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**PI ReToF-MS TPD measurements of unirradiated ices**

To elucidate the reaction product(s), the TPD experiments were first conducted with unprocessed acetaldehyde and acetaldehyde‑2,2,2‑d3 ices at a photon energy of 10.49 eV (Fig. S3). As acetaldehyde polymerizes at low temperatures, these experiments are necessary to probe potential (protonated) acetaldehyde clusters as well as other impurities of the acetaldehyde. Fig. S3 shows the desorption profiles of mass-to-charge ratios between 40 and 200 for temperatures ranging from 80 K to 320 K for these measurements. While the main impurity of acetaldehyde‑d4 is found at a mass-to-charge ratio of 64, most probably corresponding to a C2D4O2 isomer, the only impurity all three samples have in common is found at mass-to-charge ratios of 117, 123, and 126 for CH3CHO, CD3CHO, and CD3CDO ices, respectively. These different masses indicate the empirical formula of the impurity to be C5H9O3 (C5D6H3O3 for acetaldehyde‑2,2,2‑d3), which points to a protonated cluster, e.g. of methylglyoxal (CD3COCHO) and acetaldehyde. Otherwise, no notable signals appear in the TPD profiles.

**Ratio determination for D2O + CH3CHO ice**

Deuterium oxide and the acetaldehyde isotoplogues were condensed onto the silver substrate through two separate gas deposition arms with partial pressures amounting to 3×10-8 Torr and 3×10-9 Torr for deuterium oxide and acetaldehyde, respectively. The thickness of the ice was determined to be 950 ± 50 nm by laser interference measurements. To determine the ratio of constituents in the ice, the integrated absorption of each acetaldehyde IR absorption feature shown in Fig. S6 was compared to that of the 500 nm thick neat acetaldehyde ice to determine the column density and corresponding thickness of the acetaldehyde in the ice. In this analysis the absorption peak at 1720 cm-1 was neglected as it changed drastically in shape in the mixed ice and its evaluation lead to a thickness more than twice of that derived from any other absorption feature. This analysis lead to a thickness of 220 ± 30 nm for acetaldehyde and correspondingly 730 ± 60 nm for deuterium oxide. Assuming densities of 0.78 g cm-3 and 1.05 g cm-3for acetaldehyde and deuterium oxide, respectively, this translates to column densities of (2.3 ± 0.3)×1017molecules cm‑1 and (2.3 ± 0.2)×1018 molecules cm-1,respectively, corresponding to a ratio of (10±1):1.

**Formation of acetaldehyde oligomers**

Upon irradiation, oligomers of acetaldehyde molecules form. In the experiments reported here they consist of up to four acetaldehyde molecules and are detected at *m/z* = 94, *m/z* = 141, and *m/z* = 188 with decreasing signal strength as molecular mass grows. Additionally, strong signals can be seen at m/z = 95, m/z = 142, and m/z = 189, corresponding to protonated acetaldehyde oligomers. The abundance of protonated oligomers in electron irradiated acetaldehyde ice also provides evidence of the suppressed formation of the vinoxy radical, which releases deuterium compared to the formation of the acetyl radical, which releases hydrogen. If both radicals formed at roughly equal abundance, this would be reflected in the relative amounts of protonated and deuteronated oligomers assuming these radicals to be the main source of hydrogen and deuterium. However, protonated acetaldehyde dimers (*m/z* = 95) are detected at a much higher signal strength than the deuteronated dimers (*m/z* = 96), the latter amounting to 9% of the signal at mass 95, as shown in Fig. S7. The deuterium needed to form the deuteronated dimers could be provided by release in the formation of ketene-d2 (CD2CO).

**Formation of acetone**

Another radical-radical reaction product detected in the TPD experiment is acetone‑d6 (CD3COCD3) at *m/z* = 64, as shown at 10.49 eV in Fig. S8. To validate the empirical formula, the desorption profile of *m/z*= 58 of irradiated acetaldehyde ice is also shown. Acetone can form from the reaction of the acetyl radical (CD3ĊO) with the methyl (ĊD3) radical:

|  |  |  |  |
| --- | --- | --- | --- |
| CD3CHO |  | ĊD3 + HĊO | (3a) |
| CD3CHO + H |  | ĊD3 + CO + H2 | (3b) |
| CD3ĊO + ĊH3 |  | CD3COCD3 | (4) |

As seen for the diacetyl, the same desorption profile is also detected at *m/z*= 63 at about 20% signal strength and at *m/z*= 62 with even lower signal strength, which is another indication of H/D exchange in the sample. Again, no additional desorption event is seen at *m/z*= 63 for propionaldehyde (CD3CD2CHO) which forms in the reaction of the methyl and the vinoxy radical. Similar to the formation of diacetyl, the formation of acetone from acetaldehyde is endoergic, but steps (3b) and (4) are both exoergic.

Even though the formation of the methyl radical should also produce the formyl radical (HĊO, step 3a above), no reaction products involving the formyl radical are detected. As the recombination of the acetyl and the formyl radical is exoergic and proceeds barrierless, this indicates that either the formyl radical exclusively reacts with hydrogen to form carbon monoxide and molecular hydrogen, which is endoergic (RG = ‑373 kJ mol-1), that the formation of methyl only proceeds from the acetyl radical to directly form methyl and carbon monoxide (step 3b), or that triple fragmentation to methyl, hydrogen and carbon monoxide is the dominating channel as seen in the gas phase photolysis experiments at 248 nm[1].

**Table S1.** Data used to calculate the irradiation dose of acetaldehyde‑2,2,2‑d3 (CD3CHO)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  |  | | --- | --- | | **irradiation current, I (nA)** | **15 ± 2** | | **initial kinetic energy of the electrons, Einit** | **5 keV** | | **total number of electrons** | **(2.8 ± 0.3)×1013** | | **average penetration depth, l\* (nm)** | **310 ± 30** | | **density of the ice, ρ (g cm-3)** | **0.87 ± 0.09** | | **average kinetic energy of transmitted electrons, Etrans\* (keV)** | **1.6 ± 0.2** | | **average kinetic energy of backscattered electrons, Ebs\* (keV)** | **3.3 ± 0.3** | | **fraction of transmitted electrons, ftrans\*** | **0.07 ± 0.01** | | **fraction of backscattered electrons, fbs\*** | **0.34 ± 0.03** | | **irradiated area, A (cm2)** | **1.0 ± 0.1** | | **dose per acetaldehyde molecule (eV)** | **0.31 ± 0.06** | | **total # molecules processed** | **(3.5 ± 0.5)×1017** | | Notes: **\*CASINO output values** | | |

**Table S2.** Observed infrared absorption features and their assignments before irradiation of acetaldehyde ice (CH3CHO) at 5 K.

|  |  |  |
| --- | --- | --- |
| Absorption cm-1 | Assignment[2] | Approximate type of mode[2] |
| 3417 | 24 | overtone |
| 3123 | 4 + 6 | combination |
| 3001 | 1 | as(CH3) |
| 2964 | 11 | (CH3) |
| 2916 | 2 | s(CH3) |
| 2858 | 6 | overtone |
| 2843 | 6 | overtone |
| 2759 | 3 | (CH) |
| 2736 | 3 | (CH) |
| 2598 | 4 + 9 | combination |
| 2466 | 7 + 8 | combination |
| 2234 | 7 + 9 | combination |
| 2003 | 8 + 9 | combination |
| 1769 | 9 | overtone |
| 1726 | 4 | (CO) |
| 1718 | 4 | (CO) |
| 1680 | 4 (CH313CHO) | (13CO) |
| 1641 | 8 + 10 | combination |
| 1546 | 14 | overtone |
| 1430 | 12 / 5 | (CH3) / as(CH3) |
| 1406 |  + 10 | combination |
| 1392 | 6 | (CH) |
| 1347 | 7 | s(CH3) |
| 1123 | 8 | r(CH3) |
| 1107 | 8 (13CH3CHO) | r(13CH3) |
| 886 |  + 15 | combination |
| 772 |  | (CH) |

**Table S3.** Observed infrared absorption features and their assignments before irradiation of acetaldehyde‑2,2,2‑d3 ice (CD3CHO) at 5 K.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Absorption cm-1 | | Assignment[2] | Approximate type of mode[2] | |
| 3405 | 24 | | overtone |
| 3112 | 4 + 5 | | combination |
| 2853 | 5 | | overtone |
| 2749 | 1 | | (CH) |
| 2252 | 2 | | as(CD3) |
| 2228 | 11 | | (CD3) |
| 2118 | 3 | | s(CD3) |
| 2085 |  + 8 | | combination |
| 1890 | 6 + 9 | | combination |
| 1728 | 4 | | (CO) |
| 1711 | 4 | | (CO) |
| 1397 | 5 | | (CH) |
| 1138 |  | | (CC) |
| 1029 | 7 | | as(CD3) |
| 963 | 8 | | s(CD3) |

**Table S4.** Masses observed in the PI-ReToF-MS data of electron irradiated acetaldehyde and acetaldehyde‑2,2,2‑d3, corresponding empirical formula and tentative assignment based on deuterium and hydrogen content.

|  |  |  |  |
| --- | --- | --- | --- |
| **CH3CHO** | **CD3CHO** | **Formula** | **Assignment** |
| 42 | 44 | C2D2O | Ketene (CD2CO) |
| 43 | 46 | C2D3O | Fragment of 62 and 92 |
| 44 | 47 | C2D3HO | Acetaldehyde (CD3CHO) |
| 58 | 62 | C2D6O | Acetone (CD3COCD3) |
| 72 | 78 | C4D6H2O | ? |
| 86 | 92 | C4D6O2 | Diacetyl (CD3COCOCD3) |
| 88 | 94 | C4D6H2O2 | (CD3CHO)2 |
| 89 | 95 | C4D6H3O2 | (CD3CHO)2H |
| 101 | 107 | C5D6H3O2 | (CD3CHCO)H(CD3CHO) |
| 103 | 109 | C5D6H5O2 | (CD3CH2CHO)H(CD3CHO) |
| 117 | 123 | C5D6H3O3 | (CD3COCOH)H(CD3CHO) |
| 131 | 140 | C6D9H2O3 | (CD3COCOCD3)H(CD3CHO) |
| 132 | 141 | C6D9H3O3 | (CD3CHO)3 |
| 133 | 142 | C6D9H4O3 | (CD3CHO)3H |
| 145 | 154 | C7D9H4O3 | (CD3CHCO)H(CD3CHO)2 |
| 149 | 158 | C6D9H4O4 | (CD3CHO)2H(CD3COOH) |
| 159 | 171 | C8D12H3O3 | (CD3COCOCD3)H(C4D6H2O) |
| 176 | 188 | C8D12H4O4 | (CD3CHO)4 |
| 177 | 189 | C8D12H5O4 | (CD3CHO)4H |
| 203 | 215 | C8D12H5O5 | (CD3CHO)3H(CD3COOH) |

