Electronic Supplementary Material (ESI) for RSC Advances.

Monocyclic and bicyclic CO_4: How stable can they be?

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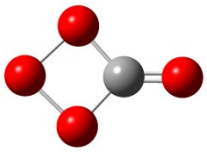
SI1: The structures, energies of the oligomers of isomer ^{1}**1** and ^{1}**1** at the B3LYP/aug-cc-pVTZ level.

SI Table 1: Relative Energies (kcal mol^{-1}) of ^{1}**TS1**, **U**^{1}**TS1**, ^{1}**TS2**, **U**^{1}**TS2** and products $\mathbf{CO_2}$+$^1\mathbf{O_2}$.

SI1: The structures, energies of the oligomers of isomer **^{1}1** and **^{1}1** at the B3LYP/aug-cc-pVTZ level.

Isomer ^{1}1

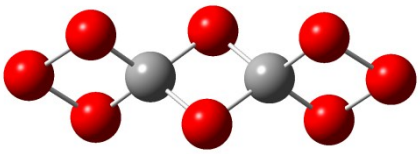


8	0.000000	0.000000	1.730283
6	0.000000	0.000000	0.556836
8	0.000000	1.011963	-0.363948
8	0.000000	-1.011963	-0.363948
8	0.000000	0.000000	-1.420015

Sum of electronic and zero-point Energies=-338.924477

Oligomers of isomer ^{1}1

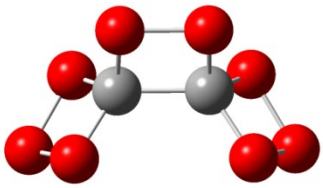
CO head-to-tail:



8	-0.000047	-0.000222	-1.013672
6	0.975804	-0.000013	-0.000179
8	1.912244	1.019585	-0.000304
8	1.912279	-1.019567	-0.000025
8	2.968463	0.000027	0.000267
8	0.000053	0.000152	1.013676
6	-0.975816	-0.000024	0.000171
8	-1.912277	-1.019558	0.000313
8	-1.912240	1.019587	-0.000003
8	-2.968466	0.000023	-0.000245

Sum of electronic and zero-point Energies=-677.778939

CO head-to-head:



8	0.748595	1.645692	-0.000061
6	0.780435	0.246817	0.000016
8	1.509950	-0.356658	1.022059
8	1.509819	-0.356847	-1.022039
8	2.242315	-1.117299	0.000038
8	-0.748597	1.645696	-0.000108
6	-0.780404	0.246772	0.000006
8	-1.509793	-0.356887	-1.022025
8	-1.509899	-0.356684	1.022063
8	-2.242415	-1.117205	0.000056

Sum of electronic and zero-point Energies=-677.668074

SI Table 1: Relative Energies (kcal mol^{-1}) of **^{1}TS1**, **U^{1}TS1**, **^{1}TS2**, **U^{1}TS2** and products **CO_2+$^1O_2$**.

	^{1}TS1[U^{1}TS1]^a	**^{1}TS2[U^{1}TS2]^a**	**CO_2+$^1O_2$^{a}**
B3LYP/aug-cc-pVTZ+ZPVE	31.6[20.3]	68.2[50.8]	-29.5[-57.8]
G3B3	36.9	69.1	-33.6
CBS-QB3	37.0	69.1	-32.0
G4	37.1	68.3	-33.5
W1BD	35.2	65.5	-32.3
CCSD(T)/aug-cc-pVTZ// B3LYP/aug-cc-pVTZ+ZPVE	36.6[22.8]	68.7[53.8]	-30.9[-51.1]
CCSD(T)/aug-cc-pVQZ// B3LYP/aug-cc-pVTZ+ZPVE	36.6[23.2]	69.0[54.8]	-31.7[-51.6]
CCSD(T)/CBS// B3LYP/aug-cc-pVTZ+ZPVE	36.6[23.5]	69.3[55.6]	-32.3[-52.0]
CASPT2(18e,12o)/aug-cc-pVTZ// B3LYP/aug-cc-pVTZ+ZPVE	[28.8]	[46.7]	[-43.8]
CASPT2(18e,12o)/aug-cc-pVQZ// B3LYP/aug-cc-pVTZ+ZPVE	[28.7]	[47.9]	[-44.6]
CASPT2(18e,12o)/CBS// B3LYP/aug-cc-pVTZ+ZPVE	[28.7]	[48.8]	[-45.2]

[a]The energy in the brackets from the open shell single point calculations based on the open shell geometries.