	C1	C2	C3	C4	C5	C6	C7	H1	H2	Н3	Н4	Н5
C1	30031		C-13 labeled 12-qubit system Cl H1									
C2	57.56	8787	C ₇ H ₆ Cl ₂ SO ₃ Cl H ₃									
C3	-2.03	32.70	6248	,	0 2	3		5 4			C3	→ H3
C4	-0.96	0.50	0	10334				6 7		c2/		H2
C5	-1.14	2.80	1.11	33.07	15746		0				H 4	
C6	5.54	-1.70	0	-3.53	-33.50	34382		H5				
C7	0.97	37.48	0.94	-29.02	-21.75	34.57	11932	0=			ЭН	
H1								3310			711	
H2								0	2468			
Н3								0.18	-12.41	2158		
H4								-0.68	1.28	6.00	2692	
H5								8.46	-1.06	-0.36	1.30	3649