LIF excitation and emission spectra of CdAr van der Waals complexes: Novel possibilities

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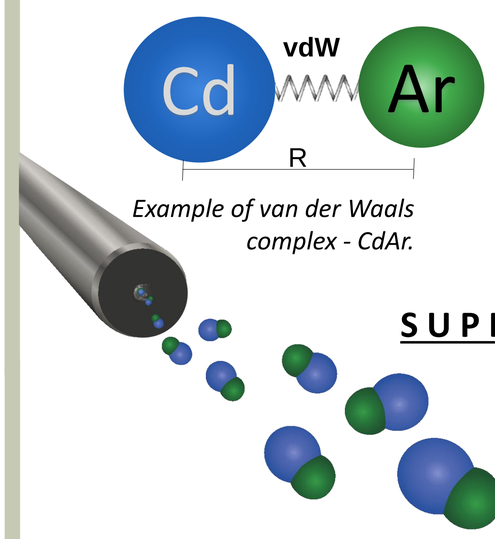
van der Waals complexes in supersonic beam



Example of van der Waals complex - CdAr.

VAN DER WAALS COMPLEXES

van der Waals (vdW) diatomic complexes constitute the simplest model for theoretical and experimental studies of vdW interactions [1].

SUPERSONIC BEAM

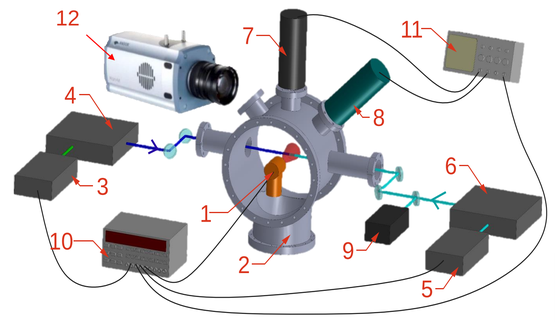
The supersonic expansion technique provides a source of rotationally and vibrationally **cold molecules** which are weakly bound in their **ground** states. It is widely used method in laser spectroscopy of molecules [1].

Experimental scheme

Two types of detection are used in the experiment:

→ **Excitation spectra**
Photomultipliers to measure total laser induced fluorescence (LIF) signal

→ **Emission spectra**
Spectrograph with CCD camera (working range 200 – 975 nm)



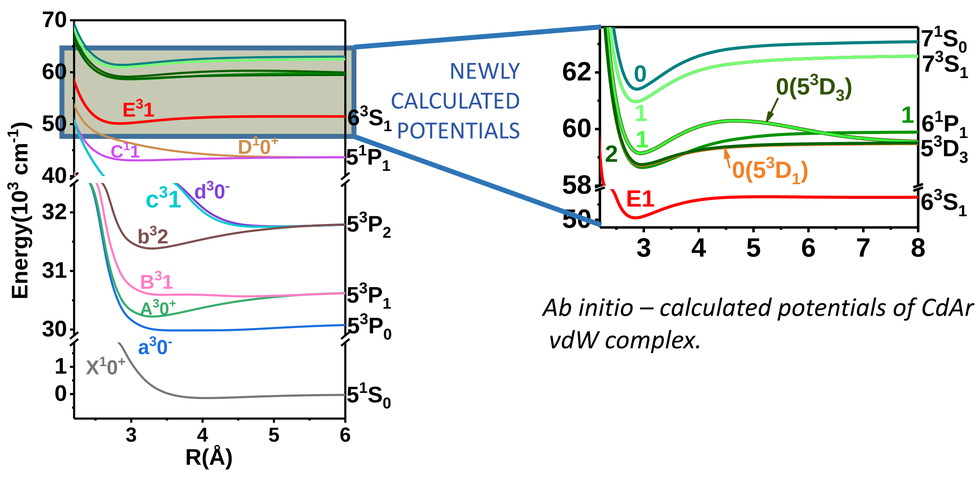
Experimental scheme used in excitation and emission spectroscopy of CdAr vdW complexes in supersonic beam using optical – optical double resonance (OODR) method [3].

