Spectroscopic Studies of Gas-Phase ArCH(D) Van der Waals (vdW) Complexes: II. Observation and Analysis of B-X Electronic Transitions of ArCD

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13. ABSTRACT (Maximum 200 words)

The ArCD van der Waals (vdW) complex has been generated in the gas phase by the 248-nm photolysis of $CDBr_3$ entrained in a supersonic jet of argon. Rotationally resolved spectra associated with the complex have been observed by laser-induced fluorescence in the vicinity of the CD $B^2\Sigma$ - $X^2\Pi$ (1,0) band near 366 nm. Bands at 27310.7 cm^{-1} and 27327.8 cm^{-1} are rotationally analyzed using computer simulations and assigned as transitions to the B state $(1,0^0,0)$ and $(1,1^P,0)$ vibrational levels, respectively. The vibronic structure of the ArCD excited states has also been analyzed using a model based on hindered internal rotation. The results are compared to those reported for ArCH.

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1. INTRODUCTION

In recent years, there has been a considerable interest in characterizing van der Waals (vdW) complexes formed by a diatomic radical and a rare-gas atom. Representative studies of such systems are given in references [1–15]. Complexes involving the CH radical are of particular interest. The radical plays an important role in atmospheric and interstellar chemistry and mediates a wide variety of reactive processes in combustion and flames. Numerical modeling of these various environments depends on the measurement and/or theoretical calculation of numerous bimolecular reaction rates involving many different collisional partners. A prerequisite for deriving reaction rates is a representation of the intermolecular potential surface on which the interaction takes place. However, generating a potential function that adequately represents the surface can be quite difficult, particularly for reactive collisions. Spectroscopic investigations of rare gas - CH(D) systems are a step in this direction.

In a recent study, we reported the observation of laser excitation spectra associated with gas-phase ArCH where the electronic states of the complex correlate with the $^1S_0$ state of Ar and the $X^2\Pi_r$ and $B^2\Sigma^-$ states of CH [2]. It was found that the ground state geometry was T-shaped, while the B state was linear. The ground state geometry was inferred based on the similarity between the observed rotational energy level structure and that of bent triatomic molecules. The geometry of the excited state was based on a tentative vibronic assignment and a modeling of the energy separation between the proposed bending levels assuming a hindered internal rotation description [14]. Here, we report the observation and analysis of rotationally resolved spectra of the ArCD vdW complex, excited in the region of the CD $B^2\Sigma^- - X^2\Pi$ (1,0) band. The results are compared to those obtained for the ArCH complex.

2. EXPERIMENTAL

The molecular beam apparatus used to obtain the spectra reported in this report has been described previously [3]. The ArCD complexes were formed via a supersonic free jet expansion. $CDBr_3$ vapor was entrained in Ar gas and expanded into a vacuum chamber through an extender channel mounted on a pulsed valve (Jordan Co.). The backing pressure for the expansion was nominally 100–120 psi. CD radicals were generated in the early stages of the expansion by photolyzing the $CDBr_3$/Ar mixture with the focused output of an excimer laser (Lambda Physik, EMG 150 MSC) operating at 248 nm. (Comparable ArCD signals were obtained using $CDBr_2Cl$ as a precursor.) Typical pulse energy at the photolysis region was approximately 10 mJ. Laser-induced fluorescence was used to probe the ArCD and

CD products in the region of the CD $B^2\Sigma^- - X^2\Pi$ (1,0) band near 366 nm. The probe beam was directed normal to the photolysis laser beam and molecular beam a few millimeters from the extender channel. Tunable laser radiation with a nominal pulse energy of 5 mJ was generated using a XeCl excimer pumped dye laser (Lumonics Hyper EX-400 and Hyper DYE-300) operating with PBD dye. In this wavelength region, the line width of the probe laser is approximately 0.09 cm^{-1}. The ArCD complex was also probed in the vicinity of the CD $B^2\Sigma^- - X^2\Pi$ (0,0) transition near 388 nm, but poor signal-to-noise (S/N) levels precluded an analysis of the rotational energy level structure. Under similar experimental conditions, the S/N ratio for the ArCD complexes probed near the CD (0,0) and (1,0) bands was a factor of 5–10 weaker than that for the ArCH complexes probed near the CH (0,0) and (1,0) bands. The fluorescence from the ArCD transitions excited in the region of the CD $B^2\Sigma^- - ^2\Pi$ (1,0) band was monitored near the CD $B^2\Sigma^- - ^2\Pi$ (1,1) transition centered at 401 nm. The fluorescence was band-pass filtered by a 0.25-m monochromator (McPherson, Model 218) and detected with a photomultiplier tube (EMI-9789-QA). After amplification, the output signal was directed to a gated integrator (Stanford Research Systems) with a PC interface for data acquisition. The spectra were calibrated with a wavemeter (Candela, Model LS-1) whose calibration was crosschecked by measuring the $P_1(1)$ and $R_2(1)$ CH rotational frequencies and comparing them to previously established values [16–17]. Absolute wavenumbers could be determined to ±0.7 cm^{-1}, and wavenumber differences could be measured to 0.09 cm^{-1}.

