Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material for:-

The application of inelastic neutron scattering to investigate the interaction of methyl propanoate with silica

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Table S1: Crystal data, data collection and refinement methods for methyl propanoate.

Crystal data
$C_4H_8O_2$
M_r = 88.11
Triclinic, $P\bar{1}$ Z = 4
a = 5.9523 (5) Å
b = 6.7864 (5) Å
c = 12.7209 (11) Å
α = 87.987 (3)°
β = 89.585 (3)°
γ = 84.399 (4)°
V = 511.08 (7) Å^3

Mo $K\alpha$ radiation, λ = 0.71073 Å
μ = 0.09 mm^{-1}
T = 150 K
0.80 × 0.10 × 0.10 mm

Data collection
Nonius KappaCCD diffractometer
Absorption correction: Multi-scan
DENZO/*SCALEPACK* [9]
T_{min} = 0.62, T_{max} = 1.00
6235 measured reflections

1996 independent reflections

1419 reflections with $I > 2.0\sigma(I)$
R_{int} = 0.041

Refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.212
S = 0.88
1996 reflections
157 parameters

0 restraints
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

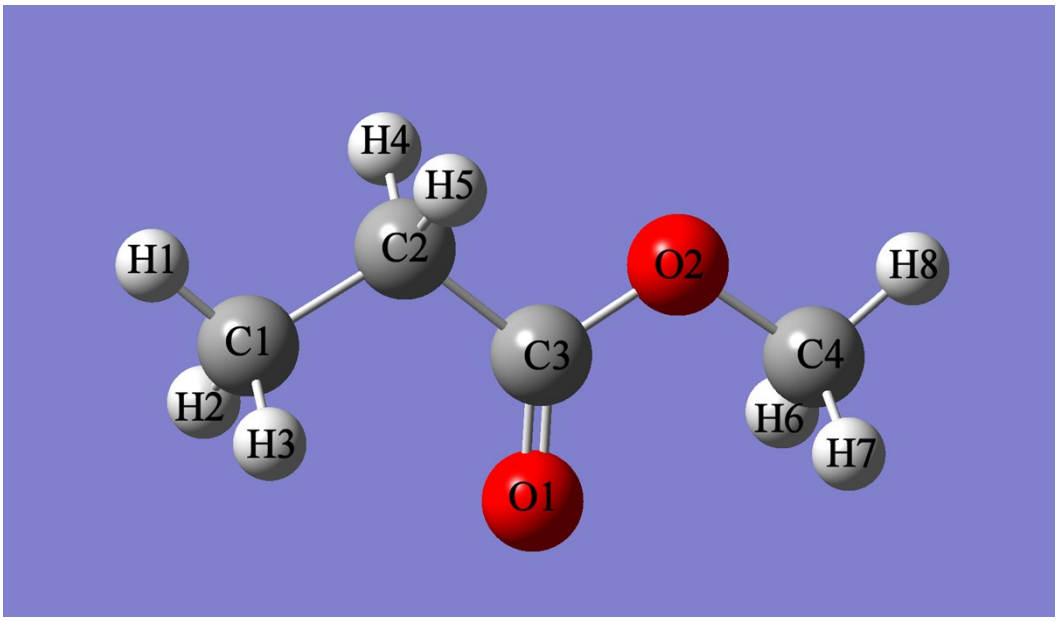

Figure S1: Numbering scheme for methyl propanoate.

Table S2: Observed and calculated structural parameters for methyl propanoate. In the crystal the almost planar molecule is called C_s and the skew molecule is called C_1.

	Crystal				Gas phase	
	Experimental		Computational			
	X-ray at 150 K		CASTEP		Gaussian 03	
	C_s	C_1	C_s	C_1	C_s	
Distance / Å						
C1–C2	1.516	1.492	1.526	1.529	1.523	
C2–C3	1.492	1.497	1.513	1.512	1.511	
C3=O1	1.203	1.202	1.219	1.221	1.211	
C3–O2	1.346	1.333	1.357	1.354	1.352	
O2–C4	1.449	1.443	1.449	1.447	1.435	
C1–H1					1.092	
C1–H2					1.091	
C1–H3					1.091	
C2–H4					1.095	
C2–H5					1.095	
C4–H6					1.090	
C4–H7					1.090	
C4–H8					1.087	
Bond angle / º						
C1–C2–C3	112.9	114.4	113.1	113.6	112.4	
C2–C3–O1	111.4	111.6	111.4	111.1	110.6	
C2–C3=O2	126.2	125.5	125.8	126.0	125.9	
C3–O1–C4	115.2	116.9	115.1	116.5	114.1	
H1–C1–C2			109.5	110.4	110.6	
H1–C1–H2			108.5	108.1	108.5	
H1–C1–H3			108.6	108.3	108.5	
H2–C1–H3			107.7	108.6	107.5	
H3–C2–H4			105.7	106.2	105.8	
H8–C4–O1			105.9	104.7	105.4	
H8–C4–H6			110.8	111.0	110.7	
H8–C4–H7			110.6	110.5	110.7	
H6–C4–H7			109.8	109.9	109.0	
Dihedral angle / º						
C1–C2–C3–O1	179.9	159.7	179.3	154.3	180.0	
C2–C3–O1–C4	179.3	179.9	179.1	177.8	180.0	

