Supplementary Material (ESI) for Chemical Communications

Supporting Information: B602116F

Table 1: Calculations are done at B3LYP/LANL2DZ and at HF/6-31G level of theory.

Molecules	Mulliken overlap populations		Wiberg Bond Index in the NAO basis.	
	B3LYP/LANL2DZ	HF/6-31G	B3LYP/LANL2DZ	HF/6-31G
C_2H_6	0.252	0.252	1.047 (σ=1.001, π=0.046)	1.026
C_2H_4	0.596	0.593	2.053(σ=1.008, π=1.045)	2.034
C_2H_2	1.007	1.067	2.997(σ=0.997, π=2.000)	2.990
C_2	0.728	0.652	3.828(σ=1.827, π=2.001)	3.723
N_2	0.573	0.376	3.020 (σ=0.994, π=2.026)	3.029
N_2^{2+}	0.302	-0.086	3.652 (σ=1.652, π=2.000)	3.675
B_2H_2 ($^1\sum_g^+$)	0.725	0.798	2.491(σ=0.659, π=1.832)	2.414
B_2H_2 ($^1\sum_g^-$)	0.707	0.740	1.994(σ=0.994, π=1.000)	1.999
$Fe_2(CO)_6$	-0.003	0.235	0.864(σ=0.055, π=0.809)	0.740

Table 2: Electron densities at bond mid point are calculated at B3LYP/LANL2DZ level of theory.

Molecules	Electron density at bond mid point (in a.u)
C_2	0.2690
C_2H_2	0.3741
C_2H_4	0.3064
C_2H_6	0.2198
$Fe_2(CO)_6$	0.1041