Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Guanine Tetrads: An IRMPD Spectroscopy, Energy Resolved SORI-CID, and Computational Study of M(9-ethylguanine)$_4^+$ (M=Li, Na, K, Rb, Cs) in the Gas Phase

by

Mohammad Azargun and Travis D. Fridgen

Department of Chemistry, Memorial University, St. John's, NL, Canada, A1B 3X7

*author to whom all correspondence should be addressed at tfridgen@mun.ca

Figure S1. Profiles of the computed structures of the $M(9eG)_4^+$ complexes computed using B3LYP/6-31+G(d,p) with Def2SVPD on the metal centres. The calculations are also empirically corrected for dispersion.

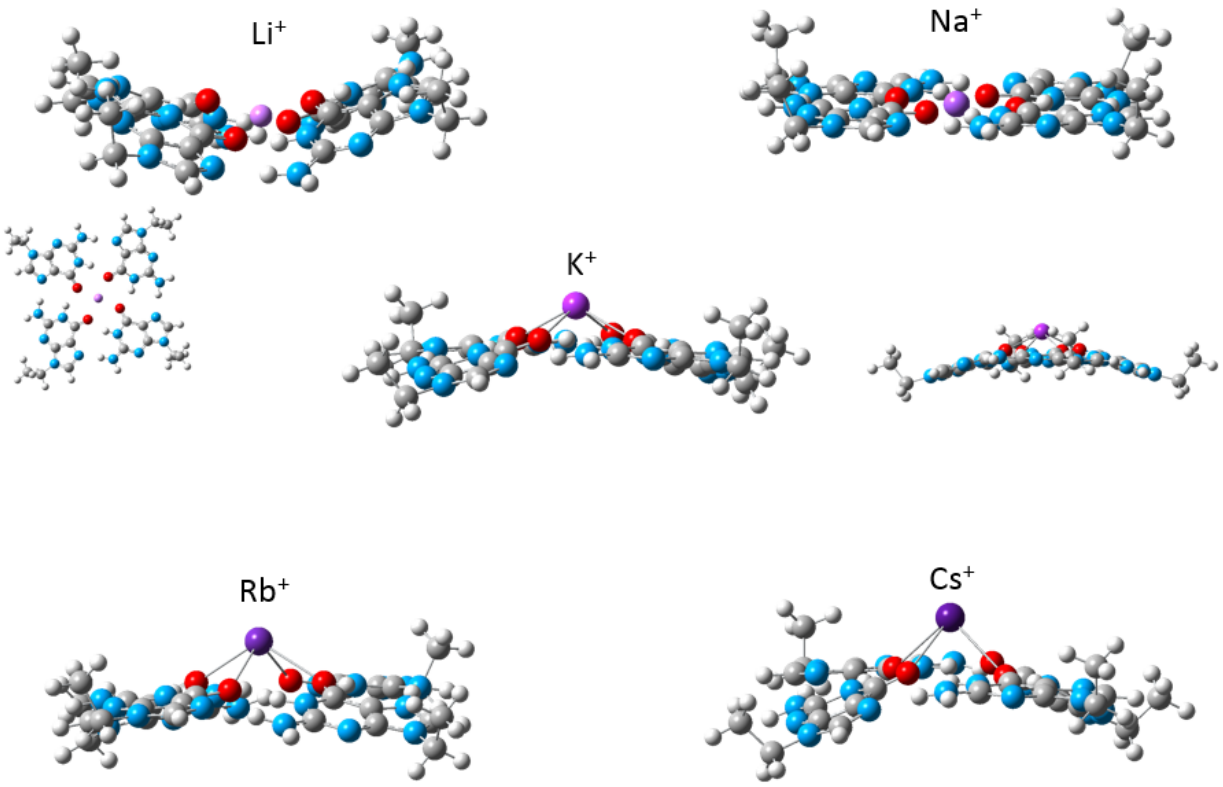

Figure S2a) Comparison of computed IR spectra for three isomers of $Na(9eG)_4^+$ with the experimental IRMPD spectra.

