Electronic Supplementary Information for

Radiation-induced transformations of matrix-isolated ethanol molecules at cryogenic temperatures: a FTIR study

Pavel V. Zasimov, Elizaveta V. Sanochkina, Daniil A. Tyurin, and Vladimir I. Feldman*

Department of Chemistry, Lomonosov Moscow State University, 119991 Moscow, Russia

*Corresponding author, e-mail: feldman@rad.chem.msu.ru (V.F.)

Table S1 Main absorption maxima (cm^{-1}) of the C_2H_5OH and C_2D_5OH isolated molecules in the noble-gas matrices. Tentative assignments are in italic. Multiple features most probably are due to the effect of matrix site splitting.

Approximate assignment	Ne	Ar	Kr	Xe	Gas phase[S1]
		C_2H_5OH			
OH_{str}	3679.7$_A$	3660.2$_A$	*3666.5*	3642.0	3676.1
	3677.4$_G$	3655.2$_G$	3650.0$_A$	3639.7sh	3667.1
			3646.6$_G$		3658.6
					3656.2
$CH_{3\ a\text{-}str}$ A″	3000.6	3000.2	2994.6	2996.9	2989.4
	2994.7	2995.0	2989.2	2989.7	
	2990.0		2985.3		
$CH_{3\ a\text{-}str}$	2985.7	2984.4	2981.1	2981.0	–
			2977.9		
$CH_{3\ s\text{-}str}$	2955.0	2953.0	*2948.2*	2943.2	–
	2942.2	2938.9	2934.8	2928.5	
$CH_{2\ a\text{-}str}$ A″	2920.4	2917.1	2908.1	2903.4	2900.5
	2914.8	2912.6	2901.7		
$CH_{2\ s\text{-}str}$	2902.7	2899.5	2896.5	2892.3	–
	2896.8	*2889.0sh*	2892.7	2885.8	
				2880.6sh	
$CH_{2\ scis}$	1492.6	1487.2	*1487.6*	1482.9	–
			1484.1		
$CH_{3\ a\text{-}deform}$	1465.3	1463.3	1460.6	*1456.8*	1453.3
					1449.9
$CH_{3\ a\text{-}deform}$ A″	1449.0	1445.0	1443.3	1440.4	–
$CH_{2\ wag}$	*1427.0*	1416.6	1415.9	1413.9	–
	1413.8				
$CH_{3\ s\text{-}deform}$	*1379.3*	1371.5	1369.4	1367.4	1393.7
	1373.0				
OH_{deform}	*1253.2*	*1254.7*	*1251.1*	*1251.2*	1241.3
	1241.3	*1252.1*	1237.6	1238.2	
		1239.5			
$CH_{2\ rock}$ + $CH_{3\ rock}$ A″	1159.3	1160.2	–	–	–
CCO_{str} + $CH_{3\ rock}$	*1103.0*	*1102.7*	*1101.5*	*1101.3*	1089.2
	1091.0	*1095.9*	*1094.6*	*1092.6*	
	1072.8	*1091.7*	*1089.5*	*1088.9*	
		1083.5	1082.8	1082.5	
		1077.0		1074.7sh	
CCO_{str} + $CH_{3\ rock}$	1028.2	1025.1	1030.6	1032.5sh	1037.6
	1020.1	1016.6	1023.8	1031.5	1027.6
	1017.0sh	*1009.3*	1021.8	1027.1	
	1012.9		1015.8	1022.6sh	
CCO_{str}	891.6$_A$	889.3$_A$	*898.2*	898.4sh$_A$	891.5
	889.8$_G$	886.4$_G$	887.9$_A$	895.0$_G$	883.0
	886.9sh$_G$	884.6sh$_G$	885.0$_G$		879.4
			882.5sh$_G$		
$CH_{2\ rock}$ + $CH_{3\ rock}$ A″	814.5	811.9	809.3	817.4	801.0

