Supporting Information for

The vibrational CD spectra of propylene oxide in liquid xenon: A proof-of-principle CryoVCD study that challenges theory

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Content:

1. Comparison of experimental spectra

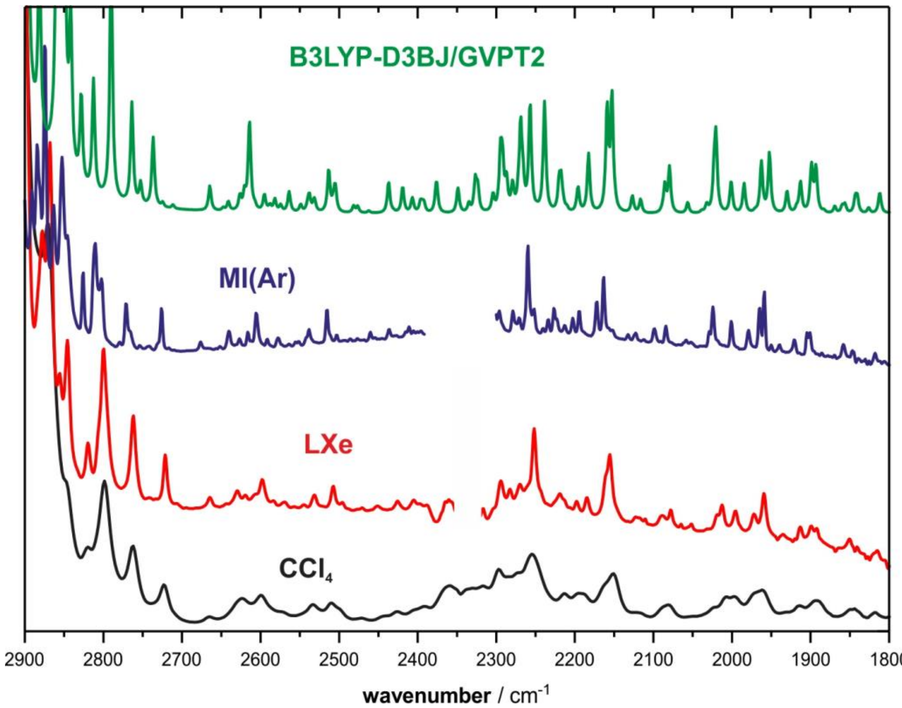

Figure S1. Comparison of the spectral range 2900-1800 cm^{-1} of PO in the different environments.

2. Additional computational data

Table S1. Mode assignments for the GVPT2 calculation of PO at B3LYP-D3BJ/6-311++G(3df,3pd)

