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Complexes of Carbon Dioxide with Dihalogenated Ethylenes: Structure, Stability and Interaction

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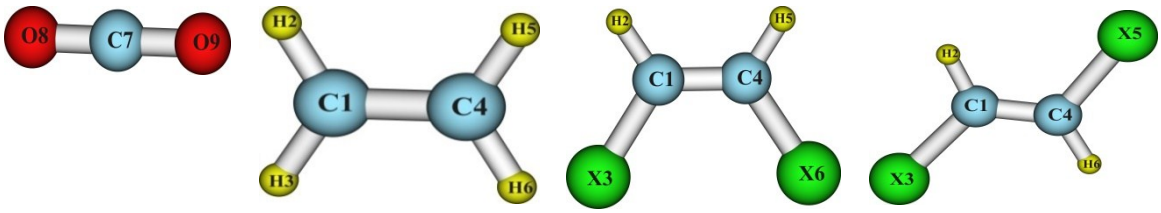


CO_2 CH_2=CH_2 *cis*-XCH=CHX *trans*- XCH=CHX

Figure S1. Stable structures of CH_2=CH_2, *cis*-XCH=CHX and *trans*-XCH=CHX (X = F, Cl, Br), and CO_2

Table S1. Selected parameters of C_2H_4 and CO_2 at MP2/aug-cc-pVDZ

Monomers	**C_2H_4**		**Monomer**	**CO_2**	
	Calculated[a)]	Experiment[b)]		Calculated[a)]	Experiment[b)]
$\angle H_2C_1H_3$	117.4°	117.6°	∠O8C7O9	180	180
$\angle H_2C_1C_4$	121.3°	121.2°	C7O8(O9)	1.180	1.162
$r(C_1\text{-}C_4)$	1.35 Å	1.339 Å			
$r(C_1\text{-}H_{2(3)})$ or $r(C_4\text{-}H_{5(6)})$	1.09 Å	1.086 Å			

[a)] Results calculated at the MP2/aug-cc-pVDZ level of theory

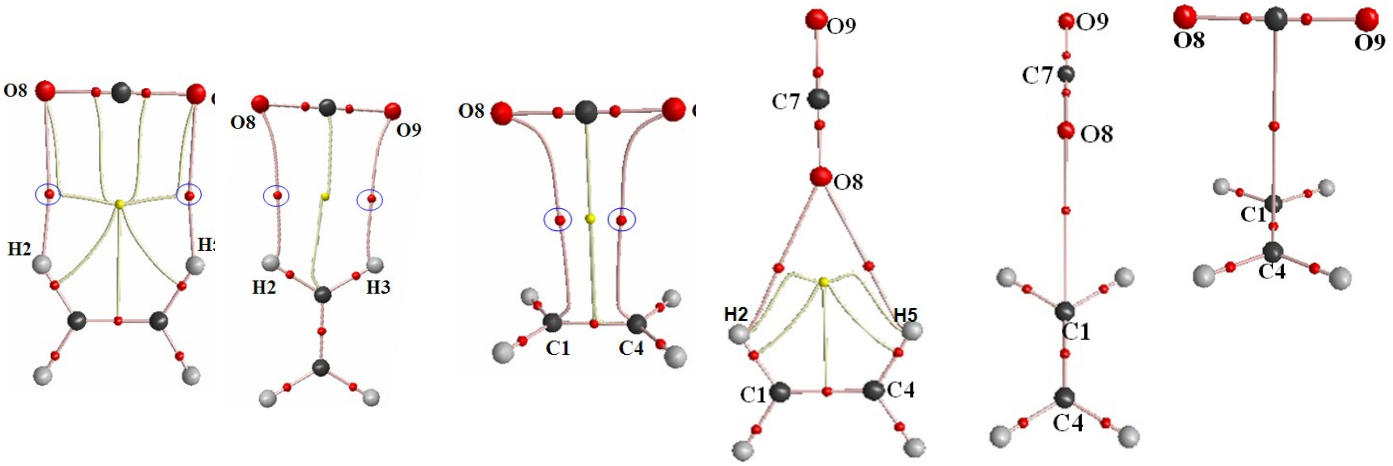
[b)]Experimental results taken from http://webbook.nist.gov/chemistry and http://cccbdb.nist.gov

Table S2. Selected parameters of *cis*-XCH=CHX and *trans*-XCH=CHX (X=F, Cl, Br) at MP2/ aug-cc-pVDZ and corresponding experimental results

		XCH=CHX, with X= F, Cl, Br					
		Calculated[a)]			Experiment[b)]		
		F	**Cl**	**Br**	**F**	**Cl**	**Br**
cis-XCH=CHX	$\angle C_1C_4X3$	122.3°	124.3°	125.1°	121.1°	124.2°	-
	$\angle H_2C_1C_4$	122.7°	126.6°	120.2°	124.0°	123.2°	-
	$R(C_1\text{-}C_4)$	1.34 Å	1.35 Å	1.35 Å	1.324 Å	1.317 Å	-
	$R(C_1\text{-}H_2)$	1,09 Å	1.09 Å	1.09 Å	1,089 Å	1.101 Å	-
	$R(C_1\text{-}X_3)$	1.36 Å	1.73 Å	1.88 Å	1.335 Å	1.717 Å	-
trans-XCH=CHX	$\angle C_1C_4X_3$	119.5°	120.9°	121.01°	119.3°	123.8°	-
	$\angle H_2C_1C_4$	125.8°	123.9°	124.0°	129.2°	-	-
	$R(C_1\text{-}C_4)$	1.34 Å	1.35 Å	1.35 Å	1.329 Å	1.354 Å	-
	$R(C_1\text{-}H_2)$	1.09 Å	1.09 Å	1.09 Å	1.080 Å	1.075 Å	-
	$R(C_1\text{-}X_3)$	1.36 Å	1.74 Å	1.89 Å	1.344 Å	1.718 Å	-

[a] Results calculated at the MP2/aug-cc-pVDZ level of theory

[b]Experimental results taken from http://webbook.nist.gov/chemistry and http://cccbdb.nist.gov



P1 **P2** **P3** **P4** **P5** **P6**

Figure S2. Topological analysis of complexes of ethylene and CO_2

The Cartesian coordinates for all optimized structures:

P1
C,0.1854712686,0.,0.1540951812
H,0.2112045779,0.,0.9386848353
H,1.146649709,0.,-0.6747647379
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C,-2.2410988948,0.,2.6469382356
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O,-3.2588514152,0.,2.0492296662
P2
C,-0.3398854535,0.,-0.1801290663
H,-0.2794666821,0.,0.9115606076
H,0.5974276309,0.,-0.7430508671
C,-1.5320557283,0.,-0.811943453
H,-1.5965266244,0.,-1.903029517
H,-2.4711443444,0.,-0.2527137447
C,2.6879219941,0.,1.4245178084

O,3.2401317655,0.,0.3814720058
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P3
C,0.,0.6750909606,-1.8955517327
H,-0.9331241184,1.244413106,-1.8963001371
H,0.9331241184,1.244413106,-1.8963001371
C,0.,-0.6750909606,-1.8955517327
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