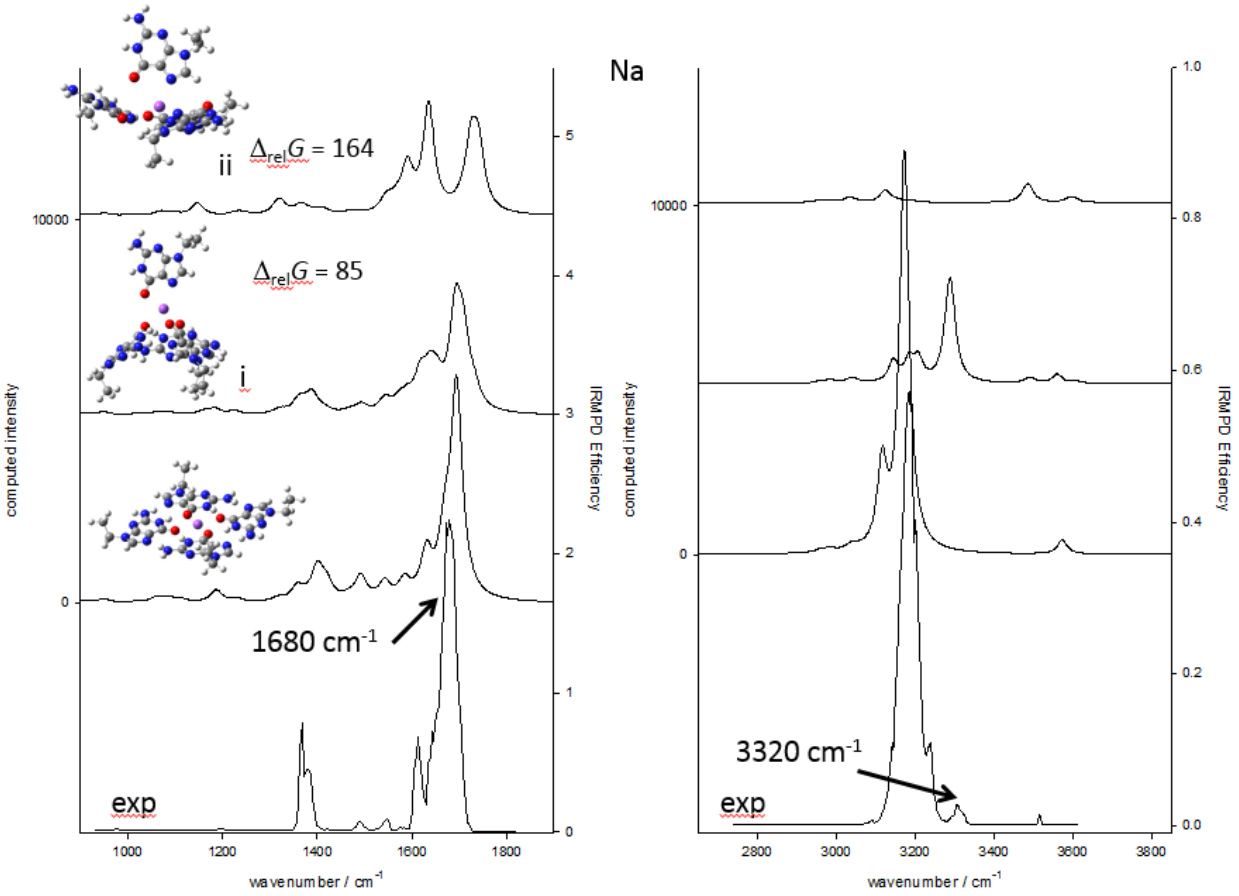

Figure S2b) Comparison of computed IR spectra for three isomers of $Li(9eG)_4^+$ with the experimental IRMPD spectra.

