

Supplementary Material

The Eight Lowest-Energy Vibrational States of Benzonitrile: Analysis of Coriolis and Darling-Dennison Coupling by Millimeter-wave and Infrared Spectroscopy

Maria A. Zdanovskaia,^a Marie-Aline Martin-Drumel,^{b,c} Zbigniew Kisiel,^d Olivier Pirali,^{b,c}

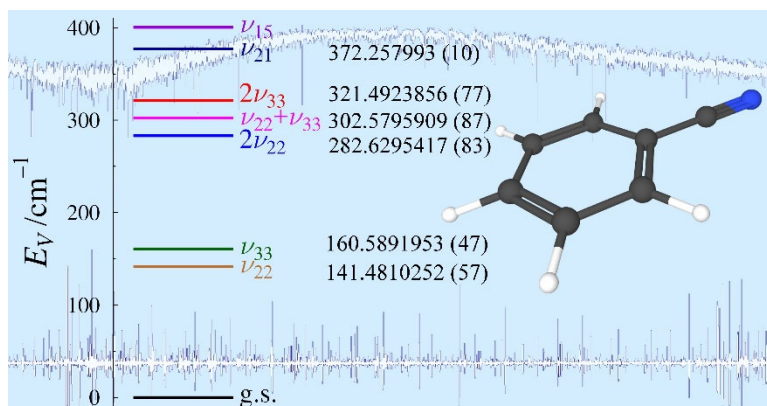
Brian J. Esselman,^a R. Claude Woods,^{a,*} Robert J. McMahon^{a,*}

^a *Department of Chemistry, University of Wisconsin–Madison, Madison, Wisconsin 53706, USA*

^b *AILES Beamline, Synchrotron SOLEIL, l'Orme des Merisiers, Saint-Aubin, 91192 Gif-sur-Yvette cedex, France*

^c *Institut des Sciences Moléculaires d'Orsay, UMR8214 CNRS, Université Paris-Sud, Bât. 210, 91405 Orsay cedex, France*

^d *Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland*



* Corresponding authors.

E-mail addresses: rcwoods@wisc.edu (R.C. Woods), robert.mcmahon@wisc.edu

(R.J. McMahon)

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Used to compute the Darling-Dennison interaction term and anharmonic energies of the $v_{22} = 2$ and $v_{33} = 2$ overtone states.

The screenshot displays the following keywords and their descriptions:

- states**: The number of states to be examined.
- 2**: (Value for states)
- print full vibration vpt2 dd calc**: Output estimate of W .
- Type of frequency calculation**
- Calculate Darling-Dennison resonance-relevant values**

A detailed explanation box on the right states: "Each line contains the $3N-6$ (33) vibrationally excited states of benzonitrile. The value for each of these denotes the number of quanta of that fundamental, from lowest to highest energy. In this case, the states of interest are $\nu_{22} = 2$ and $\nu_{33} = 2$."

Table S1. Infrared Transitions Excluded from Six-State Least-Squares Fit

Upper rotational level	Upper vibrational state	Lower rotational level	Lower vibrational state	Frequency (cm ⁻¹)
49 _{46,3}	$\nu_{33} = 2$	48 _{45,4}	$\nu_{33} = 1$	186.790845
50 _{46,4}	$\nu_{33} = 2$	49 _{45,5}	$\nu_{33} = 1$	186.888208
48 _{48,0}	$\nu_{33} = 2$	47 _{47,1}	$\nu_{33} = 1$	187.789794
49 _{48,1}	$\nu_{33} = 2$	48 _{47,2}	$\nu_{33} = 1$	187.886901
50 _{48,2}	$\nu_{33} = 2$	49 _{47,3}	$\nu_{33} = 1$	187.984463
51 _{48,3}	$\nu_{33} = 2$	50 _{47,4}	$\nu_{33} = 1$	188.082165
52 _{48,4}	$\nu_{33} = 2$	51 _{47,5}	$\nu_{33} = 1$	188.179455
53 _{48,5}	$\nu_{33} = 2$	52 _{47,6}	$\nu_{33} = 1$	188.277194
54 _{48,6}	$\nu_{33} = 2$	53 _{47,7}	$\nu_{33} = 1$	188.374734
55 _{48,7}	$\nu_{33} = 2$	54 _{47,8}	$\nu_{33} = 1$	188.472531
57 _{48,9}	$\nu_{33} = 2$	56 _{47,10}	$\nu_{33} = 1$	188.668517
58 _{48,10}	$\nu_{33} = 2$	57 _{47,11}	$\nu_{33} = 1$	188.766483
59 _{48,11}	$\nu_{33} = 2$	58 _{47,12}	$\nu_{33} = 1$	188.864671
60 _{48,12}	$\nu_{33} = 2$	59 _{47,13}	$\nu_{33} = 1$	188.963241
61 _{48,13}	$\nu_{33} = 2$	60 _{47,14}	$\nu_{33} = 1$	189.061318
62 _{48,14}	$\nu_{33} = 2$	61 _{47,15}	$\nu_{33} = 1$	189.159800
63 _{48,15}	$\nu_{33} = 2$	62 _{47,16}	$\nu_{33} = 1$	189.258451
53 _{50,3}	$\nu_{33} = 2$	52 _{49,4}	$\nu_{33} = 1$	189.377656
65 _{48,17}	$\nu_{33} = 2$	64 _{47,18}	$\nu_{33} = 1$	189.455981
54 _{50,4}	$\nu_{33} = 2$	53 _{49,5}	$\nu_{33} = 1$	189.475225
55 _{50,5}	$\nu_{33} = 2$	54 _{49,6}	$\nu_{33} = 1$	189.572883
56 _{50,6}	$\nu_{33} = 2$	55 _{49,7}	$\nu_{33} = 1$	189.671005
63 _{50,13}	$\nu_{33} = 2$	62 _{49,14}	$\nu_{33} = 1$	190.358457
64 _{50,14}	$\nu_{33} = 2$	63 _{49,15}	$\nu_{33} = 1$	190.457042
66 _{50,16}	$\nu_{33} = 2$	65 _{49,17}	$\nu_{33} = 1$	190.654609
67 _{50,17}	$\nu_{33} = 2$	66 _{49,18}	$\nu_{33} = 1$	190.753730
68 _{50,18}	$\nu_{33} = 2$	67 _{49,19}	$\nu_{33} = 1$	190.852433
69 _{50,19}	$\nu_{33} = 2$	68 _{49,20}	$\nu_{33} = 1$	190.951687
70 _{50,20}	$\nu_{33} = 2$	69 _{49,21}	$\nu_{33} = 1$	191.050853
71 _{50,21}	$\nu_{33} = 2$	70 _{49,22}	$\nu_{33} = 1$	191.150107
72 _{50,22}	$\nu_{33} = 2$	71 _{49,23}	$\nu_{33} = 1$	191.249626