		C_2D_5OH			
OH $_{str}$	3686.7_{A}	3660.6_{A}	*3666.5*	3642.6	3676.1
	3680.0_{G}	3655.6_{G}	3649.9_{A}	3640.4sh	
			3646.9_{G}		
$CD_{3\ \text{a-str}}$ A″	2252.0	2256.4	2251.6	2252.0	2233.6
	2244.3	2246.7	2242.4	2246.3	
	2240.4	2231.3	2239.6	2242.4	
	2236.0		2231.8	2236.2	
				2232.7sh	
$CD_{3\ \text{a-str}}$	*2211.6*	*2208.1*	*2205.3*	*2206.4*	–
	2201.7				
$CD_{2\ \text{a-str}}$ A″	2186.2	2194.3	*2195.8*	2171.2	2185.0
	2184.0	2191.0	2190.0sh	2170.6	
	2175.6		2186.1		
			2178.2		
$CD_{3\ \text{s-str}}$	2142.8	2141.6	2137.8	*2144.7*	–
				2134.6	
$CD_{2\ \text{s-str}}$	2126.4	2121.9	2120.5	2114.7	–
	2123.9	2111.7	2118.8	2104.1	
	2111.6	2105.9	2107.4	2095.1	
	2106.2	2103.6	2101.2	2089.5	
	2102.9	2098.5	2093.5	2076.7	
	2096.0	2086.3	2084.2sh	2072.5	
	2084.2	2078.9	2081.0	2065.9	
	2080.3		2078.5sh		
			2076.5sh		
?	2033.5	2029.0sh	2022.8	2022.9	–
	2027.1	2026.7	2018.2	2017.2	
	2021.7	2022.1			
?	1316.3	1315.0	1316.5	1319.0sh	–
			1313.6	1314.3	
$CD_{3\ \text{s-deform}}$	*1285.3*	*1276.5*	–	*1277.8*	1286.2
	1279.2				
?	*1192.0*	*1189.2*	*1166.3*	*1186.1*	1185.0
	1182.8	*1177.2sh*	*1163.3*	*1180.6*	
	1180.6	*1169.0*			
	1166.5	*1166.6*			
		1162.0			
$CD_{2\ \text{wag}}$	1144.6	1143.3	1160.9	1143.6	1155.1
	1138.7sh	1136.1	1150.3	1128.4	1141.7
	1131.4	1129.2	1142.1	1124.9sh	1123.5
	1125.6	1121.2sh	1133.5	1114.7	
	1118.6sh	1118.2	1126.9		
	1114.8	1115.0sh	1119.6		
	1109.5		1115.1		
$CD_{3\ \text{a-deform}}$	*1091.5*	*1097.7*	*1098.3*	*1094.5*	1067.6
	1086.8	*1094.9*	*1093.7*	1070.0	1064.0
	1073.2	1071.2sh	1073.6	1066.1	
	1070.9	1068.4	1067.1	1061.4	
	1066.7	1064.4	1062.6		

$CD_{2\ scic}$	1060.3	1057.1	1055.2	1055.6	1057.8
	1058.1		1053.9sh	1052.2	1053.8
				1050.9sh	
$CD_{3\ a\text{-}deform}$ A″	1051.4	1049.6	1048.4	1045.7	–
$CH_{2\ rock}$ + $CH_{3\ rock}$ A″	984.7	981.4	980.4	–	–
	982.0	975.8	974.0		
	973.0	971.8	971.7		
OH_{deform}	964.1	965.8	963.6	965.7	967.7
	959.7	961.2	959.4sh	963.2sh	965.7
	957.5sh			960.6	
				956.4	
CCO_{str} + $CD_{3\ rock}$	*922.0*	*920.4*	*919.3*	904.8	902.7
	907.4	*910.1*	*908.4*	890.3	889.4
	905.5sh	*905.0*	*902.3*	887.0	882.6
	903.5sh	*903.0*	892.1		878.4
	894.8	892.2	886.5		
	889.6	887.7	881.6sh		
	884.3	883.2			
	881.7				
CCO_{str}	744.4_A	742.8_A	*745.8*	749.9_A	744.0
	741.0_G	739.2_G	742.4_A	743.4_G	
			738.3_G		

A – anti-conformer; G – gauche-conformer; sh – shoulder.

