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Corrigendum

Corrigendum to “New REMPI observations and analyses for Rydberg and ion-pair states of HI” [J. Mol. Spectrosc. 290 (2013) 5–12]

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1. Introduction

This article presents a comprehensive overview of Rydberg and ion-pair states for HI in the two-photon excitation region of 69,600–72,300 cm^{-1}. There are two errors in the paper that need to be addressed. These are associated with (i) the wavelength calibration and (ii) the assignment of the $d^3\Pi_0(1)$ Rydberg state spectrum.

2. Calibration

Table 3 in Ref. [1] includes band origins (ν^0) and rotational parameters (B_v and D_v) for all the observed states in the energy region of concern. The calibration of the spectrum was based on observed atomic iodine (2 + 1) REMPI peaks. Only few atomic peaks are found in the region of 69,600 and 70,900 cm^{-1}. Therefore, some of the band origins in that region were not clearly determined. Later identification of weak atomic lines in the region of the Q lines of the $H(1)$ state spectrum allowed more precise determinations of the rotational line positions. See Table 1 for corrected values of band origins. Accordingly, Q rotational lines of the $k^3\Pi_0(1)$ state spectrum, have also been reassigned (see Table 2).

3. Reassignment of the $d^3\Pi_0(1)$ Rydberg state spectrum

A Rydberg state spectrum was observed with band origin of 70991.6 cm^{-1}. It had not been observed previously. The most probable reasons why the spectrum had gone unnoticed are (i) that its Q branch are found right in the midst of a strong iodine atomic line (in REMPI) and (ii) its other rotational branches are very weak.

The original rotational analysis of the spectrum incorrectly suggested a Rydberg state of $\Omega = 0$. This is incorrect, since the spectrum exhibits R and P lines, which excludes an $\Omega = 0$ state and implies either an $\Omega = 1$ or $\Omega = 2$ Rydberg state. A revised rotational analysis, revealed that the state is in fact an $\Omega = 1$ state with a band origin of $\nu^0 = 70989.0$ cm^{-1}.

Additionally, the first P line of the spectrum was incorrectly assigned. It is actually the first and only visible S line of the $V^1\Sigma^+(m+6)$ ion-pair state spectrum with band origin of 70952.3 cm^{-1}. A peak observed at 70967.4 cm^{-1}, on the other hand, is reassigned to the first and only visible P line.

Table 1
Corrections of band origins (ν^0) along with the values presented in the original paper and given by Ginter et al. [2].

	ν^0 (cm^{-1}) corrected	ν^0 (cm^{-1}) Ginter et al.	ν^0 (cm^{-1}) Hrodmarsson et al.
$f^3\Delta_1$ (0)	69689.0	69687.9	69699.9
$V^1\Sigma^+$ (m + 4)	69909.9	69909.9	69903.3
$F^1\Delta_2$ (0)	70229.7	70228.3	70223.6
$E^1\Sigma^+$ (1)	70242.2	70242.1	70236.1
$k^3\Pi_0$ (1)	70322.9	70320.4	70310.8
$V^1\Sigma^+$ (m + 5)	70517.3	70512.0	70511.0
$m^3\Delta_2$ (0)	70841.6	70837.6	70841.5
$H^1\Sigma^+$ (1)	70855.5	70850.5	70866.3

Table 2
Corrections of Q line positions of the $k^3\Pi_0$ (1) state as presented in Ref. [1].

J	$k^3\Pi_0$ (1)–Q lines – corrected	$k^3\Pi_0$ (1) – Q lines – Ref. [1]
0	70322.9	70310.8
1	70320.6	70308.6
2	70315.1	70304.0
3	70307.7	70296.4
4	70296.8	70286.1
5	70284.7	70274.7

Table 3
Rotational lines due to two-photon resonance transitions to a reassigned $n^3\Pi_1$ (0) Rydberg state of HI.

J'	P	Q	R
1		70989.5	70998.5
2	70967.4	70989.3	71009.2
3		70988.0	71024.6
4		70986.8	71039.4
5		70985.7	71051.5
6		70984.6	71059.0
7		70983.0	
8		70981.5	

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The intensities of the I^+ lines are generally found to be marginally larger than those of the HI^+ lines. This excludes a $\Omega = 2$ state. On the other hand, the intensity ratios are found to be very similar to those of other $^3\Pi$ states, e.g. $k^3\Pi_1$ and $m^3\Pi_1$ [1–4]. The state of concern does, however, not correlate with any vibrational progressions of previously observed $^3\Pi_1$ states [5,6]. Therefore, we assign the spectrum to the $n^3\Pi_1(0)$ Rydberg state with the electron configuration $(\sigma^2\pi^3)5d\pi$. Rotational assignments are presented in Table 3.

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