ν_{anharm} / cm^{-1}	D	R	Assignment
198.9	7.13	3.21	1(1)
369.0	47.56	-13.52	2(1)
390.4	78.04	-8.96	1(2)
412.5	0.47	-0.15	3(1)
568.6	0.03	0.02	2(1)-1(1)
608.9	0.15	0.01	3(1)-1(1)
738.4	0.31	0.05	2(2)
754.6	42.64	12.89	+ 97.7% 4(1) + 2.3% 3(1)-2(1)
784.4	1.18	0.11	+ 97.7% 3(1)-2(1) + 2.3% 4(1)
824.5	206.78	3.48	5(1)
826.4	0.84	0.29	3(2)
893.6	14.47	26.95	6(1)
952.7	60.52	-34.92	7(1)
956.2	1.74	-1.37	4(1)-1(1)
1018.9	26.24	4.48	+ 98.4% 8(1) + 1.6% 9(1)
1022.6	0.01	-0.02	5(1)-1(1)
1094.8	0.06	-0.14	6(1)-1(1)
1109.9	29.89	-7.69	+ 98.4% 9(1) + 1.6% 8(1)
1123.7	0.30	-0.19	4(1)-2(1)
1131.4	10.34	7.72	10(1)
1141.6	8.65	-11.27	11(1)
1153.1	1.43	-0.59	7(1)-1(1)
1165.5	2.24	0.55	12(1)
1166.5	0.47	-0.17	4(1)-3(1)
1192.7	0.58	-0.31	5(1)-2(1)
1218.7	0.46	-0.44	8(1)-1(1)
1236.4	0.11	-0.18	5(1)-3(1)
1263.9	0.03	0.01	6(1)-2(1)
1269.1	22.94	-8.88	13(1)
1306.4	0.16	0.02	9(1)-1(1)
1307.3	0.54	-0.51	6(1)-3(1)
1321.5	0.10	-0.02	7(1)-2(1)
1330.2	0.00	0.01	10(1)-1(1)
1338.3	0.03	0.04	11(1)-1(1)
1364.0	0.20	-0.12	12(1)-1(1)
1364.6	0.88	-0.07	7(1)-3(1)
1374.6	8.32	2.12	14(1)
1389.1	0.68	0.04	8(1)-2(1)
1402.1	57.56	13.12	15(1)
1431.8	2.41	0.63	8(1)-3(1)
1444.1	13.78	1.78	16(1)
1457.1	14.09	-1.48	+ 97.8% 17(1) + 2.2% 9(1)-2(1)
1469.3	0.74	-0.02	13(1)-1(1)
1477.6	1.29	0.31	+ 97.8% 9(1)-2(1) + 2.2% 17(1)
1484.6	7.43	2.79	+ 85.4% 18(1) + 11.8% 4(2) + 2.9% 10(1)-2(1)
1500.9	0.20	0.09	+ 96.3% 10(1)-2(1) + 2.2% 4(2) + 1.6% 18(1)
1511.5	0.43	0.04	11(1)-2(1)
1511.7	6.26	2.51	+ 86.0% 4(2) + 13.1% 18(1)
1521.5	0.12	0.03	9(1)-3(1)
1534.8	0.28	-0.07	12(1)-2(1)
1544.0	0.06	0.01	10(1)-3(1)
1554.1	0.15	0.00	11(1)-3(1)
1573.9	0.02	0.00	14(1)-1(1)
1577.6	1.73	0.06	5(1)-4(1)
1578.2	0.01	0.00	12(1)-3(1)
1600.4	0.08	0.03	15(1)-1(1)
1637.9	0.02	0.04	13(1)-2(1)
1643.9	0.40	0.13	16(1)-1(1)
1647.1	1.22	0.36	5(2)
1648.5	0.33	-0.27	6(1)-4(1)
1655.0	0.63	-0.14	17(1)-1(1)
1681.0	0.04	0.04	13(1)-3(1)
1686.9	0.03	0.01	18(1)-1(1)
1703.8	1.34	0.03	7(1)-4(1)
1718.4	0.04	-0.01	6(1)-5(1)
1743.1	0.02	0.02	14(1)-2(1)
1770.4	0.12	-0.05	15(1)-2(1)
1774.8	0.13	-0.03	8(1)-4(1)
1776.3	0.21	0.07	7(1)-5(1)
1786.8	0.05	-0.05	6(2)
1787.5	0.12	-0.01	14(1)-3(1)

Table S2. Harmonic frequencies, dipole and rotational strength calculated using different functionals.

