H_3^+ in the electronic triplet state

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January 16, 2006

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Hirschfelder J. Chem. Phys. 6, 795 (1938) Pfeiffer, Huff, Greenawalt & Ellison J. Chem. Phys. 46, 821 (1967) Kawaoka & Borkman J. Chem. Phys. 54, 4234 (1971) Schaad & Hicks J. Chem. Phys. 61, 1934 (1974) stable electronic state: $a^{3}\Sigma_{\mu}^{+}$ Ahlrichs, Votava & Zirc J. Chem. Phys. 66, 2771 (1977) Wormer & de Groot J. Chem. Phys. 90, 2344 (1989) Preiskorn, Frye & Clementi J. Chem. Phys. 94, 7204 (1991)



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"No accurate calculations of vibration-rotation levels ... have been published, and no spectroscopic observations have been reported, which involve the ${}^{3}\Sigma_{u}^{+}$ state. Such calculation and observations would be extremely interesting." McNab, *Adv. Chem. Phys.* **89**, 1 (1995)

"It is possible that amongst the many H_3^+ lines that have been observed in hydrogen plasmas, some will belong to the ${}^3\Sigma_u^+$ state of H_3^+ . But in the absence of a full potential energy surface for this state and sophisticated ro-vibrational calculations, these transitions will remain among the many that have yet to be assigned."

Tennyson, Rep. Prog. Phys. 57, 421 (1995)



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 Friedrich, Alijah, Xu & Varandas, *Phys. Rev. Lett.* 86, 1183 (2001)
 Sanz, Roncero, Tablero, Aguado & Paniagua, *J. Chem. Phys.* 114, 2182 (2001)

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Potential energy surfaces

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upper branch: dissociation: $2H(^{2}S) + H^{+}$, $-1.0000 E_{h}$ energy minimum (D_{3h}) : $-1.034590E_{h}$ at $3.610 a_{0}$ lower branch: dissociation: $H_{2}^{+}(^{2}\Sigma_{g}^{+}) + H(^{2}S)$, $-1.1026 E_{h}$ energy minimum $(D_{\infty h})$: $-1.11610627E_{h}$ at $2.454 a_{0}$



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Comparison of ab initio calculations

Introduction	group	r/a_0	E_{min}/E_{h}	basis
Surfaces	Schaad & Hicks	2.457	-1.114 22	21
Molecular orbitals	Wormer & de Groot	2.45	-1.114 66	60 ^{a)}
Characteristics of	Ahlrichs, Votava & Zirc	2.4568	-1.115 678 7	45
the surfaces Comparison of <i>ab</i>	Preiskorn, Frye & Clementi	2.454	-1.116 102 7	102 ^{<i>b</i>})
<i>initio</i> calculations	Friedrich, Alijah, Xu & Varandas	2.4537	-1.116 061	165
Representations of	Sanz, Roncero, Tablero,			
potential energy surfaces	Aguado & Paniagua	2.454	-1.116 106 27	489 ^{c)}
Ro-vibrational states	^{a)} only 42 functions used for PES			

Roon the lower sheet

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^{b)} Hylleraas-Cl

^{c)} only 108 functions used for PES

Tunneling Barrier: 11.78 mE_h = 2585 cm⁻¹ (Wormer & de Groot) 11.84 mE_h = 2598 cm⁻¹ (Friedrich *et al.*) 12.03 mE_h = 2640 cm⁻¹ (Sanz *et al.*)

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Acknowledgements

Friedrich, Alijah, Xu & Varandas, *Phys. Rev. Lett.* **86**, 1183 (2001) $V(\rho, \theta, \phi) = V_{Coulomb} + V_{D_{3h}}(\rho) + \frac{\sum_{ij} a_{ij}(\rho) \sin^{i} \theta \sin^{j} 3\phi}{1 + \left[\sum_{ij} b_{ij}(\rho) \sin^{i} \theta \sin^{j} 3\phi\right]^{2}}$

Sanz, Roncero, Tablero, Aguado & Paniagua, *J. Chem. Phys.* **114**, 2182 (2001)

 $V(\mathbf{R}) = V_{DIM}(\mathbf{R}) + V^{(3)}(\mathbf{R})$

Cernei, Viegas, Alijah & Varandas J. Chem. Phys. **118**, 2637 (2003) J. Chem. Phys. **120**, 2053 (2004) Chem. Phys. **308**, 2085 (2005)

$$V_{u/l}(\mathbf{R}) = \sum_{i} V^{(1)} + \sum_{i} V^{(2)}_{u/l}(R_i) + V^{(3)}_{u/l}(\mathbf{R})$$
$$V^{(3)}_{u/l}(\mathbf{R}) = P_1(\mathbf{R}) \pm \Gamma_2 P_2(\mathbf{R})$$

