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QUANTUM-CHEMICAL ANALYSIS OF COMPLEXES FORMED BETWEEN Ar AND HCl ISOTOPOLOGUES: STUDYING SOLVATION EFFECTS USING AIM, RDG, AND NCI METHODS

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Abstract. In this study, the spectroscopic properties and intermolecular interactions of the HCl molecule and its isotopologues ($H^{35}Cl$, $H^{37}Cl$, $D^{35}Cl$ and $D^{37}Cl$) in a liquid argon (Ar) solvation environment were investigated at the MP2/aug-cc-pVTZ theoretical level. The calculated harmonic vibrational frequencies were corrected using scaling factors of 0.95 for HCl and 0.96 for DCl. The results indicated that the increase in reduced mass due to isotopic substitution (hydrogen to deuterium) leads to an increase in the moment of inertia and a decrease in the rotational constant (B ~ 1/I). It was determined that the HCl molecule retains its rotational motion in the liquid argon medium, and a Q branch is formed under the influence of this environment. Furthermore, it was observed that within the vibrational band range of the DCl molecule, the number of rotational transitions and the intensity of the Q branch for the deuterated isotopologues ($D^{35}Cl$ and $D^{37}Cl$) are higher compared to HCl. AIM, RDG, and NCI analyses confirmed that the interactions for the Ar···HCl complex exhibit a van der Waals character.

Keywords: AIM analysis, DCl, HCl isotopologues, IR spectroscopy, isotope effect, liquid argon, RDG, rotational constant.

Ar va HCl izotopologlari o‘rtasida hosil bo‘lgan komplekslarning kvant-kimyoviy tahlili: AIM, RDG va NCI usullari yordamida solvatatsiya effektlarini o‘rganish

Annotatsiya. Ushbu ishda HCl molekulasi va uning izotopologlari ($H^{35}Cl$, $H^{37}Cl$, $D^{35}Cl$ va $D^{37}Cl$) ning suyuq argon (Ar) solvatatsiya muhitidagi spektroskopik xossalari hamda molekulalararo o‘zaro ta’sirlari MP2/aug-cc-pVTZ nazariy darajada o‘rganildi. Hisoblangan garmonik tebranish chastotalari HCl uchun 0,95 va DCl uchun 0,96 masshtablash koeffitsiyentlari yordamida tuzatildi. Natijalar shuni ko‘rsatdiki, izotop almashinuvi (vodorodning deyteriyga almashishi) natijasida keltirilgan massa ortishi inertsiya momentining oshishiga va aylanish doimiysining kamayishiga olib keladi (B ~ 1/I). Aniqlanishicha, HCl molekulasi suyuq argon muhitida o‘z aylanish harakatini saqlab qoladi va ushbu muhit ta’sirida Q qanot (Q branch) hosil bo‘ladi. Bundan tashqari, DCl molekulasining tebranish diapazonida deyteriylangan izotopologlar ($D^{35}Cl$ va $D^{37}Cl$) uchun aylanish o‘tishlari soni (HCl tebranish diapozonida) hamda Q qanot intensivligi HCl ga nisbatan yuqoriroq ekanligi kuzatildi. AIM, RDG va NCI tahlillari Ar···HCl kompleksidagi o‘zaro ta’sirlar van-der-Vaals tabiatga ega ekanligini tasdiqladi.

Kalit so‘zlar: AIM tahlili, DCl, HCl izotopologlari, IK (IR) spektroskopiya, izotop effekti, suyuq argon, RDG, aylanish doimiysi.

Квантово-химический анализ комплексов, образованных между Ar и изотопологами HCl: исследование эффектов сольватации с использованием методов AIM, RDG и NCI

