Can $Na_2[B_{12}H_{12}]$ be a decomposition product of $NaBH_4$?

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NMR calculations

Calculated parameters

The NMR chemical shielding and the electric field gradient tensor (EFG) were calculated. Generally, the NMR properties are very sensitive to atomic positions, which make NMR a very useful experimental technique for structure analysis and validation. The accuracy of the NMR ab-initio calculations were very sensitive to the K-point sampling of the first Brillouin zone and also heavily depended on the accuracy of the optimized structures. The calculated NMR properties are reported below. The isotropic chemical shielding (Iso) in ppm is defined as the trace of the shielding tensor:

$$\sigma_{iso} = \frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3}$$

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This is an absolute value of the isotropic chemical shielding, not relative to a standard. The anisotropy chemical shielding (Aniso) is defined as:

$$\Delta = \sigma_{zz} - \sigma_{iso}$$

The asymmetry parameter (Asym) is defined as:

$$\eta = \frac{\sigma_{xx} - \sigma_{yy}}{\Delta}$$

The quadrupole coupling constant is the largest component of the diagonalized EFG tensor, it is de-fined as:

$$C_Q = \frac{eQV_{zz}}{h}$$

where Q is the nuclear quadrupole moment. The quadrupolar asymmetry parameter (Eta) is defined as:

$$\eta_Q = \frac{V_{xx} - V_{yy}}{V_{zz}}$$

In general, the EFG values and the asymmetry parameters can be compared directly with experiments. The isotropic chemical shifts require some analysis because the program reports absolute chemical shielding whereas the experimental results concern with shifts relative to a known standard.

$Na_2[B_{12}H_{12}]$ cubic structure

The supercell contained 4 formula units, which means 104 atoms ($4Na_2B_{12}H_{12}$). While the isotropic shielding of H is almost the same for all the H atoms, boron atoms showed a doublet, and Na simply one signal.

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 |         Chemical Shielding and Electric Field Gradient Tensors
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Nucleus		Shielding tensor			EFG Tensor	
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
H	1	29.27	13.69	0.27	1.384E-01	0.08
H	2	29.33	12.20	0.30	1.382E-01	0.06
H	3	29.27	13.69	0.27	1.384E-01	0.08
H	4	29.33	12.20	0.30	1.382E-01	0.06
H	5	29.27	13.69	0.27	1.384E-01	0.08
H	6	29.33	12.20	0.30	1.382E-01	0.06
H	7	29.27	13.69	0.27	1.384E-01	0.08
H	8	29.33	12.20	0.30	1.382E-01	0.06
H	9	29.27	13.69	0.27	1.384E-01	0.08
H	10	29.33	12.20	0.30	1.382E-01	0.06
H	11	29.27	13.69	0.27	1.384E-01	0.08
H	12	29.33	12.20	0.30	1.382E-01	0.06
H	13	29.27	13.69	0.27	1.384E-01	0.08
H	14	29.33	12.20	0.30	1.382E-01	0.06
H	15	29.27	13.69	0.27	1.384E-01	0.08
H	16	29.33	12.20	0.30	1.382E-01	0.06
H	17	29.27	13.69	0.27	1.384E-01	0.08
H	18	29.33	12.20	0.30	1.382E-01	0.06
H	19	29.27	13.69	0.27	1.384E-01	0.08
H	20	29.33	12.20	0.30	1.382E-01	0.06
H	21	29.27	13.69	0.27	1.384E-01	0.08
H	22	29.33	12.20	0.30	1.382E-01	0.06
H	23	29.27	13.69	0.27	1.384E-01	0.08
H	24	29.33	12.20	0.30	1.382E-01	0.06

