SPECTROSCOPIC CHARACTERIZATION OF Be_2^+ ($X^2\Sigma_u^+$) AND THE IONIZATION ENERGY OF Be_2

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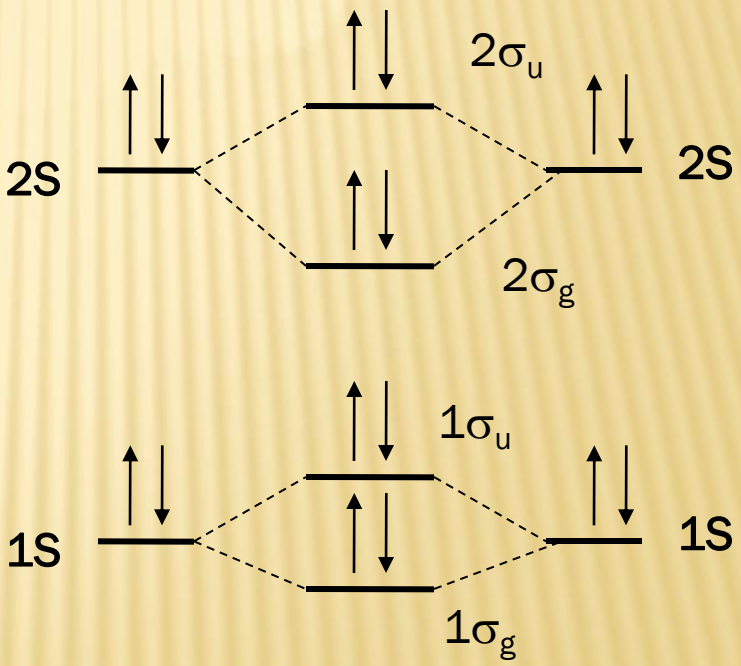
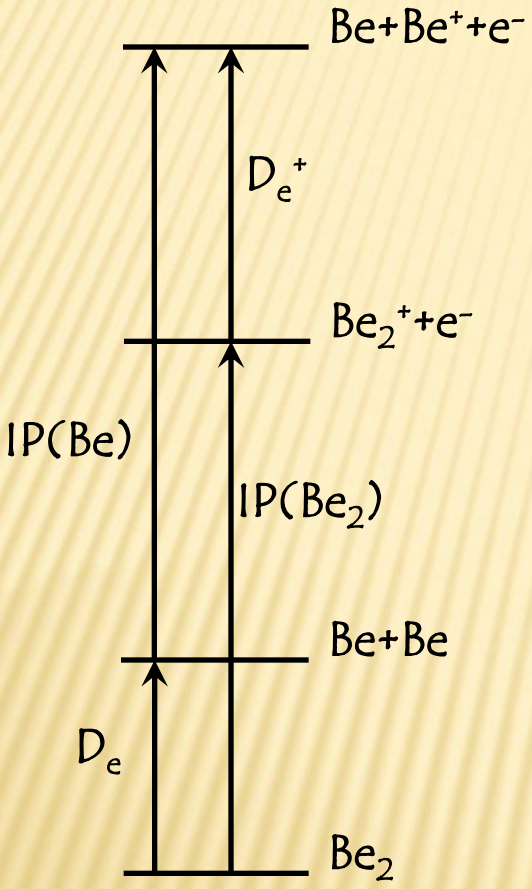
Why? Be dimer is a very complicated system...

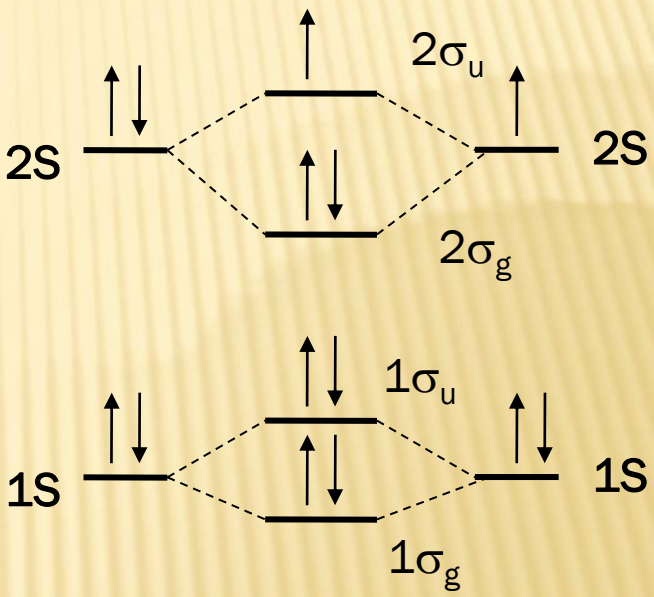
	D_e (cm^{-1})	R_e (Å)	w_e (cm^{-1})
Ar_2	92	3.83	26
Mg_2	430	3.97	51
Be_2	929.7	2.45	275.8
Li_2	8440	2.67	351