**Table S5.** Calculated ionization energies (IE) and relative energies (Erel) for possible reaction products from reactions of two acetyl‑d3 radicals (*m/z* = 92). Values given in parentheses are experimentally determined ionization energies.

|  |  |  |  |
| --- | --- | --- | --- |
| Structure | Name | IE (eV)a | Erel (kJ mol1)b |
| c-hydroxybut | *cis*-3-hydroxybut-3-en-2-one | 9.40 | 16 |
| t-hydroxybut | *trans*-3-hydroxybut-3-en-2-one | 9.39 | 47 |
| **C:\Users\Fabian\AppData\Local\Microsoft\Windows\INetCache\Content.Word\t-biacetyl.jpg** | *trans*-diacetyl | 9.25  (9.23-9.30)[3,4] | 0 |
| t-butadienediol | *trans*-buta-1,3-diene-2,3-diol | 8.95 | 83 |
| c-butadienediol | *cis*-buta-1,3-diene-2,3-diol | 8.77 | 90 |

**Notes.**

aRelative ionization potential by CCSD(T)/CBS with B3LYP/cc-pVTZ zero-point energy correction in eV.  
bRelative energy by CCSD(T)/CBS with B3LYP/cc-pVTZ zero-point energy correction in kJ mol-1

**Table S6.** Calculated ionization energies (IE) and relative energies (Erel) for possible reaction products from reactions of one acetyl‑d3 radical with one vinoxy‑2,2‑d2 radical (*m/z* = 91).

|  |  |  |  |
| --- | --- | --- | --- |
| Structure | Name | IE (eV)a | Erel (kJ mol‑1)b |
| H:\My Drive\Astro\Acetaldehyde\Calc\cropped\e-hydroxybut3ene2one.jpg | (*E*)-4-hydroxybut-3-en-2-one | 10.34 | -4 |
| z-hydroxybut3ene2one | (*Z*)-4-hydroxybut-3-en-2-one | 9.98 | 43 |
| c-oxobutanal | *cis*-3-oxobutanal | 9.96 | 22 |
| **t-oxobutanal** | *trans*-3-oxobutanal | 9.58 | 22 |
| z-3hydroxybut2enal | (*Z*)-3-hydroxybut-2-enal | 9.34 | 40 |
| e-3hydroxybut2enal | (*E*)-3-hydroxybut-2-enal | 9.34 | 43 |
| t-hydroxybut3enal | *trans*-3-hydroxybut-3-enal | 9.23 | 63 |
| c-hydroxybut3enal | *cis*-3-hydroxybut-3-enal | 8.68 | 61 |
| c-buta-1,2-diene-1,3-diol | *cis*-buta-1,2-diene-1,3-diol | 8.50 | 156 |

**Notes.**

aRelative ionization potential by CCSD(T)/CBS with B3LYP/cc-pVTZ zero-point energy correction in eV.  
bRelative energy by CCSD(T)/CBS with B3LYP/cc-pVTZ zero-point energy correction in kJ mol-1

**Table S7.** Calculated ionization energies (IE) and relative energies (Erel) for possible reaction products from reactions of two vinoxy‑2,2‑d­2 radicals (*m/z* = 90).

|  |  |  |  |
| --- | --- | --- | --- |
| Structure | Name | IE (eV)a | Erel (kJ mol‑1)b |
| c-succinaldehyde | *cis*-succinaldehyde | 10.37 | 56 |
| **t-succinaldehyde-c2** | *trans*-succinaldehyde C2 | 10.22 | 54 |
| t-succinaldehyde-ci | *trans*-succinaldehyde Ci | 10.19 | 54 |
| e-4hydroxy3enal | (*E*)-4-hydroxybut-3-enal | 9.07 | 77 |
| z-4hydroxy3enal | (*Z*)-4-hydroxybut-3-enal | 9.00 | 76 |
| 1z3z-butadienediol | (1*Z*,3*Z*)-buta-1,3-diene-1,4-diol | 7.74 | 113 |
| 1z3e-butadienediol | (1*Z*,3*E*)-buta-1,3-diene-1,4-diol | 7.64 | 94 |
| 1e3e-butadienediol | (1*E*,3*E*)-buta-1,3-diene-1,4-diol | 7.61 | 96 |

**Notes.**

aRelative ionization potential by CCSD(T)/CBS with B3LYP/cc-pVTZ zero-point energy correction in eV.  
bRelative energy by CCSD(T)/CBS with B3LYP/cc-pVTZ zero-point energy correction in kJ mol-1

**Table S8.** Reaction energies for all reactions considered in this study

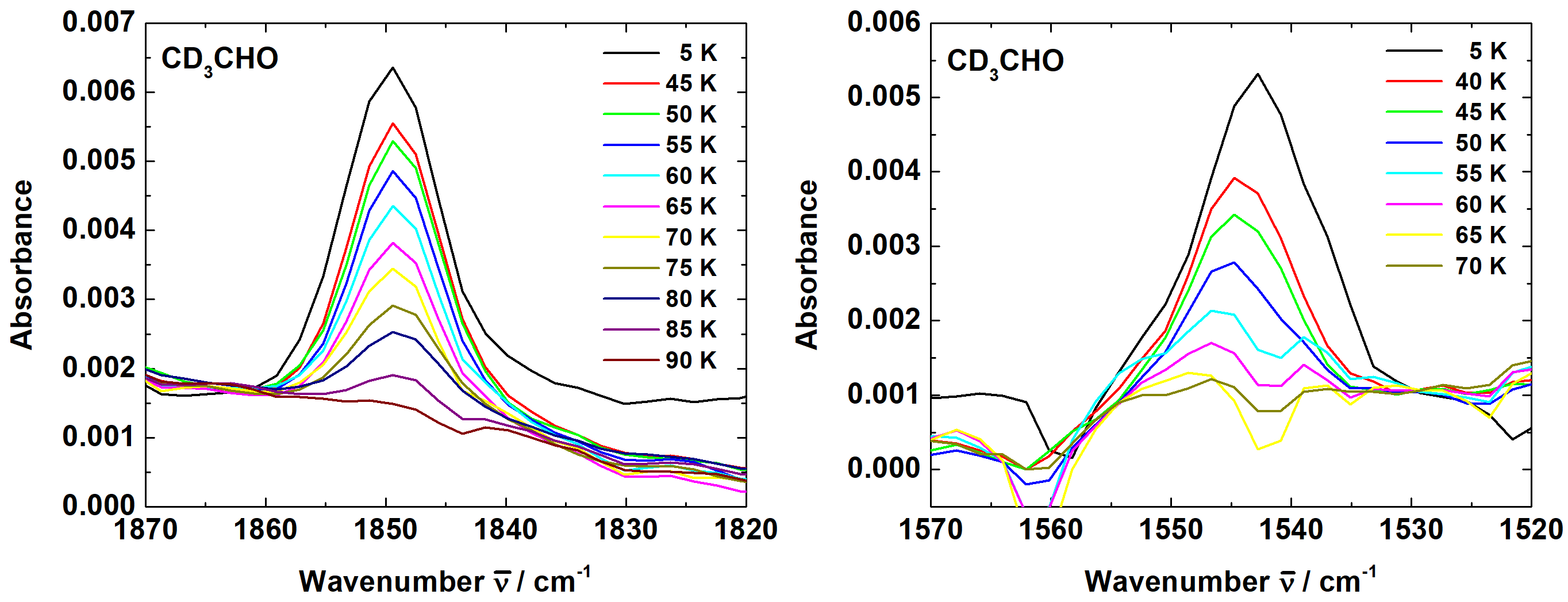
|  |  |  |
| --- | --- | --- |
| Reaction | | ΔRGa kJ mol-1 |
| CH3CHO | CH3CO + H | 377 |
| CH3CHO + H | CH3CO + H2 | -59 |
| CH3CO + CH3CO | CH3COCOCH3 | -303 |
| 2 CH3CHO | CH3COCOCH3 + 2 H | 451 |
| 2 CH3CHO | CH3COCOCH3 + H2 | 15 |
| CH3CHO | CH3 + HCO | 359 |
| CH3CHO | CH3 + CO + H | 423 |
| 2 CH3CHO | CH3COCH3 + H + HCO | 384 |
| 2 CH3CHO | CH3COCH3 + CO + H2 | 11 |
| CH3CO | CH3 + CO | 45 |
| CH3CHO + H | CH3 + CO + H2 | -13 |
| CH3CO + CH3 | CH3COCH3 | -352 |
| CH3CO + HCO | CH3COCHO | -305 |
| CHO + H | CO + H2 | -373 |
| CHO | H + CO | 63 |
| CH3CHO | CH2CO + 2H | 559 |
| CH3CHO | CH2CO + H2 | 123 |
| CH3CO | CH2CO + H | 182 |
| CH3CO + H | CH2CO + H2 | -254 |
| CH3CHO + CH2CO | CH3COCOCH3 | -107 |

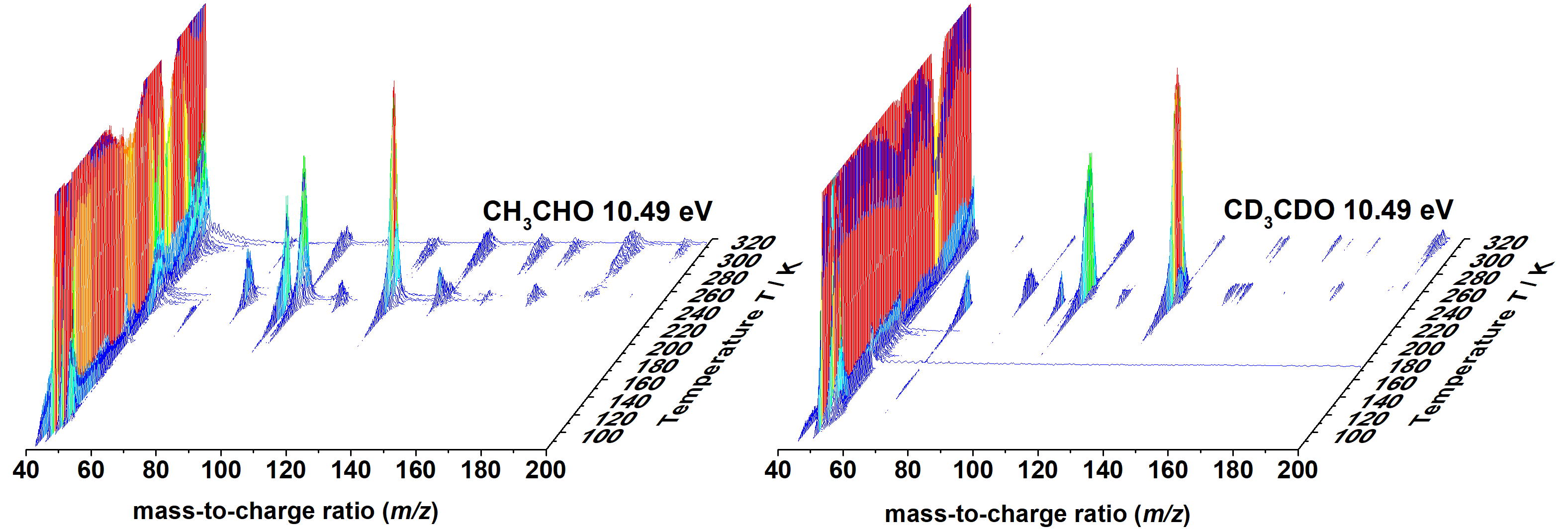
**Notes**: a values taken from http://webbook.nist.gov/chemistry