Аннотация. В данной работе спектроскопические свойства и межмолекулярные взаимодействия молекулы HCl и её изотопологов ($H^{35}Cl$, $H^{37}Cl$, $D^{35}Cl$ и $D^{37}Cl$) в условиях сольватации в жидком аргоне (Ar) были исследованы на теоретическом уровне MP2/aug-cc-pVTZ. Рассчитанные гармонические колебательные частоты были скорректированы с использованием масштабных коэффициентов 0,95 для HCl и 0,96 для DCl. Результаты показали, что увеличение приведённой массы вследствие изотопного замещения (водорода на дейтерий) приводит к увеличению момента инерции и уменьшению вращательной постоянной (B ~ 1/I). Установлено, что молекула HCl сохраняет вращательное движение в среде жидкого аргона, при этом под влиянием данной среды формируется Q-ветвь. Кроме того, было обнаружено, что в диапазоне колебательной полосы молекулы DCl число вращательных переходов и интенсивность Q-ветви для дейтерированных изотопологов ($D^{35}Cl$ и $D^{37}Cl$) выше по сравнению с HCl. Анализы AIM, RDG и NCI подтвердили, что взаимодействия в комплексе Ar···HCl имеют ван-дер-ваальсов характер.

Ключевые слова: AIM-анализ, DCl, изотопологи HCl, ИК-спектроскопия, изотопный эффект, жидкий аргон, RDG, вращательная постоянная.

1. **Introduction.** In recent decades, the study of weak intermolecular interactions has become one of the key research areas in quantum chemistry and molecular spectroscopy [1–3]. In particular, the nature of hydrogen bonding, dipole–dipole, and van der Waals interactions, as well as their contributions to the stability of molecular systems, has been extensively investigated in both theoretical and experimental studies [4–6]. These interactions play an important role in a wide range of phenomena, from biological systems to atmospheric processes [7].

In the literature, weakly bound complexes, especially those isolated in inert gas environments, are considered ideal model systems for studying intermolecular interactions in their "pure" form [8]. In particular, studies on complexes formed with rare gases such as argon, krypton, and xenon have shown that their bonding is primarily governed by dispersion and electrostatic interactions [9,10]. Simple systems such as the Ar···HCl complex provide an excellent opportunity for a detailed analysis of these interactions and serve as important benchmarks for testing the accuracy of theoretical models [11,12].

The diatomic HCl molecule and its isotopologues ($H^{35}Cl$, $H^{37}Cl$, $D^{35}Cl$, $D^{37}Cl$) represent classical model systems for studying vibrational–rotational coupling [13–15]. Previous studies have shown that the infrared spectra, rotational constants, and vibration–rotation interaction constant (α_e) of HCl significantly depend on isotopic substitution [16,17]. In addition, an increase in reduced mass leads to an increase in the moment of inertia, which in turn results in a decrease in the rotational constant [18]. These relationships are clearly reflected in the positions and intensities of spectral lines.

Numerous studies on solvation effects in inert gas media have demonstrated that even very weak intermolecular interactions can significantly influence vibrational frequencies and rotational parameters [19,20]. For example, the formation of a complex between HCl and argon leads to a slight elongation of the H–Cl bond, resulting in a red shift of the vibrational frequency [21]. At the same time, complex formation causes a decrease in the rotational constant and a redistribution of spectral line intensities [22].

From a theoretical point of view, modern quantum chemical methods play a crucial role in the investigation of such systems. In particular, density functional theory and ab initio methods enable accurate determination of molecular geometries, energies, and vibrational properties [23]. The use of

scaling factors to correct calculated vibrational frequencies is a common practice to improve agreement with experimental data [24,25]. For a deeper analysis of intermolecular interactions, Atoms in Molecules and Reduced Density Gradient approaches are widely applied [26–28]. The AIM method allows characterization of bonding based on the topology of electron density [29], whereas the RDG approach provides a visual and quantitative description of weak interactions [30].

Despite these advances, a comprehensive study of the Ar···HCl complex at the level of isotopologues, particularly considering solvation effects using AIM and RDG analyses, remains insufficiently explored. This gap highlights the relevance of the present work.

In this study, the formation of the Ar···HCl complex, along with its structural and energetic properties and the effects of isotopic substitution and solvation, is investigated using quantum chemical calculations. The optimized geometry, binding energy, infrared spectral characteristics, and the nature of intermolecular interactions are analyzed using AIM analysis and RDG analysis methods.

2. **Methods.** In this study, the electronic structure and spectroscopic characteristics of the HCl molecule and its isotopologues were investigated using both experimental measurements and quantum-chemical calculations.

