A Study of the Conformational Isomerism of 1-Iodobutane by High Resolution Rotational Spectroscopy

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Abstract

The first microwave study of 1-iodobutane, performed by Steinmetz et al. in 1977, led to the determination of the $B + C$ parameter for the anti-anti- and gauche-anti-conformers. Nearly 40 years later, this reinvestigation of 1-iodobutane, by high-resolution microwave spectroscopy, led to the determination of rotational constants, centrifugal distortion constants, nuclear quadrupole coupling constants (NQCCs), and nuclear-spin rotation constants belonging to both of the two previously mentioned conformers, in addition to the gauche-gauche-conformer, which was observed in this frequency regime for the first time. Comparisons between the three conformers of 1-iodobutane and other iodo- and bromoalkanes are made, specifically through an analysis of the nuclear quadrupole coupling constants belonging to the iodine and bromine atoms in the respective chemical environments.

Keywords: rotational spectroscopy, nuclear quadrupole coupling tensor, conformations, iodine, haloalkane, FTMW

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Introduction

It has been commonly accepted that the electric field gradient of a nucleus remains unchanged in most simple molecules even as they take on different conformations or as they form van der Waals complexes. A field gradient caused by a charge is proportional to $1/r^3$, where r is the distance from the charge to the nucleus. It is presented by Townes and Dailey[1] and outlined in Gordy and Cook[2], how the field gradient found at a nucleus can be assumed to have been produced by the bonds made by that atom. This analysis was originally for bonding p orbitals, but was later extended to include hybrid orbital contributions by Novick in 2011[3]. This unchanging nature of a field gradient was recently used to correctly determine the structure of HOD–N₂O[4].

The assumption that the field gradient will remain unchanged upon the formation of a complex, conformational change, or isotopic substitution has, of course, exceptions. Choosing N₂O and the complexes it forms as an example[5–16], it was shown repeatedly that there are subtle changes in the electronic environment of near atoms as complexes are formed. For HCCH...N₂O[5, 7], as studied by Leung and coworkers, it was shown that in forming the complex there is a significant change in the electric field gradient of the central nitrogen, while the field gradient at terminal nitrogen remained unchanged. Through molecular multipole analysis, the authors showed that this change is caused by redistribution of electrons about the central nitrogen.

To observe changes in electronic structure from perturbations smaller in magnitude than those observed upon forming a van der Waals complex, such as conformational changes, a more sensitive nucleus is required to act as a probe for this change. Iodine, with its large nuclear electric quadrupole moment, $-69.6(12) fm^2$ [17] for ¹²⁷I, compared to the ¹⁴N value of $2.001(10) fm^2$ [18], makes the observed nuclear quadrupole coupling constants significantly more sensitive to small changes in electron distribution near the iodine nucleus. For example, in a recent study of iodobenzene and the Ne-iodobenzene complex[19], there is a $< 0.3\%$ change in the iodine NQCC upon forming the complex with

neon. We have recently reported a small, but significant, change in electronic structure from carbon-13 isotopic substitution in 2-iodobutane[20].

Continuing a series of studies on the subtle changes in electric structure determined by changes in nuclear quadrupole coupling constants, we report
35 here on the conformational effects on a terminal iodine group in a hydrocarbon chain.

Experimental

The high-resolution rotational spectrum of 1-iodobutane was measured from 7-13 GHz with a chirped-pulse Fourier transform microwave (FTMW) spectrom-
40 eter. Detailed specifications of this spectrometer, which is based on the design of Pate and coworkers[21], have been presented previously[22]. In short, a chosen microwave center frequency, ν , and a 6 μ s linear frequency sweep are mixed from DC to 1 GHz. The resulting radiation, $\nu \pm 1$ GHz, is broadcast directly into a vacuum chamber through a microwave horn antenna. This transmitted
45 radiation then induces a polarization in the coincident molecular beam. A second microwave horn antenna collects the free induction decay (FID) after a 1 μ s delay. With the aid of a Tektronix TDS6124C Digital Oscilloscope, the FID is fast Fourier transformed and directly digitized. A total of 800,000 points, over a time of 20 μ s, are collected from the FID. On average, the molecular rotational
50 transitions have a line width of 80 kHz with an uncertainty of $|8|$ kHz in the center frequency.

