VAN DER WAALS MOLECULES CONSISTING OF AGGRESSIVE ELEMENT Zn: TOWARDS HIGH RESOLUTION

UNIWERSYTET JAGIELLOŃSKI W KRAKOWIE

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Zn_2 MOLECULE

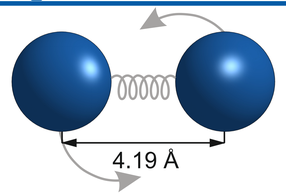

FIG. 1. Scheme of Zn_2 molecule. Equilibrium distance in its ground state is marked.

As 12-group metal, **zinc** is characterised by closed-shell electronic configuration and it is a good candidate to form **van der Waals molecules**. However, due to experimental difficulties, **Zn_2** has been less intensively investigated as compared with Hg_2 and Cd_2 [1].

Due to extremely low dissociation energy of **Zn_2** (242 cm^{-1} in its ground state [2]), spectroscopy of the molecule requires rotational and vibrational cooling. In our laboratory, **cooling molecules in supersonic beam** is applied.

Zn_2 POTENTIAL

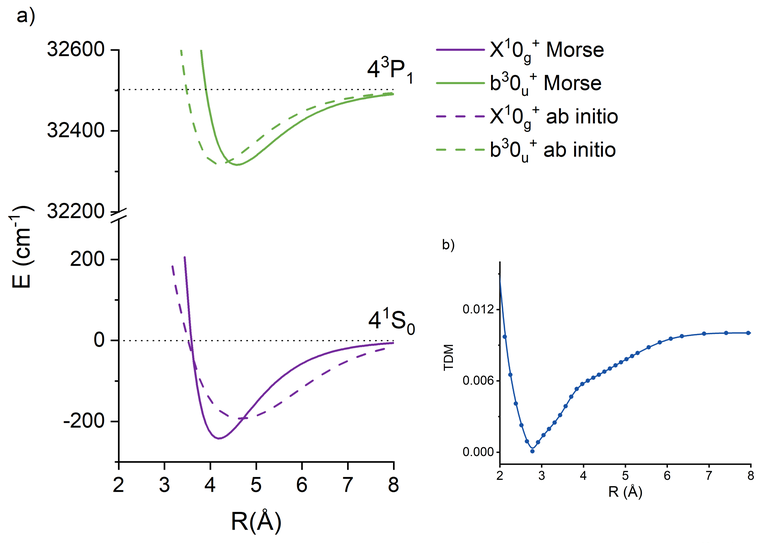

FIG.2. a) Morse (solid lines) and *ab initio* calculated (dashed lines) potentials of the $b^3 0_u^+ (4^3P_1)$ and $X^1 0_g^+ (4^1S_0)$ states in Zn_2. Both ab initio and Morse potential of the $X^1 0_g^+ (4^1S_0)$ are from [2]. Parameters of Morse potential of the $b^3 0_u^+ (4^3P_1)$ are from current study (see Table 1). b) *Ab initio* calculated transition dipole moment for the $b^3 0_u^+ (4^3P_1) \leftarrow X^1 0_g^+ (4^1S_0)$ transition.

ACKNOWLEDGEMENTS

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EXPERIMENTAL SETUP

Difficulties in obtaining zinc vapours under sufficient partial pressure:

- **high melting point of zinc** (692.7 K)
- **degradation of stainless-steel elements** in contact with zinc

construction of new source-module of molecular beam

DETAILS ABOUT DESIGN OF THE SOURCE-MODULE FOR AGGRESSIVE ELEMENTS ARE INCLUDED IN POSTER **N15**: *SUPERSONIC MOLECULAR BEAM SOURCE-MODULE FOR MOLECULES CONSISTING OF HIGHLY AGGRESSIVE ELEMENTS.*

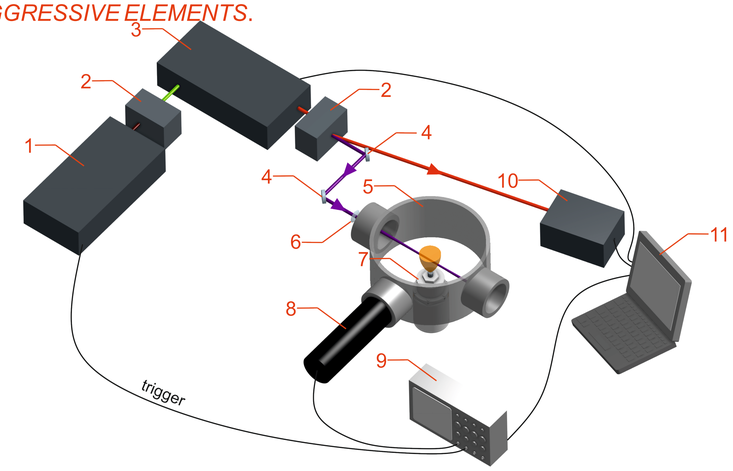

FIG. 3. Experimental set-up for LIF excitation spectroscopy of Zn_2 produced in supersonic molecular beam. 1) Nd+:YAG laser, 2) second harmonic generator, 3) pulsed dye laser, 4) mirror, 5) vacuum chamber, 6) lens, 7) source-module, 8) photomultiplier, 9) oscilloscope, 10) wavemeter, 11) computer.