2.1. Experimental and Computational Methods

Experimental investigations were conducted in both the gas phase and liquid Ar solvation environment at a temperature of 90 K using a Fourier-transform infrared (FTIR) spectrometer. The absorption spectra of the samples were recorded with high precision to compare the experimental data with theoretical results. On the computational side, the geometric parameters and vibrational frequencies of all molecular systems were optimized at the MP2/aug-cc-pVTZ level of theory Specifically, harmonic vibrational frequencies were corrected using scaling factors of 0.95 for HCl and 0.96 for DCl. These values are consistent with the standards recommended in the literature for the chosen level of theory.

2.2. Analysis of Spectroscopic Parameters

To evaluate the rotational motion and isotope effects of the molecules, the following physical quantities and relations were calculated:

Reduced mass (M): Determined based on the formula (1)

$$M = \frac{m_1 \cdot m_2}{m_2 + m_1} \qquad (1)$$

Moment of inertia (I): Calculated using the relation (2)

$$I = Mr^2 \qquad (2)$$

Rotational constant (B_e): Found using the equation (3)

$$B_e = \frac{h}{8\pi^2 Ic} \qquad (3)$$

Vibration-rotation interaction: The dependence of the rotational constant on the vibrational quantum number was accounted for via the formula (4)

$$B_\vartheta = B_e - \alpha_e(\vartheta + \frac{1}{2}) \qquad (4)$$

Frequencies for branches: Rotational transition frequencies in the R, Q, and P branches were determined using the following classical relations (5), (6) and (7):

For the R-branch:

$$\nu_R = \nu_0 + 2B' + (3B' - B'')J'' + (B' - B'')(J'')^2 \qquad (5)$$

For the Q-branch:

$$\nu_Q = \nu_0 + (B' - B'') \cdot J \cdot (J+1) \qquad (6)$$

For the P-branch:

$$\nu_P = \nu_0 - 2B'' - (3B'' - B')J' + (B' - B'')(J')^2 \qquad (7)$$

Intensity of spectral lines: The intensity (A) of the rovibrational spectral lines was determined by the population of rotational levels (N_J), concentration (c), and transition probability ($S_{J'' \to J'}$).

The basis set superposition error (BSSE) was taken into account when calculating the binding energy (E_{bond}).

3. Results and discussion.

3.1. Vibrational–Rotational Spectra

The infrared spectra of the HCl molecule isotopologues ($H^{35}Cl$, $H^{37}Cl$, $D^{35}Cl$, $D^{37}Cl$) recorded in liquid argon at 90 K exhibit well-resolved rovibrational structures consisting of P-, Q-, and

R-branches. The presence of a pronounced Q-branch indicates that the rotational motion of the molecules is partially preserved in the cryogenic argon environment.

The infrared spectra of HCl and DCl isotopologues in liquid argon are shown in figure 1.

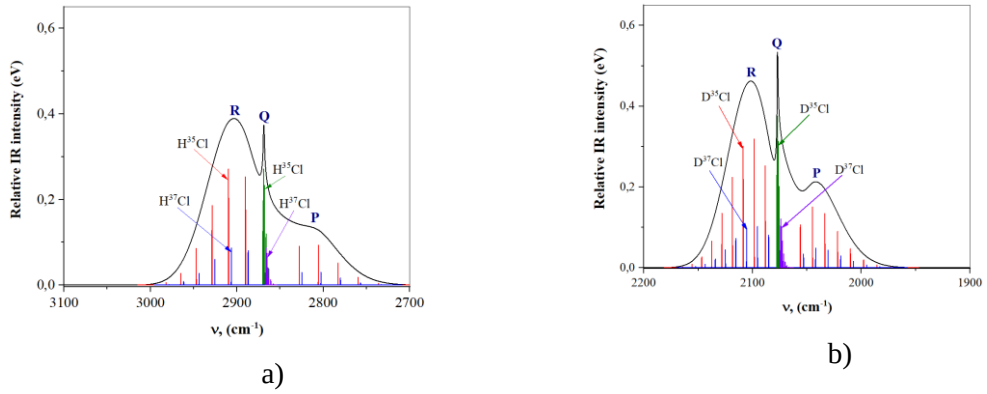

Figure 1. Infrared absorption spectra of HCl (a) and DCl (b) isotopologues calculated in a liquid argon environment at 90 K. The red, blue, green, and purple lines correspond to $H^{35}Cl$ ($D^{35}Cl$) and $H^{37}Cl$ ($D^{37}Cl$) isotopologues, showing the rotational structure in the R-, Q-, and P-branches.