3. RESULTS/DISCUSSION

Figure 1 presents a survey fluorescence excitation spectrum obtained near the CD $B^2\Sigma^- - ^2\Pi$ (1,0) band. This spectrum has not been corrected for variation in laser intensity or detection sensitivity. The sharp features at low energies are CD B-X (1,0) rotational lines. To the blue of these transitions is a sequence of broad, red-shaded features (A–H) associated with the ArCD complex. A broad continuum is also observed in this region and is presumably associated with bound-free transitions of the complex. At higher resolution, partially resolved rovibronic transitions are observed for features A and B, but not for features C–H.

Good empirical fits of bands A and B were obtained using a model based on Σ-Σ type transitions [2]. In this model, the term values for the ground state rotational energy levels are calculated using the expressions

$$F_1''(N) = B''N(N+1) + 0.5\gamma''N \qquad (1a)$$

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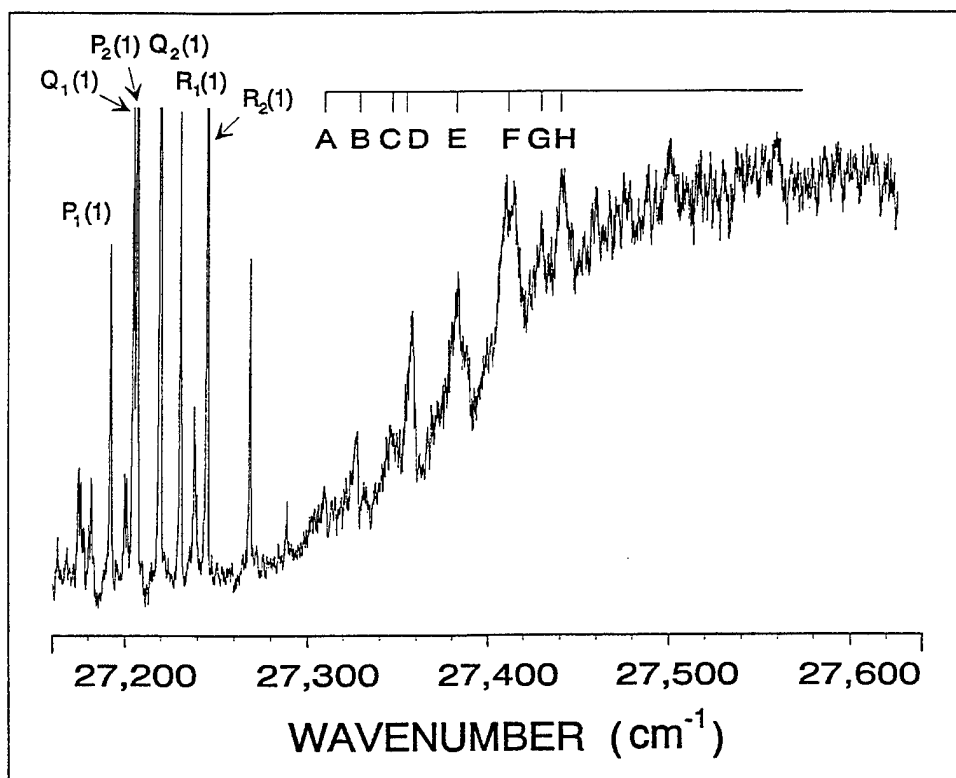
Figure 1. <u>Laser-induced fluorescence scan of ArCD excited near the CD $B^2\Sigma^- - ^2\Pi$ (1,0) band.</u>

