. ABSTRACT (MAXIMUM 200 WORDS)

Several new cyclopropenes were synthesized and evaluated as new High Energy Density Material (HEDM) candidates. An optimized synthetic route to [1.1.1]propellane was developed and several bicyclo[1.1.1]pentanes were prepared and evaluated as HEDM materials. Preliminary work toward the preparation and study of bicyclo[1.1.1]pentyl carbenes under inert gas matrix isolation conditions was undertaken. Several new prismane derivatives were prepared and their structures determined by X-ray crystallography.

14. SUBJECT TERMS

high energy density materials; strained ring; cyclopropenes; matrix isolation; hydrocarbons; bicyclo[1.1.1]pentanes; [1.1.1]propellane; bicyclo[1.1.1]pentylcarbenes; prismanes

15. NUMBER OF PAGES

18

16. PRICE CODE

SAR

17. SECURITY CLASSIFICATION OF REPORT

Unclassified

18. SECURITY CLASSIFICATION OF THIS PAGE

Unclassified

19. SECURITY CLASSIFICATION OF ABSTRACT

Unclassified

20. LIMITATION OF ABSTRACT

Standard Form 298 (Rev 2-89) Prescribed by ANSI Std 239-18 298-102
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Introduction</td>
<td>1</td>
</tr>
<tr>
<td>Synthesis of Novel Cyclopropenes as Potential HEDM</td>
<td>1</td>
</tr>
<tr>
<td>Synthesis of Bicyclo[1.1.1]pentanes Derived from [1.1.1]propellane</td>
<td>4</td>
</tr>
<tr>
<td>Synthesis and Study of Bicyclo[1.1.1]pentylicarbene</td>
<td>6</td>
</tr>
<tr>
<td>Synthesis of Prismane Derivatives</td>
<td>7</td>
</tr>
<tr>
<td>References</td>
<td>11</td>
</tr>
</tbody>
</table>
LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure No.</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>VT-NMR Experiment</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>Free Energy Coordinate Diagram of Chair Interconversion</td>
<td>3</td>
</tr>
</tbody>
</table>

LIST OF TABLES

<table>
<thead>
<tr>
<th>Table No.</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Comparison of Selected Bond Lengths in 2</td>
<td>4</td>
</tr>
<tr>
<td>2</td>
<td>Comparison of Bond Lengths in 16</td>
<td>9</td>
</tr>
<tr>
<td>3</td>
<td>Experimental and Calculated Bond Lengths in 36</td>
<td>11</td>
</tr>
</tbody>
</table>
GLOSSARY

1H  proton
Ac₂O  acetic anhydride
AcO  acetate
Br₂  bromine
Bu₃SnH  tributyltin hydride
CH₂Br₂  methylene bromide
CH₂Cl₂  methylene chloride
CH₂OH  hydroxymethyl
CH₃  methyl
CH₃Li  methyl lithium
CH₃O  methoxy
CHBr₃  bromoform
CO₂  carbon dioxide
H₂O  water
HCl  hydrogen chloride
HEDM  high energy density materials
HgO  mercuric oxide
hv  light
HNO₃  nitric acid
HO⁻  hydroxide
Iₛₚ  specific impulse
KMnO₄  potassium permanganate
MCSCF  multiconfiguration self-consistent-field
MEK  methyl ethyl ketone
MnO₂  manganese oxide
Ms  methanesulfonyl
MsCl  methanesulfonyl chloride
N₂  dinitrogen
Na/K  sodium/potassium alloy
NaBH₄  sodium borohydride
NaI  sodium iodide
NaIO₄  sodium periodate
NaOH  sodium hydroxide
NCS  N-chlorosuccinimide
NH₂NH₂  hydrazine
NMO  N-morpholine oxide
NMR  nuclear magnetic resonance
ORTEP  Oak Ridge Thermal Ellipsoid Plot
OsO₄  osmium tetroxide
PBr₃  phosphorus tribromide
RO  alkoxy
SOCl₂  thionyl chloride
t-BuLi  tertiary butyl lithium
t-BuOH  tertiary butanol
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Chemical Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>TEBA</td>
<td>tetraethylbenzylammonium chloride</td>
</tr>
<tr>
<td>THF</td>
<td>tetrahydrofuran</td>
</tr>
<tr>
<td>TiCl₄</td>
<td>titanium tetrachloride</td>
</tr>
<tr>
<td>VT</td>
<td>variable temperature</td>
</tr>
<tr>
<td>Zn</td>
<td>zinc</td>
</tr>
<tr>
<td>ΔHf</td>
<td>enthalpy of formation</td>
</tr>
</tbody>
</table>
Introduction