	H	25	29.27	13.69	0.27	1.384E-01	0.08
	H	26	29.33	12.20	0.30	1.382E-01	0.06
	H	27	29.27	13.69	0.27	1.384E-01	0.08
	H	28	29.33	12.20	0.30	1.382E-01	0.06
	H	29	29.27	13.69	0.27	1.384E-01	0.08
	H	30	29.33	12.20	0.30	1.382E-01	0.06
	H	31	29.27	13.69	0.27	1.384E-01	0.08
	H	32	29.33	12.20	0.30	1.382E-01	0.06
	H	33	29.27	13.69	0.27	1.384E-01	0.08
	H	34	29.33	12.20	0.30	1.382E-01	0.06
	H	35	29.27	13.69	0.27	1.384E-01	0.08
	H	36	29.33	12.20	0.30	1.382E-01	0.06
	H	37	29.27	13.69	0.27	1.384E-01	0.08
	H	38	29.33	12.20	0.30	1.382E-01	0.06
	H	39	29.27	13.69	0.27	1.384E-01	0.08
	H	40	29.33	12.20	0.30	1.382E-01	0.06
	H	41	29.27	13.69	0.27	1.384E-01	0.08
	H	42	29.33	12.20	0.30	1.382E-01	0.06
	H	43	29.27	13.69	0.27	1.384E-01	0.08
	H	44	29.33	12.20	0.30	1.382E-01	0.06
	H	45	29.27	13.69	0.27	1.384E-01	0.08
	H	46	29.33	12.20	0.30	1.382E-01	0.06
	H	47	29.27	13.69	0.27	1.384E-01	0.08
	H	48	29.33	12.20	0.30	1.382E-01	0.06
	B	1	114.03	-18.76	0.11	-9.129E-01	0.09
	B	2	113.07	-19.82	0.14	-8.941E-01	0.06
	B	3	114.03	-18.76	0.11	-9.129E-01	0.09

	B	4	113.07	-19.82	0.14	-8.941E-01	0.06
	B	5	114.03	-18.76	0.11	-9.129E-01	0.09
	B	6	113.07	-19.82	0.14	-8.941E-01	0.06
	B	7	114.03	-18.76	0.11	-9.129E-01	0.09
	B	8	113.07	-19.82	0.14	-8.941E-01	0.06
	B	9	114.03	-18.76	0.11	-9.129E-01	0.09
	B	10	113.07	-19.82	0.14	-8.941E-01	0.06
	B	11	114.03	-18.76	0.11	-9.129E-01	0.09
	B	12	113.07	-19.82	0.14	-8.941E-01	0.06
	B	13	114.03	-18.76	0.11	-9.129E-01	0.09
	B	14	113.07	-19.82	0.14	-8.941E-01	0.06
	B	15	114.03	-18.76	0.11	-9.129E-01	0.09
	B	16	113.07	-19.82	0.14	-8.941E-01	0.06
	B	17	114.03	-18.76	0.11	-9.129E-01	0.09
	B	18	113.07	-19.82	0.14	-8.941E-01	0.06
	B	19	114.03	-18.76	0.11	-9.129E-01	0.09
	B	20	113.07	-19.82	0.14	-8.941E-01	0.06
	B	21	114.03	-18.76	0.11	-9.129E-01	0.09
	B	22	113.07	-19.82	0.14	-8.941E-01	0.06
	B	23	114.03	-18.76	0.11	-9.129E-01	0.09
	B	24	113.07	-19.82	0.14	-8.941E-01	0.06
	B	25	114.03	-18.76	0.11	-9.129E-01	0.09
	B	26	113.07	-19.82	0.14	-8.941E-01	0.06
	B	27	114.03	-18.76	0.11	-9.129E-01	0.09
	B	28	113.07	-19.82	0.14	-8.941E-01	0.06
	B	29	114.03	-18.76	0.11	-9.129E-01	0.09
	B	30	113.07	-19.82	0.14	-8.941E-01	0.06

B	31	114.03	-18.76	0.11	-9.129E-01	0.09
B	32	113.07	-19.82	0.14	-8.941E-01	0.06
B	33	114.03	-18.76	0.11	-9.129E-01	0.09
B	34	113.07	-19.82	0.14	-8.941E-01	0.06
B	35	114.03	-18.76	0.11	-9.129E-01	0.09
B	36	113.07	-19.82	0.14	-8.941E-01	0.06
B	37	114.03	-18.76	0.11	-9.129E-01	0.09
B	38	113.07	-19.82	0.14	-8.941E-01	0.06
B	39	114.03	-18.76	0.11	-9.129E-01	0.09
B	40	113.07	-19.82	0.14	-8.941E-01	0.06
B	41	114.03	-18.76	0.11	-9.129E-01	0.09
B	42	113.07	-19.82	0.14	-8.941E-01	0.06
B	43	114.03	-18.76	0.11	-9.129E-01	0.09
B	44	113.07	-19.82	0.14	-8.941E-01	0.06
B	45	114.03	-18.76	0.11	-9.129E-01	0.09
B	46	113.07	-19.82	0.14	-8.941E-01	0.06
B	47	114.03	-18.76	0.11	-9.129E-01	0.09
B	48	113.07	-19.82	0.14	-8.941E-01	0.06
Na	1	572.97	-23.76	0.00	8.186E-01	0.00
Na	2	572.97	-23.76	0.00	8.186E-01	0.00
Na	3	572.97	-23.76	0.00	8.186E-01	0.00
Na	4	572.97	-23.76	0.00	8.186E-01	0.00
Na	5	572.97	-23.76	0.00	8.186E-01	0.00
Na	6	572.97	-23.76	0.00	8.186E-01	0.00
Na	7	572.97	-23.76	0.00	8.186E-01	0.00
Na	8	572.97	-23.76	0.00	8.186E-01	0.00