Table S2 Absorption maxima (cm^{-1}) of the species produced under X-ray radiolysis of the C_2H_5OH/Ng and C_2D_5OH/Ng 1:1000 (Ng = Ne, Ar, Kr, or Xe) samples. Tentative assignments are in italic.

Species	Assignment	Ne[a]	Ar	Kr	Xe	Ref.
			C_2H_5OH			
CH_3CHO	$2\nu_6$	–	2841.0	2842.9	2823.4	S2, S3
				2838.2	2822.0	
				2833.9		
	$\nu_5+\nu_6$	–	–	–	2803.7	
	$\nu_5+\nu_7/\nu_7+\nu_{12}$	2753.3	2751.1	2752.0	2743.2	
				2745.7		
	CH_{str}	2719.8	2730.0	2725.6sh	2731.5	
		2716.7	2726.5	2723.4	2716.3sh	
			2719.5	2719.4sh	2713.8	
				2711.8		
	CO_{str}	1733.5	*1728.3*	1740.8	1735.6	
		–	–	*1726.4*		
	$CH_{3\ d\text{-}deform}$			–	1423.9	
					1419.9	
	$CH_{3\ s\text{-}deform}$	1352.7	1352.5	1349.4	1345.5	
			1349.3	1347.0		
	CC_{str}	1117.7	1123.9	1121.7	1122.7	
		1114.7	1120.3	1118.6	1116.1	
			1116.0	1113.8		
			1111.6	1109.9		
	CCO_{deform}	509.6	515.2	*516.8*	515.4	
				515.1	512.1	
				510.3		
				505.7		
CH_2CHOH	OH_{str}	*3629.0*	*3625.4*	*3609.2*	–	S2, S4, S5
			3621.2	*3607.1*		
			3616.7			
			3609.4			
	CC_{str}	*1669.0*	*1672.0*	–	–	
		1666.8	*1667.4*			
		1665.4	*1665.2*			
		1662.7	*1661.9*			
	Mixed mode	*1078.1*	*1079.2*	*1078.8*		
	CH_2CH_{OPLA}	817.0	823.0	821.3	*814.6sh*	
			817.6	816.0	*812.8*	
					804.0	
$C_2H_2\cdots H_2O$	$CH_{a\text{-}str}$	3252.2	3239.8	3234.0	–	S2, S6
		3247.8				
	OH_{bend}	1598.9	1593.1	1591.1		
		1596.3sh		1588.2		
	$CH_{a\text{-}bend}$	778.9sh	*786.1*	*782.7*		
		776.6				
		772.9				
		770.8				

$CH_3CO^{\bullet}$	CO $_{str}$ [b]	–	–	*1881.0*	1880.2	S2, S5,
				1847.7	1876.3	S7, S8
					1844.4	
	$CH_{3\ deform}$			*1321.5*	1318.4	
$H_2CCO–H_2$	$CH_{2\ s\text{-}str}$	3078.2	3071.7	3066.6sh	3056.0	S2, S9
			3069.8sh	3062.6	3052.5	
			3067.7			
	CO $_{str}$	2150.3	2148.1	2143.9	2139.3	
	$CH_{2\ scis}$	1386.8	1381.7	1378.0	1375.0	
	$CH_{2\ rock\text{-}opla}$	592.3	–	–	–	
	CO $_{rock\text{-}opla}$	527.5	524.5			
H_2CCO	$CH_{2\ s\text{-}str}$	3069.1	3062.8	*3049.4*	*3040.7*	S2, S7,
	CO $_{str}$	2150.3	2142.2	2139.8	*2136.7*	S10, S11
	$CH_{2\ scis}$	1386.8	–	–	–	
	$CH_{2\ rock\text{-}opla}$	592.3				
	CO $_{rock\text{-}opla}$	527.5				
$HCCO^{\bullet}$	CCO $_{deform}$	2023.9	*2031.2*	2028.1	2021.0sh	S2, S12, S13
		2018.6sh	2022.1	2026.1	2016.4	
		2015.4sh	2019.6sh	2019.6	*2013.7sh*	
CCO	CO $_{str}$	1972.6	1973.5	1970.3	1966.5	S2, S14
		1967.2				
H_2CO	$CH_{2\ a\text{-}str}$	–	2865.3	2854.1	–	S15–S17
	$CH_{2\ s\text{-}str}$		2797.6	2787.6		
	CO $_{str}$		1740.8	1738.8		
	$CH_{2\ scis}$		1498.0	1494.3		
	$CH_{2\ wag}$		1169.6	1166.5		
$HCO^{\bullet}$	CH $_{str}$	2482.2	2481.3	2475.4	2444.8	S18−S20
			2478.3sh	2468.0		
	CO $_{str}$	1866.2	1862.8	1861.9	1858.8	
				1859.7	1856.8	
	HCO $_{deform}$	–	1086.2	1081.2	*1076.3*	
					1073.5	
CO	CO $_{str}$	2143.5sh	2137.6	2135.7	2132.4	S7, S21
		2141.2			2130.9sh	
CH_4	$CH_{3\ d\text{-}str}$	3020.3	3026.0	3019.3	3019.5	S22
			3020.8sh	3016.4	3012.5	
					3006.7	
	$CH_{3\ d\text{-}deform}$	1308.7	1305.6	1308.7	1309.4	
				1305.3sh	1303.8	
				1303.0	1300.6	
				1300.4		
$CH_3^{\bullet}$	$CH_{3\ OPLA}$	607.3	606.5	609.3	*602.7*	S7, S23
				604.0		