This final technical report covers work from September 1, 1994 to August 31, 1997 that was sponsored under F04611-94-K-0056 through the Air Force Research Laboratory (AFRL) Propulsion Directorate Edwards Site (formerly Operating Location-AC Phillips Laboratory), at Edwards AFB, CA. The objectives of this work were to 1) synthesize and study the properties of strained-ring cyclopropenes for potential application as high energy density materials (HEDM), 2) synthesize and study the properties of bicyclo[1.1.1]pentanes derived from [1.1.1]propellane, and 3) study carbene rearrangements of bicyclo[1.1.1]pentyl carbeneen under matrix isolation conditions. In spite of severe funding cuts in years two and three of the contract all of these objectives were still met. Because of this work, several novel molecules are under development as promising high energy fuels.

This report will be divided into several sections. The first part will concentrate on the synthetic work with cyclopropenes and their potential as high energy density compounds. The second section will focus on efforts in the preparation of bicyclo[1.1.1]pentanes derived from [1.1.1]propellane. The third section will describe the computational and experimental results in the study of bicyclo[1.1.1]pentylcarbeneen. The final section will detail results in the area of prismanes.

Synthesis of Novel Cyclopropenes as Potential HEDM

On a per carbon basis, cyclopropene is one of the most energetic hydrocarbons that can be synthesized and manipulated. Cyclopropene itself has ΔH_f = 66 kcal/mol and a strain energy of 55 kcal/mol. The parent compound and substituted derivatives which have fewer than two substituents on the methylene carbon tend to be unstable. They undergo polymerization via an ene reaction. However, cyclopropenes that have two groups at the methylene carbon can be quite robust. For instance, 3,3-dimethylcyclopropene can be heated to 100°C for extended periods without decomposition. These compounds are being investigated as potential high energy fuels and fuel additives.

Two of the new compounds that were prepared in this study are shown in Schemes 1 and 2.

Two of the new compounds that were prepared in this study are shown in Schemes 1 and 2.

The synthesis of 1 is shown in Scheme 3. The bisdiene was prepared using modifications of literature preparations. Addition of dibromocarbene using phase transfer conditions produced the bis(dibromocyclopropane). Tin hydride reduction followed by base induced elimination produced the biscyclopropene 1 in good overall yield. The compound is a liquid at room temperature and is moderately sensitive to oxygen or Lewis acids.
Scheme 3

A conformational study of 1 was undertaken by dynamic $^1$H nuclear magnetic resonance (NMR). At room temperature the $^1$H NMR for 1 consists of 2 sharp peaks. Upon cooling, each of these peaks broadens and resharpenes into two peaks. At 500 MHz, the coalescence temperature for the methylene protons was -70°C. The spectra are shown in Figure 1.

Figure 1. VT-NMR Experiment
The free energy of activation for the site exchange process in 1 is 8.8 kcal/mol. This can be compared with cyclohexane (10.8 kcal/mol) and 1,1,4,4-tetramethylcyclohexane (11.4 kcal/mol). The transition structure for conversion of the chair form of cyclohexane to give the twist boat form, the half twist chair form, was located using HF/6-31G* calculations. The barrier is calculated to be 12.2 kcal/mol. In a similar manner, the analogous transition structure was calculated for the biscyclopropene 1. The barrier is calculated to be 9.8 kcal/mol, in good agreement with the value derived from dynamic NMR measurements. A diagrammatic representation of this process is shown in Figure 2.

\[
\Delta G^\ddagger = 8.8 \text{ kcal/mole}
\]

Cyclohexane \( \Delta G^\ddagger = 10.8 \text{ kcal/mole} \)

1,1,4,4-Tetramethylcyclohexane \( \Delta G^\ddagger = 11.4 \text{ kcal/mole} \)

**Figure 2. Free Energy Coordinate Diagram of Chair Interconversion**

The caged-ring compound 2 was prepared in a manner similar to that of 1. Investigators found that the precursor diene could be prepared much more easily using the Lombardo reagent than the literature method (3 steps, 52% yield). Dibromocarbene addition followed by reduction and base induced elimination produced the biscyclopropene 2, which was a crystalline solid with mp 44-46°C. This biscyclopropene was much more sensitive to oxygen than compound 1. (See Scheme 4.)
The structure of 2 was confirmed by single crystal X-ray analysis. An ORTEP\(^1\) is shown in Scheme 5. A comparison of the experimental and HF/6-31G* calculated structure is included in Table 1. The agreement is outstanding. The calculated density is 1.26 g/cc.