Early controversy over an inner "deep" minimum or an outer shallow minimum.

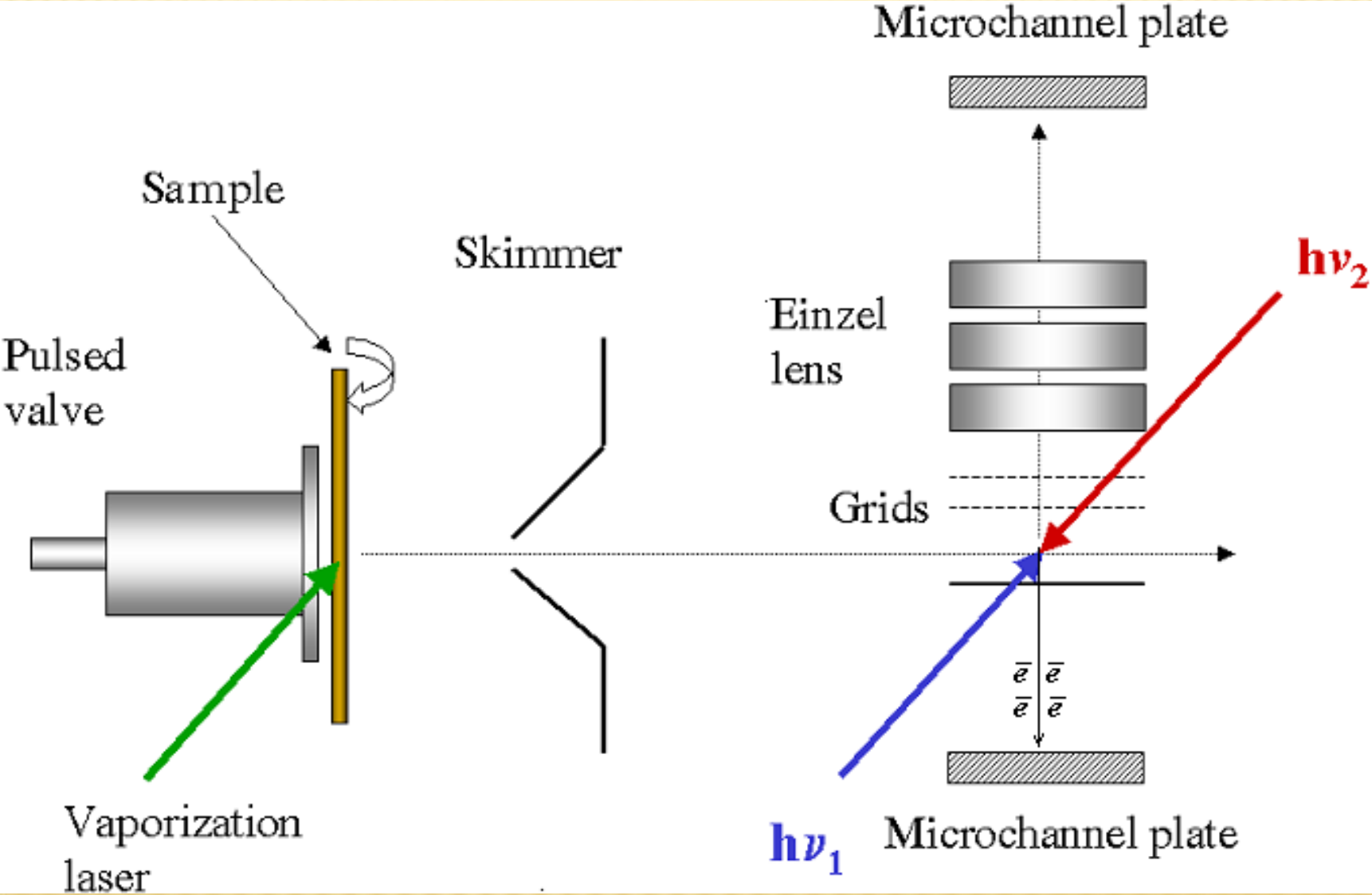
Why + ?