**Table S9.** Wavelengths and nonlinear media used to generate the different photoionization photon energies

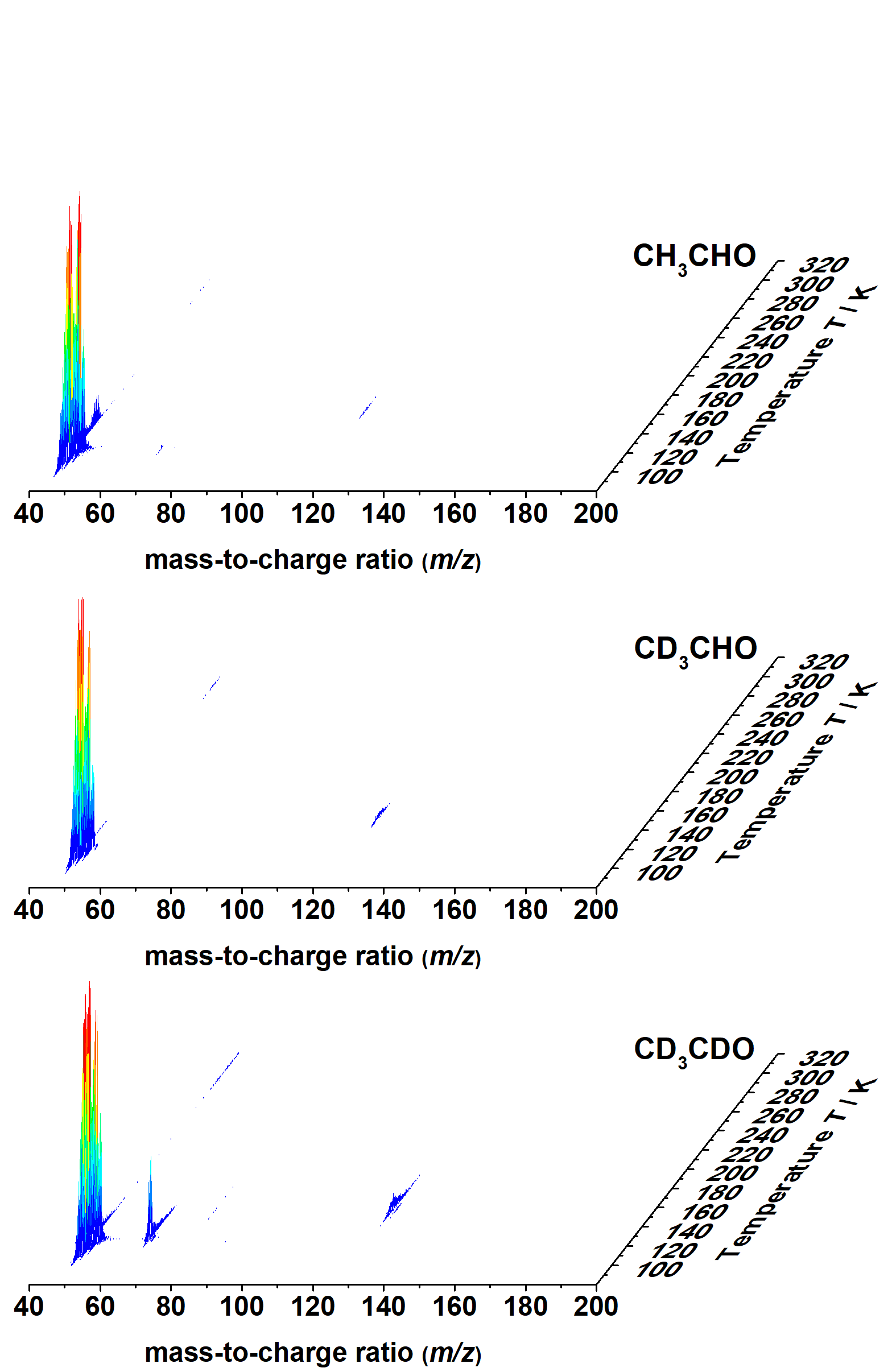
|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | Photoionization energy / eV | 10.49 | 10.11 | 9.50 | 9.30 | 9.10 |
|  | Wavelength / nm | 118.2 | 122.6 | 130.51 | 133.3 | 136.2 |
| 1 | Wavelength / nm | 355 | 202.316 | 202.316 | 222.566 | 222.566 |
| Nd:YAG (1) | Wavelength / nm | 355 | 532 | 532 | 355 | 355 |
| Dye laser (1) | Wavelength / nm | - | 606.948 | 606.948 | 445.132 | 445.132 |
| Dye (1)*a* |  |  | Rh mix | Rh mix | C 450 | C 450 |
| 2 | Wavelength / nm | - | 578 | 450 | 673 | 607 |
| Nd:YAG (2) | Wavelength / nm | - | 532 | 355 | 532 | 532 |
| Dye laser (2) | Wavelength / nm | - | 578 | 450 | 673 | 607 |
| Dye (2)*a* |  |  | P 597 | C 450 | P 1 | Rh mix |

**Notes: *a*** Rh mix: Rhodamine 610 + Rhodamine 640, C 450: Coumarin 450,  
 P 597: Pyrromethene 597, P 1: Pyridine 1

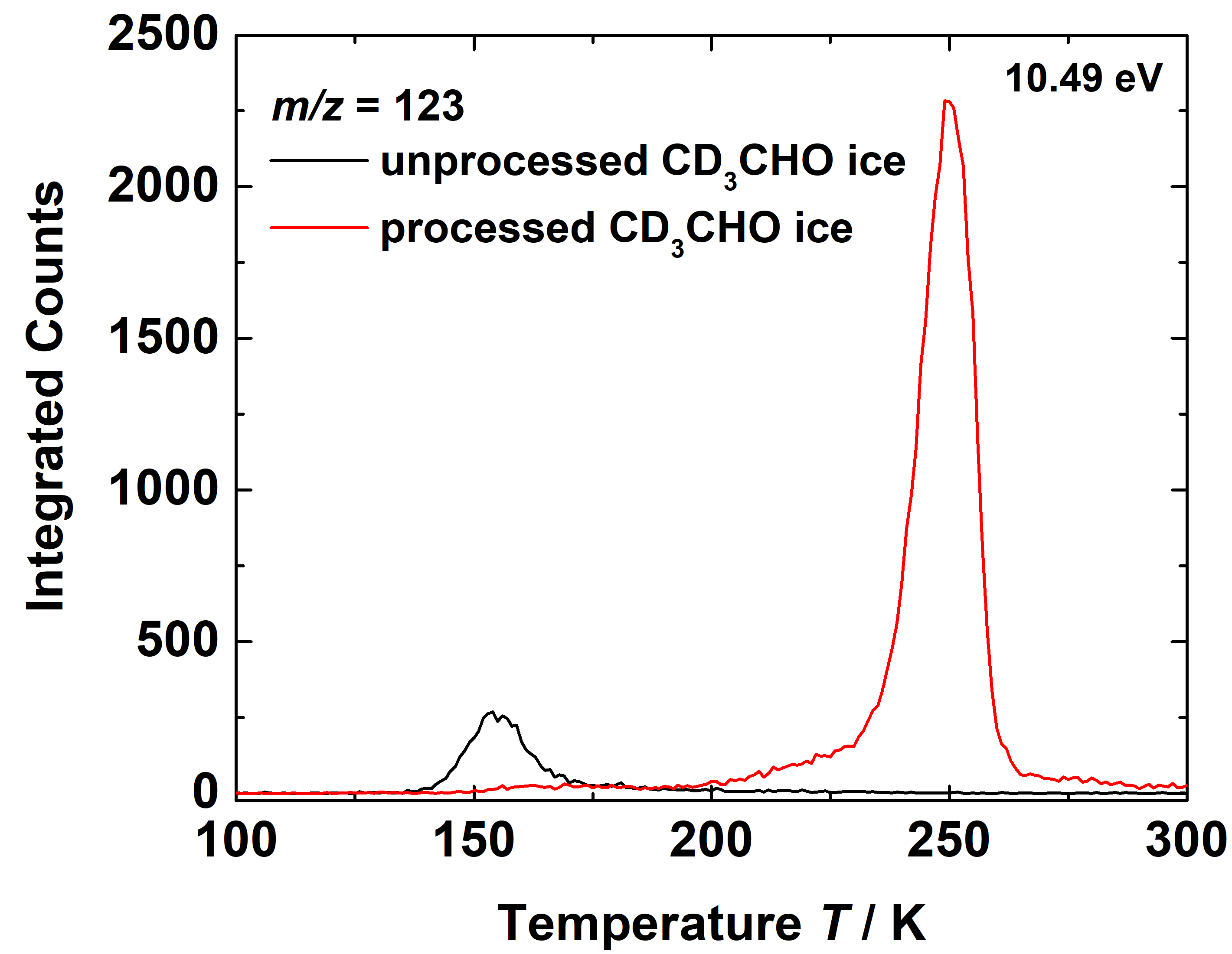
 **Figure S1.** Temperature-dependent FTIR spectra of the two radicals found in the experiments.