**Table 1. Comparison of Selected Bond Lengths in 2**

<table>
<thead>
<tr>
<th>Bond</th>
<th>X-ray(Å)</th>
<th>HF/6-31G*</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1-C2</td>
<td>1.554</td>
<td>1.553</td>
</tr>
<tr>
<td>C9-C10</td>
<td>1.567</td>
<td>1.568</td>
</tr>
<tr>
<td>C11-C14</td>
<td>1.505</td>
<td>1.494</td>
</tr>
<tr>
<td>C14-C15</td>
<td>1.273</td>
<td>1.281</td>
</tr>
<tr>
<td>C11-C15</td>
<td>1.488</td>
<td>1.488</td>
</tr>
</tbody>
</table>

![Scheme 5](image)

**Synthesis of Bicyclo[1.1.1]pentanes Derived from [1.1.1]propellane**

A second area of study concerns the conversion of [1.1.1] to stable high energy materials. A number of bicyclo[1.1.1]pentanes are shown in Schemes 6–10, along with their calculated performance values.

\[
\Delta H_f = 83 \text{ kcal/mol} \\
I_{sp} = 316.6 \\
\text{Scheme 6}
\]

\[
\Delta H_f = 51 \text{ kcal/mol} \\
I_{sp} = 313.9 \text{ sec} \\
\text{Scheme 7}
\]

\[
\Delta H_f = 45 \text{ kcal/mol} \\
I_{sp} = 311.2 \\
\text{Scheme 8}
\]

\[
\Delta H_f = 95 \text{ kcal/mol} \\
I_{sp} = 309.9 \\
\text{Scheme 9}
\]

\[
\Delta H_f = 26 \text{ kcal/mol} \\
I_{sp} = 308.0 \\
\text{Scheme 10}
\]
The remarkably direct Szeimies synthesis\textsuperscript{2} of [1.1.1]propellane (3) has allowed the investigation of many reactions of this compound on a preparative scale. The Szeimies method involves addition of dibromocarbene, formed by base induced dehydrobromination of bromoform, to commercially available 3-chloro-2-(chloromethyl)-1-propene (4) followed by methyl lithium induced ring closure of 1,1-dibromo-2,2-bis(chloromethyl)cyclopropane (5). (See Scheme 11.)

\[
\begin{align*}
\text{Cl} & \quad \text{Cl} \quad \text{HCB}_{3} \quad \text{Br} \quad \text{Cl} \quad \text{Br} \quad \text{Cl} \quad \text{CH}_{3}\text{Li} \\
\text{4} & \quad \text{5} & \quad \text{3}
\end{align*}
\]

Scheme 11

While this method is brief, literature yields for the dibromocarbene addition reaction are modest (30\% of recrystallized material), and the work-up is time-consuming due to emulsions. Additionally, 3-chloro-2-(chloromethyl)-1-propene is expensive. Procedures have been developed\textsuperscript{3} that allow the preparation of large quantities of 4 and 5 in good yields.

The synthesis of 3-chloro-2-(chloromethyl)-1-propene (4) can be accomplished by the direct chlorination of methallyl chloride, but the yields are low and purification involves a tedious spinning band distillation. A much more satisfactory method is described in a recent report\textsuperscript{4} starting with pentaerythritol (6). Pentaerythritol is converted to a 2.8:1 mixture of trichloride 7 and tetrachloride 8 using 3.08 equivalents each of pyridine and thionyl chloride. Without purification, the crude mixture of chlorides is oxidized with hot nitric acid. Unreacted tetrachloride 8 may be recovered unchanged from the oxidation while the trichloride 7 is converted to the carboxylic acid 9. The overall yield of crude acid 9 is 55\% from 6. Heating the crude acid 9 to 210\degree C allows for smooth decarboxylation and elimination of HCl and gives a virtually quantitative yield of pure alkene 4. (See Scheme 12.)

\[
\begin{align*}
\text{HO} & \quad \text{OH} \quad \text{SOCl}_{2} \quad \text{Cl} \quad \text{Cl} \quad \text{Cl} \quad \text{Cl} \\
\text{6} & \quad \text{7} & \quad \text{8} & \quad \text{9} \\
\text{HNO}_{3} & \quad \Delta & \quad \text{Cl} \quad \text{CO}_{2}\text{H} & \quad \text{Cl} \quad \text{CO}_{2}\text{H} \quad \text{Cl} \\
\text{4} & \quad \text{50\% overall yield}
\end{align*}
\]