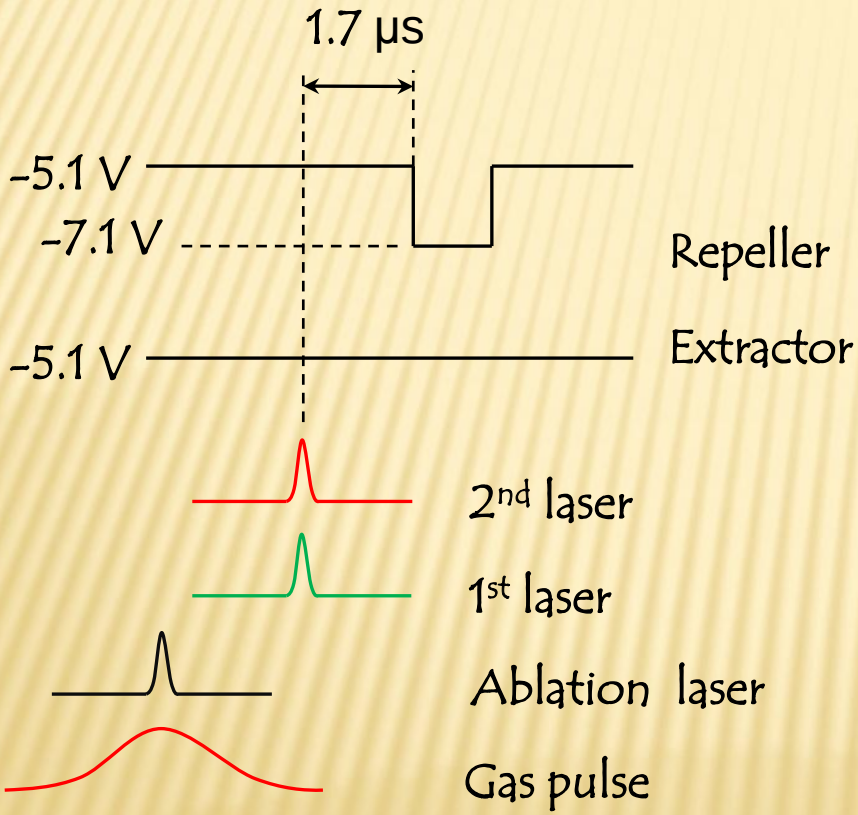


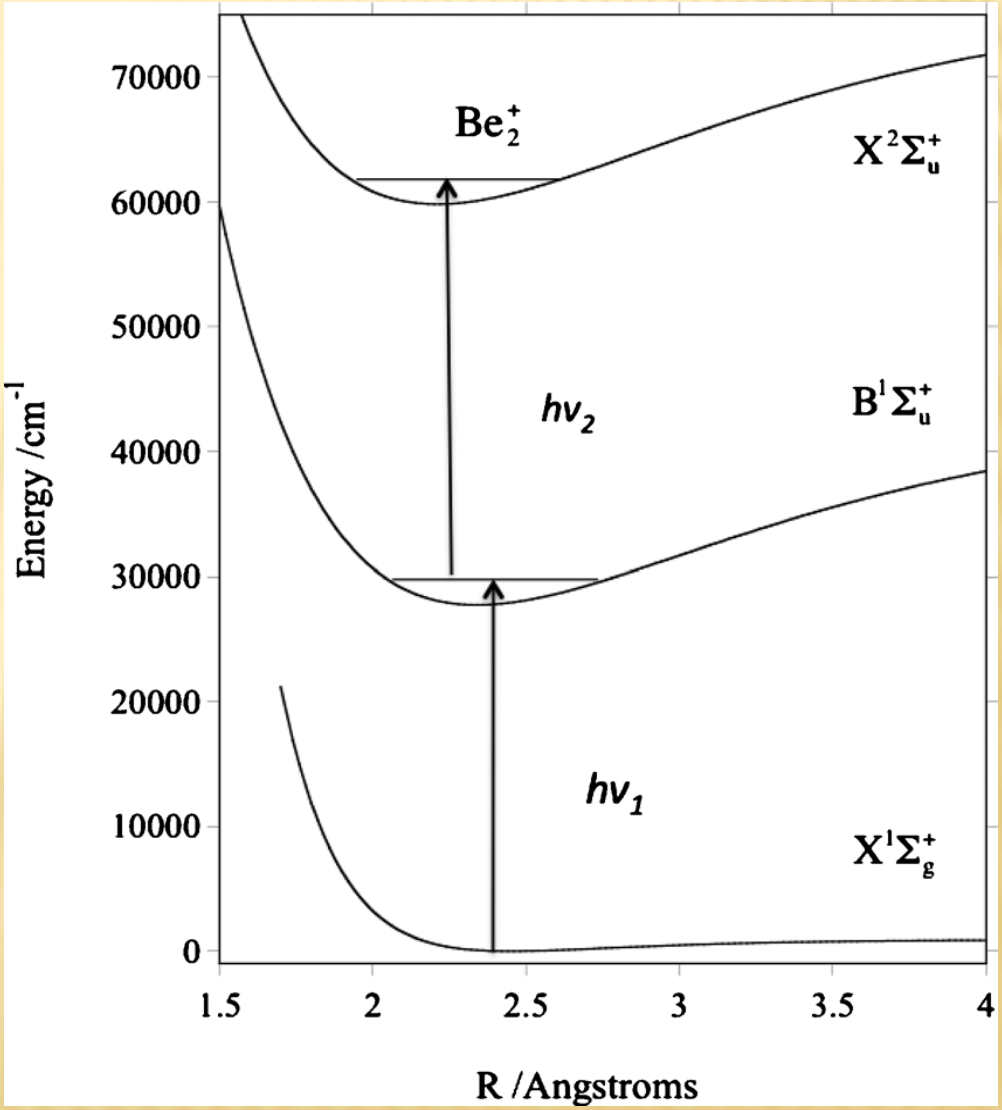
	D_e^+ (cm^{-1})	R_e (Å)	$\Delta G_{1/2}$ (cm^{-1})
Be_2^+ exp	16321(40)		498(20)
Be_2^+ theor	16684	2.211	516