$Na_2[B_{12}H_{12}]$ **monoclinic structure**

The supercell contained two formula units, and hence 52 atoms. The NMR shielding followed the symmetry. In fact, each B_{12} unit showed different shielding values: (112.19 and 112.07), (113.92 and 113.93), 114.71. Accordingly, the hydrogen atoms showed different shielding values too.

Chemical Shielding and Electric Field Gradient Tensors						
Nucleus		Shielding tensor			EFG Tensor	
Species	Ion	Iso(ppm)	Aniso(ppm)	Asym	Cq(MHz)	Eta
H	1	29.08	15.53	0.23	1.414E-01	0.05
H	2	29.22	15.50	0.14	1.356E-01	0.06
H	3	29.17	12.35	0.28	1.373E-01	0.05
H	4	29.42	12.12	0.14	1.402E-01	0.07
H	5	29.21	15.28	0.35	1.368E-01	0.07
H	6	29.31	14.83	0.32	1.393E-01	0.07
H	7	29.08	15.53	0.23	1.414E-01	0.05
H	8	29.22	15.50	0.14	1.356E-01	0.06
H	9	29.17	12.35	0.28	1.373E-01	0.05
H	10	29.42	12.12	0.14	1.402E-01	0.07
H	11	29.21	15.28	0.35	1.368E-01	0.07
H	12	29.31	14.83	0.32	1.393E-01	0.07
H	13	29.08	15.53	0.23	1.414E-01	0.05
H	14	29.22	15.50	0.14	1.356E-01	0.06
H	15	29.17	12.35	0.28	1.373E-01	0.05
H	16	29.42	12.12	0.14	1.402E-01	0.07

	H	17	29.21	15.28	0.35	1.368E-01	0.07
	H	18	29.31	14.83	0.32	1.393E-01	0.07
	H	19	29.08	15.53	0.23	1.414E-01	0.05
	H	20	29.22	15.50	0.14	1.356E-01	0.06
	H	21	29.17	12.35	0.28	1.373E-01	0.05
	H	22	29.42	12.12	0.14	1.402E-01	0.07
	H	23	29.21	15.28	0.35	1.368E-01	0.07
	H	24	29.31	14.83	0.32	1.393E-01	0.07
	B	1	112.07	-18.75	0.10	-1.001E+00	0.05
	B	2	114.71	-20.47	0.29	-8.728E-01	0.09
	B	3	113.93	-20.34	0.21	-9.210E-01	0.09
	B	4	112.19	-20.59	0.23	-8.888E-01	0.05
	B	5	113.92	-19.58	0.27	-9.192E-01	0.13
	B	6	112.68	-19.85	0.12	-9.252E-01	0.03
	B	7	112.07	-18.75	0.10	-1.001E+00	0.05
	B	8	114.71	-20.47	0.29	-8.728E-01	0.09
	B	9	113.93	-20.34	0.21	-9.210E-01	0.09
	B	10	112.19	-20.59	0.23	-8.888E-01	0.05
	B	11	113.92	-19.58	0.27	-9.192E-01	0.13
	B	12	112.68	-19.85	0.12	-9.252E-01	0.03
	B	13	112.07	-18.75	0.10	-1.001E+00	0.05
	B	14	114.71	-20.47	0.29	-8.728E-01	0.09
	B	15	113.93	-20.34	0.21	-9.210E-01	0.09
	B	16	112.19	-20.59	0.23	-8.888E-01	0.05
	B	17	113.92	-19.58	0.27	-9.192E-01	0.13
	B	18	112.68	-19.85	0.12	-9.252E-01	0.03
	B	19	112.07	-18.75	0.10	-1.001E+00	0.05

