Electronic Supplementary Material

Computational insights into CH$_3$MX (M = Cu, Ag and Au; X = H, F, Cl, Br and I)

Zhengguo Huang*   Yuan Yuan   Le Sun   Xiaohong Wang   Yuying Li

Tianjin Key Laboratory of Structure and Performance for Functional Molecules; Key Laboratory of Inorganic-Organic Hybrid Functional Materials Chemistry (Tianjin Normal University), Ministry of Education; College of Chemistry, Tianjin Normal University, Tianjin 300387, People's Republic of China

Table S1. The selected frequencies of the CH$_3$X (X = H and halogens) and CH$_3$M (M = coinage metals) calculated at the B3LYP level of theory [a].

	CH$_4$	CH$_3$F	CH$_3$Cl	CH$_3$Br	CH$_3$I	CH$_3$Cu	CH$_3$Ag	CH$_3$Au
CH$_3$, deform	1338.7 (12)	1481.3 (1)	1375.8 (12)	1324.5 (20)	1273.5 (28)	1132.4 (39)	1103.7 (62)	1201.6 (50)
CH$_2$, sys stretch	3033.0 (0)	3032.5 (33)	3072.8 (23)	3082.2 (16)	3087.1 (11)	3031.8 (21)	3055.5 (22)	3048.6 (11)
CH$_2$, asys stretch	3135.0 (22)	3111.9 (28)	3167.3 (4)	3185.6 (1)	3195.0 (0)	3124.2 (5)	3156.2 (3)	3150.2 (1)
v (C-Au)						544.6 (3)	453.8 (2)	540.0 (0)

[a] Frequencies are in cm^{-1} and intensities (in parentheses) are in km·mol^{-1}.

* Corresponding author. E–mail address: hsxyhzg@126.com