

AUTODETACHMENT LIFETIMES OF SMALL DIANIONS

THOMAS SOMMERFELD, *Theoretische Chemie, Universität Heidelberg, Im Neuenheimer Feld 229, 69120 Heidelberg, Germany*; FRANCESCO TARANTELLI, *Dipartimento di Chimica, Università di Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy*.

Almost all small dianions known from condensed phases are unstable with respect to electron autodetachment in the gas phase. These dianions show rare-gas-like closed-shell electronic ground states and represent a new type of metastable system. Here we discuss the ab initio calculation of energies and *lifetimes* of temporary closed-shell systems. Some methodological issues are briefly discussed, in particular, there is no “natural” choice of orbital set for metastable closed-shell states and therefore no unique one-particle level. Applications to O^{2-} , C_2^{2-} , CN_2^{2-} , and CO_3^{2-} are presented.