Supplementary Information for

Formation of hydroxy, cyano and ethynyl derivatives of C_4H_4 isomers in the interstellar medium

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Table S1: Relative energies (in kcal/mol) for the cyclobutadiene, butatrieno **and** vinylacetylene. ZPV energies included

Sistema	M08HX	CC-F12//M08HX	B2PLYPD3	CC-F12//B2PLD	CCSD(T)-F12	CCSD(T)/CBS[a]	CCSD(T)/cc-pVTZ[b]
c-C_4H_4	36.20	33.22	38.68	33.06	32.97	33.68	33.40
H_2CCCCH_2	5.34	7.64	6.18	7.74	9.03	7.64	7.70
$H_2CCHCCH$	0.00	0.00	0.00	0.00	0.00	0.00	0.00

[a]From reference **24**, computed on the B3LYP/cc-pVTZ optimized geometries

[b]From reference **21**, computed on the B3LYP/6-311++G(3df,3dp) optimized geometries

Figure S1:

Geometrical parameters for C_4H_4 isomers and OH, CN, and CCH, radicals, calculated at the M08HX/aug-cc-pVTZ, MPWB1K/aug-cc-pVTZ (in parentheses), B2PLYPD3/aug-cc-pVTZ (in brackets) and CCSD(T)-F12/cc-pVTZ-F12 (in curly bracket) levels. **Experimental values for H_2CCCCH_2, $H_2CCHCCH$[40], CCH[42], CN, and OH[41] are given in blue.** Distances are given in Angstroms. **Relative energies for C_4H_4 isomers are also given at the M08HX/aug-cc-pVTZ, B2PLYPD3/aug-cc-pVTZ (in brackets) and CCSD(T)-F12/cc-pVTZ-F12 (in curly bracket) levels.**