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- Hyperspherical
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- Spectroscopic
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$$\begin{split} |\Psi_{A}^{\pm}\rangle &\sim |\Psi_{I}^{\pm}\rangle + |\Psi_{II}^{\pm}\rangle + |\Psi_{III}^{\pm}\rangle \\ |\Psi_{E,\xi}^{\pm}\rangle &\sim |\Psi_{I}^{\pm}\rangle + \omega |\Psi_{II}^{\pm}\rangle + \omega^{2}|\Psi_{III}^{\pm}\rangle \\ |\Psi_{E,\eta}^{\pm}\rangle &\sim |\Psi_{I}^{\pm}\rangle + \omega^{2}|\Psi_{II}^{\pm}\rangle + \omega |\Psi_{III}^{\pm}\rangle \quad ; \quad \omega = e^{\frac{2\pi i}{3}} \end{split}$$

$$|\Psi^{\pm}
angle = rac{1}{\sqrt{2}} |v_1 v_2^{|\ell|} v_3
angle \,\,\, (|N\ell
angle \pm |N-\ell
angle)$$

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Method of hyperspherical harmonics

Wolniewicz, J. Chem. Phys. 90, 371 (1988)

Schrödinger equation:

$$\left\{ T(\rho) + \frac{\Lambda^2(\Omega)}{2\mu\rho^2} + V(\rho,\theta,\phi) - E_k \right\} \Phi_k(\rho,\Omega) = 0$$

Hyperspherical harmonics:

$$\Lambda^2 \Psi = K(K+4) \Psi$$
 ; $-i \frac{\partial}{\partial \phi} \Psi = \frac{\nu}{2} \Psi$

Expansion:

$$\Phi_k(\rho, \Omega) = \sum_j \Psi_j(\Omega) R_{jk}(\rho)$$

Coupled radial equations:

$$\left[\sum_{j} \left(T(\rho) + \frac{K(K+4)}{2\mu\rho^2}\right)\delta_{jk} + \langle \Psi_j | V | \Psi_k \rangle - E_k \delta_{jk}\right] R_{jk}(\rho) = 0$$

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Spectroscopic assignment of hyperspherical states

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Alijah, Wolniewicz & Hinze, *Molec. Phys.* **85**, 1125 (1995) Features: wavefunctions not needed, Dunham fits not needed

hyperspherical states $\implies S_N \times I \iff$ spectroscopic states

Algorithm:

- Given a set of hyperspherical states $|\Gamma, J, n\rangle$, where Γ denotes permutation-inversion symmetry in $S_N \times I$
- Given the symmetry properties, Γ , of spectroscopic states $|v_1, v_2, \dots, J\rangle$

loop over vibrational quantum numbers v_i

• determine band origin, $|v_1, v_2, ..., J = 0\rangle$, choosing a hyperspherical state with appropriate Γ

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Algorithm: continuation

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loop over J

- find $|\Gamma, J, n\rangle$ that represents $|v_1, v_2, ..., J\rangle$ subject to
 - correct Γ

•
$$E(J+1) > E(J)$$

• observation of trends within families of states: $|v_1, v_2, ..., J\rangle$, $|v_1 + 1, v_2, ..., J\rangle$, $|v_1 + 2, v_2, ..., J\rangle$, ... where ν_1 denotes the totally symmetric vibration



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Results for H_3^+: I

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Alijah, Viegas, Cernei & Varandas, J. Mol. Spectrosc. 221, 163 (2003) 560 ro-vibrational states identified ($J \leq 10$)



Ro-vibrational states

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Results for H_3^+ : II





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Results for H⁺₃: III



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Results for D_3^+ : vibrational states

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Cuervo-Reyes, Rubayo-Soneira, Aguado, Paniagua, Tablero, Sanz & Roncero, *Phys. Chem. Chem. Phys.* **4**, 6012 (2002)



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Results for H_2D^+ : ro-vibrational states

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Alijah & Varandas, J. Phys. Chem. A (2006)

Isomers: HDH⁺

 HHD^+ $(H_{[1]}H_{[2]}D^+ \text{ and } H_{[2]}H_{[1]}D^+)$



Ro-vibrational states

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HDH⁺: irregular rotational structure