****

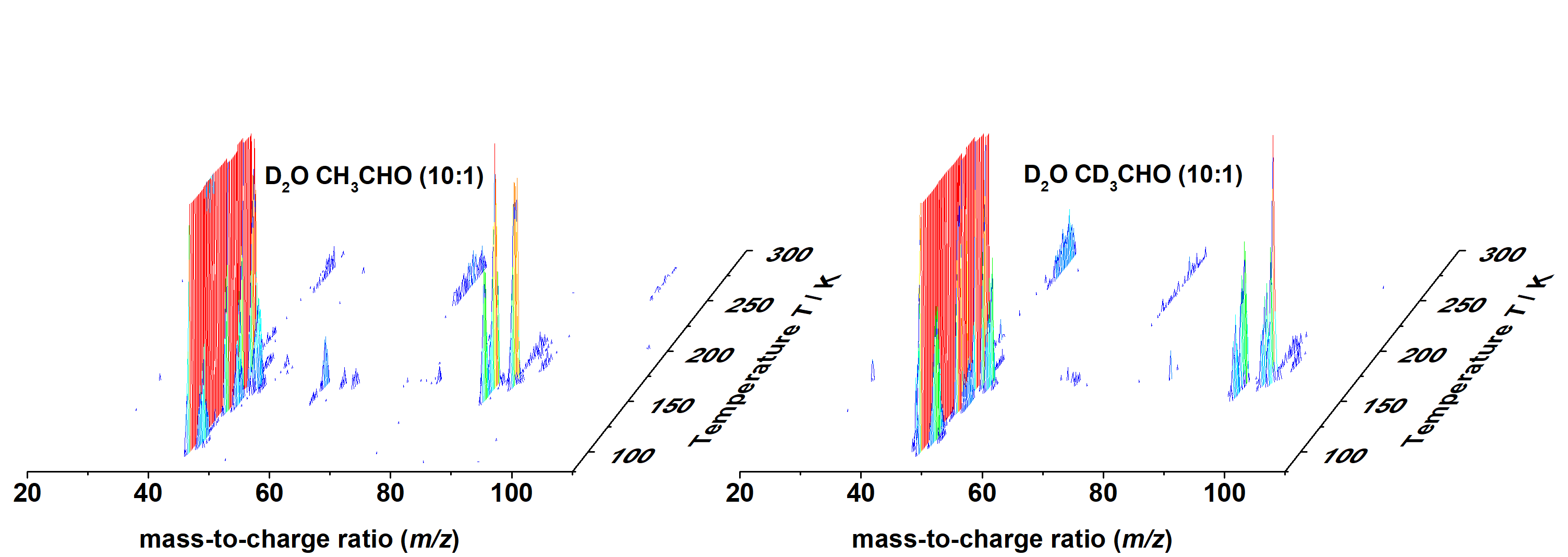
**Figure S2.** Temperature-dependent PI-ReToF mass spectra of acetaldehyde and acetaldehyde-d4 after irradiation with a dose of 0.31 eV molecule-1.Spectra were recorded at 10.49 eV.



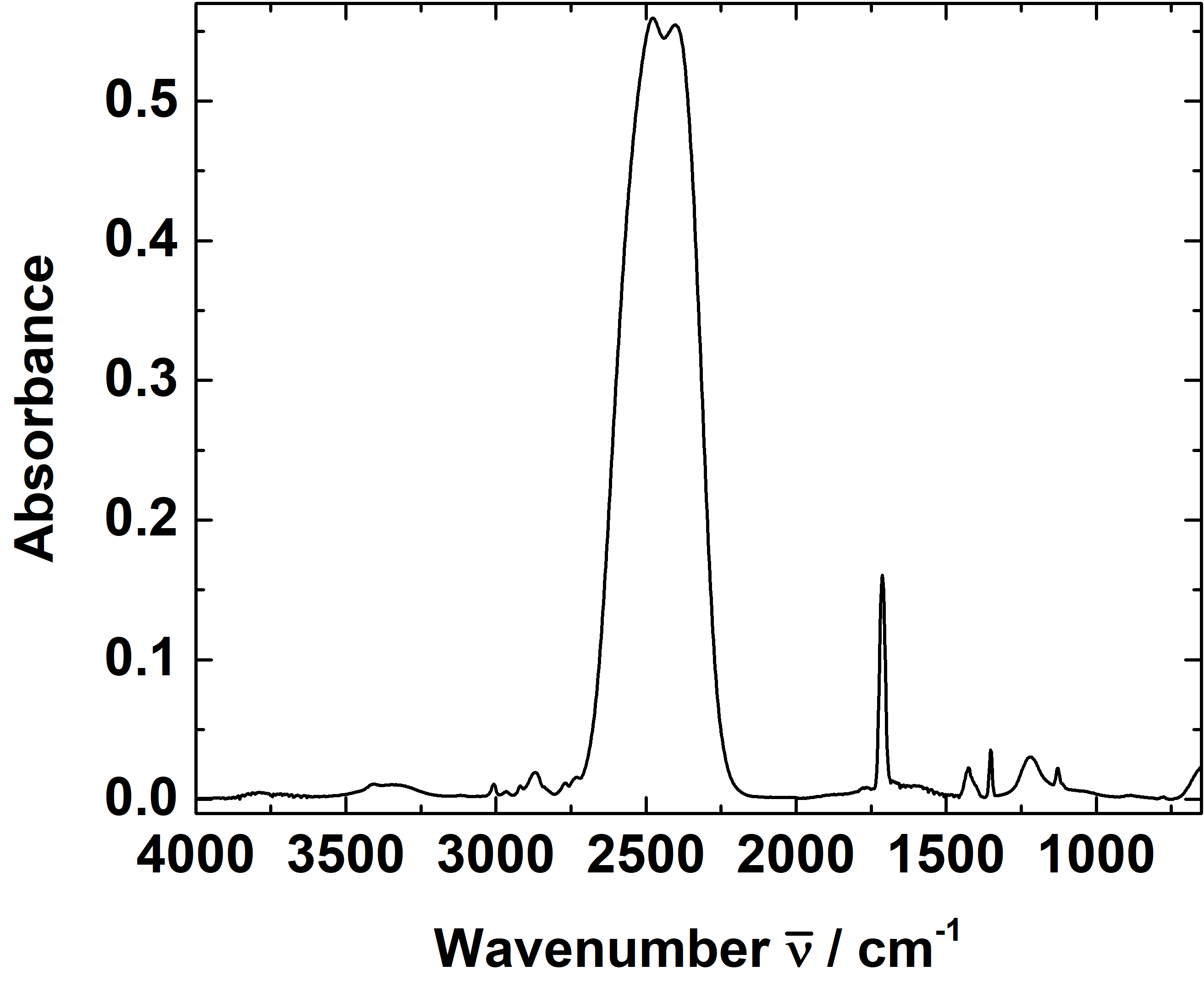
**Figure S3.** Temperature-dependent PI-ReToF mass spectra of acetaldehyde, acetaldehyde‑d4 and acetaldehyde‑2,2,2‑d3 recorded at 10.49 eV.



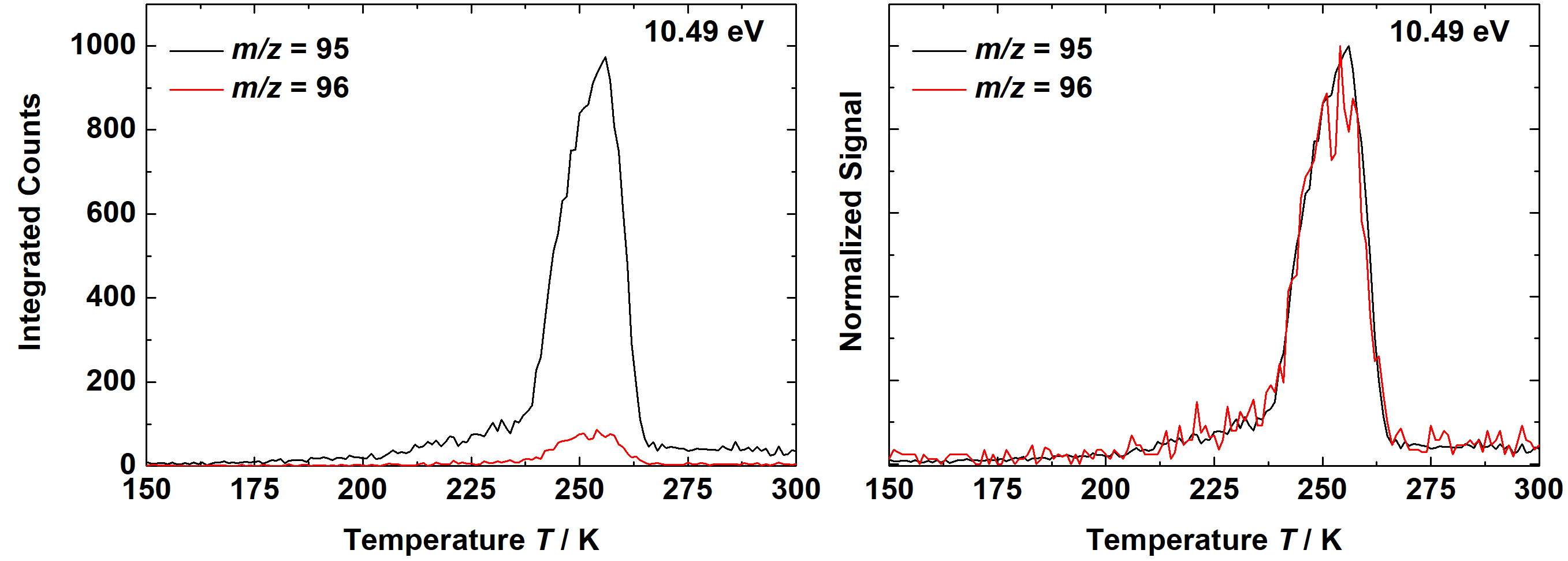
**Figure S4**. ReToF MS Sublimation profile of the main impurity of acetaldehyde‑2,2,2‑d3 (C5D6H3O3, *m/z* = 123) of unprocessed and processed ices recorded at 10.49 eV.



**Figure S5.** Temperature-dependent PI-ReToF mass spectra for 10:1 mixtures of deuterium oxide and acetaldehyde (left), and deuterium oxide and acetaldehyde-d3 (right).



**Figure S6.** FTIR spectrum of the 10:1 mixture of deuterium oxide and acetaldehyde.



**Figure S7.** Temperature Programmed Desorption profiles of protonated (black lines) and deuteronated (red lines) acetaldehyde dimers forming in the irradiated acetaldehyde‑2,2,2‑d3 ice.

A close up of a logo

Description automatically generated

**Figure S8.** PI-ReToF sublimation profiles of *m/z*= 62, 63, and 64 after electron irradiation of acetaldehyde‑2,2,2‑d3, and *m/*z = 58 after electron irradiation of acetaldehyde. The inset shows a zoom into smoothed data of the *m/z* = 62 TPD profile. Spectra were recorded at a photon energy of 10.49 eV.

