Supplementary information

Structural Studies of 1,1-Dimethyl-2-Oxy-1-Silacyclohexane by Means of Matrix Isolation Infrared Absorption Spectroscopy

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Table S1. Infrared (Ar matrix, gas phase, liquid) Raman (liquid) and DFT calculated bands in cm^{-1} (intensities (normalized a.u. for Ar matrix and km/mol for DFT) in parenthesis) of 1,1-dimethyl-2-oxy-1-silacyclohexane(DOS) (*chair*) conformer

Raman		Infrared				Mode description
	gas	liquid	Ar	Ar matrix	Calculated	
	3242	3213 br.				
	2974.0		2973.5	2973.5 (0.16) br.	3102.5 (12.2)	CH_3 as. str.
	2969.1		2970.3	2970.3 (0.14)	3095.4 (19.1)	CH_3 as. str.
2960.5	2965.5	2956	2966.5	2966.5 (0.11) br	3093.7 (10.1)	CH_3 as. str.
			2962.0	2962.0 (0.09)	3089.2 (9.6)	CH_3 as. str.
	2943 br. sh.		2944.6	2944.6 (0.20)	3059.7 (68.5)	CH_2 as. str.
			2938.0	2938.0 (0.10)	3056.9 (7.7)	CH_2 as. str.
	2937.4					
2929.0						
	2933.4					
	2928.9					
	2926.1					
2902.0	2924 br.	2919	2934.2	2934.2 (0.24)	3054.0 (66.2)	CH_2 as. str.
				2928.7 (0.20)		
				2916.6 (0.13)	3041.5 (54.3)	CH_2 as. str.
2888.0		2884	2910.1	2910.1 (0.08)		
			2880.5	2880.5 (0.06)	3025.7 (6.0)	CH_3 sym. str.
			2883.0	2883.0 (0.05) br. sh.	3021.6 (6.0)	CH_3 sym. str.

			2873.7	2873.7 (0.10)	3013.4 (15.6)	CH_2 sym. str.
			2871.5	2871.5 (0.09)	3011.5 (15.5)	CH_2 sym. str.
	2893.1					
	2865.1 sh.					
2856.6	2859.5	2851	2864.2	2864.2 (0.17)	3002.3 (24.7)	CH_2 sym. str.
				2856.8 (0.21)	2974.0 (51.4)	CH_2 sym. str.
				2847.2 (0.06)		
2728.8	2733	2726,4	2733 br.w.	2733 ()		
		1514.0				
1478.3		1476.0	1478.5	1478.5 (0.03)	1516.7 (1.8)	CH_2 b.
1459.5		1454.3	1459.5	1459.5 (0.04)	1500.4 (3.7)	CH_2 b.
1442.7			1442.5	1442.5 (0.06)	1480.3 (7.1)	CH_2 b.
	1442	1440				
				1430.3 (0.03)	1469.5 (6.1)	CH_2 b. (CH_3 group)
				1419.7 (0.02)	1463.1 (1.3)	CH_2 b. (CH_3 group)
				1417.4 (0.01)	1459.5 (3.3)	CH_2 b.
				1409.3 (0.01)	1455.6 (1.8)	CH_2 b.
				1403.2 (0.02)	1451.6 (2.0)	CH_2 b.
	1412.2	1403				
	1385.4 R					
	1378.1 Q	1376.6	1378.6	1378.6 (0.04)	1408.5 (6.7)	CH_2 w.

	1372.6 P					
				1359.0 (0.01)		
1350.0		1346.5	1348.2	1348.2 (0.01)	1379.9 (2.0)	CH_2 w. + CH_2 tw.
	1339.8 R					
	1333.9 Q	1329.5	1333.3	1333.3 (0.03)	1367.7 (3.7)	CH_2 w. + CH_2 tw.
	1327.8 R					
1285.8	1286.0	1285.5	1287.1	1287.1 (0.05)	1315.6 (3.2)	CH_2 w. + CH_2 tw.
				1279.8 (0.02)		
				1274.3 (0.03)		
	1263.9		1263.2	1263.2 (0.17)	1295.8 (30.0)	CH_3 sym. b.
1259.4	1259.7	1260.0	1255.9	1255.9 (0.39)	1291.7 (38.8)	CH_3 sym. b.
1244.2	1255.2	1248.6	1250.1	1250.1 (0.55)	1288.4 (16.4)	CH_3 sym. b. + CH_2 tw.
	1247 br. sh.		1244.9	1244.9 (0.02)	1270.4 (1.1)	CH_2 r. + CH_2 tw.
1201 br.			1197.5	1197.5 (0.01) br		
	1178.1 R					
1171.5	1173.5 Q	1168.3	1172.8	1172.8 (0.22)	1193.6 (21.7)	CH_2 r. + C-O str. + CH_2 w.
	1167.6 P					
				1169.7		
1163.9						
	1148.0					
1138.2	1143.3	1134.8	1140.0	1140.0 (0.53)	1162.0 (67.3)	C-C str.
	1140.0					
1108.1						

