DEUTERIUM ARRAY MEMO #055

MASSACHUSETTS INSTITUTE OF TECHNOLOGY
HAYSTACK OBSERVATORY
WESTFORD, MASSACHUSETTS 01886

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Telephone: 978-692-4764
Fax: 781-981-0590

To: Deuterium Array Group

From: Alan E.E. Rogers

Subject: The theoretical D line strength

The expected D1 line strength is estimated from the quantum mechanics of the D1 atom. In practice we are only interested in the relative opacities of D1 and H for a given abundance ratio n_D/n_H however, lets work from first principles. The probability of spontaneous decay, also frequently called the "Einstein A" coefficient can be calculated from (see Condon and Shortley equation 7^4 (3))

$$A = \frac{64\pi^4 \upsilon^3 M \left|\mu_0\right|^2}{3hc^3 g_a}$$

where υ = frequency Hz
h = Plank's constant = 6.626×10^{-27} erg s
c = velocity of light = 2.9979×10^{10} cm s^{-1}
$\mu_0^2 = \left(\frac{eh}{4\pi mc}\right)^2 = 8.6 \times 10^{-41}$ erg^2 $gauss^{-2}$
g_a = upper state degeneracy = $2F_a + 1$

M is the sum of matrix elements squared.

For hydrogen:

S = ½ electron spin
I = ½ proton spin

And the vector F = I + S takes on the value of 0 from the ground state and 1 for the upper 3 states whose projections M_F = -1, 0, 1 are 21 cm above the ground state.

The matrix elements squared (from Townes equations 5-65 and 5-66) are

$$\left|\mu\right|^2 = \frac{4\left[\left(I + \tfrac{1}{2}\right)^2\right]\mu_0^2}{\left(2I+1\right)^2} \; when \; \Delta m_F = 0$$

and

$$|\mu|^2 = \frac{2\left(I+\tfrac{1}{2}\right)\left(I+\tfrac{3}{2}\right)\mu_0^2}{\left(2I+1\right)^2}$$

and all 3 possible transitions have values of $|\mu|^2 = |\mu_0|^2$ so that

A=2.86×10^{-15} for Hydrogen

And this value can be found in many places and to my knowledge has never been in dispute.

For deuterium

S = ½ electron spin
I = 1 deuteron spin

For deuterium F takes on the values of ½ for the ground states and 3/2 for those states 327 MHz above ground. The ground state splits into a doublet with m_F = -½, ½ and the upper state momentum vector takes on 4 projections m_F = -3/2, -½, ½, 3/2 and the matrix elements are no longer just equal to the Bohr magneton μ_0 squared.

The values are given by

$$\frac{4\left[\left(\tfrac{3}{2}\right)^2 - m_F^2\right]}{9} \text{ for } \Delta m_F = 0$$

$$\frac{2\left(\tfrac{3}{2} \pm m_F\right)\left(\tfrac{5}{2} \pm m_F\right)}{9} \text{ from } \Delta m_F = \pm 1$$

and take on the values of

$$8/9 \text{ for } \Delta m_F = 0, |m_F| = \tfrac{1}{2}$$
$$4/3 \text{ for } |\Delta m_F| = 1; m_F = \tfrac{1}{2}$$
$$4/9 \text{ for } |\Delta m_F| = 1; m_F = -\tfrac{1}{2}$$
$$g_a = 2(3/2) + 1 = 4$$

for a sum over all 6 possible transitions of 16/3

so that

$$A_D = \frac{64\pi^4\upsilon^3\mu_0^2\,(16/3)}{12hc^3} = 4.6\times10^{-17}\text{ sec}^{-1}$$

This value has been in contention.

Shklovsky (page 258) gives a value of 6.6×10^{-17} sec^{-1} and a relative opacity ratio $\tau_D/\tau_H \approx 0.4 \quad n_D/n_H$ while Weinreb points out errors in Shklovsky's equations and quotes a new value of 4.65×10^{-17} sec^{-1} which comes from Field. The value assumed by Weinreb results an opacity ratio of $\tau_D/\tau_H \approx 0.3 \quad n_D/n_H$.

Sandy Weinreb also mentions that Field's calculation has been checked by Alan Barrett.

The optical depth τ is given by

$$\tau = \frac{hc^2 A_{a\to b} g_a}{8\pi k \upsilon T_{ex} \sum g} \int_0^L Nf(\upsilon, e)\, de$$

where T_{ex} = excitation temperature

So that the ratio τ_D/τ_H is given by

$$\frac{\tau_D}{\tau_H} = \left(\frac{g}{\sum g}\right)_D \left(\frac{\sum g}{g}\right)_H \left(\frac{A_D}{A_H}\right)\left(\frac{\upsilon_H}{\upsilon_D}\right)^2 (n_D/n_H)$$

on the assumption that the line is only broadened by Doppler so that the Doppler widths are proportional to frequency.

With the revised value of A_D the ratio is reduced to $\tau_D/\tau_H \approx 0.27 \quad (n_D/n_H)$.

In a more recent paper Gould calculates the Einstein A coefficients for H and D and gets a value of A = 4.69675×10^{-17} sec^{-1} in his table 1, which is close the value of Field. Gould includes some small corrections to A which presumably result in a more accurate value. Using Gould's values the opacity ratio is $(\tau_D/\tau_H) = 0.272(n_D/n_H)$.

References:

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