			C_2D_5OH			
CD_3CDO	$CD_{3\ s\text{-}str}$	–	–	*2124.9* *2122.6*	*2118.6*	S2, S3
	CD_{str}	*2062.4* *2060.2* *2054.7*	*2061.6*	*2056.6*	*2069.1* *2054.3* *2050.9* *2049.1*	
	CO_{str}	*1735.5* *1724.6*	*1746.3* *1733.8* *1732.2* *1726.9*	1731.5 1728.8 1725.0	1726.9	
	CD_{bend}	*1154.8*	*1154.5*	*1156.3*	1152.7	
	$CD_{3\ s\text{-}deform}$	1026.8	1024.9	*1022.4*	1019.2	
	CC_{str}	943.9 *940.3* *934.5*	939.5	937.4	939.1	
	CCO_{deform}	*443.7* 436.7	*442.2* 433.3	*443.3* *432.4*	*442.1* *439.5* *429.6*	
CD_2CDOD	*OD_{str}*	*2684.4*	*2679.8* *2676.9sh*	*2667.1*	*2654.9*	S4
CD_2CDOH	OH_{str}	–	*3626.9* *3623.3* *3615.5*	*3609.2* *3607.1*	–	S2, S4
	CC_{str}	*1595.6* *1585.3* *1578.4*	*1598.6* *1597.1* *1590.0* *1581.6*	*1595.3* *1593.8* *1587.7*	*1592.5* *1584.8*	
	Mixed mode	926.7 923.3	924.2	922.5	920.9 916.3sh	
	CD_2CD_{OPLA}	651.6	653.4sh 651.5 649.9sh	651.5 649.8	648.0 646.4	
$C_2D_2 \cdots HDO$	*OD_{str}*	*2713.8*	*2714.6*	–	–	S6
	OH_{bend}	*1399.6*	*1401.0*	*1400.5*		
$HCCD \cdots D_2O$	*$CD_{a\text{-}str}$*	*2547.3* *2541.4*	*2542.2*	–	–	S6
$DCCH \cdots D_2O$	*$CD_{a\text{-}str}$*	*2591.4*	*2578.3*	*2573.6*	–	S6
	$CH_{a\text{-}bend}$	*729.7*	*729.3*	*725.3*		
$C_2D_2 \cdots D_2O$	$OD_{a\text{-}str}$	*2769.8*	*2775.0*	*2766.9*	–	S2, S6
	$CD_{a\text{-}str}$	2414.1	2411.0	*2405.7*	*2401.0*	
	OH_{bend}	*1180.7*	*1176.2*	*1173.0*	–	
	$CD_{a\text{-}bend}$	*516.5* *510.7*	*514.3*	*512.9*		
$CD_3CO^{\bullet}$	CO_{str}	–	–	*1862.2*	1859.4	S2, S7, S8
	$CD_{2\ scis}$			–	*1022.0* *1020.9sh*	

