

G2 Atomization Energies With Chemical Accuracy

Bathélemy Pradines,¹ Anthony Scemama,¹ Julien Toulouse,² Pierre-François Loos,^{1, a)} and Emmanuel Giner²

¹*Laboratoire de Chimie et Physique Quantiques (UMR 5626), Université de Toulouse, CNRS, UPS, France*

²*Laboratoire de Chimie Théorique, Université Pierre et Marie Curie, Sorbonne Université, CNRS, Paris, France*

I. INTRODUCTION

II. RESULTS

A. The case of C₂ and the comparison with the F₁₂ methods.

^{a)}Corresponding author: loos@irsamc.ups-tlse.fr

TABLE I. Dissociation energy (D_e) in kcal/mol of the C_2 molecule computed using FCIQMC, CIPSI, FCIQMC+F₁₂, CIPSI+LDA_{HF} and CIPSI+LDA_{HF-val} (valence only interaction and density) in the Dunning cc-pVXZ (VXZ) basis sets.

	FCIQMC	CIPSI	FCIQMC+F ₁₂	CIPSI+LDA _{HF}	CIPSI+LDA _{HF-val}	CIPSI+PBE _{HF}	CIPSI+PBE _{HF-val}
V2Z	130.0	132.0	142.3	141.9	142.9	142.7	145.6
V3Z	139.9	140.3	145.3	142.8	145.5	142.7	146.7
V4Z	-	143.6	-	145.8	146.2	145.3	147.0
V5Z	-	144.3	-	145.1	146.1	144.9	146.5
			Estimated exact				
			146.9				