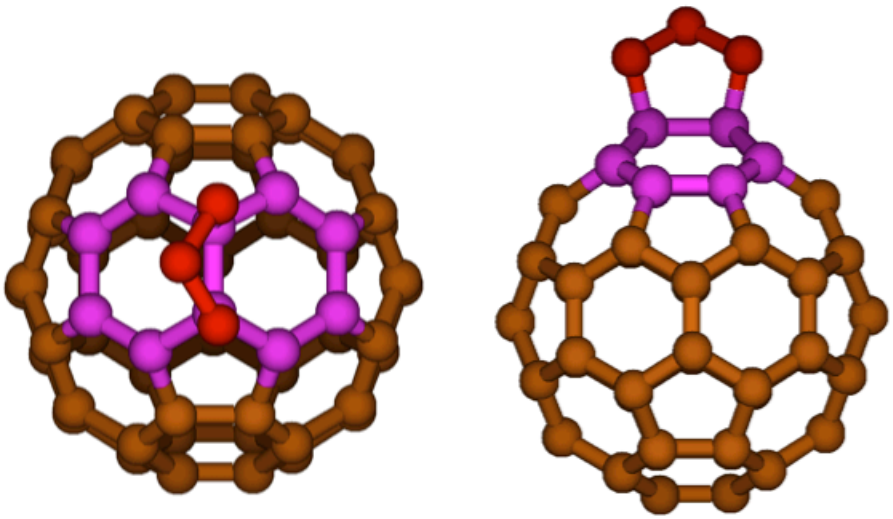
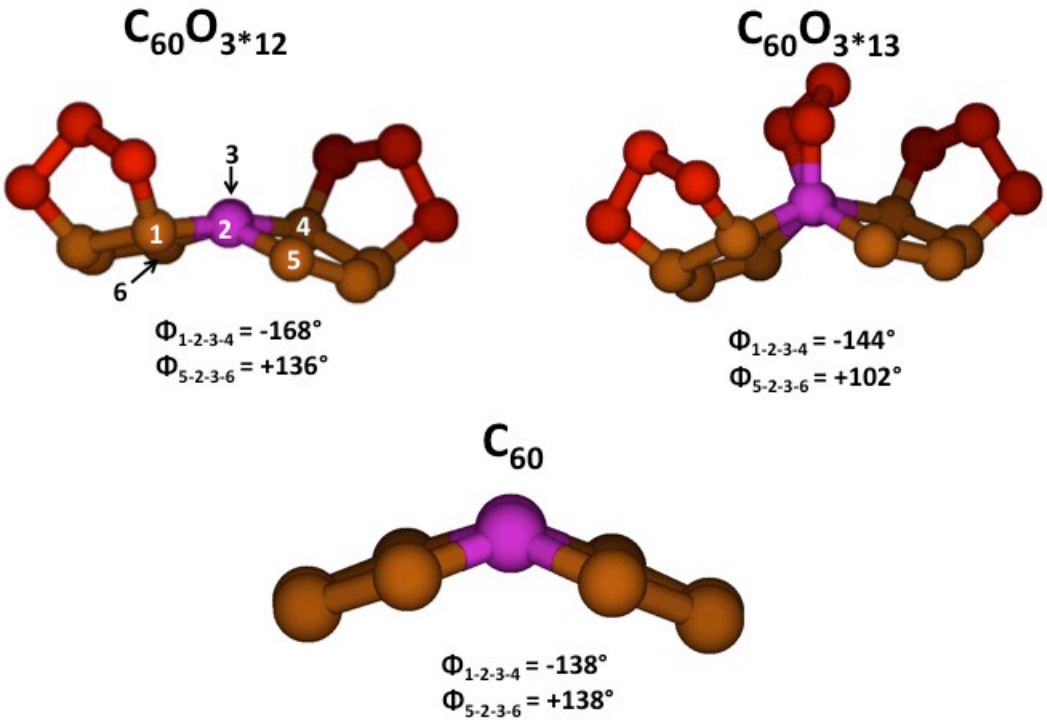
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