and

$$F_2''(N) = B''N(N+1) - 0.5\gamma''(N+1),\tag{1b}$$

where N is an integer quantum number and B is the effective rotational constant. The terms containing γ'' were included to allow for Coriolis coupling related splitting in the ground state. Justification for these functional forms is provided in Lemire et al. [2]. Following the treatment by Chang et al. [9], the excited state term values are given by

$$F_1'(N) = B'N(N+1) + 0.5\mu N\tag{2a}$$

and

$$F_2'(N) = B'N(N+1) - 0.5\mu(N+1).\tag{2b}$$

In equations 2a and 2b, μ may be further expanded as

$$\mu = (\kappa\rho^2/(N(N+1))) + \gamma',\tag{3}$$

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where κ is the coefficient for the spin-rotation term associated with vibronic levels and ρ is the projection of the vibrational angular momentum on the axis of the complex. The selection rule $\Delta N = \pm 1$ leads to six branches, which we label P_1, P_2, P_{12}, R_1, R_2, and R_{12}.

Features **A** and **B** were recorded at an effective resolution of 0.09 cm^{-1}. In contrast to the ArCH B-X spectra, where the R and P branches were clearly observed at this resolution, lower S/N levels prevent a straightforward assignment of these features. Rather, the initial assignment was based on correspondence with the results obtained for ArCH. This procedure is justified because, considered as a pseudodiatom, the reduced masses (μ) of ArCD and ArCH are similar ($\mu_{Ar\text{-}CD} = 10.0$ vs. $\mu_{Ar\text{-}CH} = 9.8$). Thus, the rotational energy level structure and rotational constants of these complexes should be comparable. This is in contrast to the case of CD vs. CH, where the reduced mass of CD ($\mu_{CD} = 1.71$) is much larger than that of CH ($\mu_{CH} = 0.92$), and, consequently, the two have much different rotational energy level separations.

To verify assignments, obtain rotational constants, and determine the band origins, graphical simulations were generated using a multivariable computer program based on the energy level expressions and selection rules given previously, and $\Sigma\text{-}\Sigma$ line strengths. Besides the spectroscopic constants of the ground and excited states, the program variables included the laser line width and the population of the ground state based on a Boltzmann distribution. It was found that the correspondence with ArCH bands was not sufficient to confidently assign the rotational spectra. Thus, it was further assumed that both **A** and **B** originated from the same ground state. This assumption is based on the fact that the complexes were generated in a free jet expansion with a temperature of approximately 10 K.

Figure 2 presents a comparison of the experimentally obtained spectrum for feature **A** and two simulations, labeled S_1 and S_2, based on different rotational assignments. Both simulations reasonably reproduce the band. The simulation labeled S_1 is based on $B'' = 0.172 \pm 0.004$ cm^{-1}, $B' = 0.107 \pm 0.004$ cm^{-1}, and $\gamma'' \leq (\pm)0.019$ cm^{-1}, while S_2 is based on $B'' = 0.168 \pm 0.004$ cm^{-1}, $B' = 0.102 \pm 0.004$ cm^{-1}, and $\gamma'' = (\pm)0.035$ cm^{-1}. Both simulations yield a band origin value of 27310.7 cm^{-1}.

