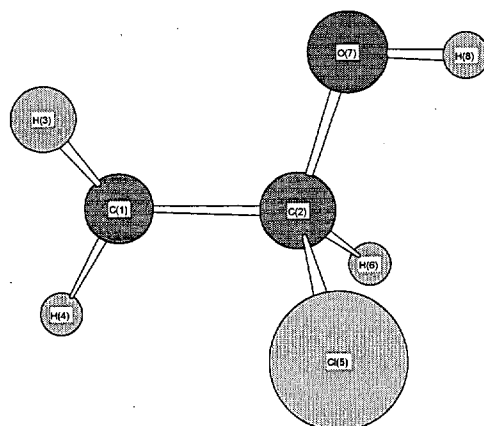
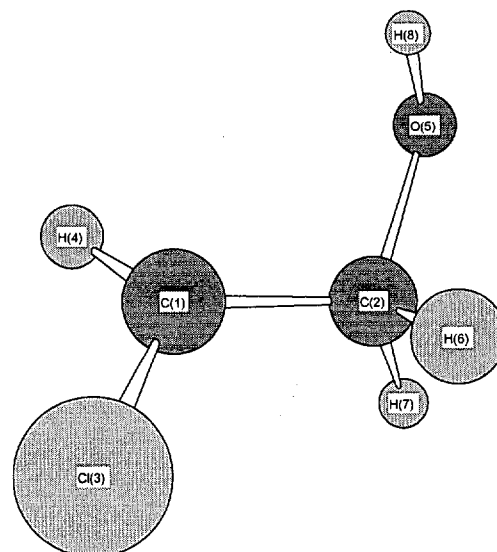


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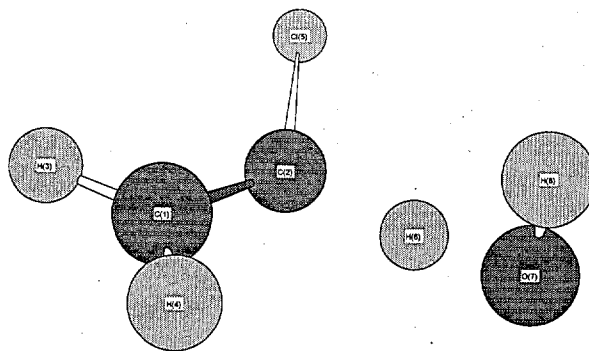
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Bond Length (Å)		Bond Angle (°)		Dihedral Angle (°)	
C2-C1	1.474				
H3-C1	1.083	H3-C1-C2	119.3		
H4-C1	1.081	H4-C1-C2	119.9	H4-C1-C2-H3	-162.0
Cl5-C2	1.848	Cl5-C2-C1	107.9	Cl5-C2-C1-H3	88.9
H6-C2	1.089	H6-C2-C1	112.8	H6-C2-C1-H3	-156.7
O7-C2	1.388	O7-C2-C1	114.6	O7-C2-C1-H3	-34.5
H8-O7	0.975	H8-O7-C2	108.1	H8-O7-C2-C1	56.0

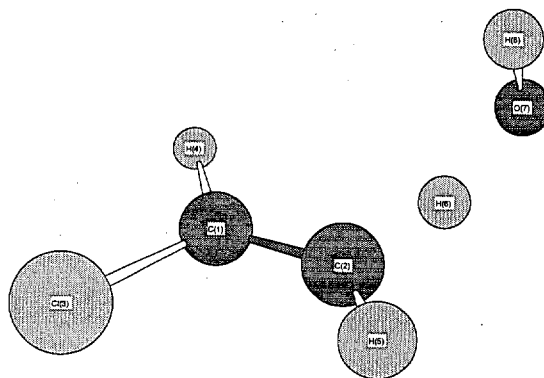
Figure 1S (a) – Vinyl Chloride – OH Adduct (α site)

Bond Length (Å)		Bond Angle (°)		Dihedral Angle (°)	
C2-C1	1.491				
Cl3-C1	1.712	Cl3-C1-C2	118.6		
H4-C1	1.083	H4-C1-C2	120.4	H4-C1-C2-Cl3	-153.0
O5-C2	1.422	O5-C2-C1	110.7	O5-C2-C1-Cl3	-167.0
H6-C2	1.099	H6-C2-C1	109.9	H6-C2-C1-O5	-42.3
H7-C2	1.097	H7-C2-C1	111.2	H7-C2-C1-H6	76.2
H8-O5	0.972	H8-O5-C2	107.0	H8-O5-C2-C1	64.2

Figure 1S (b) – Vinyl Chloride – OH Adduct (β site)