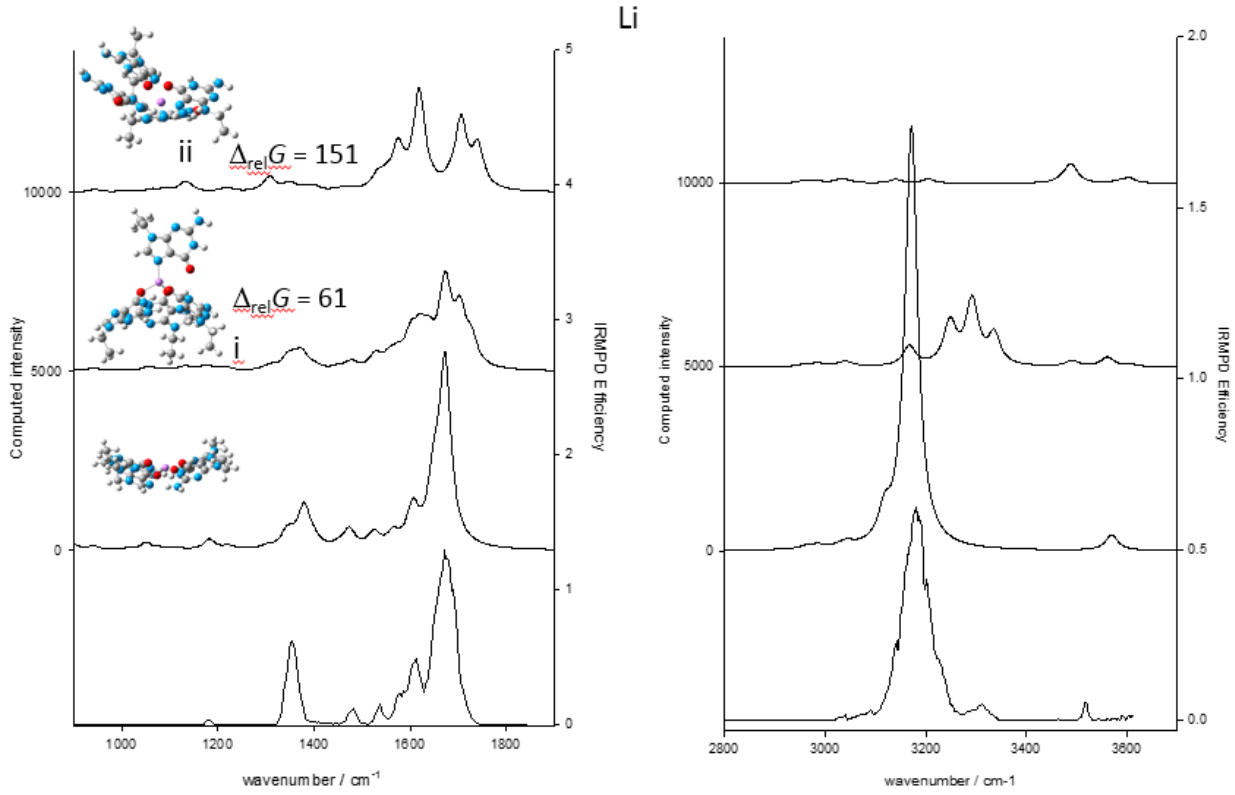

Figure S2c) Comparison of computed IR spectra for three isomers of $K(9eG)_4^+$ with the experimental IRMPD spectra.

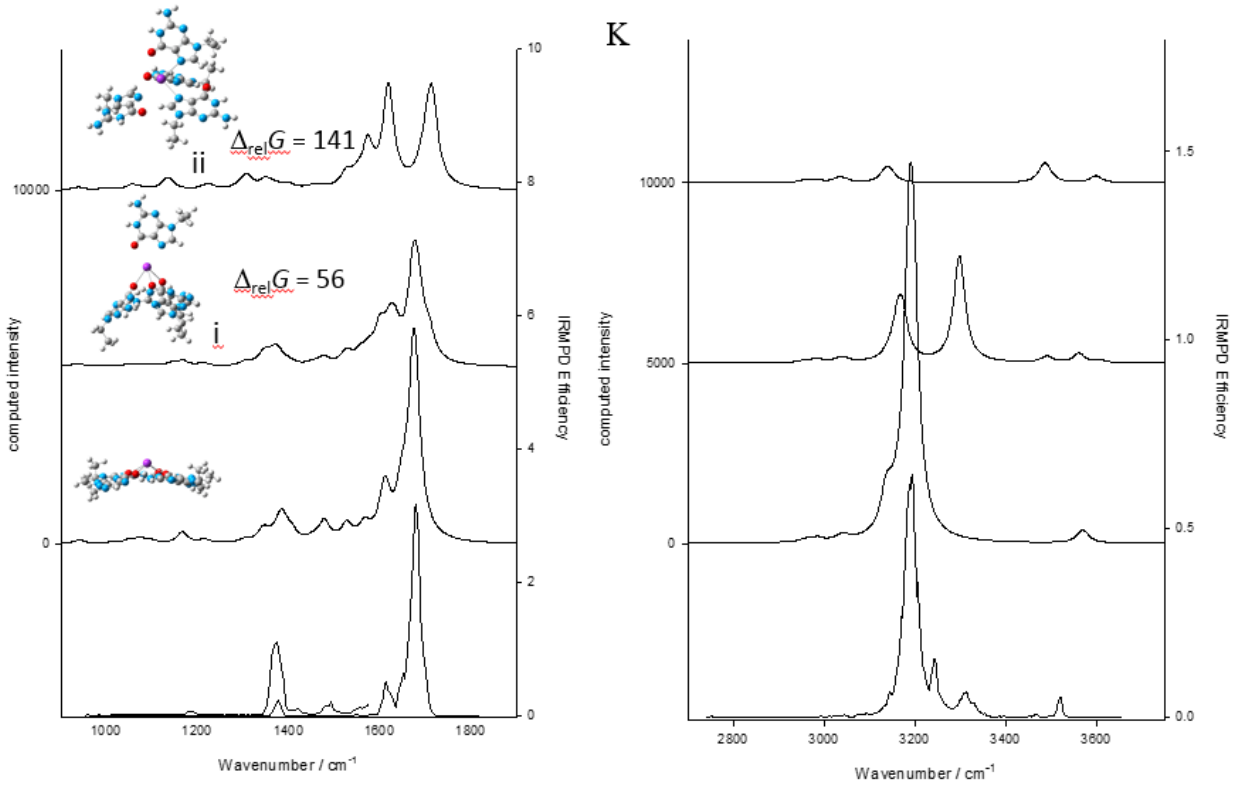

Figure S3. Energy resolved intensity profiles for SORI-CID of the $M(9\text{-eG})_4^+$ complexes.