To differentiate between S_1 and S_2, we attempted to simulate feature **B** using the two sets of (B'', γ'') values obtained from the analysis of feature **A**. A better fit of the feature was obtained using the (B'', γ'') values employed in S_1 ($B'' = 0.172 \pm 0.004$ cm^{-1}, $\gamma = 0.019$ cm^{-1}). However, this fit did not reproduce several lines observed from 27,323 through 27,327 cm^{-1}. These "extra" lines may be associated
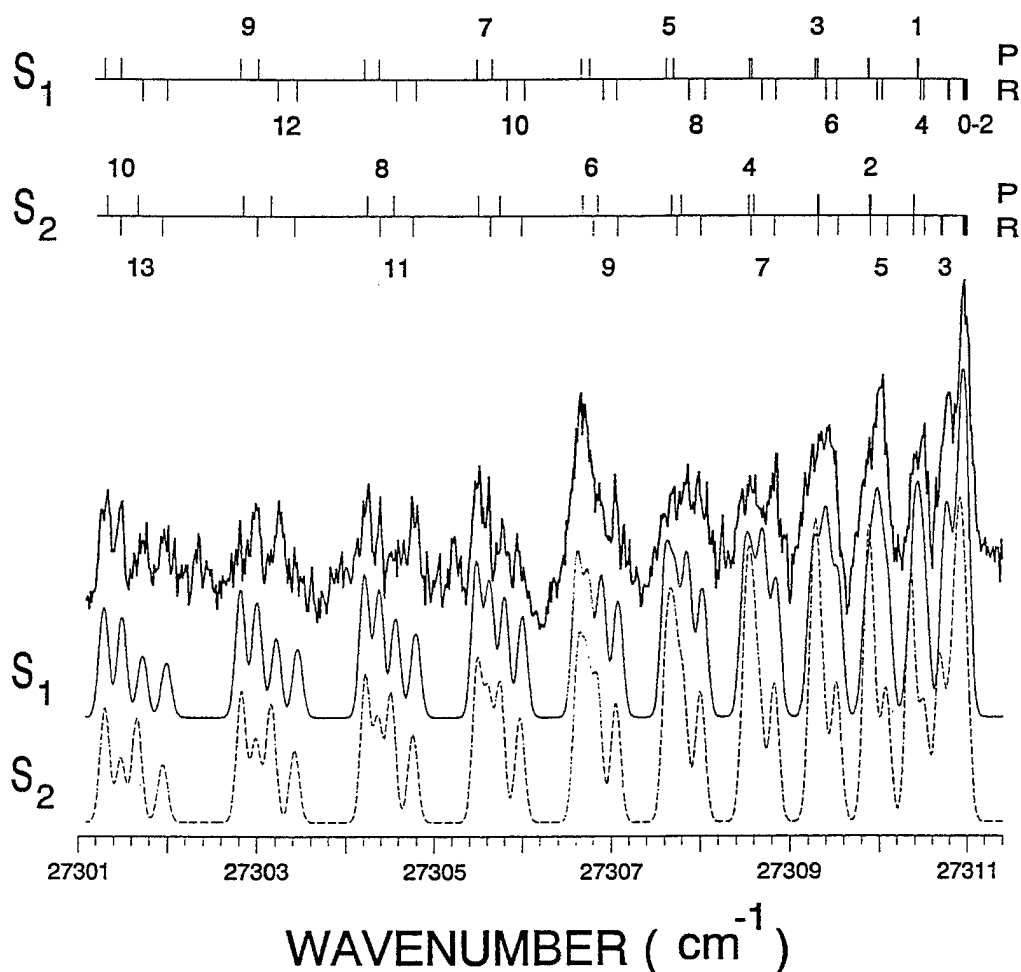
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Figure 2. Laser-induced excitation spectrum and simulations (---) of the feature labeled A in Figure 1 in the region of the CD $B^2\Sigma^--^2\Pi$ (1,0) transitions. (Simulations S_1 and S_2 are based on two different rotational assignments. S_1 yields rotational constant values of $B'' = 0.172 \pm 0.004$ cm^{-1}, $B' = 0.107 \pm 0.004$ cm^{-1}, and $\gamma'' = 0.195$ cm^{-1}; while S_2 yields values of $B'' = 0.168 \pm 0.004$ cm^{-1}, $B' = 0.102 \pm 0.004$ cm^{-1}, and γ''. Both simulations yield a band origin value of 27310.7 cm^{-1}.)

with other products formed in the jet or another ArCD band, so we cannot rule out the assignment based on S_1 on this basis alone. Using $B'' = 0.172$ cm^{-1} and $\gamma'' = 0.019$ cm^{-1}, the best simulation of feature B yields a value of $B' = 0.112 \pm 0.004$ cm^{-1} for the excited state rotational constant and a value of 27327.8 cm^{-1} for the band origin. The ground state B'' values obtained from the analysis of features A and B correspond to an average Ar-CD center of mass separation (R_o'') of 3.13 Å, which is similar to the R_o'' value of 3.11 Å reported for the ground state of the ArCH complex. The R_o' values fall in the range of those reported for ArCH, 3.97–4.61 Å, and indicate that the Ar-CD vdW bond is lengthened upon electronic excitation.

