Theoretical Study of the Reactive Intermediate 
$\text{Si}_2\text{Me}_4[(\eta^5\text{-C}_5\text{H}_4)\text{Fe(CO)}_2]^{2-}$

Juvencio Robles$^{2,3}$ and Jorge Cervantes$^{2,4}$

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In two previous papers (King et al., J. Organomet. Chem. 19, 327, 1969; Pannell et al., Organometallics 9, 859, 1990), the synthesis and X-ray structure of the two tetramethyl disilyl complexes $[(\eta^5\text{-C}_5\text{H}_4)\text{Fe(CO)}_2]_2\text{Si}_2\text{Me}_4$ (I) and $\text{Si}_2\text{Me}_4[(\eta^5\text{-C}_5\text{H}_4)\text{Fe(CO)}_2\text{CH}_3]_2$ (II) were reported. Complex II is obtained from I [2]. However, attempts to form other derivatives from I have generally failed. In the chemical process to get II from I, an intermediate complex, $\text{Si}_2\text{Me}_4[(\eta^5\text{-C}_5\text{H}_4)\text{Fe(CO)}_2]^{2-}$ (III), is probably formed. This is similar to complex II without the two methyl groups bonded to the Fe atoms. Therefore, a theoretical study that may shed some light on the intermediate structure, stability, and reactivity is justified. We have developed theoretical studies consisting of extended Huckel electronic structure calculations on the simulated intermediate geometry. The results obtained from these calculations suggest that it might be stable enough to form during reactions of complex I. The more reactive sites, which suggest reaction alternatives, are pointed out.

KEY WORDS: Theoretical; extended Huckel; molecular mechanics; silyl organometallic complexes.

INTRODUCTION

Structures of two tetramethyldisilyl complexes, $[(\eta^5\text{-C}_5\text{H}_4)\text{Fe(CO)}_2]_2\text{Si}_2\text{Me}_4$ (I) (see Fig. 1) and $\text{Si}_2\text{Me}_4[(\eta^5\text{-C}_5\text{H}_4)\text{Fe(CO)}_2\text{CH}_3]_2$ (II) (see Fig. 2), have been recently determined [1, 2]. Complex II is obtained from

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2Facultad de Química, Universidad de Guanajuato, Noria Alta s/n, Guanajuato, Gto., 36050, México.
3On sabbatical leave from Departamento de Química, Universidad Autónoma Metropolitana-Iztapalapa, 09340 D.F., México.
4To whom correspondence should be addressed.

79
I by using a base treatment [lithium diisopropylamide (LDA) at 0°C], in tetrahydrofuran (THF) solution. This seems to induce the tetramethyl disilyl double group migration, cleaving the Fe–Si bonds. During this process, an intermediate, Si₂Me₄[(η⁵-C₅H₅)Fe(CO)₂]₂⁻Li₂⁺ (III) (see Fig. 3), is probably formed. Thereafter, direct methylation yields complex II. Similar results have been obtained in the case of base treatments of other group 14 organometallic complexes [3–6].

We have tested several routes to obtain other organometallic derivatives using complex III, but they have failed so far. A better understanding of the suggested intermediate, in terms of stability and reactivity, might provide