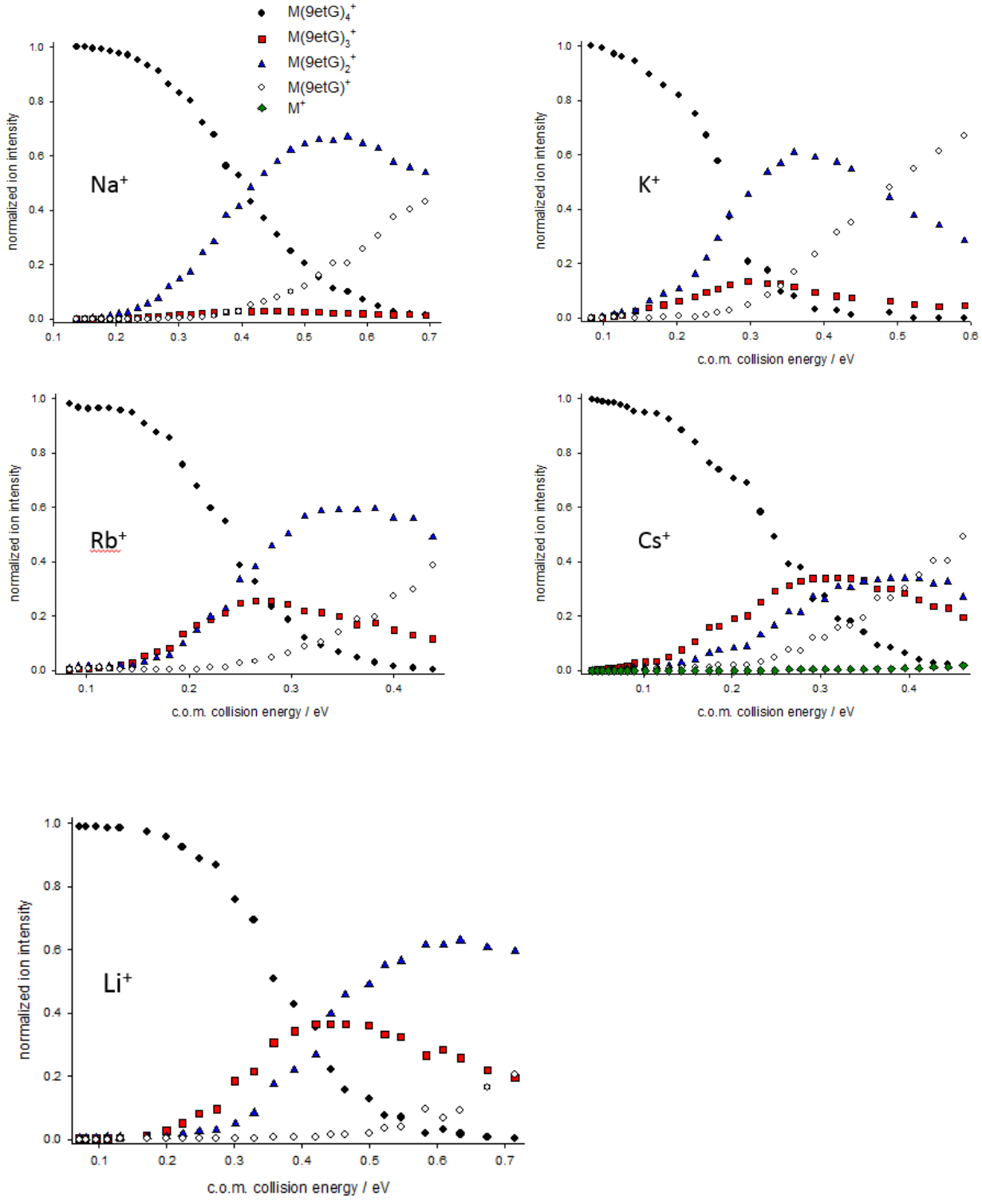

Figure S4. Energy-resolved G-tetrad intensity profiles for the SORI-CID of $M(9eG)_4^+$ with a) a reservoir pressure of 5 mbar and b) a reservoir pressure of 15 mbar with Ar.