RESULTS

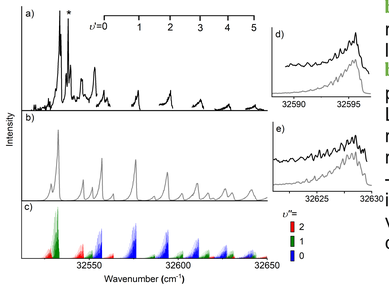

FIG. 4. a) Experimental LIF excitation spectra of the $b^3 0_u^+ (4^3P_1) \leftarrow X^1 0_g^+ (4^1S_0)$ transition in **Zn_2** recorded using new source-module. Unidentified line is marked with an asterisk. b) Simulation of the $b^3 0_u^+ (4^3P_1)$, $\upsilon' \leftarrow X^1 0_g^+ (4^1S_0)$, υ'' transitions with parameters: T_{vib} =150K, T_{rot}=10K, Gaussian and Lorentzian convolutions 0.1 cm^{-1} (FWHM) of rotational components, Morse-function representation for the $b^3 0_u^+ (4^3P_1)$ and $X^1 0_g^+ (4^1S_0)$ - state potentials. c) Intensities of all individual Zn_2 isotopologue components within each of the $\upsilon' \leftarrow \upsilon''$ vibrational band (see colour legend) which constitutes the shaded profiles in b).

BIRGE - SPONER PLOT

The excited-state vibrational frequency (ω_e') and anharmonicity ($\omega_e' x_e'$) were determined using a Birge-Sponer (BS) plot method and were somewhat different from those obtained previously (see Tab.1).

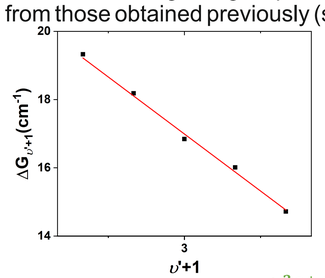

Fig.5. Birge - Sponer plot for the $b^3 0_u^+ (4^3P_1)$ state in Zn_2.

Table 1. The $b^3 0_u^+ (4^3P_1)$ and $X^1 0_g^+ (4^1S_0)$ - state potentials in Zn_2.

	$b^3 0_u^+ (4^3P_1)$	$X^1 0_g^+ (4^1S_0)$
ω_e (cm^{-1})	**20.3±0.1** [a] 20.6±0.1 [b]	25.90±0.45 [b]
$\omega_e x_e$(cm^{-1})	**0.557±0.020** [a] 0.58±0.01 [b]	0.69±0.03 [b]
R_e(Å)	4.58±0.01 [b]	4.19±0.01 [b]

[a] This work
[b] Strojecki et al. [2]

ROTATIONAL PROFILES

FIRST DETECTION OF ROTATIONAL PROFILES IN Zn_2

Simulations of the experimental LIF excitation spectra were performed using **LEVEL** [3] (vibrational structure) and **PGOPHER** [4] (rotational structure) packages.

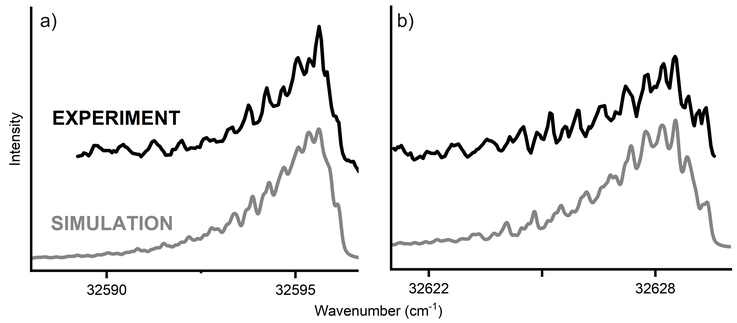

FIG.6. Experimental (black) and simulated (gray) rotational-isotopologue structure of b) υ'=2← υ''=0 and e) υ'=4← υ''=0 bands. Details related to simulations are described in caption of Fig. 4.

REFERENCES

[1] J. Dudek, K. Puczka, T. Urbańczyk and J. Koperski, *High-temperature continuous molecular beam source for aggressive elements: an example of zinc*, in preparation

[2] M. Strojecki, M. Ruszczak, M. Krośnicki, M. Łukomski, and J. Koperski, Chem. Phys. **327**, 229 (2006).

[3] R.J. Le Roy, J. Quant. Spectrosc. Radiat. Transf. **186**, 167 (2017)

[4] C.M. Western, J. Quant. Spectrosc. Radiat. Transf. **186**, 221 (2017)