	C1	C2	C3	C4	C5	C6	C7	H1	H2	Н3	Н4	H5	
C1	30020	C-13 labeled 12-qubit system											
C2	57.58	8779	Dichloro-cyclobutanone										
C3	-2.00	32.70	6245				CI	C ₅	$-C_4$	S		H ₃	
C4	0	0.30	0	10333							C_3	H_2	
C5	-1.25	2.62	1.11	33.16	15745				7	C ₂			
C6	5.54	-1.66	0	-3.53	33.16	34381			H ₅		H ₄		
C7	1.25	37.48	0.94	29.02	-21.75	34.57	11928		0	0	Н		
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				
Н3	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		
Н5	7.87	-8.35	3.35	8.13	2.36	8.52	148.5	8.46	-1.06	-0.36	1.30	3649	
T1	8.015	3.611	1.834	3.722	12.95	8.157	3.636	3.831	2.128	2.278	2.654	3.472	
T2	1.611	0.877	1.122	0.792	1.143	1.912	0.531	0.337	N/A	N/A	0.318	0.276	