Using the notation (v_1, r^ρ, v_s), where v_1 is the quanta of CD stretch, r is the quanta of bend/hindered internal rotation of CD with respect to Ar, ρ is the projection of the vibrational angular momentum on the intermolecular axis of the complex, and v_s is the quanta of CD-Ar stretch, the features labeled **A** and **B** are assigned as $(1,0^0,0)$ and $(1,1^\rho,0)$, respectively. These assignments are based on a comparison with the results obtained for ArCH. One observation is considered important in this regard: the small but definite increase in the B' value for the higher energy transition. For ArCH, the B' value for the level assigned as $(0,1^0,0)$ was also slightly larger than the B' value for the $(0,0^0,0)$ level (0.114 v. 0.111 cm^{-1}). These results would be realized in the case where the D/H atom points away from the argon atom in the vibrationless state, and introducing the bending/hindered internal rotation reduces the Ar-CD center-of-mass separation. For feature **B**, ρ could not be determined from the rotational analysis. Spectral simulation in which κ was varied over a considerable range ($-2B'' \leq \kappa \leq 2B''$) did not qualitatively affect the fits.

In order to gain further insight into the nature of the ground state intermolecular potential, and aid in the rotational assignment of feature **A,** we have analyzed the spectroscopic data in terms of a general model based on hindered internal rotation which neglects bend-stretch coupling. The model was developed by Dubernet, Flower, and Hutson [14] and later expanded by Chang et al. [9] to include the Coriolis coupling interaction. The intermolecular potential of the complex is modeled by

$$V_{inter} = \Sigma_{l,m}\, V_{l,m}\, (R)C_m^{\,l}\, (\theta,0) = V_{1,0}\, C_0^{\,1}(\theta,0) + V_{2,0}\, C_0^{\,2}(\theta,0) + V_{2,2}\, C_2^{\,2}(\theta,0) + \ldots \qquad (4)$$

where θ is the angle between the monomer and complex axis, and $V_{l,m}$ (R) are coefficients of the renormalized spherical harmonic expansion terms [$C_m^{\,l}\, (\theta,0)$]. These coefficients are varied to reproduce the energy level structure separations observed in the spectra. For the following discussion, we restrict ourselves to expansion terms with $l \leq 2$.

For the ArCH(D) ground state, the geometry of the intermolecular potential is reflected in the Coriolis splitting of the rotational levels. Each end-over-end rotational state (N) correlates with a pair of degenerate, parity doublets $N = J \pm 1/2$. The degeneracy of this state is lifted for $V_{l,m}$ not equal to zero. The energy levels for a $V_{l,m}$ combination were calculated by diagonalizing the effective Hamiltonian derived by Chang et al. [9]. The functional form of the ground state energy levels, equations (1a) and (1b), is particular to the case of a potential dominated by $V_{2,m}$ terms and with $V_{1,0} = 0$. For ArCH, γ'' was observed to be ($\pm$)0.021 cm^{-1}. Assuming that the barriers to hindered internal rotation for the ArCH

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and ArCD complexes are similar, there do not exist expansion coefficients which yield $\gamma''_{ArCH} =$ $(\pm)0.021$ cm^{-1} and $\gamma''_{ArCD} \leq 0.034$ cm^{-1}. Thus, the γ (≤ 0.019 cm^{-1}) obtained from the simulation labeled S_1 is not consistent with equal barriers for ArCH and ArCD in this description. The γ (0.035 cm^{-1}) obtained from simulation S_2 is consistent with this expectation. Plots of the solutions for $\gamma_{ArCH} =$ $(\pm)0.021$ cm^{-1} and $\gamma_{ArCD} = (\pm)0.035$ cm^{-1} are presented in Figure 3. In this figure, the solutions for each case form a closed curve in the $V_{2,0}$–$V_{2,2}$ plane. Agreement between these sets of solutions is only observed at $V_{2,0} = 20$ cm^{-1}, $V_{2,2} = -28$ cm^{-1}, and $V_{2,0} = -28$ cm^{-1}, $V_{2,2} = 28$ cm^{-1}. The uncertainties in $V_{2,0}$ and $V_{2,2}$ are estimated to be approximately ± 7 cm^{-1} and ± 3 cm^{-1}, respectively. It is interesting to note that the solution corresponds to $V_{l,m}$ combination in each set for which $|V_{2,2}|$ is a maximum. Dagdigian et al. [18] have shown that V_{22} is negative for the case of a CH $^2\Pi$ monomer in a π^1 configuration inelastically scattered from a rare gas atom. Thus, the solution $V_{2,0} = 20$ cm^{-1}, $V_{2,2} =$ -28 cm^{-1} describes the intermolecular potential if such an analysis is warranted. Figure 4 shows the ground state A″ and A′ potential energy surfaces corresponding to this solution. While it is recognized that the uncertainty in assigning the rotational structure of feature A leaves room for doubt about this description, the T-shaped geometry for the A″ state and the lack of a barrier to internal rotation for the A′ surface are in agreement with the results obtained from multireference configuration interaction calculations reported by Alexander et al. [19].

