

Supplementary Information for:

Infrared spectra reveal box-like structures for a pentamer and hexamer of mixed carbon dioxide-acetylene clusters

by

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Table S1. Calculated structure of the lowest-energy isomer of $(\text{CO}_2)_3\text{-(C}_2\text{H}_2)_2$ (principal axis system atomic coordinates in Å).

Atom	a	b	c
C	-2.70383	-0.00004	-0.00052
O	-2.70436	-0.00229	1.16049
O	-2.70330	0.00221	-1.16153
C	0.76023	-2.06214	-0.00283
O	1.91620	-2.17026	-0.00265
O	-0.39573	-1.95403	-0.00300
C	0.76015	2.06217	0.00311
O	1.91612	2.17030	0.00349
O	-0.39581	1.95402	0.00273
C	1.59787	0.00342	-2.38449
H	2.64895	0.00316	-2.24768
C	0.40459	0.00371	-2.53982
H	-0.64648	0.00396	-2.67663
C	1.59653	-0.00337	2.38516
H	2.64766	-0.00308	2.24883
C	0.40318	-0.00371	2.53994
H	-0.64796	-0.00400	2.67628