The experimental band centers were determined as $\nu_0(H^{35}Cl) = 2869.93$ cm^{-1}, $\nu_0(H^{37}Cl) = 2866.82$ cm^{-1}, $\nu_0(D^{35}Cl) = 2077.80$ cm^{-1}, and $\nu_0(D^{37}Cl) = 2074.75$ cm^{-1}. The observed isotopic shifts are consistent with the expected dependence of vibrational frequency on reduced mass. Specifically, substitution of hydrogen by deuterium leads to a significant decrease in vibrational frequency due to the increase in reduced mass.

The frequencies and relative intensities of rovibrational transitions for HCl isotopologues are listed in Table 1.

Table 1. Rovibrational transition frequencies (ν, cm^{-1}) and relative intensities (A) for HCl isotopologues in liquid argon at 90 K, corresponding to the R-, Q-, and P-branches of the infrared absorption bands.

	$H^{35}Cl$					
	ν(R)	**A(R)**	**ν(P)**	**A(P)**	**ν(Q)**	**A(Q)**
	2890,142	0,37885	2849,112	0	2869,93	0,189425
	2909,748	0,407362	2827,688	0,135787	2869,324	0,407362
	2928,748	0,279102	2805,658	0,139551	2868,112	0,348878
	2947,142	0,12851	2783,022	0,077107	2866,294	0,179915
	2964,93	0,04072	2759,78	0,027147	2863,87	0,06108
	2982,112	0,008993	2735,932	0,006424	2860,84	0,014132
	2998,688	0,001394	2711,478	0,001046	2857,204	0,002266
	3014,658	0,000152	2686,418	0,000119	2852,962	0,000255
	3030,022	1,18E-05	2660,752	9,47E-06	2848,114	2,01E-05
0	3044,78	6,5E-07	2634,48	5,32E-07	2842,66	1,12E-06
	$H^{37}Cl$					
	2886,974	0,12115	2846,062	0	2866,82	0,060575
	2906,524	0,130268	2824,7	0,043422	2866,216	0,130268
	2925,47	0,089252	2802,734	0,044626	2865,008	0,111565
	2943,812	0,041096	2780,164	0,024658	2863,196	0,057534
	2961,55	0,013022	2756,99	0,008681	2860,78	0,019532
	2978,684	0,002876	2733,212	0,002054	2857,76	0,004519
	2995,214	0,000446	2708,83	0,000334	2854,136	0,000725
	3011,14	4,88E-05	2683,844	3,81E-05	2849,908	8,15E-05
	3026,462	3,78E-06	2658,254	3,03E-06	2845,076	6,43E-06

0	3041,18	2,08E-07	2632,06	1,7E-07	2839,64	3,58E-07
$D^{35}Cl$						
	2088,324	0,37885	2067,052	0	2077,8	0,189425
	2098,624	0,47804374	2056,08	0,159348	2077,576	0,478044
	2108,7	0,45104984	2044,884	0,225525	2077,128	0,563812
	2118,552	0,33563079	2033,464	0,201378	2076,456	0,469883
	2128,18	0,20168768	2021,82	0,134458	2075,56	0,302532
	2137,584	0,09912235	2009,952	0,070802	2074,44	0,155764
	2146,764	0,04014376	1997,86	0,030108	2073,096	0,065234
	2155,72	0,01346276	1985,544	0,010471	2071,528	0,022438
	2164,452	0,00375115	1973,004	0,003001	2069,736	0,006377
0	2172,96	0,00087044	1960,24	0,000712	2067,72	0,001503
$D^{37}Cl$						
	2085,238	0,12115	2064,04	0	2074,75	0,060575
	2095,504	0,153266	2053,108	0,051089	2074,528	0,153266
	2105,548	0,145359	2041,954	0,07268	2074,084	0,181699
	2115,37	0,109004	2030,578	0,065402	2073,418	0,152606
	2124,97	0,066182	2018,98	0,044122	2072,53	0,099274
	2134,348	0,032949	2007,16	0,023535	2071,42	0,051777
	2143,504	0,013552	1995,118	0,010164	2070,088	0,022022
	2152,438	0,004628	1982,854	0,003599	2068,534	0,007713
	2161,15	0,001316	1970,368	0,001053	2066,758	0,002238
0	2169,64	0,000313	1957,66	0,000256	2064,76	0,00054

