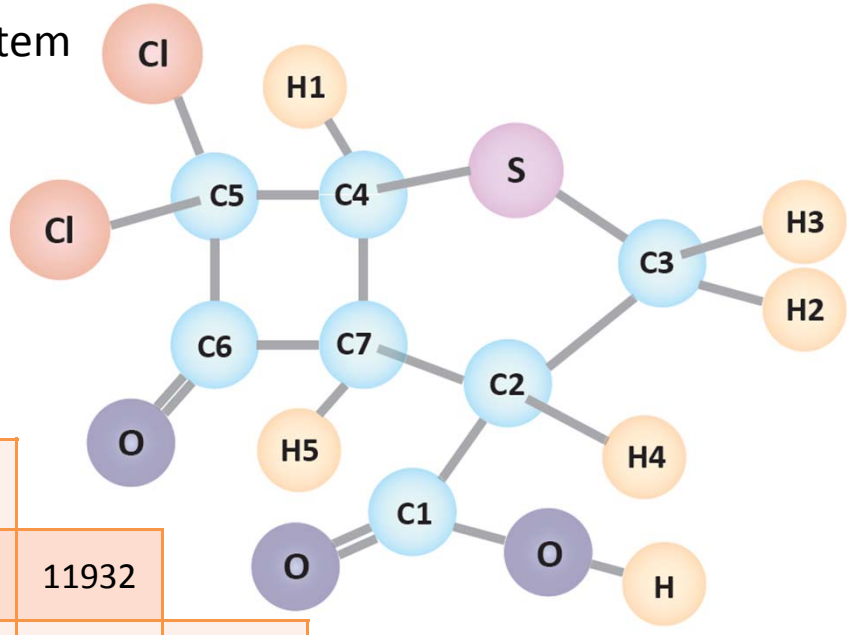
C-13 labeled 12-qubit system

$C_7H_6Cl_2SO_3$



	C1	C2	C3	C4	C5	C6	C7	H1	H2	H3	H4	H5
C1	30031											
C2	57.56	8787										
C3	-2.03	32.70	6248									
C4	-0.96	0.50	0	10334								
C5	-1.14	2.80	1.11	33.07	15746							
C6	5.54	-1.70	0	-3.53	-33.50	34382						
C7	0.97	37.48	0.94	-29.02	-21.75	34.57	11932					
H1	0	0	2.36	166.6	4.06	5.39	8.61	3310				
H2	4.41	1.86	146.6	2.37	0	0	0	0	2468			
H3	1.81	3.71	146.6	2.37	0	0	0	0.18	-12.41	2158		
H4	13.19	133.6	6.97	6.23	0	5.39	3.78	-0.68	1.28	6.00	2692	
H5	7.87	8.35	3.35	8.13	2.36	8.52	148.5	8.46	-1.06	-0.36	1.30	3649