4. SUMMARY/CONCLUSION

The ArCD vdW complex has been detected near the CD B$^2\Sigma^-$–$^2\Pi$ (1,0) band by laser-induced fluorescence. Rotationally resolved spectra of the complex have been recorded and analyzed by computer simulations and a model based on hindered internal rotation. The analysis, coupled with the results from spectroscopic and numerical studies of ArCH, indicates that the ground state interaction between CH(D) (X$^2\Pi$) and Ar(^1S_o) has A″ symmetry and has a (global) minimum associated with a (nearly) T-shaped configuration. We anticipate that these results will provide a useful foundation/starting point for future efforts to characterize the potential energy surfaces for reactive collisional (combustion) systems involving the CH radical.
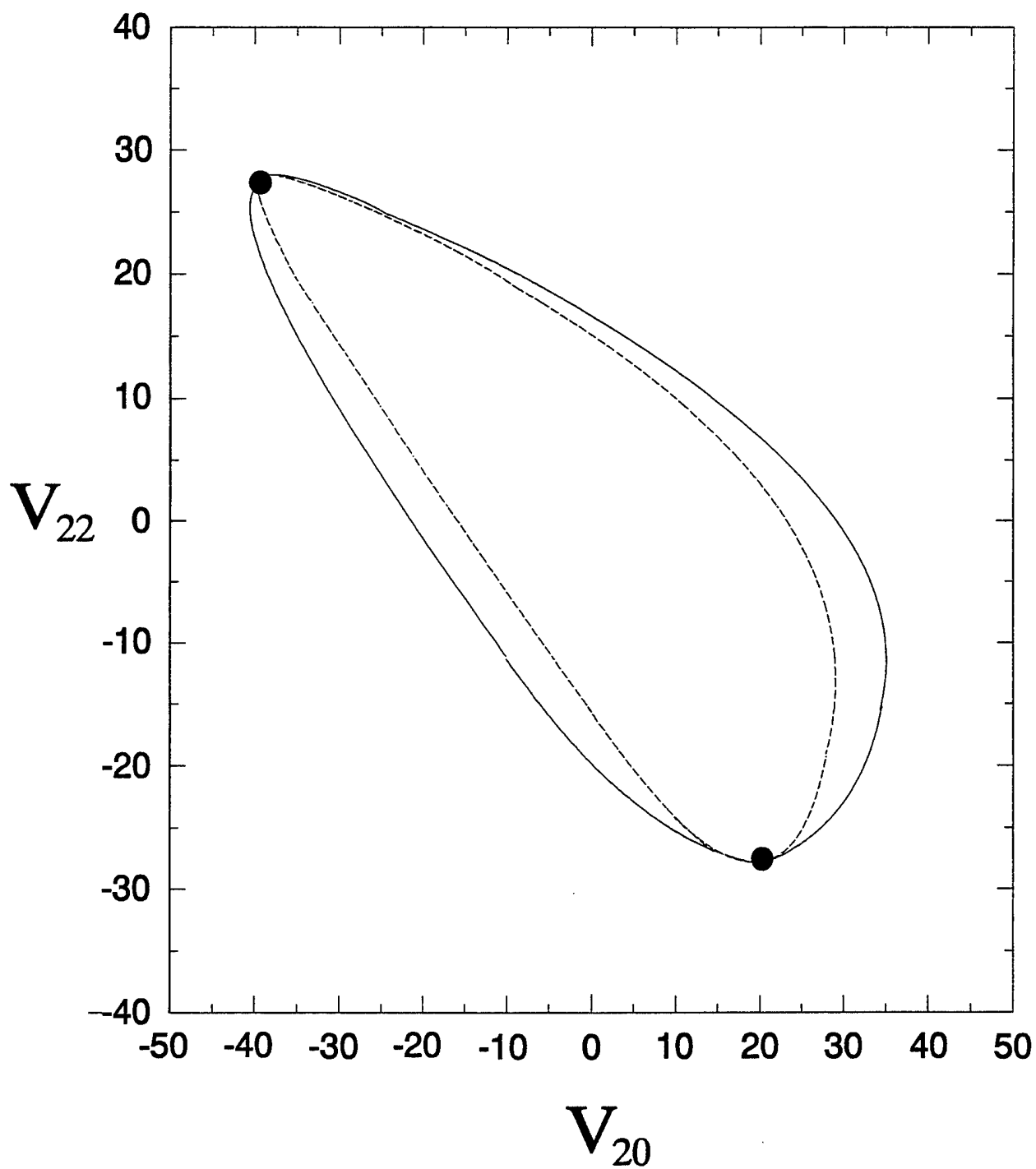
Figure 3. A plot of the $V_{2,0}$ and $V_{2,2}$ coefficients of the renormalized spherical harmonic expansion used to model intermolecular potential.
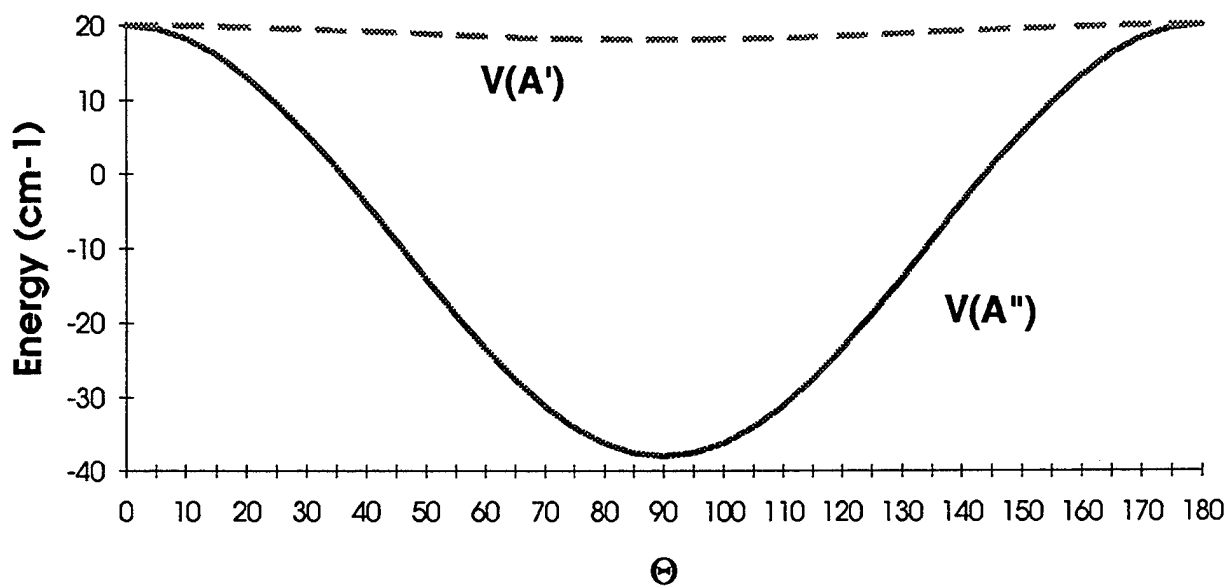
Figure 4. Angular dependence of the ArCH(D) (X,A″) and (X,A′) potential energy surfaces corresponding to $V_{2,0} = 20$ cm^{-1}, $V_{2,2} = -28$ cm^{-1}.

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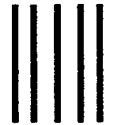**(DO NOT STAPLE)**

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