



QUADRUPOLE TRANSITIONS OF THE HYDROGEN MOLECULAR ION HD^+

BEKBAEV A.K.,
AZNABAYEV D.T. AND KOROBOV V.I.

FFK-2019

10-14 June 2019, Hungary, Tihany

EXTERNAL ELECTROMAGNETIC FIELD

The interaction Hamiltonian of a system of particles with external electromagnetic field

$$H_{\text{int}} = - \sum_{\alpha} \frac{Z_{\alpha} e}{m_{\alpha}} \mathbf{P}_{\alpha} \cdot \mathbf{A}(\mathbf{R}_{\alpha}, t)$$

$$\mathbf{A}(\mathbf{R}, t) = \mathbf{A}_0 e^{i(\mathbf{k} \cdot \mathbf{R} - \omega t)} + \mathbf{A}_0^* e^{-i(\mathbf{k} \cdot \mathbf{R} - \omega t)}$$

$$\mathbf{E}(\mathbf{R}, t) = \mathbf{E}_0 e^{i(\mathbf{k} \cdot \mathbf{R} - \omega t)} + \mathbf{E}_0^* e^{-i(\mathbf{k} \cdot \mathbf{R} - \omega t)}, \quad \mathbf{E}_0 = i\omega \mathbf{A}_0$$

$$H_{\text{int}}^{(E2)} = - \frac{i}{\hbar} \sum_{\alpha} \frac{Z_{\alpha} e}{2\omega} T_{ij}^{(2)}(t) [R_{\alpha i} R_{\alpha j}, H^{NR}].$$

Table 1.
Numerical results for selected E2 transitions in HD⁺.
The values of Einstein coefficients A (s⁻¹).
The notation a[b]=a x 10^b

$$A_{fi} / t_0^{-1} = \frac{\alpha^5}{15(2L+1)} \left((E_{v'L'}^{NR} - E_{vL}^{NR}) / \epsilon_0 \right)^5 \times \left(\langle v' L' \| Q^{(2)} \| vL \rangle / (ea_0^2) \right)^2$$

v	L0-L2	L1-L3	L2-L4
0-0	0.1746981877 [+1]	0.2352024926 [+1]	0.2825913216 [+1]
0-1	-0.3169487105 [0]	-0.4036315242 [0]	-0.4572667471 [0]
0-2	-0.2597618842 [-1]	-0.3650742061 [-1]	-0.4533028550 [-1]
0-3	-0.3787353177 [-2]	-0.5704824190 [-2]	-0.7528318299 [-2]
1-0	-0.3678591092 [0]	-0.5175435528 [0]	-0.6480637188 [0]
1-1	0.1963390433 [+1]	0.2642204024 [+1]	0.3172459014 [+1]
1-2	-0.4661992982 [0]	-0.5920186399 [0]	-0.6686065859 [0]
1-3	-0.4752729562 [-1]	-0.6646098936 [-1]	-0.8213519161 [-1]
2-0	-0.2120519992 [-1]	-0.2584869195 [-1]	-0.2751840406 [-1]
2-1	-0.5449109727 [0]	-0.7681000442 [0]	-0.9634452746 [0]
2-2	0.2194315968 [+1]	0.2951795753 [+1]	0.3542094991 [+1]
2-3	-0.5933725328 [0]	-0.7513312591 [0]	-0.8458270609 [0]
3-0	-0.2292316023 [-2]	-0.2377455837 [-2]	-0.1999203293 [-2]
3-1	-0.3952106062 [-1]	-0.4857067890 [-1]	-0.5222915024 [-1]
3-2	-0.6985466306 [0]	-0.9865685885 [0]	-0.1239616409 [+1]
3-3	0.2441044525 [+1]	0.3282524086 [+1]	0.3936879159 [+1]
4-0	-0.3238441606 [-3]	-0.2386686001 [-3]	-0.5786957000 [-4]
4-1	-0.5070081092 [-2]	-0.5394531817 [-2]	-0.4740864875 [-2]
4-2	-0.6013397271 [-1]	-0.7447744156 [-1]	-0.8083912007 [-1]
4-3	-0.8438040527 [0]	-0.1194078703 [+1]	-0.1503012248 [+1]
5-0	-0.4494524018 [-4]	-0.3598135563 [-5]	0.7648344183 [-4]
5-1	-0.8390039054 [-3]	0.6835939619 [-3]	-0.3012548283 [-3]
5-2	-0.8861109716 [-2]	0.9643458554 [-2]	-0.8791150170 [-2]
5-3	-0.8353495618 [-1]	0.1042251783 [0]	-0.1141243838 [0]
6-0	-0.3178282158 [-6]	0.2350516658 [-4]	0.5452930512 [-4]
6-1	-0.1464020877 [-3]	-0.3904918877 [-4]	0.1320463770 [-3]
6-2	-0.1671251202 [-2]	-0.1467374501 [-2]	-0.8453830652 [-3]
6-3	-0.1385693606 [-1]	-0.1538875613 [-1]	-0.1447275066 [-1]
7-0	0.5470986148 [-5]	0.1739547685 [-4]	-0.3170145271 [-4]
7-1	-0.1531366944 [-4]	0.4274418459 [-4]	-0.1214389267 [-3]
7-2	-0.3465573099 [-3]	-0.1677461223 [-3]	-0.1387808493 [-3]
7-3	-0.2923643838 [-2]	-0.2721764469 [-2]	0.1838662380 [-2]
8-0	0.4743591531 [-5]	0.1101624783 [-4]	0.1813113443 [-4]
8-1	0.8577059743 [-5]	0.3977369306 [-4]	0.7840099109 [-4]
8-2	-0.6058714178 [-4]	0.4586826818 [-4]	0.1970189345 [-3]
8-3	-0.6956350105 [-3]	-0.4413531941 [-3]	0.3693969762 [-4]
9-0	0.3358278593 [-5]	0.6838445256 [-5]	-0.1063676339 [-4]
9-1	0.1059478407 [-4]	0.2797836199 [-4]	-0.4824475314 [-4]
9-2	0.3629459214 [-5]	0.6484138983 [-4]	-0.1434061317 [-3]
9-3	-0.1602635346 [-3]	0.7491122555 [-5]	-0.2593484261 [-3]
10-0	0.2287220340 [-5]	0.4311879106 [-5]	0.6460260266 [-5]
10-1	0.8399841498 [-5]	0.1852853708 [-4]	0.2987098012 [-4]
10-2	0.1564762336 [-4]	0.5163255471 [-4]	0.9488468787 [-4]
10-3	-0.2073781857 [-4]	0.8212386904 [-4]	0.2200674374 [-3]

**THANK YOU FOR YOUR
ATTENTION!**