B	20	114.71	-20.47	0.29	-8.728E-01	0.09
B	21	113.93	-20.34	0.21	-9.210E-01	0.09
B	22	112.19	-20.59	0.23	-8.888E-01	0.05
B	23	113.92	-19.58	0.27	-9.192E-01	0.13
B	24	112.68	-19.85	0.12	-9.252E-01	0.03
Na	1	577.54	-23.63	0.17	1.548E+00	0.35
Na	2	577.54	-23.63	0.17	1.548E+00	0.35
Na	3	577.54	-23.63	0.17	1.548E+00	0.35
Na	4	577.54	-23.63	0.17	1.548E+00	0.35

Phonons calculations

We report below the wave numbers of $Na_2[B_{12}H_{12}]$ monoclinic structure, calculated via phonon analysis, using Quantum Espresso code. The number of vibrational normal modes, equal to $3N-6$, was 156, where N is the number of atoms per unit cell. Below we report the wave numbers (omega) in cm^{-1} and for each the symmetry with the additional information of IR- (I) or Raman- (R) active mode. Only one mode showed negative frequency. We found the typical stretching modes of boron-hydrogen bond in the range (2500, 2560) cm^{-1} and the characteristic modes of the icosahedral B_{12} unit.[1]

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omega(  1 -  1) =         -7.6  [cm-1]   --> A_u            I
omega(  2 -  2) =         16.4  [cm-1]   --> A_u            I
omega(  3 -  3) =         24.5  [cm-1]   --> A_u            I
omega(  4 -  4) =         45.1  [cm-1]   --> A_u            I
omega(  5 -  5) =         45.3  [cm-1]   --> A_g            R
omega(  6 -  6) =         65.5  [cm-1]   --> A_u            I
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omega(  7 -  7) =        66.3  [cm-1]   --> A_g          R
omega(  8 -  8) =        81.9  [cm-1]   --> A_g          R
omega(  9 -  9) =        88.0  [cm-1]   --> A_u          I
omega( 10 - 10) =        90.2  [cm-1]   --> A_g          R
omega( 11 - 11) =        91.5  [cm-1]   --> A_g          R
omega( 12 - 12) =        95.5  [cm-1]   --> A_u          I
omega( 13 - 13) =       103.7  [cm-1]   --> A_g          R
omega( 14 - 14) =       109.9  [cm-1]   --> A_u          I
omega( 15 - 15) =       113.5  [cm-1]   --> A_g          R
omega( 16 - 16) =       119.9  [cm-1]   --> A_g          R
omega( 17 - 17) =       137.7  [cm-1]   --> A_u          I
omega( 18 - 18) =       142.1  [cm-1]   --> A_g          R
omega( 19 - 19) =       147.8  [cm-1]   --> A_u          I
omega( 20 - 20) =       156.2  [cm-1]   --> A_g          R
omega( 21 - 21) =       157.9  [cm-1]   --> A_u          I
omega( 22 - 22) =       166.9  [cm-1]   --> A_u          I
omega( 23 - 23) =       170.3  [cm-1]   --> A_g          R
omega( 24 - 24) =       174.5  [cm-1]   --> A_g          R
omega( 25 - 25) =       532.4  [cm-1]   --> A_u          I
omega( 26 - 26) =       532.7  [cm-1]   --> A_u          I
omega( 27 - 27) =       534.6  [cm-1]   --> A_u          I
omega( 28 - 28) =       535.6  [cm-1]   --> A_u          I
omega( 29 - 29) =       536.4  [cm-1]   --> A_u          I
omega( 30 - 30) =       536.9  [cm-1]   --> A_u          I
omega( 31 - 31) =       543.5  [cm-1]   --> A_u          I
omega( 32 - 32) =       544.5  [cm-1]   --> A_u          I
omega( 33 - 33) =       549.3  [cm-1]   --> A_u          I
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omega( 34 - 34) =       550.5  [cm-1]   --> A_u           I
omega( 35 - 35) =       574.2  [cm-1]   --> A_g           R
omega( 36 - 36) =       577.1  [cm-1]   --> A_g           R
omega( 37 - 37) =       578.1  [cm-1]   --> A_g           R
omega( 38 - 38) =       578.8  [cm-1]   --> A_g           R
omega( 39 - 39) =       579.6  [cm-1]   --> A_g           R
omega( 40 - 40) =       582.4  [cm-1]   --> A_g           R
omega( 41 - 41) =       586.3  [cm-1]   --> A_g           R