1	pulsed source of molecular beam	10	digital delay generator
2	vacuum chamber	11	oscilloscope
3,5	pulsed Nd : YAG laser	12	spectrograph with CCD camera
4,6	tuneable dye laser		
7,8	photomultipliers		
9	wavemeter		

Ab initio potentials of CdAr complex

Novel potential curve of the **$E^3 1(6^3S_1)$** Rydberg state of **CdAr** vdW complex was calculated by *ab initio* method [2].

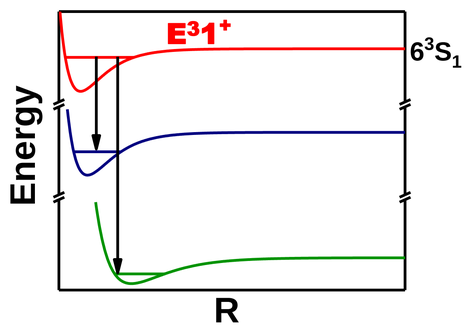
The main goal of the presented work is to determine these Rydberg - state potentials experimentally employing both LIF excitation and emission spectra, and verify accuracy of the ab initio method.



Ab initio – calculated potentials of CdAr vdW complex.

Using results of ab initio calculations, two experimental approaches were analyzed.

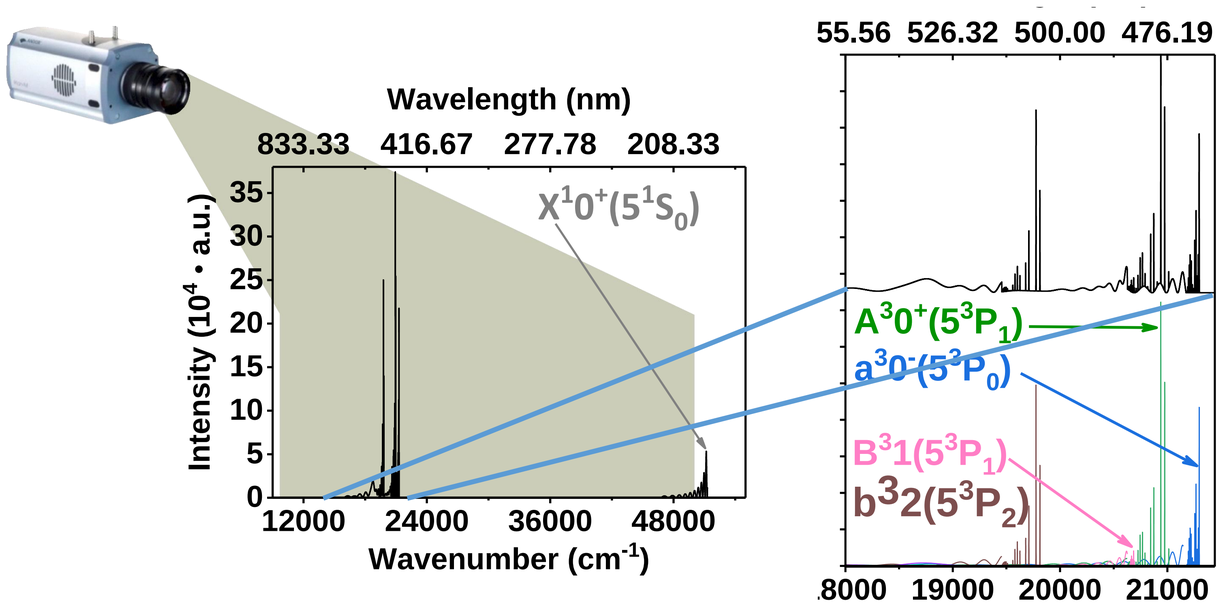
Emission from the $E^3 1(6^3S_1)$ state



Both **bound→bound** and **bound→free** transitions from the inner well of the **$E^3 1$** (v'=13) state in **$^{112}Cd^{40}Ar$** have been simulated using **LEVEL** [4] and **BCONT** [5] programs, respectively.