Mass-selected REMPI spectrometer

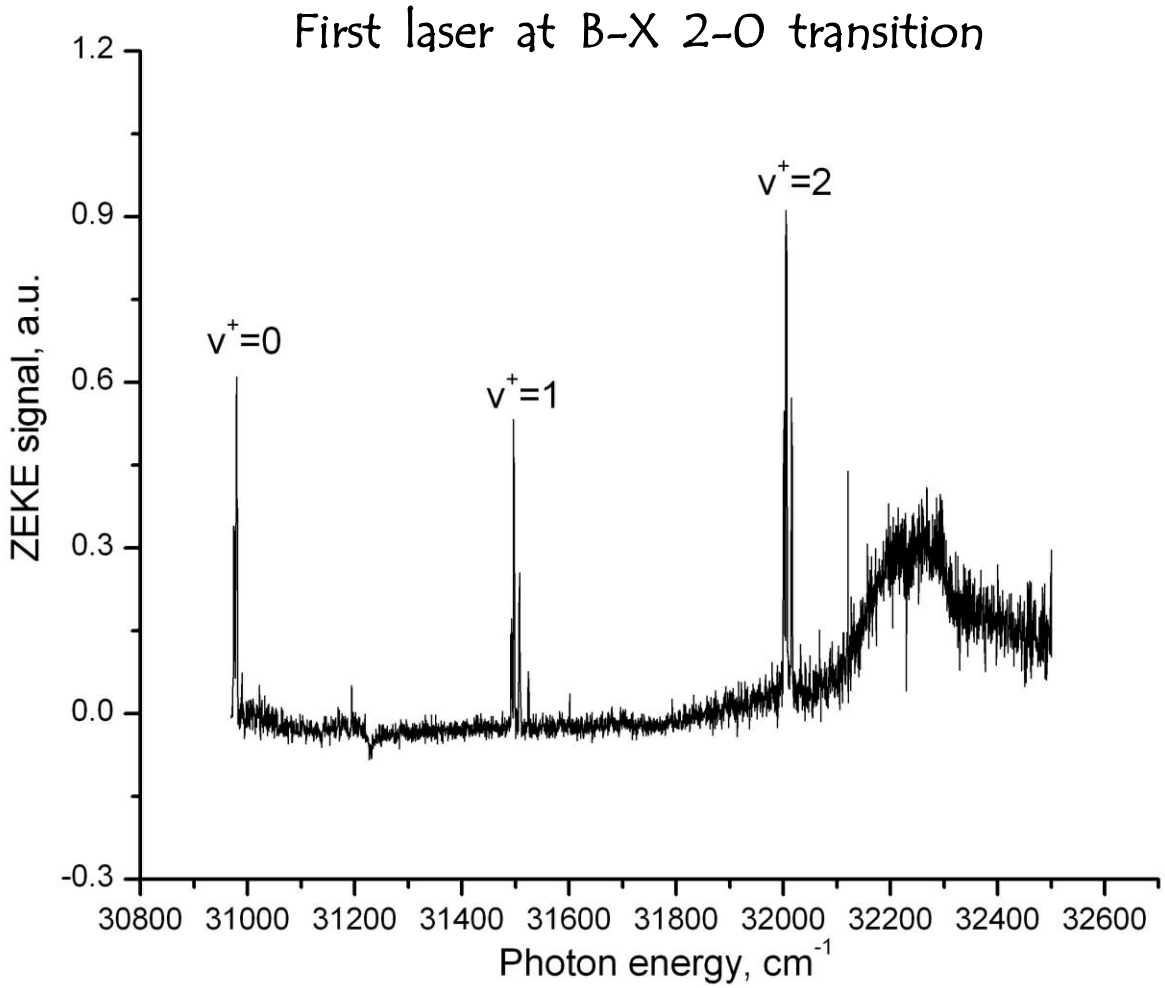


PFI-ZEKE time sequence and excitation scheme





Broad PFI-ZEKE scan of Be_2^+