	APF			APFD			B3LYP			B3LYP-D3BJ			CAM-B3LYP			MN15			PBE0			PBE0-D3BJ		
Mode	**Freq**	**D**	**R**	**Freq**	**D**	**R**	**Freq**	**D**	**R**	**Freq**	**D**	**R**	**Freq**	**D**	**R**	**Freq**	**D**	**R**	**Freq**	**D**	**R**	**Freq**	**D**	**R**
1	207.6	6.7	3.2	206.2	6.7	3.4	206.2	7.5	3.5	206.6	7.5	3.6	207.5	7.8	3.5	210.0	7.7	4.1	208.3	6.6	3.3	208.5	6.6	3.3
2	368.4	36.7	-11.1	370.8	44.7	-13.3	367.7	42.7	-12.6	368.7	43.4	-13.0	373.3	42.7	-13.0	365.8	33.3	-12.5	369.1	36.1	-11.1	369.5	36.4	-11.3
3	409.0	45.3	-5.4	410.9	37.3	-3.6	410.6	42.6	-4.8	412.0	41.7	-4.5	415.2	45.0	-5.2	399.9	53.1	-5.8	409.7	45.7	-5.5	410.2	45.3	-5.4
4	800.1	32.1	10.8	797.3	31.6	11.8	772.9	37.3	12.3	773.9	37.8	12.5	800.9	34.3	10.5	812.9	31.4	6.9	805.0	31.9	10.4	805.5	31.9	10.4
5	873.9	175.9	0.2	872.1	187.2	3.8	844.2	206.4	4.1	845.8	206.8	3.9	873.9	192.3	4.6	888.3	131.5	-12.2	879.8	169.8	-2.1	880.3	169.6	-2.4
6	907.2	14.9	27.6	912.5	11.1	25.2	907.5	11.5	25.2	908.2	11.6	25.2	918.9	10.9	24.4	902.0	35.3	39.6	908.0	17.8	29.8	908.4	18.3	30.2
7	996.1	54.8	-32.5	993.3	57.0	-34.5	973.6	62.7	-33.7	974.7	61.7	-33.7	1000.2	61.1	-32.3	1009.5	41.6	-28.9	1001.0	52.2	-32.7	1001.4	51.9	-32.8
8	1044.8	52.5	11.0	1039.2	46.2	8.6	1042.8	34.2	6.1	1043.1	34.0	6.0	1053.4	43.0	9.4	1039.8	58.3	14.1	1046.6	55.7	12.3	1046.7	55.6	12.3
9	1132.6	28.5	-6.4	1123.7	31.1	-3.7	1130.2	24.0	-6.9	1130.5	24.0	-6.9	1143.5	28.4	-6.0	1128.0	27.5	-7.1	1134.3	29.1	-6.2	1134.4	29.1	-6.2
10	1159.9	1.5	3.3	1158.5	0.1	0.1	1157.9	7.3	4.9	1157.7	6.5	5.3	1175.8	7.7	2.9	1163.5	9.3	1.0	1161.9	1.2	2.6	1161.6	1.2	2.6
11	1168.3	15.8	-11.1	1165.2	18.9	-10.9	1166.7	11.2	-12.5	1167.5	12.2	-13.1	1181.0	10.8	-12.2	1164.9	9.3	-9.2	1170.4	16.0	-10.7	1170.7	16.1	-11.0
