Title:	Radiative lifetimes of spin forbidden a1Δ → X 3Σ- and spin allowed A3Π → X 3Σ- transitions and complete basis set extrapolated ab initio potential energy curves for the ground and excited states of CH -
Authors:	Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Ab initio potential energy curves Bound state
Issue Date:	2012
Publisher:	American Institute of Physics
Citation:	Journal of Chemical Physics, 137 (21), art. no. 214314, .
Abstract:	The spin forbidden transition a1Δ → X 3Σ- in CH- has been studied using the Breit-Pauli Hamiltonian for a large number of geometries. This transition acquires intensity through spin-orbit coupling with singlet and triplet Π states. The transition moment matrix including more than one singlet and triplet Π states was calculated at the multi-reference configuration interaction/aug-cc-pV6Z level of theory. The computed radiative lifetime of 5.63 s is in good agreement with the experimental (5.9 s) and other theoretical (6.14 s) results. Transition moment values of the spin allowed A3Π → X3Σ- transition have also been calculated at the same level of theory. Calculations show that the corresponding radiative lifetime is considerably low, 2.4 × 10-7 s. Complete basis set extrapolated potential energy curves for the ground state of CH and the ground state and six low lying excited states (a1Δ, b1Σ+, two 3Π, and two 1Π) of CH- are reported. These curves are then used to calculate the vibrational bound states for CH and CH-. The computed electron affinity of CH supports the electron affinity bounds reported by Okumura [J. Chem. Phys. 85, 1971 (1986)10.1063/1.451140].
Description:	Only IISERM authors are available in the record.
URI:	http://jcp.aip.org/resource/1/jcpsa6/v137/i21/p214314_s1 (http://jcp.aip.org/resource/1/jcpsa6/v137/i21/p214314_s1) http://dx.doi.org/10.1063/1.4768873 (http://dx.doi.org/10.1063/1.4768873)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/232/3/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/123456

Show full item record (/jspui/handle/123456789/232?mode=full) (/jspui/handle/123456789/232/statistics)