Rotational structure of Be_2^+ at $v^+=1$ line

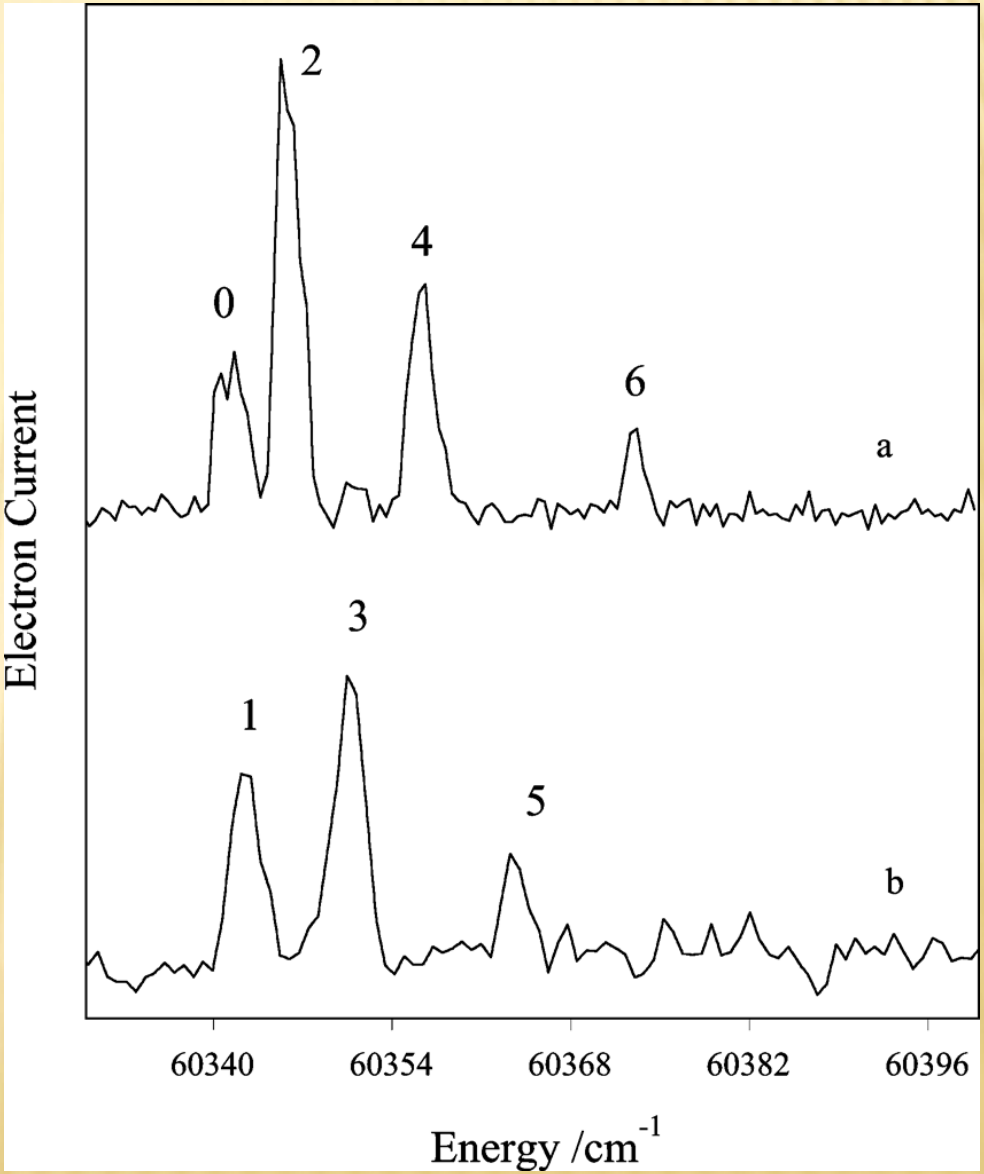
a) Excitation through B-X

2-0 R(1) line

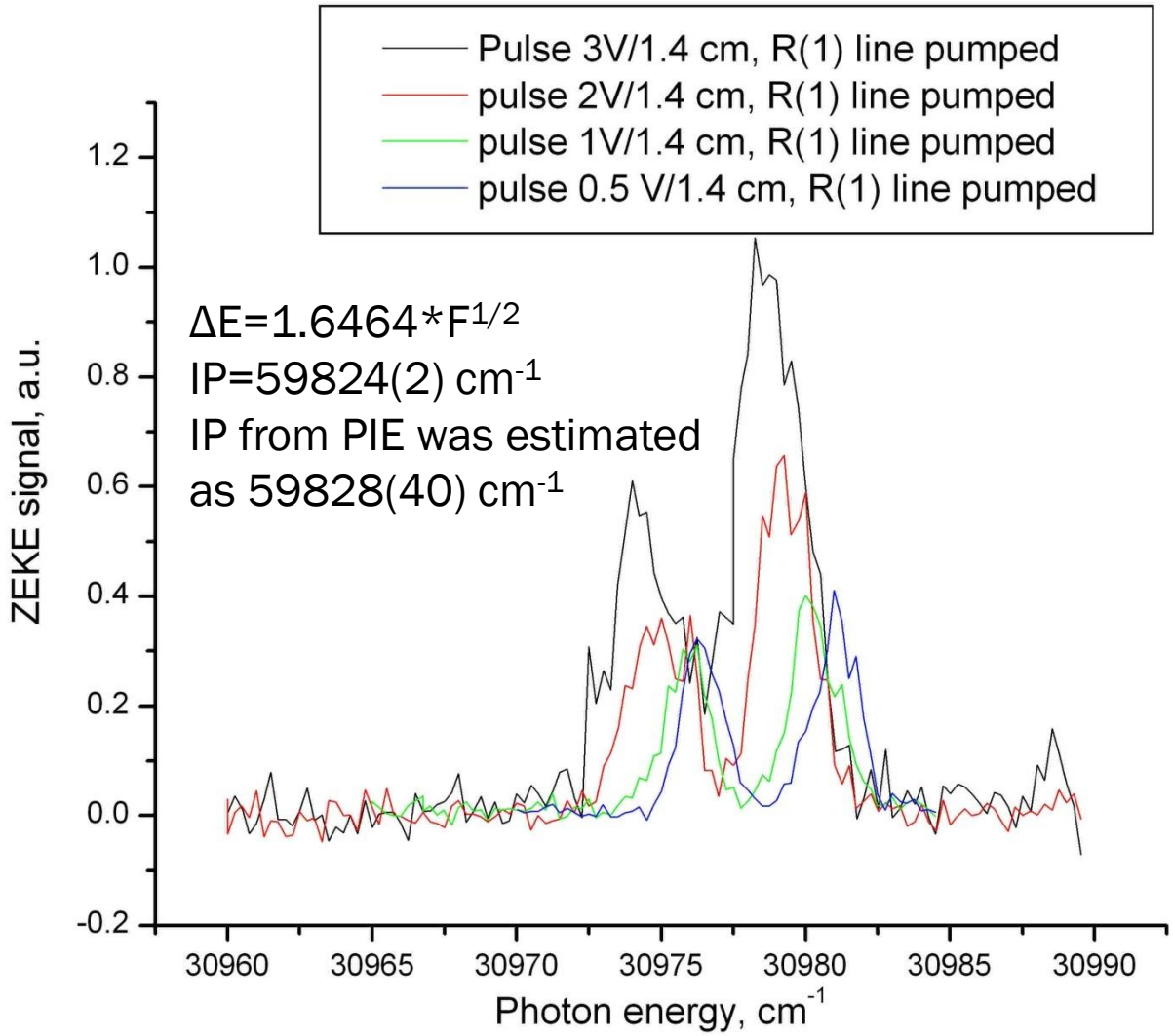
b) Excitation through B-X

2-0 R(2) line

Ground state of Be_2^+ is $X^2\Sigma_u^+$ by nuclear spin symmetry;
B_0=0.760 cm^{-1}; r_0=2.212 Å