The sample was acquired from Sigma-Aldrich[®] ($\geq 99\%$ $\text{CIH}_2\text{CH}_2\text{CH}_2\text{CH}_3$). Further purification was not necessary. The sample (bp 130-131 $^\circ\text{C}$) was contained in a glass U-form tube at room temperature and one atmosphere of dry
55 argon (99.999%, Airgas[®]) was bubbled directly through the liquid. The final mixture of carrier gas and sample was pulsed through a solenoid valve into the chamber, held at an ambient pressure of 10^{-6} Torr, allowing the molecules to undergo supersonic expansion, where the molecules become rotationally cold (1-2 K).

Using a 321G* basis set at the APFD level of theory, a coordinate scan of the C–C–C–C and C–C–C–I dihedral angles was performed, in order to identify the most probable ground state molecular geometries. Three of the lowest energy structures from the scan were optimized at the MP2 level of theory. A 6311G*
65 basis set was imported from the EMSL Basis Set Library[23, 24] specifically chosen to handle the iodine atom, while a 6311G++(2d,2p) basis set was used for the remaining carbon and hydrogen atoms. All calculations were performed with the GAUSSIAN09 Revision D suite[25]. Results from the *ab initio* optimizations are presented in Table 1. Illustrations of the corresponding structures can be
70 found in Figure 1. More on predicting the NQCCs will be discussed in the subsequent sections.

Table 1: Rotational constants and NQCCs for three conformers of 1-iodobutane as determined from *ab initio* optimization at the MP2 level of theory.

Parameters	gg	ga	aa
A (MHz)	6033	7388	15123
B (MHz)	1077	937	706
C (MHz)	1013	867	686
$^{127}\text{I}\chi_{aa}$ (MHz)	-397	-274	-682
$^{127}\text{I}\chi_{bb}$ (MHz)	74	-167	223
$^{127}\text{I}\chi_{cc}$ (MHz)	322	441	459
$^{127}\text{I}\chi_{ab}$ (MHz)	-570	-670	-511
$^{127}\text{I}\chi_{ac}$ (MHz)	-330	-109	0 ^b
$^{127}\text{I}\chi_{bc}$ (MHz)	-226	-104	0
ΔE^a (cm ⁻¹)	385	160	0

^aRelative energies from MP2 optimizations.

^b χ_{ac} and χ_{bc} are zero by symmetry.

Figure 1: Calculated structures of the anti-anti (aa)-, gauche-anti (ga)-, and gauche-gauche (gg)-conformers of 1-iodobutane from an *ab initio* optimization. The C–C–C–C and C–C–C–I dihedral angles for the aa-, ga-, and gg-species were calculated to be 180° , 180° ; 179° , 66° ; and -65° , -63° .

Spectral Assignments

All three of the lowest energy conformers obtained from the *ab initio* investigation were successfully assigned from the rotational spectrum collected in the frequency range of 7-13 GHz. A 70 MHz portion of this spectrum is shown in Figure 2. The three broadband assignments were accomplished with the help of both the AABS package[26] and Pickett’s programs, SPFIT/SPCAT[27, 28]. The final rotational constants, centrifugal distortion constants, NQCCs, and nuclear spin-rotation constants for each conformer can be found in Table 2.

Although there is a large discrepancy between the *ab initio* and experimental NQC tensors belonging to the iodine atom in each of the three species, there is at most only a 7% difference between the rotational constants obtained from the *ab initio* study and those determined experimentally. This seems to suggest that the actual geometries of the three conformers present in the molecular beam are quite similar to those that were calculated, whereas the only agreement in the NQCCs was in the trend of their respective magnitudes.

The poor *ab initio* NQCC values made the first assignment, of the gauche-conformer, quite challenging. In order to make the assignment process more efficient and less tedious, alternate methods of prediction were employed. Taking advantage of the fact that changes in the geometry of the butane chain have

Figure 2: A small portion of the experimental spectrum of 1-iodobutane is shown in black, with the final simulated spectra for the aa-, ga-, and gg-conformers shown below in green, purple, and red, respectively. The quantum numbers associated with each rotational transition are also presented above the experimental spectrum, in the form $J'_{K'_a K'_c} F' \leftarrow J''_{K''_a K''_c} F''$.

Prediction using
hybrid tensor:

Prediction
from fit:

MP2 optimization:

Figure 3: A 100 MHz portion of three different predictions of the rotational spectrum of aa-1-iodobutane. The top orange spectrum is based on a hybrid tensor (discussed in Spectral Assignments) and *ab initio* rotational constants, the middle blue spectrum is the prediction using the experimental results belonging to the aa-conformer, and the bottom orange spectrum is based completely on *ab initio* results.

