Supporting Information

Bottom-Up Synthesis of 1,1-Ethenediol (H2CC(OH)2) - the Simplest Unsaturated Geminal Diol - in Interstellar Analogue Ices

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**Table S1.** Assignments of new infrared peaks after irradiation in the CO2:CH4 ice

|  |  |  |
| --- | --- | --- |
| Band position (cm−1) | Assignment | Characterization |
| 821 | 12 C2H6 | CH3 rock |
| 958 | 7 C2H4 | CH2 wag |
| 1022 | 15 CH3OH | CO stretch |
| 1051 | 15 t-CH3COOH | CH3 rocking |
| 1078 | 4 t-HOCO | CO stretch |
| 1091 | 2 HCO | HCO bending |
| 1157 | 8 t-CH3COOH | CHO rocking |
| 1195 | 8 t-CH3COOH | CHO rocking |
| 1352 | 7 CH3CHO | CH3 deformation |
| 1373 | 6 C2H6 | CH3 symm. def. |
| 1465 | 11 C2H6 | CH3 d-def. |
| 1499 | 3 H2CO | CH2 scissor |
| 1610 | 5 H2C=CHOH | C=C stretch |
| 1640 br | 5 H2C=CHOH | C=C stretch |
| 1722 | 4 t-CH3COOH B | CO stretch |
| 1736 br |  (CO) RCHO | CO stretch |
| 1756 | 4 t-CH3COOH A | CO stretch |
| 1783 | 4 t-CH3COOH M | CO stretch |
| 1823 | 2 t-HOCO | CO stretch |
| 1842 | 2 t-HOCO | CO stretch |
| 1853 | 2 t-HOCO/3 HCO | CO stretch |
| 2093 | 1 13CO | CO stretch |
| 2140 | 1 CO | CO stretch |
| 2742 | CH RCHO | CH stretch |
| 2844 | 2+4+12 C2H6 | combination |
| 2884 | 5 C2H6 | CH3 symm str. |
| 2924 | methylacetelyne/propene | CH3 symm str. |
| 2945 | 3 CH3COOH | CH3 symm str. |
| 2962 | 1 C2H6 | CH3 symm str. |
| 2977 | 10 C2H6 | CH3 deg. str. |
| 3097 | 9 C2H4 | CH2 asymm. str. |
| 3147 | 3 CH3 | CH stretch |
| 3259 | 3 C2H2 | CH stretch |
| 3500 br | (OH) | OH stretch |

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**Table S2.** Error analysis of computed ionization energies for COMs containing oxygen atoms; adiabatic ionization energies were computed at CCSD(T)/CBS//B3LYP/cc-pVTZ level of theory + zero-point vibrational energy.

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| --- | --- | --- | --- | --- | --- |
| **Structure** | **Name** | **Experimental adiabatic ionization energy in eV** | **Lowest Computed adiabatic ionization energy**  **in eV** | **Difference to lower bound** | **Difference to upper bound** |
|  | Acetone | 9.703 ± 0.006 [1](#_ENREF_1) | 9.71 | −0.013 | −0.001 |
|  | Propanal | 9.96 ± 0.01 [1](#_ENREF_1) | 9.97 | -0.02 | 0.00 |
|  | Propylene oxide | 10.22 ± 0.02 [2](#_ENREF_2) | 10.24 | −0.04 | 0.00 |
|  | Prop-1-en-2-ol | 8.67 ± 0.05 [3](#_ENREF_3) | 8.71 | −0.09 | 0.01 |
|  | 2-Propen-1-ol | 9.67 ± 0.03 [1](#_ENREF_1) | 9.65 | −0.01 | 0.05 |
|  | (*E*)-1-Propenol | 8.64 ± 0.02 [4](#_ENREF_4) | 8.61 | 0.01 | 0.05 |
|  | (*Z*)-1-Propenol | 8.70 ± 0.03 [4](#_ENREF_4) | 8.63 | 0.04 | 0.10 |
|  | Methanol | 10.84 ± 0.01 | 10.86 | −0.03 | −0.01 |
|  | Propadienone | 9.12 ± 0.05 | 9.15 | −0.08 | 0.02 |
|  | Formaldehyde | 10.88 ± 0.01 | 10.89 | −0.02 | 0.00 |
|  | Ketene | 9.617 ± 0.003 | 9.58 | 0.034 | 0.040 |
|  | Acetaldehyde | 10.229 ± 0.0007 | 10.24 | −0.0117 | −0.0103 |
|  |  |  | Average difference | −0.019 | 0.021 |
|  |  |  | Std. deviation | 0.039 | 0.033 |
|  |  |  | Error bounds | −0.06 | 0.05 |

**Table S3.** Data used to calculate irradiation doses of methane and carbon dioxide

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
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| |  |  |  | | --- | --- | --- | | irradiation current, *I* (nA) | 50 ± 5 | | | initial kinetic energy of the electrons, *E*init | 5 keV | | | total number of electrons | (1.1 ± 0.1)×1015 | | | average penetration depth, *l*\* (nm) | 360 ± 30 | | | density of the ice, *ρ* (g cm-3) | 0.87 ± 0.09 | | | average kinetic energy of transmitted electrons, *E*trans\* (keV) | 0.8 ± 0.1 | | | average kinetic energy of backscattered electrons, *E*bs\* (keV) | 3.4 ± 0.3 | | | fraction of transmitted electrons, *f*trans\* | 0 | | | fraction of backscattered electrons, *f*bs\* | 0.37 ± 0.04 | | | irradiated area, *A* (cm2) | 1.0 ± 0.1 | | | dose per molecule (eV) | CO2  9.9 ± 1.6 | CH4  3.6 ± 0.6 | | Notes: \*CASINO output values | | | |
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**References**

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