**B3LYP/aug-cc-pVTZ Cartesian coordinates (in Å) for the molecules analyzed.**

*cis*-buta-1,3-diene-2,3-diol+

C -0.172019 1.477384 1.181224

C 0.022473 0.724339 0.047476

C -0.022473 -0.724339 0.047476

C 0.172019 -1.477384 1.181224

H 0.169833 -2.556112 1.108438

H 0.356815 -1.023496 2.140650

O -0.172019 -1.380374 -1.102953

H -0.610782 -0.866994 -1.797666

O 0.172019 1.380374 -1.102953

H 0.610782 0.866994 -1.797666

H -0.356815 1.023496 2.140650

H -0.169833 2.556112 1.108438

*cis*-buta-1,3-diene-2,3-diol

C -0.146945 0.174126 -0.047312

C -0.022792 -0.032460 1.261292

C 1.256605 0.009167 2.001650

C 2.390212 -0.549776 1.585650

H 3.296876 -0.453679 2.164376

H 2.410160 -1.122015 0.673053

O 1.203968 0.618649 3.237132

H 0.472195 1.245437 3.258871

O -1.146274 -0.231410 2.035153

H -0.903382 -0.687551 2.848644

H 0.713569 0.439033 -0.638944

H -1.110831 0.098002 -0.528279

*cis*-3-hydroxybut-3-en-2-one+

C 1.145824 1.610533 0.000000

C -0.083714 0.780975 0.000000

C 0.000000 -0.771830 0.000000

C 1.149094 -1.579923 0.000000

H 2.133316 -1.134766 0.000000

H 1.049625 -2.658238 0.000000

O -1.150694 -1.331924 0.000000

H -1.828938 -0.591298 0.000000

O -1.225329 1.170316 0.000000

H 1.755039 1.387926 0.880755

H 1.755039 1.387926 -0.880755

H 0.876879 2.662782 0.000000

*cis*-3-hydroxybut-3-en-2-one

C 1.333250 1.419879 0.000000

C 0.000000 0.721546 0.000000

C -0.084267 -0.772510 0.000000

C 0.974133 -1.586998 0.000000

H 1.974717 -1.188717 0.000000

H 0.850520 -2.659875 0.000000

O -1.353046 -1.235963 0.000000

H -1.925409 -0.447855 0.000000

O -1.051609 1.339512 0.000000

H 1.915080 1.141490 0.879261

H 1.915080 1.141490 -0.879261

H 1.168547 2.493576 0.000000

*trans*-biacetyl+

C -0.485745 -1.983720 0.000000

C 0.485745 -0.868553 0.000000

C -0.485745 0.868553 0.000000

C 0.485745 1.983720 0.000000

H -0.065873 2.922610 0.000000

H 1.122765 1.897377 0.881766

H 1.122765 1.897377 -0.881766

O -1.632088 0.710735 0.000000

O 1.632088 -0.710735 0.000000

H 0.065873 -2.922610 0.000000

H -1.122765 -1.897377 0.881766

H -1.122765 -1.897377 -0.881766

*trans*-biacetyl

C -0.401030 -1.933684 0.000000

C 0.401030 -0.664746 0.000000

C -0.401030 0.664746 0.000000

C 0.401030 1.933684 0.000000

H -0.267951 2.789208 0.000000

H 1.057369 1.960746 0.871316

H 1.057369 1.960746 -0.871316

O -1.609521 0.625490 0.000000

O 1.609521 -0.625490 0.000000

H 0.267951 -2.789208 0.000000

H -1.057369 -1.960746 0.871316

H -1.057369 -1.960746 -0.871316

*trans*-buta-1,3-diene-2,3-diol+

C -0.017061 0.183712 0.044449

C -0.013034 -0.152335 1.378788

C 1.222131 -0.155946 2.148357

C 1.250565 0.297410 3.447227

H 2.193837 0.366309 3.971202

H 0.357077 0.652320 3.938296

O 2.376738 -0.495346 1.586740

H 2.280292 -0.963508 0.745722

O -1.184808 -0.368222 1.965355

H -1.115080 -0.764202 2.845199

H 0.895243 0.437435 -0.473966

H -0.955739 0.263411 -0.486202

*trans*-buta-1,3-diene-2,3-diol

C -0.324944 1.806743 -0.257928

C 0.324944 0.664259 -0.019486

C -0.324944 -0.664259 -0.019486

C 0.324944 -1.806743 -0.257928

H -0.192285 -2.752677 -0.209602

H 1.357133 -1.805750 -0.570954

O -1.666602 -0.685539 0.226809

H -1.924226 0.151196 0.630569

O 1.666602 0.685539 0.226809

H 1.924226 -0.151196 0.630569

H -1.357133 1.805750 -0.570954

H 0.192285 2.752677 -0.209602

*trans*-3-hydroxybut-3-en-2-one+

C 1.827286 -0.638391 0.375386

C 0.724589 0.275125 -0.031372

C -0.743365 -0.138804 0.040810

C -1.695022 0.800240 0.411466

H -1.388529 1.806212 0.653772

H -2.732836 0.508552 0.506386

O -1.138812 -1.317664 -0.352263

H -0.424097 -1.962443 -0.488972

O 0.833213 1.378071 -0.505205

H 1.649522 -1.022303 1.382575

H 1.885179 -1.494947 -0.304726

H 2.774615 -0.107349 0.332967

*trans*-3-hydroxybut-3-en-2-one

C 1.448651 1.201892 0.000000

C 0.000000 0.752643 0.000000

C -0.274256 -0.726110 0.000000

C -1.520058 -1.196403 0.000000

H -2.342991 -0.500901 0.000000

H -1.715047 -2.258287 0.000000

O 0.789276 -1.592671 0.000000

H 1.621700 -1.113777 0.000000

O -0.904353 1.558317 0.000000

H 1.975936 0.834149 0.884706

H 1.975936 0.834149 -0.884706

H 1.479061 2.287367 0.000000

*cis*-buta-1,2-diene-1,3-diol+

C 0.987434 1.401204 -0.024648

C 0.938166 -0.081723 -0.008317

C -0.227349 -0.812986 -0.018456

C -1.569923 -0.682223 -0.025745

O -2.174774 0.481906 0.038193

H -3.141165 0.400610 0.020446

H -2.191723 -1.573412 -0.080243

O 2.104828 -0.662949 0.023647

H 2.048698 -1.633325 0.052960

H 1.275112 1.740371 0.976035

H 1.767048 1.725654 -0.715431

H 0.031624 1.842817 -0.285492

*cis*-buta-1,2-diene-1,3-diol

C 1.848846 1.149864 -0.075328

C 0.960689 -0.050154 0.029877

C -0.333301 -0.026993 0.222260

C -1.609821 0.022704 0.476522

O -2.572836 0.080350 -0.508964

H -3.442071 0.107449 -0.098545

H -1.997693 0.020340 1.492124

O 1.686391 -1.214133 -0.109892

H 1.082915 -1.963656 -0.050955

H 2.620081 1.111156 0.696530

H 2.353761 1.156387 -1.043189

H 1.276092 2.066065 0.034899

*cis*-3-hydroxybut-3-enal+

C 0.168277 1.052943 0.000

C 1.597588 0.557803 0.000

O 1.872777 -0.625493 0.000

H 2.389275 1.317138 0.000

C -0.873713 -0.030533 0.000

C -2.258726 0.246596 0.000

H -2.961650 -0.575531 0.000

H -2.619895 1.264908 0.000

O -0.518060 -1.260073 0.000

H 0.518922 -1.304048 0.000

H 0.017289 1.711013 0.864419

H 0.017289 1.711013 -0.864419

*cis*-3-hydroxybut-3-enal

C 0.197893 0.952964 0.372642

C 1.575044 0.546269 -0.086785

O 1.912780 -0.587826 -0.337034

H 2.312903 1.367771 -0.152424

C -0.921403 -0.008548 0.057492

C -2.119577 0.392114 -0.358848

H -2.903343 -0.325183 -0.551648

H -2.335705 1.440649 -0.491364

O -0.664829 -1.326225 0.297276

H 0.282900 -1.484890 0.156380

H 0.293198 1.069440 1.463285

H -0.025308 1.947821 -0.013167

*cis*-oxobutanal+

C 0.281880 -0.978098 -0.411026

C 1.643232 -0.349000 -0.065671

O 1.854744 0.689721 0.461444

H 2.467285 -1.025958 -0.381525

C -0.938239 -0.114721 -0.014698

C -1.017378 1.356977 -0.305592

H -0.594170 1.557845 -1.289392

H -2.052023 1.679285 -0.238202

H -0.412298 1.887389 0.433522

O -1.816754 -0.750424 0.498618

H 0.238791 -1.146983 -1.494028

H 0.231524 -1.956906 0.071043

*cis*-oxobutanal

C 0.345498 -0.802922 -0.628223

C 1.657971 -0.267364 -0.096043

O 1.788065 0.689651 0.620908

H 2.542733 -0.846470 -0.427737

C -0.913599 -0.190209 -0.022019

C -1.205163 1.252399 -0.339482

H -1.245611 1.403488 -1.420779

H -2.148526 1.548926 0.110657

H -0.394147 1.873894 0.043871

O -1.632570 -0.864801 0.677548

H 0.364335 -0.647417 -1.713727

H 0.329015 -1.882650 -0.465338

(*E*)-3-hydroxybut-2-enal+

C 1.362720 1.301682 -0.045052

H 1.399406 1.625954 -1.091601

H 2.360295 1.416885 0.378766

H 0.673311 1.965462 0.473458

C 0.917966 -0.109061 0.002098

C -0.417631 -0.558450 0.068379

C -1.552803 0.315329 0.132855

O -2.661272 -0.141682 -0.120118

H -1.437517 1.393508 0.306420

H -0.609480 -1.619832 -0.021876

O 1.790988 -1.072171 -0.005768

H 2.714751 -0.768147 0.012235

(*E*)-3-hydroxybut-2-enal

C 1.352451 1.298574 0.000

H 1.968369 1.485531 -0.883753

H 1.968369 1.485531 0.883753

H 0.536907 2.013650 0.000

C 0.876342 -0.118891 0.000

C -0.395703 -0.561306 0.000

C -1.571474 0.285802 0.000

O -2.712214 -0.136030 0.000

H -1.397624 1.378971 0.000

H -0.570454 -1.629379 0.000

O 1.861569 -1.054501 0.000

H 2.727952 -0.634328 0.000

(*E*)-4-hydroxybut-3-en-2-one+

C -2.294185 0.239334 -0.000049

C -0.796652 -0.067501 0.000013

C 0.178650 0.960474 0.000057

C 1.513419 0.678849 -0.000010

H 2.244570 1.481756 -0.000065

O 1.945319 -0.555840 -0.000002

H 2.911054 -0.634639 -0.000197

H -0.163878 1.982289 0.000078

O -0.535389 -1.279753 0.000034

H -2.496558 0.829023 0.895361

H -2.496558 0.829023 -0.895361

H -2.885652 -0.670283 -0.000422

(*E*)-4-hydroxybut-3-en-2-one

C 0.00000000 0.00000000 0.00000000

C -1.46825796 -0.34072001 0.0000

C -2.43165494 0.73631399 0.000

C -3.76182398 0.46185500 0.000

H -4.51271599 1.24401400 0.000

O -4.26846000 -0.75614000 0.000