Table S3: Observed and calculated vibrational transition energies for methyl propanoate. In the crystal the almost planar molecule is called C_s and the skew molecule is called C_1.

Experimental				Calculated					Description
Infrared			INS	Gaussian 03		CASTEP			
Gas	Liquid	Solid	Solid	Gas	Infrared intensity	Solid	Infrared intensity	Character	
cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	km mol^{-1}	cm^{-1}	km mol^{-1}		
			51			19	0.00	A_g	Translation
						39	0.00	A_g	Translation
			62			41	0.00	A_g	Translation
						44	0.00	A_g	Translation
						50	3.54	A_u	Libration
						55	6.40	A_u	Libration
						59	3.61	A_u	Translation
			81			60	0.00	A_g	Libration
						61	0.00	A_g	Libration
						63	2.94	A_u	Libration
						67	0.00	A_g	Libration
						75	0.86	A_u	Translation
						82	0.00	A_g	Translation
				29	0.00	87	0.56	A_u	C2–C3 torsion
						90	0.00	A_g	C2–C3 torsion
						92	0.00	A_g	C2–C3 torsion
						95	1.38	A_u	C2–C3 torsion
			90			103	0.71	A_u	Translation
						104	0.00	A_g	Translation
						106	1.37	A_u	Libration
			116			108	0.00	A_g	Libration
						112	0.00	A_g	Libration
						113	6.27	A_u	Libration
						124	5.98	A_u	Libration

			136			126	0.00	A_g	Libration
			162	174	1.31	160	2.15	A_u	C_1 C4 methyl torsion
			165			166	0.00	A_g	C_1 C4 methyl torsion
				147	4.81	179	1.14	A_u	C3–O1 torsion
			193			181	0.00	A_g	C3–O1 torsion
			204			185	0.00	A_g	C_s C4 methyl torsion
						189	69.95	A_u	C3–O1 torsion
						194	0.00	A_g	C3–O1 torsion
			235			213	0.88	A_u	C_s C4 methyl torsion
				215	2.01	220	0.00	A_g	C1–C2–C3 + C2–C3–O1 in-phase, in-plane bend
						221	23.11	A_u	C1–C2–C3 + C2–C3–O1 in-phase, in-plane bend
			245			228	0.00	A_g	C1–C2–C3 + C2–C3–O1 in-phase, in-plane bend
						230	11.22	A_u	C1–C2–C3 + C2–C3–O1 in-phase, in-plane bend
				233	1.88	240	1.53	A_u	C_s C1 methyl torsion
			262			242	0.00	A_g	C_s C1 methyl torsion
						242	0.00	A_g	C_1 C1 methyl torsion
						249	30.07	A_u	C_1 C1 methyl torsion
			303	343	19.91	317	68.79	A_u	C_1 C1–C2–C3 + C3–C1–C4 out-of-phase, in-plane bend
						318	0.00	A_g	C_1 C1–C2–C3 + C3–C1–C4 out-of-phase, in-plane bend
			339			329	66.67	A_u	C_s C1–C2–C3 + C3–C1–C4 out-of-phase, in-plane bend
						332	0.00	A_g	C_s C1–C2–C3 + C3–C1–C4 out-of-phase, in-plane bend
				455	0.73	428	3.52	A_u	C_1 C2–C3–O1 in-plane bend
			442			428	0.00	A_g	C_1 C2–C3–O1 in-plane bend
						438	1.80	A_u	C_s C2–C3–O1 in-plane bend