$D_2CCO–D_2$	$CD_{2\ \mathrm{s\text{-}str}}$	2270.2	2265.8	2260.3	2259.1	S2
		2265.7			2255.4	
	$\nu_3+\nu_4$	2156.5	2154.9	2151.1	2146.1	
	CO_{str}	2120.6	2118.7	2114.4	2110.3	
	$CD_{2\ \mathrm{rock\text{-}opla}}$	–	–	–	*538.4*	
	$CO_{\mathrm{rock\text{-}opla}}$			*432.2*	*429.3*	
D_2CCO	$CD_{2\ \mathrm{s\text{-}str}}$	2270.2	2260.0	2255.6	*2250.4sh*	S2, S7,
	$\nu_3+\nu_4$	2265.7	2149.2	*2145.7*	–	S10, S11
	CO_{str}	*2153.3*	2112.7	2110.1	2106.8	
		2120.6				
$DCCO^{\bullet}$	CCO_{deform}	1994.9	1993.3	1993.2sh	*1993.1*	S2, S12, S13
		1992.1	1990.0	1990.0	1989.2sh	
					1986.0	
CCO	CO_{str}	1972.8	1972.2	1969.5	1965.3	S2, S14
		1967.2		1966.3	1962.8	
HDCO	CH_{str}	–	2859.1	–	–	S15, S17
			2762.2			
			2760.3			
			2758.2			
			2734.5			
	CO_{str}		1719.0	*1716.1*		
	CHD_{scis}		1396.0	–		
D_2CO	$CD_{2\ \mathrm{a\text{-}str}}$	–	2178.6	2170.8	–	S15–S17
	$CD_{2\ \mathrm{s\text{-}str}}$		2069.3	2062.3		
	CO_{str}		1696.4	1693.6		
			1694.2			
	$CD_{2\ \mathrm{scis}}$		1099.2	1096.5		
	$CD_{2\ \mathrm{rock}}$		987.7	985.4		
	$CD_{2\ \mathrm{wag}}$		942.5	*940.8*		
$HCO^{\bullet}$	CH_{str}	–	2481.4	–	–	S15, S19–S21
	CO_{str}	1869.2	1862.8	*1860.0*		
		1866.1				
$DCO^{\bullet}$	CD_{str}	*1917.8*	1925.2	1918.9	*1922.7*	S18
		1909.9			*1910.5*	
	CO_{str}	–	1801.1	–	–	
	DCO_{deform}	852.2	849.7	*846.8*	*850.8*	
		848.6				
CO	CO_{str}	2140.9	2137.6	2135.6	2132.7	S7, S21
					2128.3sh	
CHD_3	CH_{str}	*2998.5*	*2998.5*	*2986.7sh*	–	S24
		2996.6	*2996.6*	*2984.8*		
		2991.1	*2990.9*			
		2989.9sh				
	$CD_{3\ \mathrm{rock}}$	1290.4	1288.1	*1301.2*		
			1286.9	*1297.7*		
				1295.2		
				1284.6		
	$CD_{3\ \mathrm{d\text{-}deform}}$	1032.8	*1030.2*	*1027.7*		
			1024.5	*1022.3*		
	$CD_{3\ \mathrm{s\text{-}deform}}$	1002.8	*1001.9*	*1000.2*		
			1000.1	*998.4*		

CD_4	$CD_{3\ \text{d-deform}}$	996.4 *990.4*	993.9	992.1	997.2 992.9 990.0sh	S7, S25
$CD_3^{\bullet}$	$CD_{3\ \text{OPLA}}$	457.4	455.1	454.4	*454.0*	S7, S23

sh – shoulder, OPLA – out of plane.

