Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Strong interactions between copper halides and unsaturated systems: new metallocycles? or the importance of deformation

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Supporting Information

(A total of five pages)

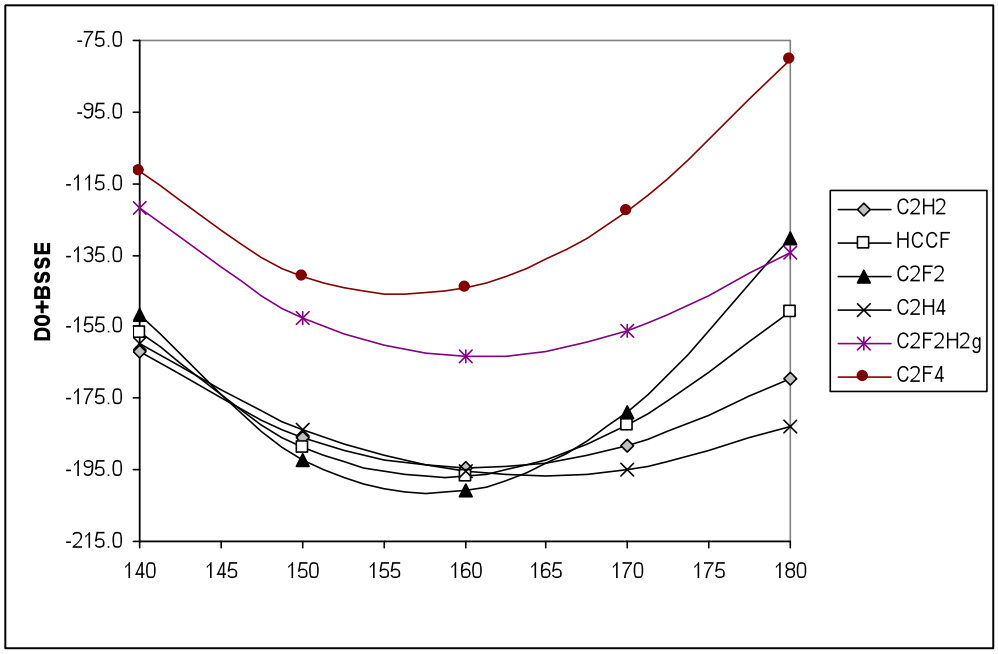

Figure S1. Variation of the dissociation energy (kJ mol^{-1}) of the complexes between CuF and fluoroacetylene and ethylene derivatives as a function of the angle α, defined in Scheme 1.

Table S1. Optimized geometry of the complexes calculated at the MP2/aug-cc-pVTZ and B3LYP/aug-cc-pVTZ computational levels (distances in Å, angles in degrees)

MP2	B3LYP
6a X X,1,1. C,1,r1,2,90. C,1,r1,2,90.,3,180.,0 H,1,r2,2,a2,3,0.,0 H,1,r2,2,a2,3,180.,0 Cu,1,r3,3,90.,2,0.,0 F,1,r4,3,90.,2,0.,0 r1=0.62816879 r2=1.67556248 r3=1.78878483 r4=3.51621979 a2=102.4310151	**6a** 6 0.000000 0.000000 0.000000 6 0.000000 0.000000 1.224090 1 0.258272 0.000000 -1.036219 1 0.258272 0.000000 2.260309 29 -1.898313 0.000000 0.612045 9 -3.669705 0.000000 0.612045
6a X X,1,1. C,1,r1,2,90. C,1,r1,2,90.,3,180.,0	**6a** 6 0.000000 0.000000 0.000000 6 0.000000 0.000000 1.224090