H -3.48113695 -1.37521201 0.000

H -2.10383590 1.76423099 0.000

O -1.83346695 -1.52812701 0.0000

H 0.24978603 0.58423900 -0.88852805

H 0.24978603 0.58423900 0.88852805

H 0.59282784 -0.91028410 0.0000

*trans*-3-hydroxybut-3-enal+

C 0.335974 0.203775 0.778382

C 1.496316 -0.344232 -0.153927

O 2.466066 0.295523 -0.362489

H 1.323656 -1.361235 -0.549442

C -0.962885 0.042695 0.122896

C -1.738219 1.118111 -0.296350

H -2.726601 0.972934 -0.713785

H -1.372624 2.127923 -0.184451

O -1.319461 -1.211538 -0.062960

H -2.150940 -1.319036 -0.553002

H 0.407390 -0.446257 1.656806

H 0.559164 1.231691 1.041457

*trans*-3-hydroxybut-3-enal

C 0.369116 0.164365 0.729844

C 1.467854 -0.300773 -0.209691

O 2.544166 0.231172 -0.287934

H 1.222250 -1.184423 -0.828437

C -0.992185 0.086482 0.107197

C -1.714100 1.135307 -0.279718

H -2.692135 1.020692 -0.728415

H -1.337385 2.137150 -0.149116

O -1.385794 -1.218435 -0.032140

H -2.236605 -1.257552 -0.483045

H 0.394153 -0.502819 1.599273

H 0.598629 1.172763 1.064536

*trans*-oxobutanal+

C 1.019932 -0.363659 0.000000

C 0.280961 -1.672830 0.000000

O -0.919017 -1.738513 0.000000

H 0.876516 -2.601816 0.000000

C 0.000000 0.768151 0.000000

C 0.481511 2.193835 0.000000

H -0.361677 2.876346 0.000000

H 1.105590 2.351661 0.882374

H 1.105590 2.351661 -0.882374

O -1.178588 0.496185 0.000000

H 1.680198 -0.296106 0.871841

H 1.680198 -0.296106 -0.871841

*trans*-oxobutanal

C 0.358935 -0.133652 -0.777325

C 1.520913 0.298386 0.098290

O 2.454320 -0.411331 0.364593

H 1.447269 1.329893 0.487245

C -0.971029 0.174624 -0.088578

C -1.852076 -0.999714 0.250020

H -2.749787 -0.662691 0.760891

H -2.122325 -1.537013 -0.662024

H -1.304847 -1.706006 0.878971

O -1.264342 1.316164 0.181112

H 0.393499 0.480875 -1.681731

H 0.475909 -1.181579 -1.043425

(*Z*)-3-hydroxybut-2-enal+

C 2.130544 -0.799918 -0.035381

H 2.846916 -0.365588 -0.736189

H 1.929219 -1.830717 -0.311944

H 2.594510 -0.794139 0.958576

C 0.892977 0.009865 0.021339

C -0.384150 -0.563733 -0.007946

C -1.571805 0.232291 -0.142393

O -2.665808 -0.265276 0.087551

H -1.495800 1.307072 -0.361385

H -0.500699 -1.627908 0.131688

O 0.960246 1.312951 0.075801

H 1.864964 1.658848 -0.001279

(*Z*)-3-hydroxybut-2-enal

C 2.213833 -0.525709 0.000000

H 2.580112 -1.056952 0.882995

H 2.638406 0.474277 0.000000

H 2.580112 -1.056952 -0.882995

C 0.720583 -0.479924 0.000000

C 0.000000 0.657418 0.000000

C -1.453517 0.711456 0.000000

O -2.087528 1.750190 0.000000

H -1.976791 -0.260463 0.000000

H 0.522862 1.602883 0.000000

O 0.091796 -1.685462 0.000000

H 0.735758 -2.400068 0.000000

(*Z*)-4-hydroxybut-3-en-2-one+

C 0.902346 1.376337 0.0000

C 0.923161 -0.149828 0.0000

C -0.188232 -1.025022 0.0000

C -1.496609 -0.633701 0.000

H -2.266351 -1.399395 0.0000

O -1.885592 0.618010 0.000

H -2.849748 0.709163 0.000

H 0.017874 -2.084320 0.000

O 2.087027 -0.592473 0.0000

H 0.365937 1.694477 0.894109

H 1.912529 1.774714 0.000

H 0.365937 1.694477 -0.894109

(Z)-4-hydroxybut-3-en-2-one

C 0.00000000 0.00000000 0.00000000

C 0.18244700 -1.50050300 0.00000

C -0.99316000 -2.39199700 0.0000

C -2.29597800 -2.08699100 0.0000

H -3.03679000 -2.87896300 0.0000

O -2.79583100 -0.82579300 0.0000

H -3.75651399 -0.85239100 0.0000

H -0.74771900 -3.44487000 0.0000

O 1.29764600 -1.99453100 0.0000

H -0.56870200 0.31816300 0.87480560

H 0.97801201 0.47361900 0.0000

H -0.56870200 0.31816300 -0.87480560

(1*E,*3*E*)-buta-1,3-diene-1,4-diol+

C 0.342006 1.814449 0.000000

C -0.336728 0.608563 0.000000

C 0.336728 -0.608563 0.000000

C -0.342006 -1.814449 0.000000

O 0.336728 -2.934076 0.000000

H -0.226747 -3.721946 0.000000

H -1.426176 -1.864372 0.000000

H 1.419927 -0.642387 0.000000

H -1.419927 0.642387 0.000000

O -0.336728 2.934076 0.000000

H 0.226747 3.721946 0.000000

H 1.426176 1.864372 0.000000

(1*E,*3*E*)-buta-1,3-diene-1,4-diol

C 0.336460 1.805514 0.000000

C -0.324032 0.645755 0.000000

C 0.324032 -0.645755 0.000000

C -0.336460 -1.805514 0.000000

O 0.324032 -3.007655 0.000000

H -0.310603 -3.727700 0.000000

H -1.419462 -1.856217 0.000000

H 1.408471 -0.678431 0.000000

H -1.408471 0.678431 0.000000

O -0.324032 3.007655 0.000000

H 0.310603 3.727700 0.000000

H 1.419462 1.856217 0.000000

(1*Z,*3*E*)-buta-1,3-diene-1,4-diol+

C 0.017752 -2.013904 0.000000

C -0.646777 -0.795535 0.000000

C 0.000000 0.437138 0.000000

C -0.715237 1.621106 0.000000

O -0.074401 2.760984 0.000000

H -0.662819 3.530573 0.000000

H -1.800760 1.637973 0.000000

H 1.081019 0.495538 0.000000

H -1.727639 -0.843064 0.000000

O 1.328444 -2.060991 0.000000

H 1.674476 -2.965219 0.000000

H -0.531045 -2.948575 0.000000

(1*Z,*3*E*)-buta-1,3-diene-1,4-diol

C -0.050008 0.000000 -0.039159

C -0.032214 0.000000 1.297380

C 1.157295 0.000000 2.119000

C 1.120110 0.000000 3.453562

O 2.264207 0.000000 4.205622

H 2.041431 0.000000 5.139339

H 0.187604 0.000000 4.007614

H 2.122343 0.000000 1.628053

H -0.997043 0.000000 1.788767

O 1.102409 0.000000 -0.783713

H 0.886294 0.000000 -1.718697

H -0.977819 0.000000 -0.596323

(1*Z,*3*Z*)-buta-1,3-diene-1,4-diol+

C 0.000000 1.644545 0.158766

C 0.000000 0.700034 1.175945

C 0.000000 -0.700034 1.175945

C 0.000000 -1.644545 0.158766

O 0.000000 -1.352021 -1.115495

H 0.000000 -2.143286 -1.674520

H 0.000000 -2.694523 0.431229

H 0.000000 -1.152270 2.158986

H 0.000000 1.152270 2.158986

O 0.000000 1.352021 -1.115495

H 0.000000 2.143286 -1.674520

H 0.000000 2.694523 0.431229

(1*Z,*3*Z*)-buta-1,3-diene-1,4-diol

C -0.113108 1.603754 0.152698

C 0.113108 0.719695 1.128833

C -0.113108 -0.719695 1.128833

C 0.113108 -1.603754 0.152698

O 0.652283 -1.276857 -1.056490

H 0.730622 -2.065400 -1.598456

H -0.104746 -2.654536 0.303383

H -0.466847 -1.150208 2.057807

H 0.466847 1.150208 2.057807

O -0.652283 1.276857 -1.056490

H -0.730622 2.065400 -1.598456

H 0.104746 2.654536 0.303383

*cis*-succinaldehyde+

C 0.245834 0.720157 0.876918

C -0.039475 1.498730 -0.407968

O -0.245834 2.658158 -0.518846

H -0.014982 0.874259 -1.350676

C -0.245834 -0.720157 0.876918

C 0.039475 -1.498730 -0.407968

O 0.245834 -2.658158 -0.518846

H 0.014982 -0.874259 -1.350676

H 0.206643 -1.284049 1.691822

H -1.334147 -0.765874 0.995919

H 1.334147 0.765874 0.995919

H -0.206643 1.284049 1.691822

*cis*-succinaldehyde

C 0.107871 0.761516 0.957861

C -0.612589 1.459543 -0.171339

o -0.107871 2.269135 -0.904522

H -1.681440 1.183380 -0.288623

C -0.107871 -0.761516 0.957861

C 0.612589 -1.459543 -0.171339

O 0.107871 -2.269135 -0.904522

H 1.681440 -1.183380 -0.288623

H 0.296044 -1.169384 1.890158

H -1.165566 -1.023383 0.915505

H 1.165566 1.023383 0.915505

H -0.296044 1.169384 1.890158

(*E*)-4-hydroxybut-3-enal+

C 0.731533 -0.788166 -0.497948

C 1.881261 -0.082738 0.391187

O 2.411478 0.898694 0.010873

H 2.122819 -0.600904 1.332562

C -0.560193 -0.637880 0.146223

C -1.503055 0.266690 -0.313051

O -2.695330 0.434939 0.178728

H -2.903421 -0.136833 0.937552

H -1.309470 0.914816 -1.160768

H -0.790858 -1.233745 1.023906

H 0.793030 -0.329674 -1.480763

H 1.061445 -1.830163 -0.527765

(*E*)-4-hydroxybut-3-enal

C 0.749299 0.742242 0.255340

C 1.785125 -0.127787 -0.428229

O 2.827838 -0.470944 0.065716

H 1.502264 -0.464896 -1.447011

C -0.539266 -0.010092 0.438337

C -1.660700 0.278164 -0.217657

O -2.854308 -0.364884 -0.114314

H -2.781820 -1.099588 0.505973

H -1.729072 1.099764 -0.919344

H -0.526194 -0.841635 1.136754

H 1.161447 1.081788 1.206623

H 0.578378 1.616034 -0.380956

*trans*-succinaldehyde/c2 cation

C 0.443848 0.614493 -0.199193

C -0.443848 1.898175 -0.308966

O -0.527563 2.672519 0.584689

H -0.963734 2.056874 -1.271200

C -0.443848 -0.614493 -0.199193

C 0.443848 -1.898175 -0.308966

O 0.527563 -2.672519 0.584689

H 0.963734 -2.056874 -1.271200

H -1.027327 -0.708084 0.713018

H -1.102830 -0.661290 -1.070372

H 1.102830 0.661290 -1.070372

H 1.027327 0.708084 0.713018