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Transition frequencies

Introduction ω/cm^{-1} molecule initial state $\Gamma_{rve}(w)$ final state $\Gamma_{rve}(w)$ Potential energy $N = 0, (0, 0^0, 0)$ H_3^+ surfaces $A_{2}^{\prime}(4)$ $N=1, (0, 1^1, 0) A_{2}^{\prime\prime}(4)$ 665.89 E'(2)N=1, $(0, 1^1, 0)-$ E''(2)Ro-vibrational states 665.89 on the lower sheet H_3^+ $N = 0, (0, 0^0, 0)$ $A_{2}^{\prime}(4)$ $N = 1, (0, 0^0, 1)$ $A_{2}^{\prime\prime}(4)$ 749.71 Localised vs. $N=1, (0, 0^0, 1)$ E''(2)E'(2)749.72 non-localised states Hyperspherical H_3^+ $N = 0, (0, 0^0, 0)$ E'(2) $N=1, (1, 0^0, 0)$ E''(2)984.12 harmonics Spectroscopic $N = 1, (0, 1^1, 0) HDH^+$ $N=0, (0, 0^0, 0)$ assignment $B_2(3)$ $B_1(3)$ 551.46 Algorithm: HDH^+ $N=0, (0, 0^0, 0)$ $N = 1, (0, 0^0, 1)$ $B_2(3)$ $B_{1}(3)$ 628.32 continuation Results for H_2^+ $N = 0, (0, 0^0, 0)$ HHD^+ $A_1(1)$ $N=1, (0, 1^1, 0) A_{2}(1)$ 638.23 Results for D_3^+ $B_2(3)$ $N=1, (0, 1^1, 0) B_1(3)$ 638.23 Results for H_2D^+ $N = 0, (0, 0^0, 0)$ HHD^+ $A_1(1)$ $N = 1, (0, 0^0, 1)$ $A_{2}(1)$ 712.13 Transition $N=1, (0, 0^0, 1)$ $B_2(3)$ $B_{1}(3)$ 712.13 frequencies HHD^+ $N = 0, (0, 0^0, 0)$ $N=1, (1, 0^0, 0)$ $A_1(1)$ $A_{2}(1)$ 879.64 Ro-vibrational states $N = 1, (1, 0^0, 0)$ $B_2(3)$ $B_{1}(3)$ 879.64 on the upper sheet Conclusions Acknowledgements $\begin{array}{ll} \mathsf{H}_3^+, \, \mathsf{D}_3^+ & \Delta J = \mathsf{0}, \pm 1 & \mathsf{A}_1' \leftrightarrow \mathsf{A}_1'', \, \mathsf{A}_2' \leftrightarrow \mathsf{A}_2'', \, \mathsf{E}' \leftrightarrow \mathsf{E}'' \\ \mathsf{H}_2\mathsf{D}^+, \, \mathsf{D}_2\mathsf{H}^+ & \Delta J = \mathsf{0}, \pm 1 & \mathsf{A}_1 \leftrightarrow \mathsf{A}_2, \, \mathsf{B}_1 \leftrightarrow \mathsf{B}_2 \end{array}$ Selection rules:

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View of the surfaces

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Vibronic Slonczewski resonance states



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Viegas, Alijah & Varandas, *J. Phys. Chem. A* **109**, 3307 (2005) Positions:



Semiclassical lifetimes: Nikitin, J. Chem. Phys. 107, 6748 (1997)

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$$egin{aligned} & v_1 v_2 GN
angle_{\pm} &= & rac{1}{\sqrt{2}} \left(\left| v_1 v_2, \ell + lpha
ight
angle \left| Nk
ight
angle \pm (-1)^N \left| v_1 v_2, -\ell - lpha
ight
angle \left| N, -k
ight
angle
ight) \ &= & rac{1}{\sqrt{2}} \left(\left| v_1 v_2 \ell
ight
angle \left| Nk
ight
angle \pm (-1)^N \left| v_1 v_2, -\ell - 2lpha
ight
angle \left| N, -k
ight
angle
ight) e^{ilpha \phi} \end{aligned}$$

10000 (000 I)

Generalized G quantum number:

$$G = |k - \ell - \alpha| = |k - j|$$
; $|j| = |\ell| + \alpha$; $\alpha = 0, 1/2$

NGP/GP correlation:

for

for $\ell = 0$ (special case)

$$egin{aligned} G_{NGP} &= 0 & \Leftrightarrow & G_{GP} = rac{1}{2} \ & G_{NGP} &= |k|
eq 0 & \Leftrightarrow & G_{GP} = G_{NGP} \pm rac{1}{2} \ & \ell
eq 0 \ & G_{GP} &= G_{NGP} + rac{1}{2} \end{aligned}$$

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Ro-vibronic cone states I



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Ro-vibronic cone states II



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Theoretical data available

- Experimental data?
 - Excitation from the ground state (X¹A'₁)
 H⁺₂(X²Σ⁺_g) + H, aligned in an external field
 H₂(b³Σ⁺_u) + H⁺

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Acknowledgements

Prof. António J. C. Varandas

Dr. Oliver Friedrich (Bielefeld)

Mihail Cernei (Coimbra)

- Luís Pedro Viegas (Coimbra)
 - Fundação para a Ciência e a Tecnologia
 - John von Neumann Institut für Computing, Jülich