Scheme 12

Optimization of the conditions for the dibromocarbene addition to alkene 4 required many trials. Finally a set of conditions was found that afforded high yields of 5 with easy workup\textsuperscript{5}. These conditions involve the combination of a catalytic amount of pinacol and dibenzo-18-crown-6 together with bromoform and 50\% aqueous sodium hydroxide solution at 40\degree C. In this way, pure crystalline cyclopropane can be obtained in yields of up to 80\%. (See Scheme 13.)
While [1.1.1]propellane shows modest stability, it is sensitive to Lewis acids, strong bases and moderate temperatures. Investigators are interested in developing methods that will allow the conversion of the high energy [1.1.1]propellane system to more kinetically stable species that still have high energy. These will be useful as high energy fuel candidates. Cleaving the central carbon-carbon bond in [1.1.1]propellane produces bicyclo[1.1.1]pentanes which are kinetically very stable, yet have 68 kcal/mol of strain energy. One attractive candidate as a high energy fuel additive is 1-t-butylbicyclo[1.1.1]pentane (10), which is available by reaction of propellane with t-butyl lithium followed by protonolysis. This molecule is a liquid at room temperature and has a boiling point of 90°C. It is a very stable compound that is unaffected by moderate temperatures or acids or bases. Geometry optimized ab initio calculations at the 6-31G* level predict a heat of formation of 26 kcal/mol. This translates to an I_p of 308 sec when combusted with liquid oxygen. Investigators are in the process of optimizing conditions for the preparation of 1-t-butylbicyclo[1.1.1]pentane so that substantial amounts can easily be prepared. A great advantage of this preparation is that it does not involve any photochemistry and only requires three synthetic steps from commercially available material.

**Scheme 14**

**Synthesis and Study of Bicyclo[1.1.1]pentylcarbenes**

A third area of study during the funding period was bicyclo[1.1.1]pentylcarbenes. There is interest in studying these systems in order to determine whether they will be stable under cryogenic inert gas matrix isolation conditions or will rearrange to strained alkenes. In many ways the bicyclo[1.1.1]pentylcarbene system is similar to the cubylcarbene-homocubene system that has received considerable study.

As a starting point, the energies and structures for singlet bicyclo[1.1.1]pentylcarbene have been determined, along with some possible rearrangement products. The computational method employed was a three configuration multiconfiguration self-consistent-field (MCSCF) wavefunction using the 6-31G* basis set. The results are shown below.
Scheme 15

It was desirable to investigate the parent carbene, so a route to the corresponding diazo compound 11 was developed. This route is shown below in Scheme 16.

Scheme 16

Initial investigations of the matrix isolation photochemistry of diazo compound 11 have indicated that there be a carbene intermediate. Unfortunately, funding cutbacks in years two and three of the contract required that this area be abandoned. With the groundwork thus laid, future work in this area is guaranteed to generate exciting results.

Synthesis of Prismane Derivatives

Prismanes are a class of polyhedranes composed of fused four-membered rings. The three smallest prismanes, [3]prismane, [4]prismane (cubane), and [5]prismane (pentaprismane) have been synthesized using a wide variety of synthetic methods.

During this study, efforts in this area have been directed toward the preparation of an unknown prismane, hexaprismane (15), a formal face-to-face dimer of benzene. Hexaprismane is predicted to have 175 kcal/mol of strain energy and a calculated $I_p$ of 313 sec. Good progress has been made toward the synthesis of hexaprismane and bishomohexaprismanedione (16) has been prepared.$^5$ Hexaprismane can be prepared using similar chemistry.

Scheme 17
The starting point for the synthesis of 16 was bishomosecoheptaprismanedione 17, which is conveniently available in eight steps8 and without resort to any chromatography starting with the Diels-Alder adduct between 5,5-dimethoxycyclopentadiene and benzoquinone. Conversion of the bishomosecoheptaprismane system of 17 to the bishomohexaprismane system was accomplished in the following manner. Dione 17 was converted to diol 18 using NaBH4, and this was converted to dimesylate 19. Dimesylate 19 was converted to diiodide 20 as a mixture of diastereomers which, when treated with Na/K alloy, produced diene 21 in good yield via Grob fragmentation. Diene 21 was converted to the highly water soluble tetral 22 in quantitative crude yield using catalytic OsO4. Treatment of crude tetral 22 with periodic acid leads to formation of 23, the doubly ring contracted product, in 60% yield. The hydroxyl groups in 23 were protected as the acetates to give 24, and the aldehyde groups were oxidized with KMnO4 to produce diacid 25. The carboxylic acid groups were converted to bromides via Hunsdiecker reaction to give 26. Treatment of 26 with lithium dispersion in t-BuOH/THF solution resulted not only in reductive debromination, as anticipated, but also reductive fragmentation to form diene 27 in 25% overall yield. Hydrolysis of 27 produced dienedione 28, which also underwent photochemical ring closure to the highly sought-after norbornadienone dimer 16. (See Scheme 18.)
The structure of 16 was determined by single crystal X-ray analysis, and some of the results are compared with those obtained from geometry optimized \textit{ab initio} calculations at the HF/6-31G* level (Table 2). The agreement is outstanding. (See Scheme 19.)