						438	0.00	A_g	C_s C2–C3–O1 in-plane bend
		575	566	582	2.17	563	13.68	A_u	C=O out-of-plane bend
						564	0.00	A_g	C=O out-of-plane bend
						571	1.71	A_u	C=O out-of-plane bend
						571	0.00	A_g	C=O out-of-plane bend
		653	650	670	3.39	640	7.70	A_u	C_s C=O in-plane bend
						640	0.00	A_g	C_s C=O in-plane bend
		671	668			661	11.22	A_u	C_1 C=O in-plane bend
						662	0.00	A_g	C_1 C=O in-plane bend
	807	805	807	824	10.02	788	108.75	A_u	Methylene rock
						788	0.00	A_g	Methylene rock
						791	7.87	A_u	Methylene rock
						792	0.00	A_g	Methylene rock
847	848	854	855	878	14.79	837	55.68	A_u	C_s C2–C3 + C3–O1 in-phase stretch
						838	0.00	A_g	C_s C2–C3 + C3–O1 in-phase stretch
						839	34.83	A_u	C_1 C2–C3 + C3–O1 in-phase stretch
						840	0.00	A_g	C_1 C2–C3 + C3–O1 in-phase stretch
968	963	962	960	1014	3.09	949	26.52	A_u	C_1 C1–C2 + O1–C4 out-of-phase stretch
						949	0.00	A_g	C_1 C1–C2 + O1–C4 out-of-phase stretch
						950	25.87	A_u	C_s C1–C2 + O1–C4 out-of-phase stretch
						951	0.00	A_g	C_s C1–C2 + O1–C4 out-of-phase stretch
1026	1022	1020	1020	1056	16.39	1005	0.00	A_g	C_s C1 methyl rock
						1006	62.24	A_u	C_s C1 methyl rock
						1011	46.34	A_u	C_1 C1 methyl rock
						1014	0.00	A_g	C_1 C1 methyl rock
1090	1085	1089	1091	1133	0.19	1066	5.03	A_u	C_s C1 methyl rock
						1068	0.00	A_g	C_s C1 methyl rock
						1071	63.97	A_u	C_1 C1 methyl rock
						1072	0.00	A_g	C_1 C1 methyl rock
				1137	9.90	1075	61.88	A_u	C_s C1–C2 + O1–C4 in-phase stretch
						1077	0.00	A_g	C_1 C1–C2 + O1–C4 in-phase stretch
						1078	27.42	A_u	C_1 C1–C2 + O1–C4 in-phase stretch

						1079	0.00	A_g	C_s C1–C2 + O1–C4 in-phase stretch
				1205	0.89	1131	1.42	A_u	C_1 C4 methyl rock
						1133	0.00	A_g	C_1 C4 methyl rock
			1166			1144	0.00	A_g	C_s C4 methyl rock
						1145	19.50	A_u	C_s C4 methyl rock
		1162		1249	270.53	1151	586.35	A_u	C2–C3 + C3–O1 out-of-phase stretch
						1153	0.00	A_g	C2–C3 + C3–O1 out-of-phase stretch
1175	1174	1175				1156	475.15	A_u	C2–C3 + C3–O1 out-of-phase stretch
						1163	0.00	A_g	C2–C3 + C3–O1 out-of-phase stretch
			1197	1227	101.73	1169	0.00	A_g	C_s C4 Methyl rock
						1171	294.22	A_u	C_s C4 Methyl rock
1200	1199	1198				1173	306.76	A_u	C_1 C4 Methyl rock
						1179	0.00	A_g	C_1 C4 Methyl rock
						1237	2.72	A_u	C_s Methylene twist
			1258	1308	0.02	1240	0.00	A_g	C_s Methylene twist
1285	1276	1261				1242	13.46	A_u	C_1 Methylene twist
						1243	0.00	A_g	C_1 Methylene twist
			1330	1415	96.41	1324	0.00	A_g	C_s Methylene wag
1357	1356	1357				1325	135.94	A_u	C_s Methylene wag
						1329	146.84	A_u	C_1 Methylene wag
						1331	0.00	A_g	C_1 Methylene wag
			1373	1457	4.67	1356	0.00	A_g	C_s C1 Methyl sym def
		1383				1360	56.18	A_u	C_s C1 Methyl sym def
						1366	55.80	A_u	C_1 C1 Methyl sym def
						1366	0.00	A_g	C_1 C1 Methyl sym def
		1417		1504	13.00	1393	124.53	A_u	C_s Methylene scissors
						1393	0.00	A_g	C_s Methylene scissors
						1404	0.00	A_g	C_1 Methylene scissors
1442	1436	1434				1405	69.29	A_u	C_1 Methylene scissors
			1423	1512	12.53	1410	57.82	A_u	C_1 C4 Methyl sym def
						1410	0.00	A_g	C_1 C4 Methyl sym def
		1444				1420	72.37	A_u	C_s C4 Methyl sym def