12	1187.6	5.9	0.6	1188.3	4.5	1.9	1188.0	3.4	0.4	1188.7	3.2	0.7	1202.8	6.5	-1.3	1185.4	13.0	-1.8	1189.5	6.5	0.7	1189.8	6.4	0.9
13	1302.1	19.0	-14.0	1294.6	16.0	-13.7	1293.9	20.6	-10.4	1294.5	20.1	-10.5	1310.5	20.1	-12.4	1294.8	21.8	-14.5	1304.5	18.9	-14.5	1304.7	18.7	-14.6
14	1395.4	11.2	2.2	1396.5	10.6	1.7	1406.7	8.9	2.4	1406.7	9.1	2.4	1415.7	10.8	2.6	1388.9	11.8	2.3	1395.3	11.8	2.3	1395.3	12.0	2.3
15	1442.2	56.6	11.3	1439.2	56.3	12.6	1437.6	60.2	14.3	1438.3	60.0	14.2	1457.8	55.2	12.9	1440.8	53.2	10.2	1444.7	55.0	10.5	1444.9	54.7	10.4
16	1474.2	17.1	1.7	1474.6	16.2	1.9	1483.0	14.9	1.7	1483.2	14.9	1.8	1489.5	17.5	2.2	1466.9	14.9	1.5	1474.0	17.5	1.7	1474.1	17.5	1.7
17	1488.9	18.2	-0.2	1490.1	18.4	-0.4	1496.8	16.2	-1.4	1497.1	16.3	-1.4	1504.0	18.5	-1.2	1481.9	17.1	0.0	1489.0	18.5	0.0	1489.2	18.5	0.1
18	1533.4	25.4	7.3	1532.6	25.6	7.6	1529.5	15.3	5.5	1529.9	15.6	5.6	1548.1	24.1	7.2	1535.3	31.8	8.0	1536.5	27.8	7.7	1536.7	28.0	7.8
19	3044.6	21.0	1.3	3044.4	20.9	1.3	3028.5	23.4	1.4	3029.9	23.4	1.4	3055.3	18.6	1.2	3073.6	22.5	1.2	3049.2	20.3	1.3	3049.8	20.2	1.3
20	3094.8	35.7	-0.9	3082.9	36.4	-0.9	3082.2	35.2	-0.1	3083.8	35.2	0.4	3109.7	30.5	0.5	3139.2	37.6	-1.1	3099.8	34.9	-0.8	3100.4	34.8	-0.7
21	3108.7	15.3	-4.6	3097.2	18.9	-3.1	3087.2	25.5	-3.0	3089.3	25.3	-3.0	3120.1	20.6	-4.1	3149.7	27.4	-5.2	3114.0	15.1	-4.7	3114.9	14.8	-4.8
22	3115.2	20.4	-2.8	3115.3	20.5	-3.7	3091.6	9.8	-5.5	3093.8	8.9	-5.9	3122.6	7.6	-4.5	3154.3	7.9	1.0	3121.3	19.7	-2.6	3122.1	19.7	-2.7
23	3136.0	35.4	6.2	3134.0	30.3	6.3	3112.9	47.0	6.4	3114.6	47.7	6.3	3141.9	40.2	5.9	3180.8	49.9	3.3	3141.3	34.6	5.9	3141.9	34.9	5.9
24	3184.0	31.7	-5.0	3171.5	33.1	-5.7	3168.3	33.6	-5.3	3170.4	33.6	-5.3	3197.7	26.7	-4.1	3234.4	35.8	-4.4	3189.5	30.9	-4.9	3190.4	30.9	-4.8

