

Spectroscopic Study of the Ng-CCl₄, O₂-CCl₄, D₂O-CCl₄ and ND₃-CCl₄ Systems.

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INTRODUCTION

The investigation of dispersion events between carbon tetrachloride molecules (CCl₄) and other atomic and molecular species have been motivated for several reasons¹. In a short way, it is observed that the interaction between CCl₄ and another atom/molecule is characterized by a van der Waals component, since that the polarizability value of CCl₄ ($\alpha = 10, 5 \text{ \AA}^3$) is expected to be much more elevated than a one of a heavy atom, for example ($\alpha = 4,04 \text{ \AA}^3$ for xenon). The CCl₄ molecule shows a high symmetry structure without permanent dipole momentum. In this work we calculated the rovibrational energies and spectroscopic constants of the carbon tetrachloride with a few atoms and molecules systems, such as He-CCl₄, Ne-CCl₄, Ar-CCl₄, O₂-CCl₄, D₂O-CCl₄ and ND₂-CCl₄.

POTENTIAL ENERGY CURVES

The Improved Lennard-Jones model (ILJ)¹, found to be suitable to formulate $V(R)$ for several systems of different nature and at increasing complexity, stands out as an interesting model that eliminates most of the original LJ model inadequacies, particularly those from short and long range. This is accomplished in an elegant fashion through the consideration of a single extra parameter. The ILJ potential functions is given by

$$V(r) = \epsilon \left[\frac{6}{n(r) - 6} \left(\frac{r_m}{r} \right)^{n(r)} - \frac{n(r)}{n(r) - 6} \left(\frac{r_m}{r} \right)^6 \right]$$

$$n(r) = \beta + 4 \left(\frac{r}{r_m} \right)^2$$

where, ϵ is the depth of the potential well, r_m the equilibrium distance and $\beta=9$ is a experimental parameter.

RESULTS AND DISCUSSION

Using the ILJ, we obtain the potential energy curves (PEC) for each considered complexes. The spectroscopic constant calculations were

determined by using two different approaches: Discrete Variable Method (DVR) and Dunham's method.

System	Method	ω_e	$\omega_e x_e$	$\omega_e y_e$	α_e	γ_e
He-CCl ₄	DVR	-	-	-	-	-
	Dunham	30.96	9.16	0.24	0.04	0.0002
Ne-CCl ₄	DVR	21.41	2.10	0.03	5.56E-07	-1.86E-08
	Dunham	21.35	2.04	0.01	0.003	6.59E-06
Ar-CCl ₄	DVR	25.58	1.10	0.005	-1.87E-07	-2.88E-08
	Dunham	25.57	1.10	0.004	0.0008	7.26E-07
O ₂ -CCl ₄	DVR	28.06	1.32	0.007	-1.12E-07	-1.00E-08
	Dunham	28.05	1.32	0.005	0.001	1.03E-06
D ₂ O-CCl ₄	DVR	39.72	2.17	0.01	-7.65E-07	-2.70E-09
	Dunham	39.70	2.15	0.01	0.002	2.25E-06
ND ₂ -CCl ₄	DVR	38.34	1.98	0.01	-1.25E-07	-1.75E-08
	Dunham	38.33	1.97	0.009	0.001	1.84E-06

From Table above, one can see an excellent agreement between the Dunham and DVR methods. One another fact that deserves special attention is that the greater contribution of harmonic part (ω_e) happens for the D₂O-CCl₄ massive system.

CONCLUSIONS

In this work, we presented the rovibrational energies and the spectroscopic constants for the systems formed between carbon tetrachloride and others atoms and molecules. Our calculations were based on potential energy curves obtained through molecular beam scattering experiments. The vibrational energy level distribution followed the pattern qualitatively expected from the nature of each system. Furthermore, it was observed that the H₂O₂-He system can remain bonded (only one vibrational state) even with a small depth of the potential well.

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¹ L.F. Roncaratti, Quantum effects in molecular scattering experiments: Characterization of the interaction in weakly bound complexes. Università Degli di Perugia, 2009.