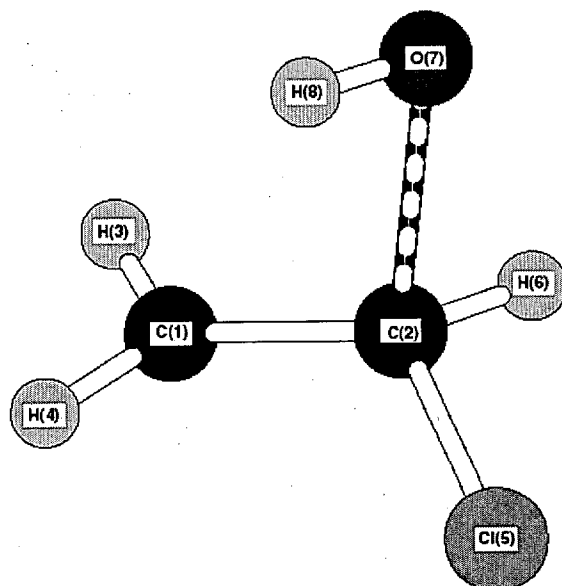


Bond Length (Å)		Bond Angle (°)		Dihedral Angle (°)	
C1-C2	1.290				
H3-C1	1.085	H3-C1-C2	122.2		
H4-C1	1.083	H4-C1-C2	119.4	H4-C1-C2-H3	179.5
C15-C2	1.709	C15-C2-C1	128.9	C15-C2-C1-H3	1.4
H6-C2	1.243	H6-C2-C1	118.7	H6-C2-C1-H3	-178.0
O7-H6	1.215	O7-H6-C2	160.0	O7-H6-C2-C1	-60.6
H8-O7	0.979	H8-O7-H6	101.1	H8-O7-H6-C2	-36.5

Figure 1S (c) – H abstraction TS (α site)

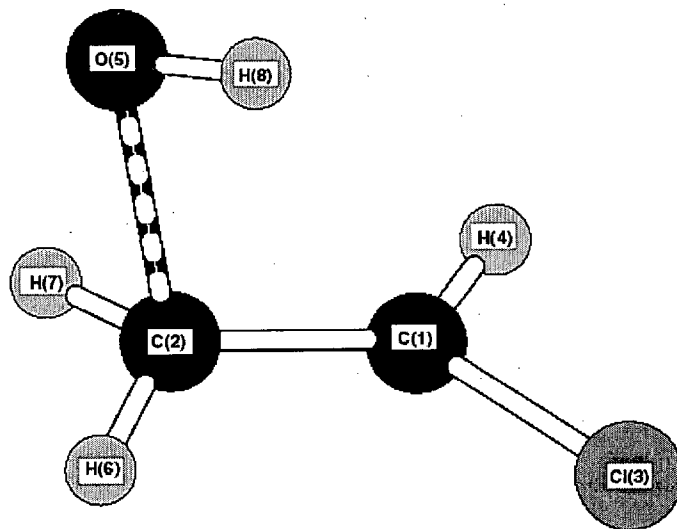
Bond Length (Å)		Bond Angle (°)		Dihedral Angle (°)	
C1-C2	1.287				
C13-C1	1.735	C13-C1-C2	123.7		
H4-C1	1.084	H4-C1-C2	123.2	H4-C1-C2-H3	-179.6
H5-C2	1.083	H5-C2-C1	129.8	H5-C2-C1-H3	-1.6
H6-C2	1.257	H6-C2-C1	115.2	H6-C2-C1-H5	179.7
O7-H6	1.197	O7-H6-C2	159.0	O7-H6-C2-C1	71.4
H8-O7	0.978	H8-O7-H6	101.5	H8-O7-H6-C2	20.7

Figure 1S (d) – H abstraction TS (β site)



Bond Length (Å)		Bond Angle (°)		Dihedral Angle (°)	
C2-C1	1.390	H3-C1-C2	119.2	H4-C1-C2-H3	-171.0
H3-C1	1.074	H4-C1-C2	121.3	Cl5-C2-C1-H3	-166.7
H4-C1	1.074	Cl5-C2-C1	117.6	H6-C2-C1-H3	-22.3
Cl5-C2	1.756	H6-C2-C1	121.8	O7-C2-C1-H3	85.5
H6-C2	1.070	O7-C2-C1	103.5	H8-O7-C2-C1	52.3
O7-C2	1.938	H8-O7-C2	92.3		
H8-O7	0.952				

Figure 1S (e) – OH addition TS (α site)



Bond Length (Å)		Bond Angle (°)		Dihedral Angle (°)	
C2-C1	1.387	Cl3-C1-C2	121.4	H4-C1-C2-Cl3	-169.8
Cl3-C1	1.733	H4-C1-C2	123.8	O5-C2-C1-Cl3	84.9
H4-C1	1.071	O5-C2-C1	106.3	H6-C2-C1-O5	-104.9
O5-C2	1.931	H6-C2-C1	119.2	H7-C2-C1-H6	-150.3
H6-C2	1.073	H7-C2-C1	117.4	H8-O5-C2-C1	-42.8
H7-C2	1.073	H8-O5-C2	99.5		
H8-O5	0.951				

Figure 1S (f) – OH addition TS (β site)