1100.2						
			1090.5	1090.5 (0.24)	1093.3 (106.5)	C-O str.
	1092.9 R					
1084.3	1088.6 Q	1078.1	1085.1	1085.1 (0.38)		
1069.5	1084.5 P					
	1056.2 R					
1049.8	1050.5 Q	1046.3	1050.9	1050.9 (0.22)	1060.4 (23.3)	C-C-C as. str.
	1045.9 P					
	1022.4 R					
1015.2	1016.3 Q	1013.3	1015.5	1015.5 (0.25)	1035.7 (27.3)	CH_2 w. + CH_2 tw.
	1011.5 P					
994.9						
982.3						
966.9						
	948.9 sh.					
940.6	942.5	939.2	942.1	942.1 (0.10)	945.1 25.3 ()	C-C, C-C, C-O str.
				939.5 (0.08)		
	927.3 R					
919.2	922.1 Q	915.8	922.0	922.0 (0.74)	933.8 (85.0)	Ring d.
	917.7 P					
900						
885.3	885.1	882.6	884.6	884.6 (0.10)	900.0 (13.1)	Ring d.
860.0						
	846.0					
839.9	841.9	832.7	841.5	841.5 (0.73)	863.7 (84.2)	Si-C str. +CH_3 r.
818.8						
					855.1 (86.8)	C-O str. +CH_3 r.
				817.2 (0.03)	819.9 (3.8)	C-C-C sym. str.
	797.5					
790.3	790.7	783.4	788.6	788.6 (1.00)	799.0 (85.3)	Si-C-H b.
	784 br.					
				784.8 (0.10)		

				779.5 (0.03)		
768 vw.						
754.7 sh.						
740.0	736.5	741	741.0	741.0 (0.09)	758.7 (8.2)	CH_3 r.
728.0	731.5	726.3	730.0	730.0 (0.10)	729.7 (21.3)	C-Si-O sym. str.
768 vw.						
				728.2 (0.08)		
698.2	696 br.	696.5	696.6	696.6 (0.08)	707.2 (7.2)	CH_2 r.
			694.3	694.3 (0.05)		
			681.0	681.0 (0.03)	687.4 (7.2)	CH_3 r.
	683.3					
679.0	676.4	674.7	674.8	674.8 (0.12)	674.5 (22.8)	C-Si str. + CH_3 r.
	668.3					
652.0			662.2	662.2 (0.02)		
		613.7				
601.5		600.4				
549.6		551				
					591.1 (1.0)	SiC_3 sym. str.
517.2		515.8	512.7	512.7 (0.05)	517.0 (4.3)	O-C-C b.
493.5						
482.1						
384.4					386.9 (2.3)	C-C-C + Si-O-C b.
353.3					353.1 (9.1)	C-C-C + C-Si-O b.
279.3					335.5 (4.7)	Ring d.
242.1					269.3 (9.1)	Ring d.
209.6					236.3 (0.3)	Ring d.
					202.6 (0.5)	Ring d.
144.7					193.8 (0.5)	H_3C-Si-CH_3 b.
					151.6 (0)	CH_3 t. sym.
					138.6 (0)	CH_3 t. as.
100.1					128.5 (0.6)	H_3C-Si-CH_3 tw.
					86.1 (0.9)	H_3C-Si-CH_3 r.

br. - band is broad with full width at half maximum more than 10 cm^{-1}

sh. - shoulder, band is overlapped with neighboring stronger band.

str. – stretching vibration

b. - bending vibration

t. - torsion vibration

tw. - twisting vibration

d. - deformation vibration

r. – rocking vibration

sym.- symmetric vibration

as. – asymmetric vibration

w. – waging vibration