

Table S1 The structure of MoTe<sub>2</sub>, CO, CH<sub>3</sub>CHO, and C<sub>6</sub>H<sub>6</sub> gases.

Structure	This study (DFT)	Reference (Experiment)	References
MoTe <sub>2</sub>	Mo-Te: 2.758	Mo-Te: 2.65	[1]
CO	C-O: 1.099	C-O: 1.128	[2]
CH <sub>3</sub> CHO	C-H: 1.217	C-H: 1.09	[3]
	C-C: 1.509	C-C: 1.54	
	C-O: 1.217	C-O: 1.20	
C <sub>6</sub> H <sub>6</sub>	C-C: 1.399	C-C: 1.39	[4]
	C-H: 1.091	C-H: 1.09	

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