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Molecular parameters for weakly bound $2_g(aa, ab)$ and $0_u^-(ab)$ states of molecular iodine and dipole moment functions of transitions to these states

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Abstract

Weakly bound valence states of 2_g symmetry, correlating with the $I(^2P_{3/2}) + I(^2P_{3/2})$ (aa) and $I(^2P_{3/2}) + I(^2P_{1/2})$ (ab) dissociation limits, as well as $0_u^-(ab)$ state, were studied using vibrationally resolved luminescence spectra corresponding to transitions from $\delta 2_u(^3P_2)$ and $g0_g^-$ $(^3P_1)$ ion-pair states, in molecular iodine, respectively, populated using a three-step three-color laser excitation scheme. Spectroscopic constants and potential energy curves of the valence states are determined for the first time. Dipole moment functions of $\delta 2_u \rightarrow 2_g(aa, ab)$ and $g0_g^- \rightarrow 0_u^-(ab)$ transitions are found to exponentially decrease.

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(Some figures may appear in colour only in the online journal)

1. Introduction

At the moment, iodine is one of the most widely investigated diatomic molecules. Its electronic states have been studied for decades by using emission and absorption spectroscopy accompanied by a variety of laser excitation techniques (see [1–28] and references within).

An iodine molecule has 20 ion-pair (IP) states, which form four tiers correlating with the $I^-(^1S_0) + I^+(^3P_{2,1,0}, {}^1D_2, {}^1S_0)$ dissociation limits, and 23 valence states, correlating with three dissociation limits $I(^2P_{3/2}) + I(^2P_{3/2})$ (aa), $I(^2P_{3/2}) + I(^2P_{1/2})$ (ab) and $I(^2P_{1/2}) + I(^2P_{1/2})$ (bb). Only four of the valence states have potential well depths exceeding $1000\ \mathrm{cm}^{-1}$ ($X0_g^+$, $A'2_u$, $A1_u$ (aa) and $B0_u^+(ab)$); the remaining 19 states are the so-called weakly bound (or shallow-bound) ones. Most of the molecular parameters of the latter have been determined by analysis of transitions to these states from IP ones (see, for example [3–9]). Spectroscopic characteristics of experimentally investigated weakly bound states can be found in the following publications: $B'0_u^-(aa)$ [3], $a1_g$ and $a'0_g^+$ (aa) [2], C (or B'')$1_u(aa)$ [4], $0_g^+(ab)$ [5], $c1_g(ab)$ [6], $c'1_g$ [7], $0_g^-(ab)$ [8], $2_u(ab)$, (3,4) $1_u(ab)$ and $0_u^-(bb)$ [9], $0_g^+(bb)$ [10], $1_u(bb)$ [11].

However, there are five states which spectroscopic characteristics are lacking in the literature: these are $2_g(aa)$, $3_u(aa)$, $0_u^-(aa)$, $2_g(ab)$ and $0_u^-(ab)$ states. Investigation of these states is complicated primarily by difficulties of population of the IP states from which transitions to these valence states may occur. Thus, parallel transitions ($\Delta\Omega = 0$) to states of 0_u^- and 2_g symmetry occur from IP states of 0_g^- and 2_u symmetry, respectively (namely, $g0_g^-$, $\delta 2_u$ and $2_u(^1D)$ states). However, until recently, there were no excitation pathways to these states efficient enough to measure luminescence spectra with a vibrationally resolved structure.

In a series of papers by Ishiwata's group devoted to excitation of IP states using perturbation-facilitated optical-optical double resonance (OODR) techniques, the population of both $g0_g^-$ and $\delta 2_u$ states was reported ([3, 12, 13]). In these