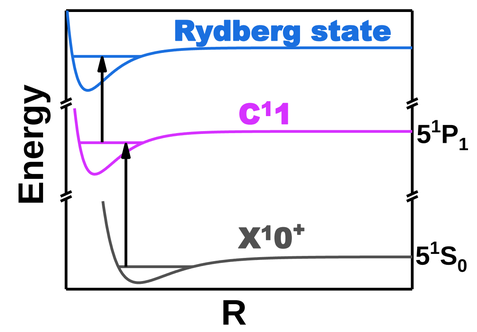
Four transitions are able to observe using spectrograph (Andor model ME5000):
$E^3 1$ →
$A^3 0^+$, **$a^3 0^-$**, **$B^3 1$**, **$b^3 2$**

Intensity of the **$E^3 1$** → **$B^3 1$** transition is reduced because of low value of **transition dipole moment (TDM)** function.



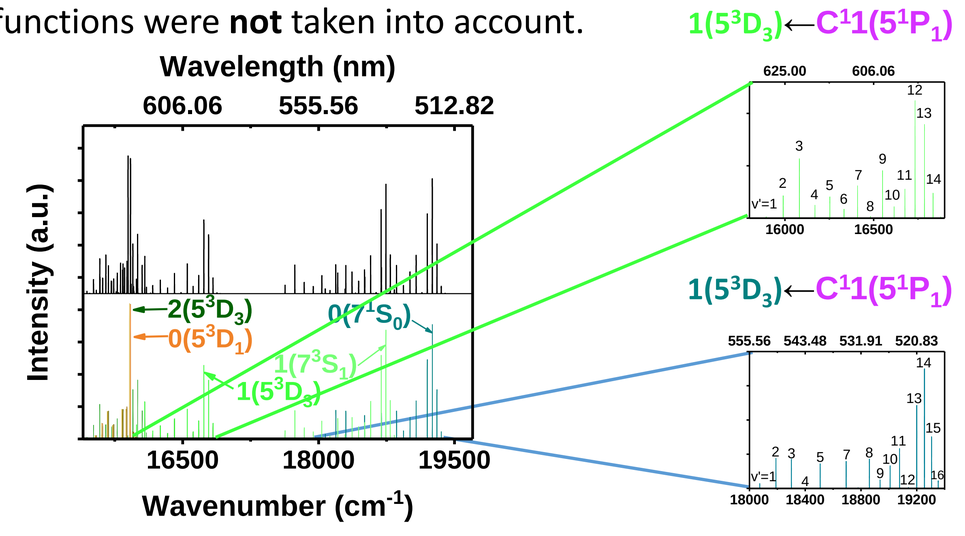
*Simulation of emission from the **$E^3 1$** state of CdAr complex. Working range of CCD camera is shown on the picture.*

Excitation to Rydberg *via* the $C^1 1(5^1P_1)$ state



A few possibilities of excitation to Rydberg states of CdAr complex using OODR method *via* the **$C^1 1$** state has been simulated using **LEVEL** [4] program.

Only **Franck – Condon** factors have been taken into consideration for calculation of intensity of transitions. Transition dipole moment functions were **not** taken into account.



Conclusions

Emission from the $E^3 1$ state: it is possible to obtain the shape of **repulsive part of the $b^3 2$ state** on the basis of spectra of bound – free transitions.

Excitation through the $C^1 1(5^1P_1)$: $1(5^3D_3) \leftarrow C^1 1$ and $0(7^1S_0) \leftarrow C^1 1$ transitions are available to obtain experimentally.

References

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