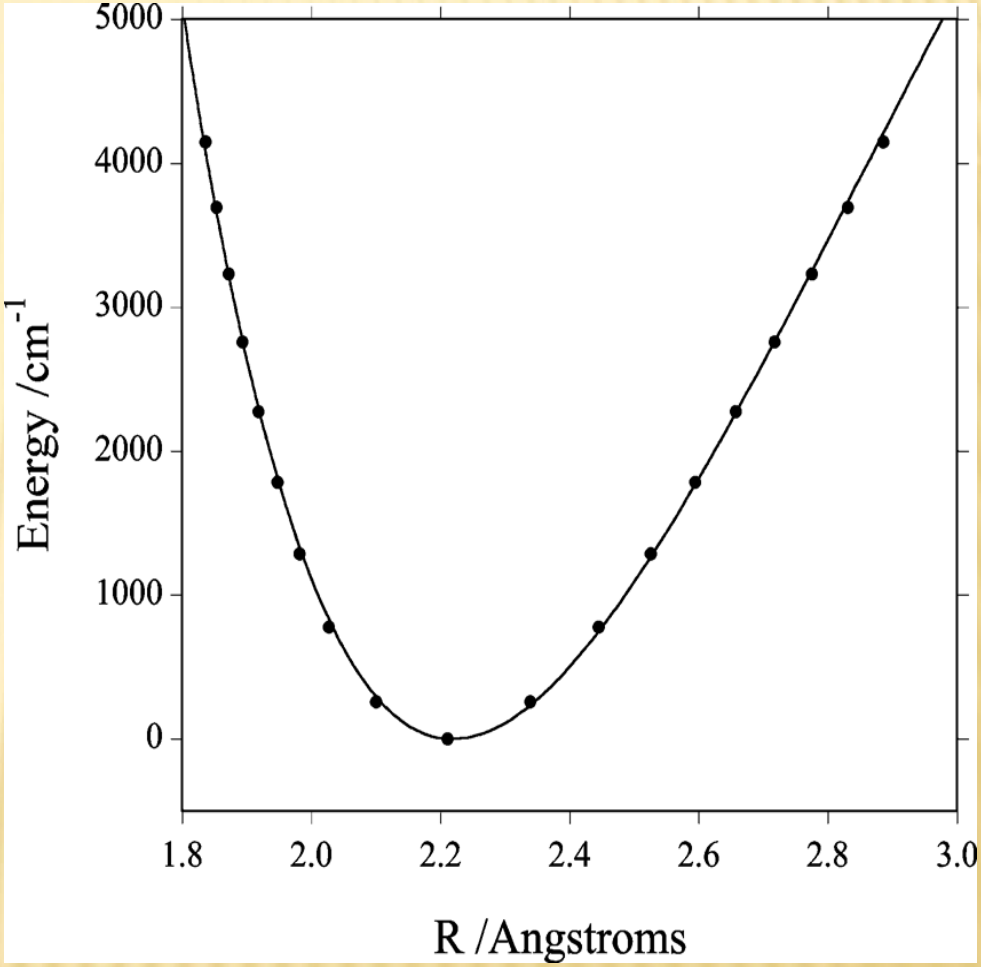
PFI-ZEKE Determination of IP of Be_2



Vibrational levels of Be_2^+

v	E (cm^{-1})	B_v (cm^{-1})
0	0.0	0.762
1	517.0	0.753
2	1024.8	0.732
3	1524.6	0.729
4	2014.7	0.717
5	2496.1	0.711
6	2968.8	0.699

B_e=0.765 cm^{-1}
α_e=0.0103 cm^{-1}
r_e=2.211 Å



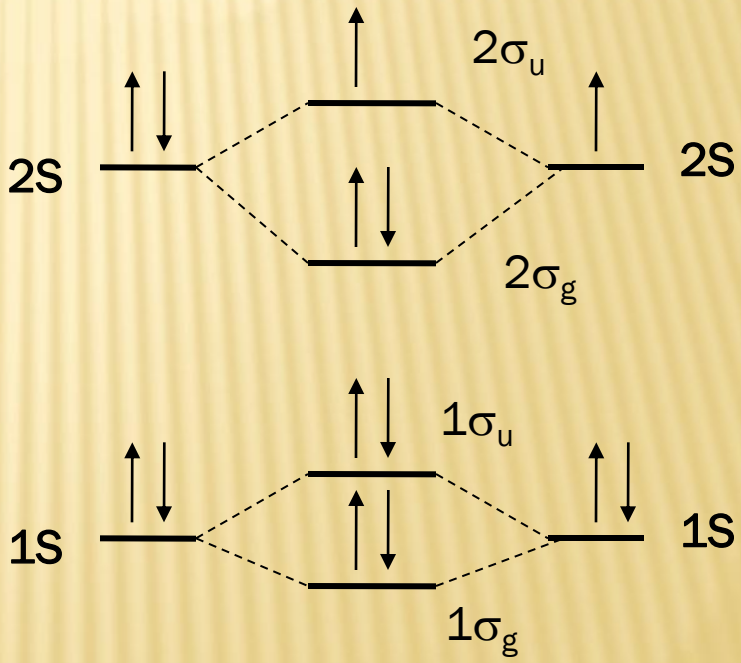
RKR inversion turning points of Be_2^+ and a Morse curve fit

Measured and calculated constants of Be_2^+

	Expt	Merritt et al.	Fischer et al.	Hogreve	Meng et al.	Srinivas and Jellinek
D_e	16 438	16 684	15 889	16 212	15 646	19 200
ω_e	525.88		502		513	
$\omega_e\chi_e$	4.44		4.2		4.2	
$\Delta G_{1/2}$	517	516	494	503.6	505	
R_e (Å)	2.211	2.211	2.231	2.236	2.249	2.21
IE_e	59 685	59 540			60 090	55 330

Molecules Isoelectronic to Be_2^+

	D_e (cm^{-1})
LiBe	2420
Li_2^-	7315
Be_2^+	16438



Conclusions

- Be_2^+ has ($X^2\Sigma_u^+$) ground state
- IP value of Be_2 is measured at 59 824(2) cm^{-1}
- D_e^+ is 16 438 (5) cm^{-1}
- Morse potential energy curve is close in form to the vibrational levels of Be_2^+
- Recent high-level and DFT theoretical calculations are in respectable agreement with Be_2^+ parameters
- Be_2^+ has uniquely high bond strength among the isoelectronic diatomic molecules Li_2^- and LiBe

Acknowledgements:
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