6b C,0.5861040621,0.,0.3615650955 C,-0.6694957132,0.,0.3254030091 F,1.7884634503,0.,-0.1137891212 H,-1.6719872211,0.,-0.0462840751 Cu,-0.048552506,0.,2.1263698665 F,0.0154679277,0.,3.8467352251	**6b** 6 0.000000 0.000000 0.000000 6 0.000000 0.000000 1.227796 9 0.427594 0.000000 -1.213189 1 0.270349 0.000000 2.260476 29 -1.869477 0.000000 0.590739 9 -3.627183 0.000000 0.428108
6c X X,1,1. C,1,r1,2,90. C,1,r1,2,90.,3,180.,0 F,1,r2,2,a2,3,0.,0 F,1,r2,2,a2,3,180.,0 Cu,1,r3,3,90.,2,0.,0 F,1,r4,3,90.,2,0.,0 r1=0.62489857 r2=1.89176523 r3=1.78814498 r4=3.50467252 a2=105.01910414	**6c** 6 0.000000 -0.614514 -1.143393 6 0.000000 0.614514 -1.143393 9 0.000000 -1.828859 -1.595361 9 0.000000 1.828859 -1.595361 29 0.000000 0.000000 0.700199 9 0.000000 0.000000 2.459047
6d X X,1,1. C,1,r1,2,90. C,1,r1,2,90.,3,180.,0 H,3,r2,1,a2,2,d2,0 H,3,r2,1,a2,2,-d2,0 H,4,r2,1,a2,2,d2,0 H,4,r2,1,a2,2,-d2,0 Cu,1,r3,3,90.,2,0.,0 F,1,r4,3,90.,2,0.,0 r1=0.6970369 r2=1.08332926 r3=1.80434981 r4=3.53377473 a2=120.54775531 d2=99.43015124	**6d** 6 0.683197 0.000000 -0.059496 6 -0.683197 0.000000 -0.059496 1 1.246441 -0.919079 -0.164890 1 1.246441 0.919079 -0.164890 1 -1.246441 0.919079 -0.164890 1 -1.246441 -0.919079 -0.164890 29 0.000000 0.000000 1.865394 9 0.000000 0.000000 3.639832
6e C,0.6597636233,0.235392989,-0.0473508372 C,-0.726555086,0.2429635307,-0.0045131801 F,1.3751321242,-0.021170338,1.0689192674 H,1.2455301383,0.0895294145,-0.94709435 H,-1.2373597201,0.0226670415,0.9236119057 H,-1.2696515171,0.1110072993,-0.931783169 Cu,-0.0471313608,2.0470742787,-0.0308362972 F,0.000271798,3.7725357604,-0.0309533397	**6e** 6 0.651328 0.163955 -0.041140 6 -0.708118 0.187657 0.000878 9 1.377207 -0.068663 1.066954 1 1.251114 0.096801 -0.940353 1 -1.235791 0.000220 0.926379 1 -1.264229 0.126590 -0.925356 29 -0.065966 2.111909 -0.031011 9 -0.005544 3.881532 -0.056351
6f C,0.6969346352,0.0394342651,0.0876455198 C,-0.6969346352,0.0394342651,0.0876455198 H,1.2601999713,-0.8729680912,-0.0685344614 F,1.3752884094,1.1617875726,-0.201590555 F,-1.3752884094,1.1617875726,-0.201590555 H,-1.2601999713,-0.8729680912,-0.0685344614	**6f** 6 0.683382 0.051497 0.022476 6 -0.683382 0.051497 0.022476 1 1.262798 -0.861222 -0.039500 9 1.376535 1.163401 -0.251500 9 -1.376535 1.163401 -0.251500 1 -1.262798 -0.861222 -0.039500
6f C,0.6969346352,0.0394342651,0.0876455198 C,-0.6969346352,0.0394342651,0.0876455198 H,1.2601999713,-0.8729680912,-0.0685344614 F,1.3752884094,1.1617875726,-0.201590555 F,-1.3752884094,1.1617875726,-0.201590555	**6f** 6 0.683382 0.051497 0.022476 6 -0.683382 0.051497 0.022476 1 1.262798 -0.861222 -0.039500 9 1.376535 1.163401 -0.251500 9 -1.376535 1.163401 -0.251500