As shown in Table 1, the rovibrational spectra of HCl isotopologues exhibit well-defined R-, Q-, and P-branch structures. The spacing between adjacent rotational lines decreases for heavier isotopologues, reflecting the increase in moment of inertia and corresponding decrease in rotational constants.

In addition, the Q-branch is clearly observed in the liquid argon environment, indicating partial preservation of rotational motion under cryogenic conditions. The relative intensities show a systematic decrease with increasing rotational quantum number, consistent with the Boltzmann distribution of population levels.

It is also observed that the Q-branch intensity is more pronounced for DCl isotopologues compared to HCl, which can be attributed to differences in rotational level population and reduced mass effects.

Analysis of rovibrational transitions shows that the spacing between spectral lines decreases for heavier isotopologues. This behavior is directly related to the increase in the moment of inertia and the corresponding decrease in rotational constants. As a result, DCl isotopologues exhibit a higher density of rotational lines compared to HCl, which is in agreement with theoretical predictions.

3.2. Rotational Constants and Vibration–Rotation Interaction

The rotational constants for the ground ($B^{//}$) and excited ($B^{/}$) vibrational states were determined from the P- and R-branch transitions. It was found that $B^{/} < B^{//}$ for all isotopologues, indicating an increase in bond length upon vibrational excitation.

The calculated and experimental spectroscopic constants of HCl isotopologues are summarized in Table 2.

Table 2. Spectroscopic constants of HCl isotopologues, including reduced mass (M), moment of inertia (I), equilibrium rotational constant (B_e), rotational constants of the ground ($B^{//}$) and excited ($B^{/}$) vibrational states, and vibration–rotation interaction constant (α_e).

Molecule	M (10^{-24} g)	I (10^{-40} g·cm^2)	B_e (cm^{-1})	$B^{/}$ (cm^{-1})	$B^{//}$ (cm^{-1})	α_e (cm^{-1})
$H^{35}Cl$	1.627	2.65	10.56	10.106	10.409	0.303
$H^{37}Cl$	1.629	2.66	10.53	10.077	10.379	0.302
$D^{35}Cl$	3.162	5.15	5.43	5.262	5.374	0.112
$D^{37}Cl$	3.172	5.17	5.41	5.244	5.355	0.111

As shown in Table 2, an increase in reduced mass from HCl to DCl isotopologues leads to a significant increase in the moment of inertia, resulting in a decrease in rotational constants. Consequently, the rotational structure becomes denser for heavier isotopologues, which is consistent with the observed infrared spectra.

The vibration–rotation interaction constant (α_e) decreases with increasing reduced mass, indicating weaker vibrational–rotational coupling in heavier isotopologues.

The vibration–rotation interaction constants (α_e) were calculated from the differences between $B^{//}$ and $B^{/}$. The obtained values show that α_e decreases significantly upon isotopic substitution (from HCl to DCl), reflecting reduced vibrational–rotational coupling in heavier isotopologues. This trend is consistent with the reduced sensitivity of heavier systems to vibrational excitation.

3.3. Effect of Solvation and Complex Formation

The formation of the Ar···HCl complex leads to noticeable changes in both structural and spectroscopic properties. The optimized geometry shows a weakly bound complex with a nearly linear Cl–H···Ar arrangement.

The optimized structure of the Ar···HCl complex in a liquid argon environment is shown in figure 2.

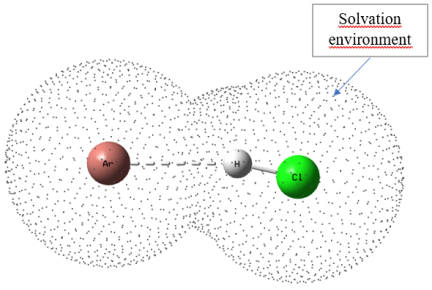

Figure 2. Structure of the Ar···HCl complex in a liquid argon environment.