*trans*-succinaldehyde/c2 neutral

C 0.417597 0.646082 -0.136721

C -0.457135 1.866977 -0.275016

O -0.457135 2.801172 0.481844

H -1.136042 1.854187 -1.154724

C -0.417597 -0.646082 -0.136721

C 0.457135 -1.866977 -0.275016

O 0.457135 -2.801172 0.481844

H 1.136042 -1.854187 -1.154724

H -1.016520 -0.736305 0.768360

H -1.096640 -0.637408 -0.997965

H 1.096640 0.637408 -0.997965

H 1.016520 0.736305 0.768360

*trans*-succinaldehyde+

C 0.391169 -0.594450 0.259117

C 0.384058 -0.590996 1.821307

O 1.396575 -0.493361 2.431658

H -0.594171 -0.713286 2.319069

C -0.391169 0.594450 -0.259117

C -0.384058 0.590996 -1.821307

O -1.396575 0.493361 -2.431658

H 0.594171 0.713286 -2.319069

H -1.431092 0.598385 0.059705

H 0.080047 1.545670 0.005198

H 1.431092 -0.598385 -0.059705

H -0.080047 -1.545670 -0.005198

*trans*-succinaldehyde

C 0.397194 -0.600519 0.276753

C 0.405270 -0.590045 1.785060

O 1.395680 -0.486166 2.460728

H -0.593441 -0.675745 2.261201

C -0.397194 0.600519 -0.276753

C -0.405270 0.590045 -1.785060

O -1.395680 0.486166 -2.460728

H 0.593441 0.675745 -2.261201

H -1.427637 0.595122 0.078280

H 0.082602 1.527778 0.051789

H 1.427637 -0.595122 -0.078280

H -0.082602 -1.527778 -0.051789

(*Z*)-4-hydroxybut-3-enal+

C 0.500822 0.399555 0.804974

C 1.498230 -0.547430 -0.048959

O 2.543635 -0.159945 -0.427089

H 1.109158 -1.565348 -0.215514

C -0.494104 0.955922 -0.094177

C -1.701555 0.349665 -0.390624

O -1.990630 -0.820909 0.122001

H -2.867742 -1.146755 -0.134649

H -2.429655 0.827352 -1.037119

H -0.286695 1.890669 -0.597802

H 0.084907 -0.264783 1.561796

H 1.145625 1.159431 1.236719

(*Z*)-4-hydroxybut-3-enal

C 0.529990 0.104072 0.711862

C 1.579197 -0.382715 -0.266327

O 2.749802 -0.105224 -0.212964

H 1.186564 -1.024802 -1.080826

C -0.532881 0.893543 0.000313

C -1.751937 0.447324 -0.286057

O -2.172914 -0.808085 0.059659

H -3.095462 -0.923994 -0.179779

H -2.475321 1.064059 -0.805421

H -0.286057 1.894307 -0.326099

H 0.082846 -0.775980 1.181434

H 1.026106 0.699531 1.478388

**B3LYP/aug-cc-pVTZ harmonic frequencies (in cm-1) for the molecules analyzed.**

*cis*-buta-1,2-diene-1,3-diol+

117.1262 191.6782 266.3152

359.8887 403.1887 464.1305

549.4904 572.1101 608.7702

624.0681 710.6812 791.2714

958.7622 959.3495 986.7263

1006.0761 1139.1263 1213.0739

1297.9229 1409.4750 1433.7361

1469.5966 1516.2366 1592.8455

3171.0923 3177.4014 3282.1574

3289.9661 3723.4508 3729.7955

*cis*-buta-1,2-diene-1,3-diol

83.7865 148.3495 254.6449

322.5566 377.4196 494.1598

500.1530 613.3441 706.1363

733.7405 745.3094 774.3202

881.3983 881.8685 960.6687

977.1929 1170.8976 1254.4010

1284.4097 1330.7490 1420.3744

1444.4853 1711.4703 1712.3681

3169.8113 3170.5876 3265.4070

3266.6088 3789.3317 3791.8704

*cis*-3-hydroxybut-3-en-2-one+

108.9589 147.1491 238.7266

277.6425 390.3993 400.1055

433.2090 598.5523 653.0285

675.3240 912.1201 968.8754

985.5917 1027.6221 1052.1894

1158.6315 1210.6858 1400.7498

1424.0584 1456.8594 1458.8794

1477.6397 1564.4468 1789.1171

3023.0367 3073.8023 3151.9153

3154.8463 3194.5433 3269.3956

*cis*-3-hydroxybut-3-en-2-one

95.9580 116.0544 281.2404

368.1144 404.1034 455.1378

602.5676 614.6698 681.4885

734.2355 735.0448 893.9466

981.3498 988.3612 1052.8667

1168.5861 1282.0419 1381.6772

1405.9504 1442.6220 1474.4827

1477.1231 1704.3656 1729.6591

3045.1394 3101.0809 3144.0992

3174.1884 3267.9806 3621.4831

*trans*-diacetyl+

21.8810 106.6671 111.1047

195.0850 197.0029 302.7265

338.9223 465.3164 478.6802

514.9206 881.5728 896.0003

1008.4694 1029.8679 1043.0503

1045.3164 1367.1885 1371.7712

1427.4145 1432.2727 1440.2327

1440.9482 1997.9101 2005.9756

3038.9604 3039.6572 3112.0320

3112.2461 3142.4244 3143.1776

*trans*-diacetyl

44.1023 101.3832 102.6632

239.2620 350.5575 360.7958

518.5448 546.5309 623.1111

682.9376 910.2076 961.1833

1013.7093 1072.6121 1135.5468

1274.0199 1388.5757 1394.2365

1455.6915 1456.7333 1456.8419

1462.0305 1776.4002 1778.6675

3042.2031 3042.2360 3093.6381

3093.9117 3148.6605 3149.2897

*trans*-buta-1,2-diene-1,3diol+

107.1685 244.0006 327.7298

385.1216 397.7739 490.7103

498.1186 564.4018 573.4094

622.5521 675.0977 797.2529

952.8426 958.2651 988.7085

1005.3223 1151.1669 1205.3019

1305.3931 1326.0881 1444.7003

1473.3198 1492.2207 1620.1408

3163.3741 3164.6499 3269.8489

3269.8510 3747.5047 3756.2312

*trans*-buta-1,2-diene-1,3-diol

107.0779 280.0174 351.1950

394.7832 412.5057 436.2002

515.1917 553.5910 715.9443

720.3943 760.7783 780.5195

862.8483 865.6943 977.7908

983.7140 1180.7133 1248.2196

1290.1234 1382.3291 1437.2142

1446.7517 1674.7811 1717.2469

3169.7331 3169.9686 3256.7859

3257.2118 3778.1026 3779.0541

*trans*-3-hydroxybut-3-en-2-one+

57.5857 110.7616 214.3533

291.9160 353.5383 474.7612

536.7156 561.8946 580.1924

640.7050 702.7805 961.4372

980.8500 1017.8659 1041.9111

1134.8365 1189.7410 1372.3537

1396.9501 1432.1826 1451.2943

1461.9525 1512.1889 1759.5136

3018.0852 3077.2401 3149.1576

3160.6795 3279.4113 3687.8398

*trans*-3-hydroxybut-3-en-2-one

49.5980 167.5817 193.9175

276.2639 393.9310 394.2396

483.7173 551.2673 644.3507

717.1052 741.9656 920.7148

951.2379 979.2777 1038.0627

1150.4019 1227.5425 1330.3879

1381.3348 1419.6397 1474.5821

1484.9397 1683.5513 1769.5144

3015.6168 3067.6415 3142.9681

3173.0546 3273.6259 3840.4576

*cis*-buta-1,2-diene-1,3-diol+

45.7715 55.2100 141.4333

220.5488 363.8873 450.6264

562.1883 595.7622 702.3547

711.9445 791.4838 987.0466

1018.0286 1034.8420 1096.7079

1247.9812 1276.3332 1345.3979

1382.6641 1421.2142 1443.0823

1467.1380 1533.0856 1691.0027

3025.9580 3090.3676 3129.8937

3166.2993 3685.6114 3723.4783

*cis*-buta-1,2-diene-1,3-diol

111.6840 119.1677 175.4997

254.7785 346.3702 382.6080

449.7826 510.7189 575.9528

591.7861 782.6253 864.7655

993.9212 1057.8278 1064.7425

1146.2657 1257.5758 1270.1921

1354.2115 1411.5942 1474.4768

1475.6185 1536.5792 2051.3194

3031.1469 3079.8509 3104.0403

3138.7476 3789.6753 3823.6241

*cis-3*-hydroxybut-3-enal+

70.6726 203.8132 320.7716

390.8365 395.9160 487.4079

501.2001 728.0149 733.5143

848.4694 900.4015 946.2758

1027.7457 1044.1903 1146.2783

1225.2954 1239.6746 1365.7948

1385.5876 1413.5236 1466.0192

1524.2232 1576.1554 1755.1689

2537.7124 3012.4474 3031.7912

3041.7889 3155.2568 3272.1936

*cis*-3-hydroxybut-3-enal

81.8382 111.6331 239.6844

374.0372 463.6755 490.5880

618.3915 697.6114 735.7086

759.9309 858.6999 860.6490

965.0952 991.4781 1041.6673

1220.5599 1272.3399 1329.6532

1365.2535 1417.5236 1427.9506

1451.9749 1725.4146 1782.0107

2913.6401 2966.6145 3083.9662

3164.4279 3252.4501 3639.0257

*cis*-oxobutanal+

55.9257 105.5096 145.5869

187.2519 319.3889 439.9852

462.4492 657.3773 711.8490

722.0893 805.4831 942.6317

988.0898 1056.1753 1093.9447

1164.2585 1237.9980 1289.8669

1357.9900 1408.2723 1438.9938

1459.5196 1700.3445 1836.1008

2854.7950 3025.9142 3043.8626

3089.8196 3110.1880 3166.9649

*cis*-oxobutanal

48.5895 101.2806 131.8353

184.2014 357.4502 480.8323

508.2404 686.9064 723.1063

787.7774 923.5100 938.5379

1045.5345 1082.6774 1189.7595

1250.3977 1311.3180 1387.1857

1417.3030 1435.9273 1469.3279

1476.2703 1781.5609 1804.1378

2888.1944 3011.3096 3031.8548

3071.8004 3089.5840 3142.2364

(*E*)-3-hydroxybut-2-enal+

97.6177 131.0342 164.2077

207.7279 395.1279 474.5365

524.5049 566.9223 655.7011

845.5389 868.7081 969.0627

1015.9463 1034.7354 1069.8399

1176.0665 1291.2665 1346.9756

1393.9404 1427.1277 1447.7460

1493.0568 1501.6409 1545.2366

3008.4417 3015.8779 3087.6673

3130.7226 3196.9375 3684.4311

(*E*)-3-hydroxybut-2-enal

129.1273 180.7407 226.6162

227.7954 392.2271 405.5475

496.9020 540.4173 554.7312

868.6555 897.0280 1011.9010

1024.5111 1066.3953 1166.7021

1203.9259 1260.8904 1369.7812

1422.8947 1445.7912 1480.4789

1483.8291 1702.2617 1733.4020

2889.8169 3020.1058 3064.0953