6g C,0.6969758648,0.0131810229,0.0908161128 C,-0.6969758648,-0.0131810229,0.0908161128 F,1.3691243655,-1.1347811083,-0.1565384228 H,1.2661563482,0.9104497206,-0.1174216725 F,-1.3691243655,1.1347811083,-0.1565384228 H,-1.2661563482,-0.9104497206,-0.1174216725 Cu,0.,0.,1.8944841897 F,0.,0.,3.6152441728	**6g** 6 0.683511 0.013319 0.025617 6 -0.683511 -0.013319 0.025617 9 1.369394 -1.131776 -0.167740 1 1.270941 0.910156 -0.122892 9 -1.369394 1.131776 -0.167740 1 -1.270941 -0.910156 -0.122892 29 0.000000 0.000000 1.953673 9 0.000000 0.000000 3.719795
6h C,0.6371145954,0.2521038118,0. C,-0.7535439053,0.2617186772,0. F,1.3593259013,0.006607326,1.0851623882 F,1.3593259013,0.006607326,-1.0851623882 H,-1.2624542714,0.0678838623,0.933501744 H,-1.2624542714,0.0678838623,-0.933501744 Cu,-0.0866052998,2.0588167818,0. F,0.0092913498,3.7783783298,0.	**6h** 6 0 0.635181 0.159696 0.000000 6 0 -0.726146 0.217198 0.000000 9 0 1.367596 -0.030573 1.082164 9 0 1.367596 -0.030573 -1.082164 1 0 -1.253236 0.078967 0.932808 1 0 -1.253236 0.078967 -0.932808 29 0 -0.124214 2.131167 0.000000 9 0 -0.013541 3.895152 0.000000
6i C,0.6746613918,0.2783412323,-0.0083002903 C,-0.7262391125,0.2786845435,-0.0385908733 F,1.3539681437,-0.0240431168,1.0829095765 F,1.3842779925,0.0363682699,-1.1059631721 F,-1.3970225262,-0.0259172488,1.0905335781 H,-1.2569153355,0.0839809627,-0.9609786573 Cu,-0.0448263807,2.078234597,-0.0310551052 F,0.0120958268,3.7943507232,-0.0285550563	**6i** 6 0.666356 0.203442 -0.003931 6 -0.707254 0.224949 -0.033921 9 1.360510 -0.056065 1.083995 9 1.391400 0.037071 -1.100522 9 -1.395569 -0.041697 1.091621 1 -1.257488 0.098670 -0.956384 29 -0.069247 2.137551 -0.037100 9 0.011292 3.896079 -0.043758
6j X X,1,1. C,1,r1,2,90. C,1,r1,2,90.,3,180.,0 F,3,r2,1,a2,2,d2,0 F,3,r2,1,a2,2,-d2,0 F,4,r2,1,a2,2,d2,0 F,4,r2,1,a2,2,-d2,0 Cu,1,r3,3,90.,2,0.,0 F,1,r4,3,90.,2,0.,0 r1=0.70302852 r2=1.32542028 r3=1.7998219 r4=3.51247609 a2=120.54955161 d2=105.05063517	**6j** 6 0.690996 0.000000 -0.056976 6 -0.690996 0.000000 -0.056976 9 1.382176 -1.102226 -0.303155 9 1.382176 1.102226 -0.303155 9 -1.382176 1.102226 -0.303155 9 -1.382176 -1.102226 -0.303155 29 0.000000 0.000000 1.847563 9 0.000000 0.000000 3.605704

Table S2. C-Cu Wiberg bond indexes (WBI) and electron densities at the BCP (ρ_b, a.u.) for B-CuF complexes (B = C_2H_2, C_2F_2, C_2H_4, HFC=CFH(E)) keeping the monomers in their equilirium conformation.

B	WBI	ρ_b
C_2H_2	0.311	0.088
C_2F_2	0.218	0.086
C_2H_4	0.261	0.084
HFC=CFH(E)	0.225	0.079