Table 2: Spectroscopic parameters of 1-iodobutane.

Parameters	gg	ga	aa
A (MHz)	5917.262(13) ^a	7532.3121(18)	15052.043(9)
B (MHz)	1162.2040(14)	970.51215(26)	732.93002(18)
C (MHz)	1082.7921(12)	896.60780(18)	711.34567(20)
D_J (kHz)	0.816(10)	0.2058(24)	0.0459(11)
D_K (kHz)	34.9(38)	45.8(4)	–
D_{JK} (kHz)	-7.18(5)	-4.450(18)	-2.867(17)
d_1 (kHz)	-0.133(12)	-0.0302(6)	–
d_2 (kHz)	–	0.0122(14)	–
χ_{aa} (MHz)	-752.593(28)	-521.973(12)	-1294.041(34)
χ_{bb} (MHz)	157.01(5)	-337.242(15)	380.05(6)
χ_{cc} (MHz)	595.58(6)	859.216(19)	913.99(7)
χ_{ab}^b (MHz)	-1116.74(13)	-1331.251(23)	-1070.28(6)
χ_{ac} (MHz)	-692.17(19)	-226.66(13)	0 ^e
χ_{bc} (MHz)	-460.66(12)	-235.95(6)	0
C_{aa} (kHz)	–	6.4(15)	15(4)
C_{bb} (kHz)	3.43(7)	0.89(27)	1.8(8)
C_{cc} (kHz)	–	1.66(26)	2.7(8)
N ^c	74	198	136
RMS ^d (kHz)	6.4	7.3	6.4

^aNumbers in parentheses give standard errors (1 σ , 67% confidence level)

in units of the least significant figure.

^bThe signs of the off-diagonal nuclear quadrupole coupling constants can not be exactly determined. It is only known that the product of the three, χ_{ab} , χ_{ac} , and χ_{bc} , must be negative. These terms are presented with signs in accordance with the *ab initio* results.

^cNumber of transitions used in the fit.

^dRoot mean square deviation of the fit, $\sqrt{(\sum [(\text{obs} - \text{calc})^2] / N)}$.

^e χ_{ac} and χ_{bc} are zero by symmetry.

a very small effect on the electric field gradient at the iodine nucleus (more on this to come later), the experimental NQC tensor of iodine in the ga-conformer was used to make predictions of the NQC tensors of iodine in both of the two remaining unassigned conformers. This predictive process was simply an exercise

95 in tensor rotation. Using QDIAG[29], the *ab initio* tensors of the two unassigned conformers were diagonalized. In doing this, the rotation matrices, specific to the *ab initio* geometries of these species, were obtained. Then, these respective rotation matrices were used to transform the experimental NQC tensor of the ga-conformer into the inertial axes systems of the gg- and aa-conformers. The

100 resulting hybrid tensors were based on *ab initio* geometries, specific to the unassigned conformers, and experimental NQCCs, belonging to the already assigned ga-conformer. To best illustrate the power of this method, the NQC tensor predictions of the aa-conformer will be used as an example. Equation (1) contains the *ab initio* tensor belonging to the aa-conformer, Equation (2) contains the

105 hybrid tensor, and Equation (3) contains the experimental tensor based only on rotational transitions belonging to the aa-conformer. It is perhaps immediately obvious that the hybrid tensor, again based on the *ab initio* geometry of the aa-conformer and the rotated experimental NQC tensor of the ga-conformer, offers a much better prediction than the purely *ab initio* tensor. To further

110 highlight this point, Figure 3 presents small portions of the rotational spectra corresponding to these respective tensors. It is worth noting here that the similarities between the NQC tensors of iodine in various iodoalkanes, such as iodoethane, t-1-iodopropane, and aa-1-iodobutane, which will be discussed later, suggest that this method can be applied to quite a large range of problems.

115 This method, based on straightforward linear algebra, can lead to very accurate predictions without the need for expensive computations.