Table S3. Anharmonic frequencies computed at various DFT levels. The modes given in bold face are the normal modes.

APF	APFD	B3LYP	B3LYP-D3BJ	CAM-B3LYP	MN15	PBE0	PBE0-D3BJ
199.1	**198.5**	**198.2**	**198.9**	**198.8**	**193.1**	**201.1**	**201.2**
368.9	**372.5**	**368.5**	**369.0**	373.5	**366.7**	**369.9**	**370.2**
388.2	388.3	387.9	390.4	**373.9**	371.6	392.7	393.2
411.2	**414.9**	**412.0**	**412.5**	**431.6**	**402.6**	**412.3**	**412.7**
568.3	571.3	567.4	568.6	573.0	559.0	571.5	571.9
611.4	612.4	609.0	608.9	660.0	596.1	614.8	615.4
738.5	745.5	737.5	738.4	748.2	733.9	740.6	741.0
781.5	**782.2**	**753.8**	**754.6**	**785.9**	771.0	783.8	784.4
783.8	790.2	783.5	784.4	806.0	**798.0**	**788.9**	**789.3**
824.3	832.8	**823.0**	**824.5**	**853.6**	806.4	826.5	827.3
853.2	**855.0**	825.5	826.4	864.8	**869.5**	**859.3**	**859.8**
894.1	**897.5**	**893.0**	**893.6**	**906.1**	**889.6**	**895.1**	**895.4**
973.2	**975.5**	**951.6**	**952.7**	**978.3**	**985.5**	**978.2**	**978.5**
984.7	982.8	954.6	956.2	986.6	992.5	991.7	992.4
1021.2	**1035.4**	**1018.6**	**1018.9**	**1030.5**	**1017.0**	**1023.2**	**1023.3**
1051.2	1052.4	1020.3	1022.6	1051.4	1061.4	1059.2	1059.8
1095.6	1098.4	1093.4	1094.8	1107.2	1085.4	1098.8	1099.2
1113.1	**1125.5**	**1109.7**	**1109.9**	**1124.7**	**1109.3**	**1115.2**	**1115.2**
1134.7	**1147.4**	1122.3	1123.7	**1142.3**	**1124.9**	**1136.8**	**1136.6**
1138.2	**1149.8**	**1125.0**	**1131.4**	1160.2	**1153.2**	**1140.7**	**1141.0**
1152.8	1155.8	**1147.4**	**1141.6**	**1165.2**	**1160.6**	1158.9	1159.6
1168.5	**1165.7**	1151.2	1153.1	**1177.7**	1164.1	**1170.2**	**1170.5**
1174.1	1176.4	**1164.8**	**1165.5**	1180.4	1179.5	1181.1	1181.6
1194.7	1193.2	1165.4	1166.5	1218.1	1200.9	1200.6	1201.5
1220.8	1226.7	1190.7	1192.7	1226.9	1210.8	1224.8	1225.1
1221.6	1233.3	1217.6	1218.7	1229.9	1236.2	1228.8	1229.4
1263.8	1269.5	1234.4	1236.4	1281.3	1257.6	1266.4	1266.9
1264.3	1271.2	1262.8	1263.9	1284.5	**1270.3**	1270.9	1271.9
1277.7	**1306.0**	**1268.3**	**1269.1**	**1287.2**	1272.0	**1280.1**	**1280.4**
1308.2	1314.1	1305.4	1306.4	1321.5	1294.6	1310.7	1311.3
1309.9	1328.9	1306.3	1307.3	1339.5	1300.8	1314.1	1314.4
1334.1	1340.5	1319.9	1321.5	1348.8	1330.2	1338.2	1338.2
1340.4	1346.4	1329.3	1330.2	1351.8	1332.3	1344.4	1344.9
1341.6	1347.5	1336.9	1338.3	1354.4	1351.8	1347.6	1348.2
1360.8	1362.4	1362.5	1364.0	1373.9	1352.1	**1364.7**	**1364.6**
1364.8	**1362.5**	1363.0	1364.6	**1385.1**	**1357.9**	1365.5	1365.9
1383.8	1389.8	**1374.4**	**1374.6**	1405.1	1384.8	1389.8	1390.6
1390.9	1407.4	1388.5	1389.1	1409.3	1387.5	1393.9	1394.2
1407.0	**1413.5**	**1401.4**	**1402.1**	**1422.7**	**1404.7**	**1409.6**	**1409.8**
1432.7	**1437.1**	1431.1	1431.8	**1452.8**	1420.5	1435.7	1436.2
1436.9	1450.0	**1443.7**	**1444.1**	1462.3	**1426.2**	**1437.0**	**1437.1**
1451.7	**1453.6**	**1456.7**	**1457.1**	**1466.5**	**1444.1**	**1452.4**	**1452.6**
1478.0	**1494.3**	1467.8	1469.3	1487.3	1466.6	1482.4	1482.9
1480.8	1504.6	1477.0	1477.6	1497.4	1474.9	1483.8	1484.1
1489.9	1506.0	**1484.1**	**1484.6**	**1505.7**	**1494.2**[a)]	**1492.9**	**1493.2**
1504.7	1515.2	1500.3	1500.9	1524.7	1503.6	1507.8	1507.9
1512.4	1520.6	1510.1	1511.5	1532.1	1505.3	1515.1	1515.6
1523.6	1539.0	1510.6	1511.7	1551.8	1511.5	1526.8	1527.3
1532.7	1547.6	1520.9	1521.5	1555.6	1527.4	1535.9	1536.4
1546.2	1559.3	1533.6	1534.8	1570.6	1540.8	1549.4	1549.6
1554.2	1561.7	1543.5	1544.0	1582.1	1542.8	1557.1	1557.9
1564.8	1562.8	1553.0	1554.1	1584.5	1550.6	1566.3	1566.4
1566.2	1563.3	1573.0	1573.9	1588.7	1563.0	1576.2	1577.1
1574.5	1581.2	1575.3	1577.6	1609.1	1594.3	1577.8	1578.5
1605.9	1611.9	1576.9	1578.2	1621.1	1598.6	1610.5	1610.9

[a)] Not in Fermi resonance!