[a] *In a Ne matrix both of H_2CCO/H_2CCO–H_2 (D_2CCO/D_2CCO–D_2) may contribute to all observed absorptions of ketene except $CH_{2\ s\text{-}str}$ ($CD_{2\ s\text{-}str}$), see Ref. S2 for details. Owing to this reason we provide the same values of absorption maxima both for H_2CCO and H_2CCO–H_2 (D_2CCO/D_2CCO–D_2).*
[b] *Fermi resonance with an overtone or a combination band, see Ref. S8 for details.*

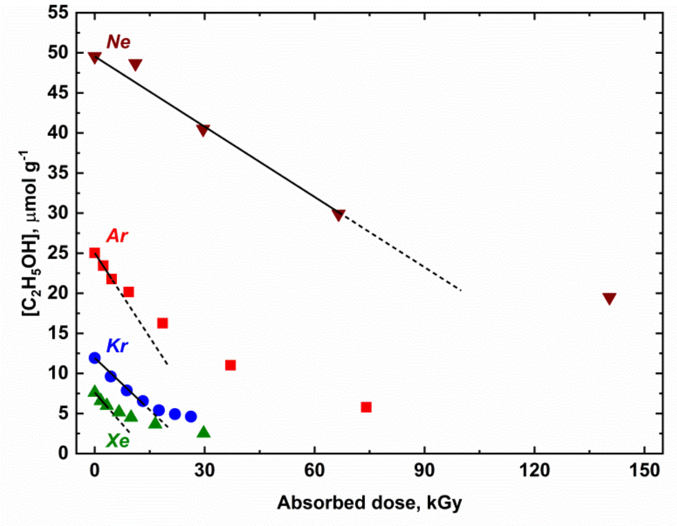

Fig. S1 Kinetics of the radiation-induced decay of ethanol molecules in the C_2H_5OH/Ng 1:1000 samples (Ng = Ne, Ar, Kr, or Xe) irradiated with X-rays. The relative concentration of ethanol in the samples irradiated to different doses was calculated by integration of the O–H $_{str}$ absorption band. The initial molar mass concentrations of C_2H_5OH were determined based on molar a mixture ratio of 1:1000. The radiation-chemical yield of the C_2H_5OH degradation estimated from initial slopes of the recorded kinetics profiles are ca. 0.29, 0.67, 0.42, and 0.51 μmol J^{-1} for Ne, Ar, Kr, and Xe, respectively, i.e. the efficiency of ethanol decomposition increases in a row Ne < Kr < Xe < Ar.

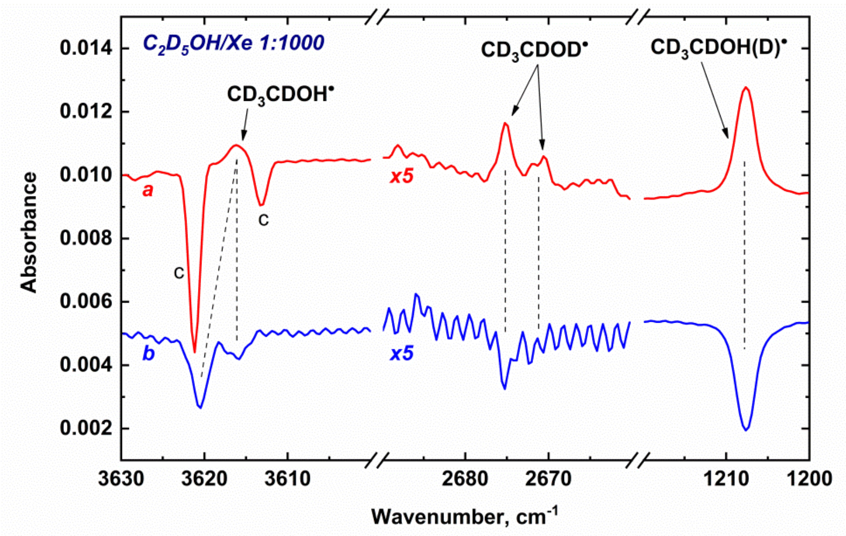

Fig. S2 Fragments of the difference FTIR spectra (recorded at 4.4 K) showing the effect of the X-ray irradiation for 5 min (*a*) and UV photolysis (254 nm) for 30 min (*b*) of the C_2D_5OH/Xe (1:1000) in the regions containing the absorptions bands assigned to the $CD_3CDOH(D)^{\bullet}$ radicals. Absorption features in the OH stretching region observed in the deposited sample and decreased upon irradiation were tentatively attributed to the ethanol dimers[S26] (marked with ‘c’).

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