omega( 42 - 42) =       586.8  [cm-1]   --> A_g           R
omega( 43 - 43) =       589.6  [cm-1]   --> A_g           R
omega( 44 - 44) =       591.9  [cm-1]   --> A_g           R
omega( 45 - 45) =       663.0  [cm-1]   --> A_g           R
omega( 46 - 46) =       664.3  [cm-1]   --> A_g           R
omega( 47 - 47) =       671.9  [cm-1]   --> A_g           R
omega( 48 - 48) =       673.7  [cm-1]   --> A_g           R
omega( 49 - 49) =       675.5  [cm-1]   --> A_g           R
omega( 50 - 50) =       676.5  [cm-1]   --> A_g           R
omega( 51 - 51) =       680.6  [cm-1]   --> A_g           R
omega( 52 - 52) =       681.5  [cm-1]   --> A_g           R
omega( 53 - 53) =       703.6  [cm-1]   --> A_u           I
omega( 54 - 54) =       704.1  [cm-1]   --> A_u           I
omega( 55 - 55) =       708.6  [cm-1]   --> A_u           I
omega( 56 - 56) =       712.0  [cm-1]   --> A_u           I
omega( 57 - 57) =       724.0  [cm-1]   --> A_u           I
omega( 58 - 58) =       731.1  [cm-1]   --> A_u           I
omega( 59 - 59) =       742.7  [cm-1]   --> A_u           I
omega( 60 - 60) =       744.4  [cm-1]   --> A_u           I
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omega( 61 - 61) =       746.7  [cm-1]   --> A_g          R
omega( 62 - 62) =       748.3  [cm-1]   --> A_u          I
omega( 63 - 63) =       750.1  [cm-1]   --> A_u          I
omega( 64 - 64) =       751.3  [cm-1]   --> A_g          R
omega( 65 - 65) =       752.5  [cm-1]   --> A_u          I
omega( 66 - 66) =       753.8  [cm-1]   --> A_g          R
omega( 67 - 67) =       754.1  [cm-1]   --> A_u          I
omega( 68 - 68) =       755.1  [cm-1]   --> A_u          I
omega( 69 - 69) =       756.3  [cm-1]   --> A_g          R
omega( 70 - 70) =       757.1  [cm-1]   --> A_g          R
omega( 71 - 71) =       757.3  [cm-1]   --> A_u          I
omega( 72 - 72) =       758.5  [cm-1]   --> A_g          R
omega( 73 - 73) =       759.6  [cm-1]   --> A_u          I
omega( 74 - 74) =       762.9  [cm-1]   --> A_u          I
omega( 75 - 75) =       767.9  [cm-1]   --> A_u          I
omega( 76 - 76) =       768.1  [cm-1]   --> A_u          I
omega( 77 - 77) =       773.5  [cm-1]   --> A_g          R
omega( 78 - 78) =       776.4  [cm-1]   --> A_g          R
omega( 79 - 79) =       783.9  [cm-1]   --> A_u          I
omega( 80 - 80) =       784.2  [cm-1]   --> A_g          R
omega( 81 - 81) =       784.6  [cm-1]   --> A_u          I
omega( 82 - 82) =       788.8  [cm-1]   --> A_g          R
omega( 83 - 83) =       806.9  [cm-1]   --> A_g          R
omega( 84 - 84) =       807.9  [cm-1]   --> A_g          R
omega( 85 - 85) =       859.4  [cm-1]   --> A_u          I
omega( 86 - 86) =       860.3  [cm-1]   --> A_u          I
omega( 87 - 87) =       871.6  [cm-1]   --> A_u          I
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omega( 88 - 88) =       872.7  [cm-1]   --> A_u          I
omega( 89 - 89) =       874.1  [cm-1]   --> A_u          I
omega( 90 - 90) =       874.3  [cm-1]   --> A_u          I
omega( 91 - 91) =       899.3  [cm-1]   --> A_u          I
omega( 92 - 92) =       900.6  [cm-1]   --> A_u          I
omega( 93 - 93) =       910.0  [cm-1]   --> A_g          R
omega( 94 - 94) =       912.5  [cm-1]   --> A_g          R
omega( 95 - 95) =       918.4  [cm-1]   --> A_g          R
omega( 96 - 96) =       919.7  [cm-1]   --> A_g          R
omega( 97 - 97) =       920.4  [cm-1]   --> A_g          R
omega( 98 - 98) =       922.3  [cm-1]   --> A_g          R
omega( 99 - 99) =       929.0  [cm-1]   --> A_u          I
omega(100 -100) =       931.7  [cm-1]   --> A_u          I
omega(101 -101) =       932.3  [cm-1]   --> A_g          R
