



# Library Indian Institute of Science Education and Research Mohali



**DSpace@IISERMohali (/jspui/)**

**/ Publications of IISER Mohali (/jspui/handle/123456789/4)**

**/ Research Articles (/jspui/handle/123456789/9)**

Please use this identifier to cite or link to this item: <http://hdl.handle.net/123456789/2611>

Title:	Study of Topological Effects Concerning the Lowest A" and the Three A' States for the CO <sub>2</sub> <sup>+</sup> Ion
Authors:	Dhindhwal, V. (/jspui/browse?type=author&value=Dhindhwal%2C+V.) Baer, M. (/jspui/browse?type=author&value=Baer%2C+M.) Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Renner–Teller (RT) CO <sub>2</sub> <sup>+</sup> Topological effects Jahn–Teller
Issue Date:	2016
Publisher:	American Chemical Society
Citation:	Journal of Physical Chemistry A, 120(19), pp.2999-3008.
Abstract:	<p>A study of the topological effects, viz., the Jahn–Teller (JT) and Renner–Teller (RT) effects, in CO<sub>2</sub><sup>+</sup> has been carried out by calculating nonadiabatic coupling terms (NACTs) at the state-averaged CASSCF level using the cc-pVTZ basis set for the lowest three A' states and one A" state along a circular contour. Using the NACTs, the privileged adiabatic-to-diabatic transformation (ADT) angles (<math>\gamma_{12}</math>) for 1A' and 2A' states of CO<sub>2</sub><sup>+</sup> have been calculated along various circular contours. Employing one of the oxygen atoms as the test particle exposed two conical intersections (ci) located on each side of the CO diatom. The main purpose of this study is to explore the possibility of forming reliable diabatic potential energy surfaces for this system. Success in achieving this goal is guaranteed by the ability to calculate quantized privileged ADT angles along closed contours covering large regions in configuration space (see, e.g., J. Phys. Chem. A 2014, 118, 6361). The calculations were carried out for two and three JT states. In most cases very nice quantization has been achieved although the calculations were frequently done, as required, for large regions in configuration space (sometimes <math>\geq 18</math> Å<sup>2</sup>). In one case, for which the quantization was not gratifying, the inclusion of the RT effect modified it considerably.</p>
URI:	<a href="https://pubs.acs.org/doi/full/10.1021/acs.jpca.5b08921">https://pubs.acs.org/doi/full/10.1021/acs.jpca.5b08921</a> ( <a href="https://pubs.acs.org/doi/full/10.1021/acs.jpca.5b08921">https://pubs.acs.org/doi/full/10.1021/acs.jpca.5b08921</a> ) <a href="http://hdl.handle.net/123456789/2611">http://hdl.handle.net/123456789/2611</a> ( <a href="http://hdl.handle.net/123456789/2611">http://hdl.handle.net/123456789/2611</a> )
Appears in	Research Articles (/jspui/handle/123456789/9)
Collections:	

Files in This Item:

File	Description	Size	Format
Need to add pdf.odt (/jspui/bitstream/123456789/2611/1/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text

[View/Open \(/jspui/bitstream/123456789/2611/1/Need%20to%20add%20pdf.odt\)](#)

[Show full item record \(/jspui/handle/123456789/2611?mode=full\)](#)

[Statistics \(/jspui/handle/123456789/2611/statistics\)](#)

Items in DSpace are protected by copyright, with all rights reserved, unless otherwise indicated.