As shown in figure 2, the argon atom is weakly bound to the hydrogen atom of HCl, forming a van der Waals complex. The interaction is primarily governed by dispersion forces, with no evidence of strong chemical bonding.

The orientation of the argon atom toward the hydrogen end of HCl suggests a weak electrostatic and dispersive interaction rather than a conventional hydrogen bond.

The optimized geometry of the Ar···HCl complex, including bond lengths and angular parameters, is presented in figure 3.

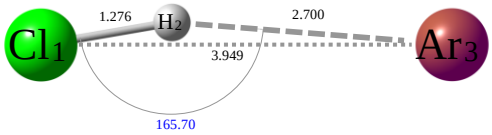

FIGURE 3. Optimized geometry of the Ar···HCl complex in a liquid argon environment. Bond lengths (Å) are shown in black, and the Cl–H···Ar angle (°) is indicated in blue.

The structure exhibits a nearly linear arrangement, characteristic of weak van der Waals complexes.

As shown in figure 3, the optimized geometry of the Ar···HCl complex reveals a weakly bound structure with a nearly linear Cl–H···Ar arrangement. The interaction leads to a slight elongation of the H–Cl bond compared to the isolated molecule, indicating a weakening of the bond upon complex formation.

The orientation of the argon atom toward the hydrogen end confirms that the interaction is primarily governed by dispersion and weak electrostatic forces rather than conventional hydrogen bonding.

While Fig. 2 provides a schematic representation of the complex, Fig. 3 shows the optimized geometry obtained from quantum chemical calculations.

The calculated binding energy ($E_{bind} \approx -0.48$ kcal/mol) confirms that the interaction is very weak and dominated by van der Waals forces.

Complex formation results in a slight elongation of the H–Cl bond, which leads to a red shift in the vibrational frequency. This shift is consistent with the weakening of the H–Cl bond due to interaction with the argon atom. Additionally, the rotational constants decrease upon complex formation, reflecting an increase in the moment of inertia of the system.

3.4. AIM Analysis

The nature of the intermolecular interaction in the complex was analyzed using Atoms in Molecules. A bond critical point (BCP) was identified between the argon atom and the hydrogen (or deuterium) atom of HCl. The electron density at the BCP ($\rho \approx 0.0064$ a.u.) and the positive value of the Laplacian ($\nabla^2\rho \approx 0.0257$ a.u.) indicate a closed-shell interaction typical of weak van der Waals forces.

A more detailed analysis of the topological properties of electron density is presented in figure 4.

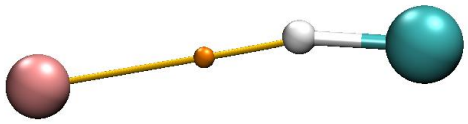

Figure 4. Topological analysis of electron density for the Ar···HCl complex based on Atoms in Molecules. The plots represent the variation of electron density and its Laplacian, confirming the weak, noncovalent nature of the intermolecular interaction.

As shown in figure 4, the electron density at the bond critical point between Ar and H(D) is low, which is characteristic of weak intermolecular interactions. The Laplacian of electron density is positive, indicating a depletion of electron density in the bonding region.

The topological parameters obtained from the Atoms in Molecules analysis are summarized in Table 3.

Table 3. Topological parameters at the bond critical point (BCP) for the Ar···HCl complex and its isotopologues obtained from AIM analysis: electron density ρ(r), Laplacian of electron density $\nabla^2\rho(r)$, kinetic energy density G(r), potential energy density V(r), and total energy density H(r).

Bond	**ρ(r) (a.u)**	**$\nabla^2\rho(r)$ (a.u)**	**G(r) (a.u)**	**-V(r) (a.u)**	**H(r) (a.u)**
Ar···H(D)	0.0064	0.0257	0.0050	0.0036	0.0014

As shown in Table 3, the electron density at the bond critical point is low ($\rho \approx 0.006$ a.u.), which is characteristic of weak intermolecular interactions.

The positive values of the Laplacian ($\nabla^2\rho > 0$) indicate electron density depletion in the bonding region, confirming a closed-shell interaction.