omega(102 -102) =       933.4  [cm-1]   --> A_g          R
omega(103 -103) =       934.4  [cm-1]   --> A_u          I
omega(104 -104) =       934.7  [cm-1]   --> A_u          I
omega(105 -105) =       939.0  [cm-1]   --> A_g          R
omega(106 -106) =       940.1  [cm-1]   --> A_g          R
omega(107 -107) =       940.4  [cm-1]   --> A_u          I
omega(108 -108) =       942.3  [cm-1]   --> A_u          I
omega(109 -109) =       946.6  [cm-1]   --> A_g          R
omega(110 -110) =       948.0  [cm-1]   --> A_g          R
omega(111 -111) =       958.9  [cm-1]   --> A_g          R
omega(112 -112) =       962.2  [cm-1]   --> A_g          R
omega(113 -113) =       967.1  [cm-1]   --> A_g          R
omega(114 -114) =       967.7  [cm-1]   --> A_g          R
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omega(115 -115) =        980.6  [cm-1]   --> A_g           R
omega(116 -116) =        981.0  [cm-1]   --> A_g           R
omega(117 -117) =        984.9  [cm-1]   --> A_u           I
omega(118 -118) =        987.1  [cm-1]   --> A_u           I
omega(119 -119) =        989.5  [cm-1]   --> A_g           R
omega(120 -120) =        989.6  [cm-1]   --> A_g           R
omega(121 -121) =        999.4  [cm-1]   --> A_g           R
omega(122 -122) =       1000.2  [cm-1]   --> A_g           R
omega(123 -123) =       1001.7  [cm-1]   --> A_u           I
omega(124 -124) =       1002.2  [cm-1]   --> A_u           I
omega(125 -125) =       1007.8  [cm-1]   --> A_g           R
omega(126 -126) =       1008.9  [cm-1]   --> A_g           R
omega(127 -127) =       1059.8  [cm-1]   --> A_u           I
omega(128 -128) =       1060.8  [cm-1]   --> A_u           I
omega(129 -129) =       1072.9  [cm-1]   --> A_u           I
omega(130 -130) =       1073.1  [cm-1]   --> A_u           I
omega(131 -131) =       1089.5  [cm-1]   --> A_u           I
omega(132 -132) =       1090.2  [cm-1]   --> A_u           I
omega(133 -133) =       2505.7  [cm-1]   --> A_u           I
omega(134 -134) =       2507.4  [cm-1]   --> A_g           R
omega(135 -135) =       2508.4  [cm-1]   --> A_u           I
omega(136 -136) =       2509.2  [cm-1]   --> A_g           R
omega(137 -137) =       2510.8  [cm-1]   --> A_g           R
omega(138 -138) =       2511.4  [cm-1]   --> A_u           I
omega(139 -139) =       2512.0  [cm-1]   --> A_u           I
omega(140 -140) =       2512.5  [cm-1]   --> A_u           I
omega(141 -141) =       2514.5  [cm-1]   --> A_g           R
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omega(142 -142) =       2517.0  [cm-1]   --> A_g            R
omega(143 -143) =       2518.3  [cm-1]   --> A_g            R
omega(144 -144) =       2518.8  [cm-1]   --> A_u            I
omega(145 -145) =       2519.6  [cm-1]   --> A_u            I
omega(146 -146) =       2521.9  [cm-1]   --> A_u            I
omega(147 -147) =       2522.8  [cm-1]   --> A_g            R
omega(148 -148) =       2524.0  [cm-1]   --> A_g            R
omega(149 -149) =       2525.3  [cm-1]   --> A_u            I
omega(150 -150) =       2530.0  [cm-1]   --> A_u            I
omega(151 -151) =       2530.5  [cm-1]   --> A_g            R
omega(152 -152) =       2538.6  [cm-1]   --> A_g            R
omega(153 -153) =       2545.5  [cm-1]   --> A_u            I
omega(154 -154) =       2549.8  [cm-1]   --> A_u            I
omega(155 -155) =       2555.6  [cm-1]   --> A_g            R
omega(156 -156) =       2559.1  [cm-1]   --> A_g            R
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References

(1) Caputo, R.; Züttel, A. *Mol. Phys.* **2009**, *107*, 1831–1842.