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Preparation and Characterization of Simple Dihalomethylidene Platinum Dihalide Complexes in Reactions of Laser-Ablated Pt Atoms with Tetrahalomethanes

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Table S1: Observed and Calculated Fundamental Frequencies for the $\text{CFCl}=\text{PtCl}_2$ and $\text{CF}_2=\text{PtCl}_2$ Methylidene Complexes in the Singlet Ground Electronic States^a

| Approximate Description | $\text{CFCl}=\text{PtCl}_2$ | | | $\text{CF}_2=\text{PtCl}_2$ | | |
|------------------------------|-----------------------------|------|-----|-----------------------------|------------------|-----|
| | obs | calc | int | obs | calc | int |
| C-F str | 1242.7 | 1252 | 356 | 1327.3 | 1333 | 684 |
| C-Cl, C-F str, ^b | 1006.2 | 994 | 331 | 1293.9 | 1276 | 216 |
| C-Cl str, CF_2 bend | | 540 | 3 | 730.1 | 731 ^b | 5 |
| C-F def | | 504 | 2 | | 573 | 7 |
| Pt-Cl str | | 367 | 69 | | 385 | 2 |
| C-F def | | 357 | 7 | | 368 | 70 |
| Pt-Cl, str, | | 344 | 0 | | 352 | 1 |
| CFX rock | | 266 | 0 | | 321 | 0 |
| F-C-X def | | 107 | 1 | | 110 | 1 |

^aFrequencies and intensities are in cm^{-1} and km/mol. Observed in an argon matrix. Frequencies and intensities computed with B3LYP/6-311++G(3df,3pd) in the harmonic approximation using the SDD core potential and basis set for Pt. Three real lower frequencies are not listed. ^bMode has some antisymmetric X-C=Pt stretching character.