It should be noted there are other methods used to make accurate predictions of NQCCs, especially for species with large quadrupoles, as shown by Professor W. C. Bailey[30]. Post-analysis, we received calculations from Professor Bai-

120 ley, which can be found in Table 3 alongside the predictions from our hybrid approach[31, 32]. These calculations involve the calibration of a specific com-

bination of level of theory and basis set, by linear regression, of the calculated
 electric field gradients versus the experimental NQCCs of a selected group of
 molecules. Once calibrated, the specific combination of level of theory and basis
 set can be applied to other systems. Upon comparison of Table 2 and Table 3,
 it can be seen that this method yields excellent results. The differences between
 the hybrid method explained previously and these calculations are small. Al-
 though it is clear that these calculations are quite accurate, the hybrid method
 can rapidly provide good predictions based on very computationally inexpensive
 optimizations.

$$\chi_{MP2} = \begin{pmatrix} -682 & -511 & 0 \\ -511 & 223 & 0 \\ 0 & 0 & 459 \end{pmatrix} \quad (1)$$

$$\chi_{hybrid} = \begin{pmatrix} -1346 & -1019 & 0 \\ -1019 & 462 & 0 \\ 0 & 0 & 884 \end{pmatrix} \quad (2)$$

$$\chi_{exp} = \begin{pmatrix} -1294.041(34) & -1070.28(6) & 0 \\ -1070.28(6) & 380.05(6) & 0 \\ 0 & 0 & 913.99(7) \end{pmatrix} \quad (3)$$

Theory

The hyperfine structure in the rotational spectrum of 1-iodobutane is a con-
 sequence of the nuclear spin of iodine ($I = \frac{5}{2}$), which allows for the observation
 of both nuclear quadrupole coupling and nuclear spin-rotation coupling. The
 respective Hamiltonians, which account for these interactions, were combined
 with both the rigid rotor and centrifugal distortion Hamiltonians. The final
 form of the Hamiltonian then becomes[20, 33–35]:

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_R + \hat{\mathcal{H}}_{CD} + \hat{\mathcal{H}}_Q + \hat{\mathcal{H}}_{SR}. \quad (4)$$

Table 3: Comparison of the two methods of prediction for the NQC tensors in 1-iodobutane.

Parameters	MP2/6311+G(d,p) ^a			Hybrid Method		
	gg	ga	aa	gg	ga ^b	aa
¹²⁷ I χ_{aa} (MHz)	-757	-546	-1317	-706	–	-1346
¹²⁷ I χ_{bb} (MHz)	164	-314	400	104	–	462
¹²⁷ I χ_{cc} (MHz)	593	860	917	602	–	884
¹²⁷ I χ_{ab} (MHz)	-1119	-1336	-1062	-1025	–	-1019
¹²⁷ I χ_{ac} (MHz)	-702	-234	0 ^c	-632	–	0 ^c
¹²⁷ I χ_{bc} (MHz)	-464	-238	0	-367	–	0

^aThese calculations were performed by Professor W. C. Bailey with the calibrated MP2/6311+G(d,p) combination[31, 32].

^bThese values were not predicted via the hybrid method, as the experimental NQC tensor of the ga-conformer was used to make the predictions for the other two conformers. Rather, the NQC tensor presented in Table 1 was used.

^cZero by symmetry.

Quantum labels for the rotational transitions belonging to 1-iodobutane are as follows: $J'_{K'_a K'_c} F' \leftarrow J''_{K''_a K''_c} F''$, where $\mathbf{F} = \mathbf{I} + \mathbf{J}$. The quantum number F is the total angular momentum quantum number that accounts for the coupling between the nuclear spin of iodine and the rotational angular momentum of the molecule.

Discussion

Table 4: Comparison of this work with the previous study of 1-iodobutane.

	Parameters	This work.	Steinmetz et al.[36]
ga	$B + C$ (MHz)	1867.11995(32)	1868.4(30) ^a
aa	$B + C$ (MHz)	1444.27569(27)	1445.3(4)
gg	$B + C$ (MHz)	2244.9961(18)	Not observed.

^aNumbers in parentheses give standard errors (1σ , 67% confidence level) in units of the least significant figure.

For the first time since 1977, 1-iodobutane was reinvestigated via microwave spectroscopy. Table 4 presents a comparison between this study and the work of Steinmetz et al.[36] In the previous low-resolution microwave study, the $B + C$ parameter was measured for the ga- and aa-conformers. Between studies, the measured values of $B + C$ are within 0.07% for both the ga-conformer and aa-conformer. In this study, the gg-conformer was spectroscopically detected in this frequency range for the first time, although previous work[36] did indicate that this species should likely be present in low abundance, as the highest energy conformer of the three.