						1424	0.00	A_g	C_s C4 Methyl sym def
						1434	0.00	A_g	C_1 C4 Methyl asym def
1467	1463	1456		1529	9.00	1435	50.02	A_u	C4 Methyl asym def
						1436	12.16	A_u	C_s C4 Methyl asym def
				1536	9.55	1439	0.00	A_g	C_s C1 Methyl asym def
						1440	0.00	A_g	C1 Methyl asym def
			1456	1540	17.70	1441	47.80	A_u	C_1 C4 Methyl asym def
						1443	0.00	A_g	C_1 C4 Methyl asym def
						1445	8.65	A_u	Methyl asym def
		1469		1544	8.53	1447	51.86	A_u	C_s C4 Methyl asym def
						1450	26.88	A_u	Methyl asym def
						1450	0.00	A_g	Methyl asym def
						1452	0.00	A_g	Methyl asym def
				1540	17.70	1453	0.00	A_g	C_s C4 Methyl asym def
						1456	11.65	A_u	C_s C1 Methyl asym def
						1461	30.01	A_u	C_1 C1 Methyl asym def
						1464	0.00	A_g	C_1 C1 Methyl asym def
1764	1737	1728		1819	172.87	1691	865.03	A_u	C_1 C=O stretch
						1694	0.00	A_g	C_1 C=O stretch
						1703	740.61	A_u	C_s C=O stretch
						1710	0.00	A_g	C_s C=O stretch

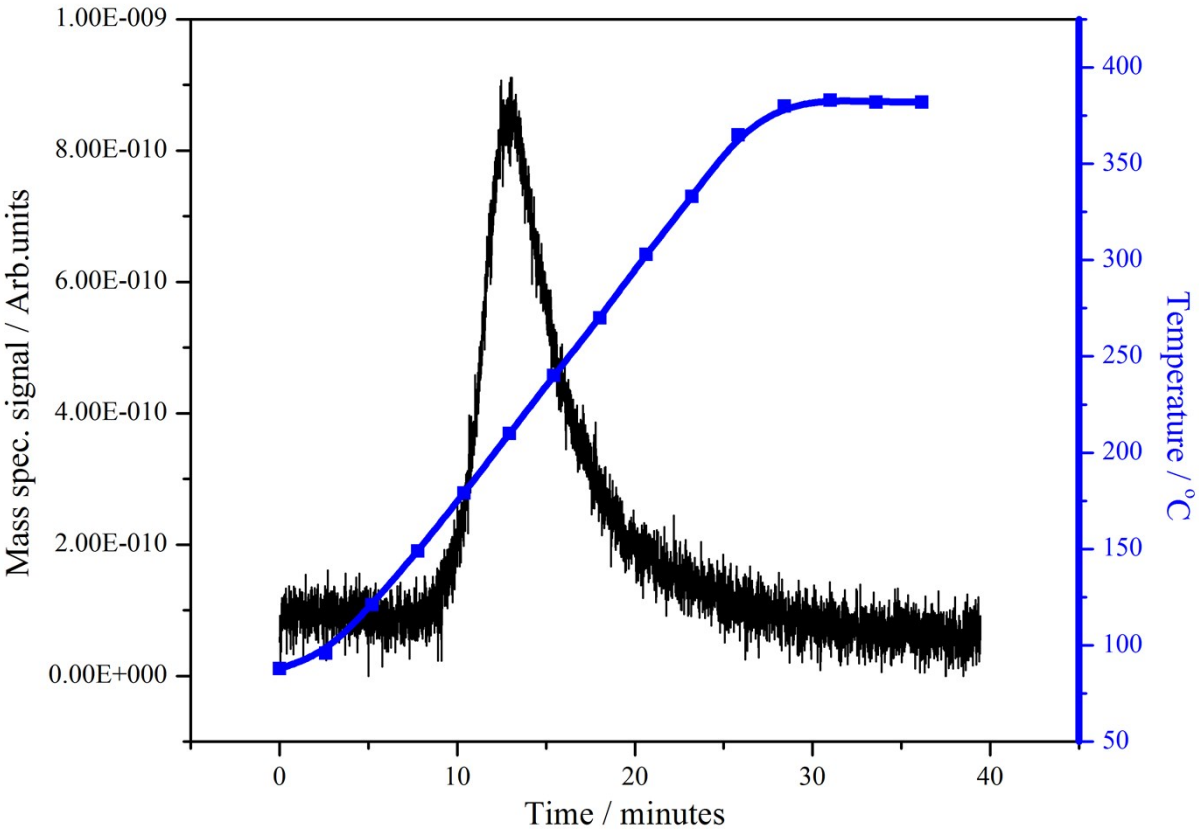

Figure S2: Temperature programmed desorption of methyl propanoate on silica.