Fourth stable radical species in X-ray irradiated sucrose

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Introduction

Sucrose is present in nearly every household as the main component of table sugar or as an ingredient of sugar-containing foodstuffs. The EPR spectrum of radicals induced by irradiation of this carbohydrate is detectable at room temperature and has several properties that make it relevant for dosimetric applications: long term stability of radicals, considerable linear dose response range and a relatively low detection limit. It is likely that dose assessment protocols could be improved if the spectrum was completely understood. Additionally, thorough characterisation of radicals enables their identification, which in turn may provide insight into the radiation chemistry of more complex sugar-containing and biologically relevant systems, e.g. DNA.

X-ray induced radicals in sucrose

Field-Frequency ENDOR at B1b

Characterisation of T4

Spectra were measured in Q band, at 110 K and in four rotation planes (to solve the Schonland ambiguity).

<table>
<thead>
<tr>
<th>T4</th>
<th>H1</th>
<th>H2</th>
<th>H3</th>
<th>H4</th>
</tr>
</thead>
<tbody>
<tr>
<td>gxx</td>
<td>2.0019</td>
<td>-0.4</td>
<td>0.570</td>
<td>0.080</td>
</tr>
<tr>
<td>gyy</td>
<td>2.0044</td>
<td>2.1</td>
<td>0.510</td>
<td>-0.851</td>
</tr>
<tr>
<td>gzz</td>
<td>2.0085</td>
<td>4.2</td>
<td>-0.777</td>
<td>-0.520</td>
</tr>
</tbody>
</table>

Ranges of values for intensity relations of T1, T2 and T3 were determined from a single crystal analysis in Ref. [2]. Relations used here: (T2+T3)/T1=1.2 and T2/T3=1.5. Determined relative double integral intensities in powder spectra:

39%×T1 + 28%×T2 + 18%×T3 + 15%×T4

Possible radical models

Inspection of the g tensor suggests that LEO should be located between a C=O group and a ring O. Its relative rhombicity δgxx=0.80, is more similar to T1's (0.70) than T2's (0.47) or T3's (0.44) [2].

A set of possible models has been devised by comparing experimental gxx and A directions to the crystallographic data.

Experimental results could not be reproduced by DFT calculations, but δgxx's of calculated g tensors and a large β-H interaction suggest that M3 is so far the best.

Conclusions

- Fourth radical species is well characterised.
- The powder spectrum of sucrose can be rather thoroughly understood.
- The model of T4 is not clear yet.

References


Acknowledgement: Authors gratefully acknowledge the financial support of the UGent Special Research Fund.