\textbf{Table 2. Comparison of Bond Lengths in 16}

<table>
<thead>
<tr>
<th>Bond</th>
<th>X-ray(Å)</th>
<th>HF/6-31G*</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1*-C4</td>
<td>1.546</td>
<td>1.546</td>
</tr>
<tr>
<td>C3-C4</td>
<td>1.530</td>
<td>1.538</td>
</tr>
<tr>
<td>C3-C7</td>
<td>1.535</td>
<td>1.536</td>
</tr>
<tr>
<td>C4-C5</td>
<td>1.574</td>
<td>1.569</td>
</tr>
<tr>
<td>C7-O1</td>
<td>1.206</td>
<td>1.183</td>
</tr>
</tbody>
</table>

Scheme 19

In an effort to synthesize a bishomoheptaprismane derivative, investigators attempted the photochemical ring closure of 21 to 29. However, the reaction failed under all conditions attempted. This failure was attributed to the 80 kcal/mol increase in strain energy that accompanies the transformation of 21 to 29. This value is above the 55 kcal/mol threshold suggested as the maximum increase in strain energy tolerated in the photoreaction. Therefore, other methods were sought to access this unknown ring system.

\textbf{Scheme 20}

Mild hydrolysis of 21 using aqueous oxalic acid gave a high yield of ketone 30. When irradiated using a medium pressure mercury arc through Pyrex\textsuperscript{TM}, 30 smoothly underwent decarbonylation/fragmentation to produce tetraene 31 in 60% yield. Further direct irradiation ($\lambda > 220$ nm) of tetraene 31 produced the [4+4]cycloadduct 32 in low yield. The identity of 32 was determined by analysis of the $^1$H and $^{13}$C NMR spectra which revealed the symmetrical nature of the compound. Diene 32 was resistant to further photochemical ring closure and yielded no traces of the homoheptaprismane ring system of 33.
Investigators were intrigued by the possibility of performing tandem Diels-Alder reactions with tetraene 31. By analogy to the pagodane synthesis, the reaction of 31 with maleic anhydride was investigated, and it was found that the reaction proceeds in excellent yield to give 34, the domino Diels-Alder adduct. Analysis of the crude reaction mixture by $^1$H NMR produced no evidence for any other isomer in the reaction. The stereochemistry of the product was confirmed by single crystal X-ray analysis, although the R factor was poor. Diene 35 was produced in modest yield via an oxidative decarboxylation. Hydrolysis of 35 gave ketone 36, which was subjected to single crystal X-ray analysis.

For comparison, the structure of 36 was calculated using ab initio molecular orbital theory at the HF/6-31G* level, and a comparison of some selected bond lengths are shown in Table 3. The agreement is quite satisfactory.
Table 3. Experimental and Calculated Bond Lengths in 36

<table>
<thead>
<tr>
<th>Bond</th>
<th>X-ray(Å)</th>
<th>HF/6-31G*</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1-C2</td>
<td>1.568</td>
<td>1.571</td>
</tr>
<tr>
<td>C1-C5</td>
<td>1.548</td>
<td>1.545</td>
</tr>
<tr>
<td>C4-C5</td>
<td>1.544</td>
<td>1.545</td>
</tr>
<tr>
<td>C5-C6</td>
<td>1.482</td>
<td>1.507</td>
</tr>
<tr>
<td>C6-C7</td>
<td>1.305</td>
<td>1.319</td>
</tr>
<tr>
<td>C4-C15</td>
<td>1.536</td>
<td>1.551</td>
</tr>
<tr>
<td>C10-C11</td>
<td>1.528</td>
<td>1.523</td>
</tr>
<tr>
<td>C11-O1</td>
<td>1.208</td>
<td>1.186</td>
</tr>
</tbody>
</table>

References