Due to the flexible nature of this molecule, the three observed conformers possess quite different rotational constants. This is most evident upon noting that the difference between the A rotational constant of the heavy atom planar aa-conformer and the highly asymmetric ga-conformer is over 9100 MHz, as seen in Table 2. As expected, the large structural differences between these

Table 5: NQC tensor of iodine in 1-iodobutane.

Parameters	gg	ga	aa
Energies (cm ⁻¹) ^a	385	160	0
χ_{zz} (MHz)	-1758.57(14) ^b	-1804.133(35)	-1815.72(6)
	-3.15% ^c	-0.64%	—
χ_{yy} (MHz)	1182.40(19)	920.04(9)	901.73(7)
	+31.13%	+2.03%	—
χ_{xx} (MHz)	576.17(16)	884.09(11)	913.99(7)
	-36.96%	-3.27%	—
η_χ ^d	0.34473(15)	0.01993(8)	-0.00675(6)

^aFrom Table 1.

^bNumbers in parentheses give standard errors (1σ , 67% confidence level) in units of the least significant figure.

^cPercentage change relative to the corresponding component of the lowest energy aa-conformer.

^d η_χ is a measure of the asymmetry of the nuclear quadrupole coupling tensor, where $\eta_\chi = \frac{\chi_{xx} - \chi_{yy}}{\chi_{zz}}$.

Table 6: NQC tensor of bromine in 1-bromobutane[37].

Parameters	gg	ga	aa
$^{79}\text{Br} \chi_{zz}$ (MHz)	536.2(5) ^a	539.7(6)	543.45(34)
$^{79}\text{Br} \chi_{yy}$ (MHz)	-264.9(6)	-264.9(20)	-269.5(6)
$^{79}\text{Br} \chi_{xx}$ (MHz)	-271.29(36)	-274.8(15)	-274.0(9)
η_{χ} ^b	-0.0119(13)	-0.018(5)	-0.0083(21)
$^{81}\text{Br} \chi_{zz}$ (MHz)	448.3(47)	451.1(9)	453.95(35)
$^{81}\text{Br} \chi_{yy}$ (MHz)	-222.0(19)	-220.2(23)	-225.5(7)
$^{81}\text{Br} \chi_{xx}$ (MHz)	-226.3(39)	-231.0(19)	-228.4(9)
η_{χ}	-0.01(1)	-0.024(7)	-0.0065(24)

^aNumbers in parentheses give standard errors (1σ , 67% confidence level) in units of the least significant figure.

^b η_{χ} is a measure of the asymmetry of the nuclear quadrupole coupling tensor,

$$\text{where } \eta_{\chi} = \frac{\chi_{xx} - \chi_{yy}}{\chi_{zz}}.$$

Table 7: A comparison of this work with similar haloalkanes.

	iodoethane[38]	t-1-iodopropane[39]	aa-1-iodobutane
$^{127}\text{I}\chi_{zz}$ (MHz)	-1815.22(85) ^a	-1814.55(55)	-1815.72(6)
$^{127}\text{I}\chi_{yy}$ (MHz)	901.71(81)	900.44(47)	901.73(7)
$^{127}\text{I}\chi_{xx}$ (MHz)	913.50(26)	914.12(44)	913.99(7)
η_{χ} ^b	-0.0065(6)	-0.0075(5)	-0.00675(6)
	bromoethane[38]	t-1-bromopropane[40]	aa-1-bromobutane[37]
$^{79}\text{Br}\chi_{zz}$ (MHz)	544.03(168)	541.6(7)	543.45(34)
$^{79}\text{Br}\chi_{yy}$ (MHz)	-270.32(166)	-267.8(7)	-269.5(6)
$^{79}\text{Br}\chi_{xx}$ (MHz)	-273.71(17)	-273.79(4)	-274.0(9)
η_{χ}	-0.0062(34)	-0.0111(12)	-0.0083(21)
	bromoethane[38]	t-1-bromopropane[40]	aa-1-bromobutane[37]
$^{81}\text{Br}\chi_{zz}$ (MHz)	453.91(203)	451.9(7)	453.95(35)
$^{81}\text{Br}\chi_{yy}$ (MHz)	-225.25(201)	223.1(7)	-225.5(7)
$^{81}\text{Br}\chi_{xx}$ (MHz)	-228.65(18)	-228.77(4)	-228.4(9)
η_{χ}	-0.0075(48)	-0.0125(16)	-0.0065(24)

^aNumbers in parentheses give standard errors (1σ , 67% confidence level) in units of the least significant figure.