3150.5848 3180.7747 3804.9090

(*E*)-4-hydroxybut-3-en-2-one+

77.3405 124.4966 170.2677

259.4201 328.0988 422.6730

498.7109 640.0039 683.4479

778.4049 872.1473 985.8884

1002.1788 1009.7639 1083.4258

1147.2267 1235.8307 1310.9080

1339.9051 1427.2834 1435.0252

1462.0893 1500.6514 1644.6789

3037.7022 3116.4325 3158.4916

3169.3165 3234.9314 3740.3548

(*E*)-4-hydroxybut-3-en-2-one

33.4620 132.3557 258.0603

374.2927 379.2868 534.9058

626.5903 726.7800 791.9010

921.1625 953.9723 990.0698

1032.0191 1055.6488 1121.5559

1227.8315 1292.1272 1382.5382

1393.0888 1463.5322 1475.7398

1489.5537 1627.7770 1684.5647

3032.6543 3077.6214 3084.8879

3140.9020 3169.0349 3210.0894

*trans*-3-hydroxybut-3-enal+

68.9795 115.3746 211.1578

394.0203 435.3903 467.7596

514.0954 615.1661 619.9779

764.3703 858.8185 914.8517

949.4830 990.7743 1021.4143

1153.4035 1180.8329 1236.2930

1306.1305 1415.5057 1447.4186

1482.5814 1515.5578 1857.0213

2939.4226 3035.1032 3151.2064

3166.6229 3262.2695 3705.2907

*trans*-3-hydroxybut-3-enal

62.9723 74.9071 208.5085

400.4141 428.3886 441.5477

523.8936 605.4761 726.8446

762.5227 837.3139 894.7210

979.0889 1033.8916 1051.6439

1185.4880 1215.5779 1290.3102

1363.7905 1415.8561 1439.9907

1463.5126 1710.8905 1800.4746

2913.7449 3012.3308 3123.3589

3149.0789 3243.4475 3794.7114

*trans*-oxobutanal+

65.5936 117.4892 220.9857

254.1205 361.2980 449.2548

519.8511 689.9392 713.4559

839.4733 905.4719 939.5973

985.2645 1071.0532 1135.4589

1194.9521 1277.2449 1316.8661

1366.0627 1388.7892 1451.0623

1460.5144 1665.1744 1747.4466

2962.0526 3030.0421 3038.4219

3059.0833 3097.9209 3172.0595

*trans*-oxobutanal

33.3959 96.8507 147.4209

220.9916 368.8026 465.1026

528.6857 591.5598 752.3438

863.9933 919.5749 966.7532

1070.3533 1085.6987 1158.4470

1218.0987 1296.3477 1387.9347

1404.8419 1452.8645 1463.7189

1472.7911 1766.9899 1807.9422

2933.5229 3027.2058 3035.4538

3078.9913 3120.1737 3141.8564

(*Z*)-3-hydroxybut-2-enal+

73.0597 126.2925 173.0480

189.2441 373.4878 449.1742

546.3854 577.9700 640.3360

818.9228 929.9677 964.1837

980.2995 1029.3102 1080.3682

1162.9843 1250.9462 1315.4940

1386.8613 1430.9550 1459.4576

1480.4866 1502.6241 1549.0134

2994.3014 3008.2568 3075.0040

3149.5551 3222.2263 3696.7252

(*Z*)-3-hydroxybut-2-enal

131.8955 179.2283 194.9301

206.1582 361.4942 385.5293

497.7900 567.1036 577.7802

846.6519 917.9360 1021.1085

1025.6851 1066.5434 1117.9843

1188.3726 1284.9329 1359.7055

1415.0304 1432.3977 1480.0852

1482.5381 1705.9424 1733.9417

2934.2442 3015.0597 3059.6243

3134.7931 3196.1578 3818.8491

(*Z*)-4-hydroxybut-3-ene-2-one+

104.4745 184.4206 212.9230

302.0397 345.0839 396.0023

552.0301 626.3586 710.4873

770.2461 840.1608 991.9487

1012.2090 1015.7998 1060.1258

1216.4181 1273.5409 1327.2456

1352.8678 1423.5705 1463.2338

1472.1692 1486.9304 1660.5324

3042.5573 3124.5998 3159.2105

3160.1949 3218.8070 3745.3453

(*Z*)-4-hydroxybut-3-ene-2-one

75.0968 168.5875 210.1191

298.3572 356.5073 417.8321

513.4369 620.5957 698.2286

798.6446 814.9694 982.9602

995.2347 1051.0661 1077.6215

1246.1575 1282.2191 1300.3974

1394.5706 1443.7657 1463.4578

1476.4503 1705.4137 1719.5764

3040.6064 3095.8542 3139.7539

3146.8338 3192.3532 3835.9275

(1*E,*3*E*)-buta-1,3-diene-1,4-diol+

117.7831 149.3028 272.5706

319.8078 397.1086 433.9254

569.5167 595.6466 622.7931

898.1030 928.4335 955.3477

1002.2132 1153.8231 1162.1055

1230.6244 1257.3593 1315.4719

1332.0180 1347.4879 1353.0951

1479.6889 1612.6581 1690.4639

3158.2747 3160.2734 3169.6401

3177.6015 3741.0666 3746.7706

(1*E,*3*E*)-buta-1,3-diene-1,4-diol

120.1449 145.0450 204.5756

230.9729 292.9331 378.7888

397.0147 428.0296 613.2618

827.2386 867.8096 910.8910

973.6572 1097.7288 1130.7033

1177.0351 1185.2570 1223.9807

1314.4861 1348.7223 1350.8229

1408.7334 1701.1405 1740.9938

3140.8250 3145.4648 3149.1417

3152.8129 3852.6042 3854.1200

(1*Z*,3*E*)-buta-1,3-diene-1,4-diol+

149.5251 164.8372 202.7499

327.3629 384.3047 520.2866

582.3354 603.3264 702.7143

844.7741 949.8198 956.8148

1001.0627 1077.9842 1162.7593

1217.3414 1261.4859 1310.5543

1330.0003 1337.2546 1362.3658

1532.0652 1598.5151 1679.2882

3156.3501 3173.3789 3186.8666

3195.0865 3741.4243 3751.1760

(1*Z*,3*E*)-buta-1,3-diene-1,4-diol

139.0695 142.8168 196.9558

249.9717 301.9157 312.8836

508.9561 533.8935 695.5267

754.5715 861.7373 918.5108

967.2251 1020.3566 1129.8190

1154.1365 1194.0200 1254.5497

1285.6796 1341.2096 1352.7361

1455.1804 1696.0032 1734.8421

3143.1138 3155.8195 3173.7388

3179.8893 3851.2137 3854.4089

(1*Z*,3*Z*)-buta-1,3-diene-1,4-diol+

13.6568 201.0117 244.3899

249.4724 450.2616 596.5033

614.1100 638.1476 760.2100

863.4548 899.4231 924.1560

991.4540 1000.0437 1083.0864

1251.4637 1265.7665 1279.0693

1339.0708 1388.3680 1482.9173

1562.6656 1610.2509 1660.0821

3161.1441 3163.7286 3182.7137

3193.1845 3735.0939 3740.6796

(1*Z*,3*Z*)-buta-1,3-diene-1,4-diol

99.4995 155.3122 232.2367

260.2144 285.0810 406.8113

542.6929 647.6126 734.1376

770.4448 857.2569 909.7783

938.6010 939.0269 1049.2778

1120.6936 1243.4401 1268.6448

1292.3175 1318.1823 1423.8423

1471.5891 1717.1537 1720.6857

3141.2142 3144.7314 3162.1691

3168.8393 3847.6486 3848.5320

*cis*-succinaldehyde+

23.7996 90.8532 138.8821

221.2766 412.6279 436.1732

515.2905 679.3803 736.1690

841.8731 893.8929 956.0929

997.4599 1091.3377 1177.1601

1236.7082 1255.1822 1260.6814

1306.8715 1321.7008 1429.0218

1437.8396 1818.3162 1835.6931

2573.2600 2682.2089 3021.7007

3027.7189 3103.8265 3107.5250

*cis*-succinaldehyde

47.0846 69.5865 106.5206

278.5929 349.1261 482.4423

528.6863 743.6618 769.8312

927.5966 957.6897 1019.1389

1090.8186 1130.5748 1210.1170

1224.2010 1339.6141 1346.9510

1416.8973 1421.0277 1460.5707

1464.2939 1801.6404 1807.8022

2870.4257 2872.1179 3015.6308

3025.0201 3079.1519 3090.6678

(*E)*-4-hydroxybut-3-enal+

51.6738 149.6489 173.6525

291.1533 331.4252 454.3085

551.0351 636.5727 708.2771

864.3164 885.6544 970.3763

1012.5862 1097.1748 1160.8184

1197.5827 1230.9634 1299.9095

1321.9891 1369.6828 1408.1441

1478.7656 1600.5549 1858.8916

2973.3819 3038.5252 3139.8287

3152.4335 3182.9189 3684.6004

(*E*)-4-hydroxybut-3-enal

57.4044 91.7704 211.4769

291.5821 378.2038 456.1028

468.2140 566.6233 834.6086

839.0627 946.6454 975.9664

1059.2007 1096.8102 1136.2911

1204.6355 1269.7872 1299.9915

1342.1443 1400.4182 1409.8289

1461.5765 1712.4030 1798.3506

2873.9658 3019.9317 3077.8512

3128.8363 3180.8714 3786.6703

*trans*-succinaldehyde+

54.5949 90.5231 92.3992

245.8371 312.7840 463.9984

490.1220 767.2305 768.1304

854.6063 897.6111 932.8929

1033.1601 1051.1310 1163.9196

1252.8959 1256.0961 1281.3972

1299.6697 1328.2586 1470.7932

1477.0448 1794.1364 1798.9114

2941.3482 2941.4131 3032.4178

3043.2285 3120.1008 3136.0013

*trans*-succinaldehyde

48.6918 72.8878 77.8346

238.7837 340.4451 480.8055

545.4405 783.7636 799.7109

939.2296 989.3765 991.2859

1103.6239 1138.5882 1206.8326

1268.8382 1301.1959 1352.0109

1416.1439 1422.1713 1466.3530

1483.2603 1800.1186 1805.6467

2875.2118 2875.5981 3015.4674

3025.2989 3084.1816 3099.2923

(*Z*)-4-hydroxy-but-3-enal+

34.7744 82.1282 211.4066

267.4517 385.9443 487.3502

616.1799 656.8351 682.4635

828.4124 920.6930 964.5821

984.6815 1045.7875 1153.3023

1184.2716 1226.4140 1278.8806

1294.2010 1326.4826 1454.1804

1500.2191 1604.0378 1861.1979

2959.7865 3071.7410 3154.1525

3171.8831 3198.7485 3723.2197

(*Z*)-4-hydroxy-but-3-enal

43.8410 68.5839 229.2541

245.5015 304.7799 493.8984

528.4959 647.9100 764.6040

836.4508 933.9483 952.4717

1038.1020 1060.5039 1113.0288

1206.6400 1280.3798 1286.3152

1296.0908 1412.1230 1428.6513

1463.5878 1732.4751 1795.9671

2881.4868 3033.1652 3090.6904

3158.2988 3188.4592 3849.7288

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