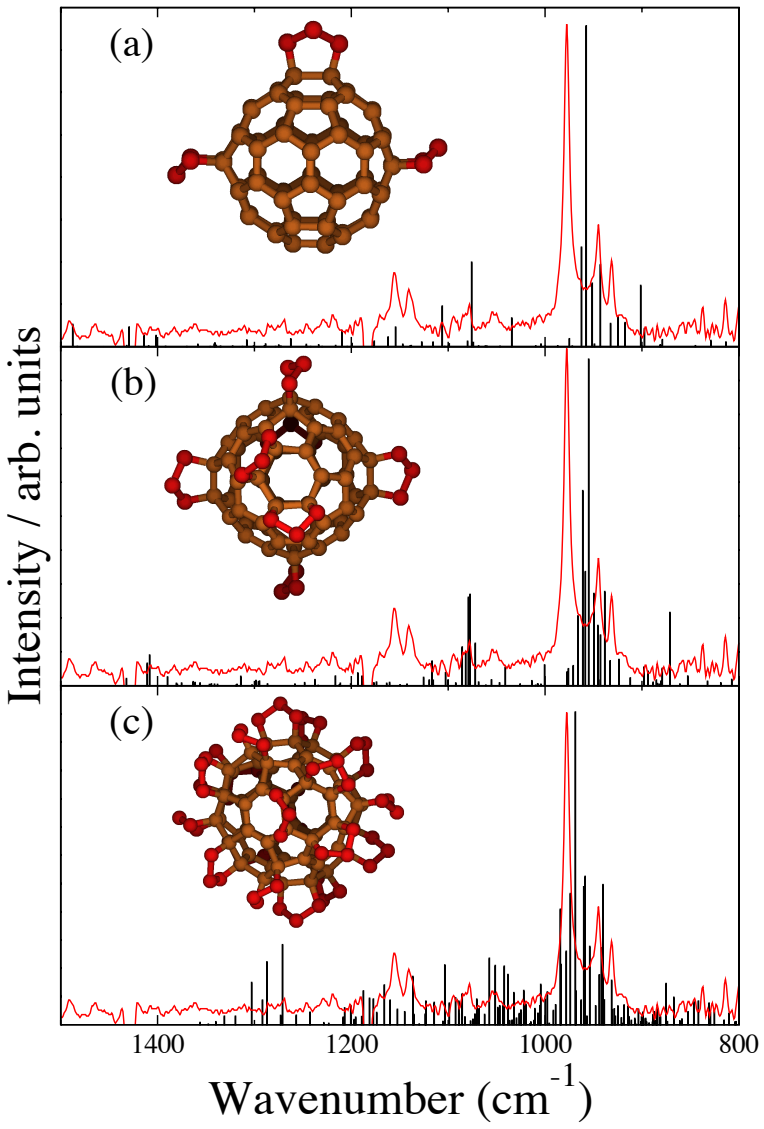
SUPPLEMENTAL INFORMATION



S1. Schematic of the partition between QM regions in the hybrid QM:QM CCSD(T)/6-311G*:B3LYP/6-31G* ONIOM calculations. In brown are carbon atoms calculated at the B3LYP/6-31G*. In pink are and red are the carbon and oxygen atoms belonging to the CCSD(T)/6-311G* layer.



S2. Structure of selected atoms in the $C_{60}O_{3*12}$, $C_{60}O_{3*13}$, and C_{60} molecules showing key C-C-C-C dihedral angles. The bond connecting the two carbon atoms that are central to the calculated dihedral angles are shown in pink for clarity.



S3. Calculated infrared spectra of (a) $C_{60}O_{3*3}$ POZ, (b) $C_{60}O_{3*7}$ POZ, and (c) $C_{60}O_{3*19}$ POZ. The red trace corresponds to the experiments of Ref. 24 after 100 L of ozone exposure to a C_{60} film. The spectra are normalized to highest peak height.

S4. Selected geometric features of stationary points along the C_{60} ozonolysis reaction pathway. The shaded cells indicate a relationship that includes non-bonded atoms.

	Distances (Å)			Angles (°)								Dihedrals (°)	
	1_C2_C	2_C3_C	$1'_O2_C$	$2_C1_C6_C$	$1'_O1_C6_C$	$1_C2_C3_C$	$1_C2_C2'_O$	$1'_O2_C2'_O$	$2'_O2_C3_C$	$2_C3_C4_C$	$3'_O3_C4_C$	$1'_O1_C6_C5_C$	$3'_O2'_O2_C3_C$
R(C_{60})	1.39	1.45	-	120.0	-	120.0	-	-	-	120.0	-	-	-
R→A	1.43	1.46	2.90	119.3	105.0	119.3	99.2	47.4	104.3	120.5	101.9	108.2	94.9
A	1.61	1.53	2.38	114.8	114.0	114.8	102.3	66.1	114.0	123.7	100.6	106.0	93.5
A→B	2.12	1.51	2.66	107.1	119.5	107.3	92.0	64.5	125.1	127.9	104.6	94.5	59.0
B	2.67	1.48	2.97	98.5	126.8	101.9	82.9	59.1	128.7	130.6	104.4	83.4	18.0
B→C	2.61	1.52	1.89	111.2	126.4	93.2	126.6	100.1	117.8	134.2	120.6	43.0	31.0
C	2.37	1.54	1.47	113.8	125.1	96.9	135.7	105.7	111.8	130.7	118.0	37.2	57.5
C→D	2.37	1.54	1.48	113.5	125.6	97.4	137.9	108.1	106.8	130.3	118.4	37.5	39.6
D	2.30	1.56	1.40	111.7	126.4	103.7	138.7	107.7	88.3	124.2	118.1	35.6	16.0
D→E	2.22	2.09	1.37	116.4	131.2	95.8	138.9	112.2	75.6	122.2	116.9	39.6	24.5
E	2.41	2.88	1.39	136.1	125.2	77.0	145.8	119.5	113.4	117.9	125.5	41.5	11.0
C→F	2.15	1.46	1.38	112.2	123.4	105.7	133.1	95.6	120.4	127.1	146.2	40.0	121.5
F	1.39	1.45	1.34	120.0	134.9	120.0	-	-	-	120.0	-	72.5	-