^b η_{χ} is a measure of the asymmetry of the nuclear quadrupole coupling tensor,

$$\text{where } \eta_{\chi} = \frac{\chi_{xx} - \chi_{yy}}{\chi_{zz}}.$$

three conformational isomers, resulting from differences in the I-C-C-C and C-C-C-C dihedral angles, do not translate to substantial variations in the chemical environment at the iodine nucleus. The most meaningful quantification of the differences between these chemical environments or more specifically, the electric field gradient at the iodine nucleus, can be made through a comparison of the various diagonalized nuclear quadrupole coupling tensors, χ , where χ is a projection of the NQC tensor in the principal axis system of the quadrupolar nucleus (e.g. iodine), as opposed to a projection of the tensor in the inertial axis system of the molecule. The advantage of comparing these diagonalized tensors is that they are all projections into an axis system which is independent of the conformation. Table 5 presents the diagonalized χ tensor of iodine in each conformer. Diagonalization was performed with QDIAG[29]. It should be noted that the χ_{zz} element is the best means of comparison because it is the projection of χ onto the z-axis of the nuclear quadrupole, which is pointed nearly along the C-I bond, whereas the orientation of the x- and y-axis are not known. While the differences in the rotated NQC tensor elements of the three conformers are small, they are never the less significant, as can be seen in Table 5. Upon inspection, only a 3.15% difference between χ_{zz} of the gg- and aa-species is observed, even though the geometry of the alkane chain is drastically different in each case. Even smaller differences in χ_{zz} , of 2.56% and 0.64%, are present when comparing the remaining two pairs of conformers, namely the gg- versus the ga-species, and the ga- versus the aa-species, respectively. This is purely a reflection of the fact that the two latter pairs of conformers possess more similar geometries than the first pair that was mentioned. This indicates that there is hardly a change in the electric field gradient at the iodine nucleus upon rather significant conformational changes.

Similar comparisons, based on a study by Kim et al., between the χ_{zz} element of χ belonging to both ^{79}Br and ^{81}Br in the gg-, ga-, and aa-species of 1-bromobutane were made[37]. These tensors are presented in Table 6. At most, a 0.7% difference between the ^{81}Br gg- and aa-species was determined, which is just over four and a half times less than the percent difference found between

the iodine gg- and aa-species. The greater differences between the χ_{zz} elements
190 of the 1-iodobutane conformers is as expected and can be explained simply by
the fact that iodine is both larger and more polarizable than bromine[41].

Additional comparisons were made between progressively longer haloalkanes,
namely iodoethane, t-1-iodopropane, aa-1-iodobutane, and the corresponding
bromine analogs. These NQCCs are presented in Table 7. In order to complete
195 Table 7, the NQCCs belonging to t-1-bromopropane were measured by high-
resolution microwave spectroscopy because these values could not be found in
the previous work on this species by Sarachman[42]. Table 7 shows clearly that
the NQC tensors of iodine in each of these progressively longer haloalkanes are
identical, within experimental error. Unsurprisingly, additional terminal carbon
200 atoms seem to have a very small effect on the electric field gradient at the iodine
nucleus. Upon investigating the differences in the bromine analogs, the same
conclusion can be realized. Although this does not necessarily present itself as
a surprise, one curious trend did emerge. If closer attention is paid to Table 7,
it can be seen that although the tensors amongst alkanes with identical halogen
205 substituents are the same, within experimental error, the tensors belonging to
iodine, ^{79}Br , and ^{81}Br are in better agreement between the ethane and butane
chains than between the ethane and propane chains or the propane and butane
chains. However, this trend remains inconclusive because the NQCCs belonging
to ^{35}Cl and ^{37}Cl in aa-1-chlorobutane have yet to be obtained. Additionally,
210 NQC tensors belonging to longer iodine- and bromine-containing alkanes have
also yet to be measured, due to the fact that collecting and measuring spectra
for progressively longer haloalkanes becomes more and more challenging.

Conclusion

The reinvestigation of 1-iodobutane by high-resolution microwave spectroscopy
215 in the frequency range of 7-13 GHz led to the determination of rotational con-
stants, centrifugal distortion constants, nuclear quadrupole coupling constants,
and nuclear-spin rotation constants for three low energy conformations. The

full NQC tensor of iodine in each conformation was obtained, which allowed for comparisons to be made between the chemical environments of these conformers,
220 as well as other similar haloalkanes.

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Supplemental Material

230 The final fit outputs for gg-, ga-, and aa-1-iodobutane are provided.

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