Electronic Supplementary Information for

Insight into structural and π-magnesium bonding characteristics of the $X_2Mg\cdots Y$ (X = H, F; Y = C_2H_2, C_2H_4 and C_6H_6) complexes

Si-Yi Li, Di Wu, Ying Li*, Dan Yu, Jia-Yuan Liu, Zhi-Ru Li

Institute of Theoretical Chemistry, Jilin University, Changchun 130023, P. R. China

E-mail: liyingedu@jlu.edu.cn

Table S1. Wiberg index of the C–C bond in the C_2H_2, C_2H_4, and C_6H_6 molecules and their complexes with X_2Mg (X = H, F).

	Bond	Wiberg bond index
C_2H_2	C≡C	3.00
$H_2Mg\cdots C_2H_2$		2.94
$F_2Mg\cdots C_2H_2$		2.95
C_2H_4	C=C	2.04
$H_2Mg\cdots C_2H_4$		1.97
$F_2Mg\cdots C_2H_4$		1.99
C_6H_6	C1–C2	1.44
$H_2Mg\cdots C_6H_6$		1.41
$F_2Mg\cdots C_6H_6$		1.41

Table S2. Selected harmonic vibrational frequencies (ν, cm^{-1}) and corresponding Raman intensities (RI, au.) of the five monomers.

	X-Mg-X sym. stretch		X-Mg-X antisym. stretch		C-C stretch	
	ν	RI	ν	RI	ν	RI
MgH_2	1634.2	496.7	1656.9	0		
MgF_2	551.4	4.9	861.1	0		
C_2H_2					1967.8	87.2
C_2H_4					1678.0	21.2
C_6H_6					1012.1	89.0

Fig. S1 The optimized geometries of the MgX_2 (X = F, H), C_2H_2, C_2H_4 and C_6H_6 molecules at the MP2/aug-cc-pVTZ level.

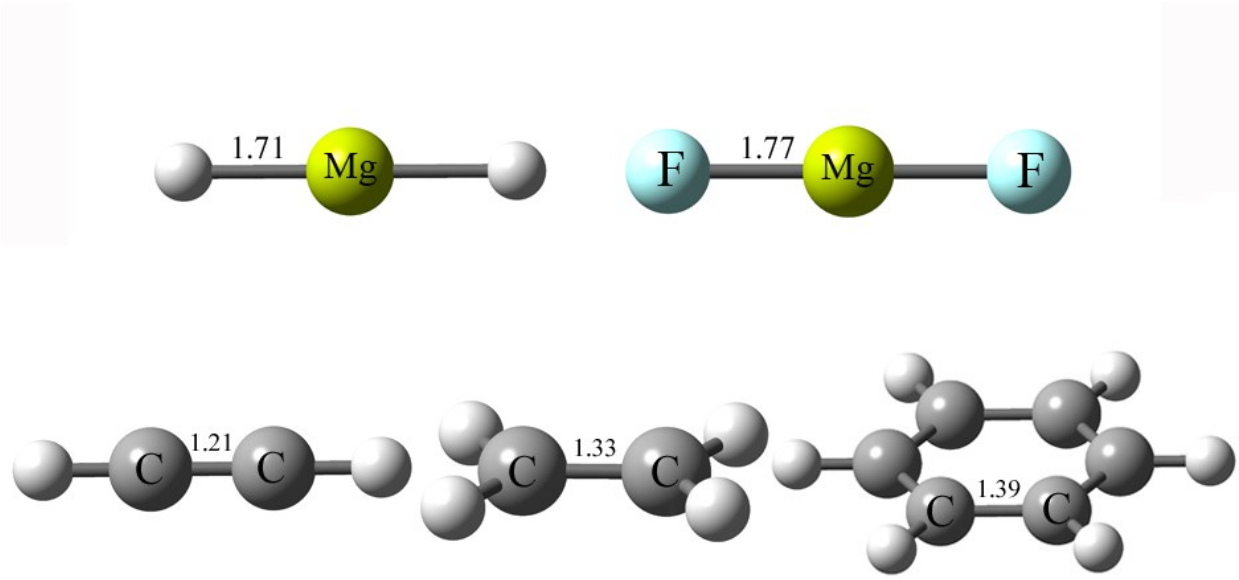
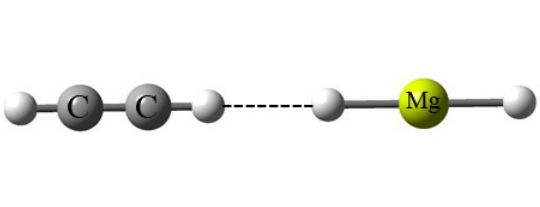
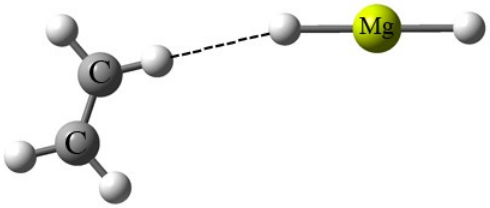


Fig. S2 The optimized hydrogen bonding complexes between the MgX_2 (X = F, H) and C_2H_2, C_2H_4 molecules at the MP2/aug-cc-pVTZ level.

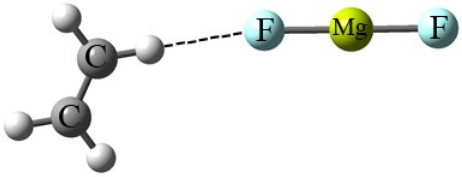


$MgH_2\cdots H_2C_2$



$MgH_2\cdots H_4C_2$

$MgF_2\cdots H_2C_2$



$MgF_2\cdots H_4C_2$