Furthermore, the total energy density H(r) was found to be positive, confirming that the interaction is noncovalent in nature. The similarity of AIM parameters across all isotopologues suggests that isotopic substitution does not significantly affect the nature of the intermolecular interaction, but rather influences the spectroscopic properties.

3.5. RDG and NCI Analyses

Additional insight into the weak interaction was obtained using Reduced Density Gradient analysis. The RDG isosurfaces reveal a green-colored region between Ar and H (or D), which is characteristic of weak dispersive interactions. The corresponding sign(λ_2)ρ values further confirm that the interaction is attractive but weak, consistent with van der Waals bonding.

The nature of intermolecular interactions in the Ar···HCl complex was further analyzed using AIM and RDG methods, as shown in figure 5.

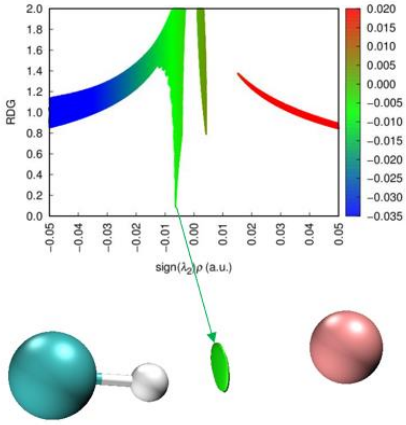

Figure 5. Visualization of intermolecular interactions in the Ar···HCl complex and its isotopologues using Atoms in Molecules and Reduced Density Gradient analyses. The RDG isosurfaces illustrate weak noncovalent interactions, while AIM analysis indicates the presence of bond critical points between Ar and H (or D).

Green regions correspond to weak van der Waals interactions, blue regions indicate attractive interactions, and red regions represent steric repulsion.

As shown in figure 5, the RDG isosurfaces reveal a green-colored region between the argon atom and the hydrogen (or deuterium) atom, which is characteristic of weak van der Waals interactions. No significant blue regions are observed, indicating the absence of strong hydrogen bonding.

The RDG analysis also shows no significant steric repulsion or strong hydrogen bonding features, supporting the conclusion that the Ar···HCl complex is stabilized primarily by dispersion forces.

Overall, the combined experimental and computational results demonstrate that the spectroscopic properties of HCl isotopologues are strongly influenced by both isotopic substitution and solvation effects. While isotopic substitution primarily affects vibrational frequencies and rotational constants, the argon environment induces subtle but measurable changes in molecular structure and interaction characteristics.

The agreement between experimental IR spectra and quantum chemical calculations, including scaled vibrational frequencies, confirms the reliability of the applied computational approach. The combined use of AIM analysis and RDG analysis methods provides a consistent and detailed description of the weak intermolecular interaction in the Ar···HCl complex.

4. **Conclusion.** As a result of the theoretical investigations conducted, the following conclusions were reached regarding the spectroscopic and structural properties of HCl and its isotopologues in a liquid argon solvation environment: The results obtained at the MP2/aug-cc-pVTZ level of theory showed that isotopic substitution (H → D) leads to an increase in the reduced mass of the molecules.

This, in turn, results in an increase in the moment of inertia and a corresponding decrease in the rotational constant (B ~ 1/I). It was determined that HCl and its isotopologues retain their rotational motion in the liquid argon medium, and the formation of a Q branch in the spectrum was identified under the influence of this environment.

It was proved that due to the smaller rotational constant in deuterated isotopologues (DCl), the number of lines corresponding to rotational transitions in their absorption bands and the intensity of the Q branch are higher compared to HCl. The central vibrational frequencies (ν_0) for HCl and its isotopologues were refined using scaling factors (0.95 and 0.96) and aligned with experimental results.

AIM, RDG, and NCI analyses confirmed that the intermolecular interactions in the Ar ··· HCl complex have the same nature for all isotopologues and are characterized as weak van der Waals interactions.It was found that the electron density ($\rho(r)$ = 0.0064 a.u.) and the binding energy (E_{bond} = -0.48 kcal/mol) for the Ar ··· HCl bond remain constant across all isotopologues, indicating that isotopic substitution does not significantly affect the stability of the complex.

The results of this research are of significant scientific importance in studying molecular dynamics and isotope effects in liquid media.

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