

Supplementary Information

Table S1. Observed frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of the parent 2-thiouracil.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'_T	F'	I''_T	F''	Obs / MHz	Obs-cal / MHz
1	1	1	0	0	0	2	1	1	1	4514.164	-0.001
						2	1	2	2	4514.164	-0.001
						2	1	0	0	4514.164	-0.002
						1	1	1	1	4514.829	-0.001
						1	1	2	2	4514.829	-0.001
						1	1	0	0	4514.829	-0.001
						2	3	2	2	4515.062	0.002
						1	2	1	1	4515.294	0.001
						1	2	2	2	4515.294	0.001
						0	1	1	1	4515.709	0.002
						0	1	2	2	4515.709	0.002
						0	1	0	0	4515.709	0.002
						2	2	1	1	4515.778	-0.002
						1	0	1	1	4516.014	0.001
						2	1	2	1	0	1
2	1	2	2	6433.870	-0.004						
2	1	0	1	6433.945	-0.005						
1	2	1	2	6434.382	-0.001						
2	0	2	1	6434.748	-0.001						
2	1	1	1	6434.884	0.002						
1	2	1	1	6434.892	0.006						
2	4	2	3	6434.982	-0.001						
1	1	1	0	6435.262	0.001						
0	2	2	1	6435.308	-0.001						
1	3	1	2	6435.430	0.001						
2	1	2	1	6435.561	-0.003						
2	3	2	2	6435.628	-0.001						
2	2	2	2	6436.114	-0.002						
2	2	0	1	6436.191	-0.001						
2	3	2	3	6436.383	-0.003						
1	1	1	1	6436.517	-0.003						
2	2	2	3	6436.872	-0.001						
3	0	3	2	1	2	2	2	2	2	4746.012	-0.003
						0	3	2	3	4746.038	-0.001
						1	3	1	3	4746.827	-0.004
						2	4	2	3	4747.376	-0.002
						2	3	2	2	4747.436	-0.003
						1	4	1	3	4747.664	-0.003
						2	5	2	4	4747.736	-0.002
						1	3	1	2	4747.876	-0.002

							0	3	0	2	4748.047	-0.00349
							2	2	2	1	4748.255	-0.00291
							2	1	2	0	4748.317	-0.00408
							2	2	0	2	4748.510	-0.00270
							2	4	2	4	4748.780	-0.00217
4	0	4	3	1	3		2	3	2	3	7212.280	-0.00803
							0	4	2	4	7212.387	-0.00540
							2	4	2	3	7213.869	-0.00703
							2	5	2	4	7213.915	-0.00608
							1	5	1	4	7214.130	-0.00726
							2	6	2	5	7214.237	-0.00732
							1	4	1	3	7214.342	-0.00619
							0	4	0	3	7214.414	-0.00787
							2	3	2	2	7214.436	-0.00677
							2	2	2	1	7214.583	-0.00587
							2	4	2	4	7214.693	-0.00699
							2	3	0	3	7215.135	-0.00664
							2	5	2	5	7215.494	-0.00727
3	1	3	2	0	2		0	3	2	3	8192.059	-0.00289
							1	3	1	3	8192.628	-0.00196
							1	3	1	2	8193.276	-0.00373
							0	3	0	2	8193.299	-0.00294
							2	5	2	4	8193.374	-0.00345
							1	4	1	3	8193.886	-0.00184
							1	2	1	1	8193.971	-0.00388
							2	4	2	3	8194.090	-0.00158
							2	3	2	2	8194.611	-0.00223
							2	3	2	3	8194.912	-0.00327
							2	4	2	4	8194.956	-0.00157
							1	2	1	2	8194.982	-0.00284

Table S2. Observed frequencies and residuals (in MHz) for the nuclear quadrupole coupling hyperfine components of the ^{34}S species in its natural abundance.

J'	K'_{-1}	K'_{+1}	J''	K''_{-1}	K''_{+1}	I'_T	F'	I''_T	F''	Obs / MHz	Obs-cal / MHz
1	1	1	0	0	0	2	1	1	1	4483.177	-0.001
						2	1	2	2	4483.177	-0.001
						2	1	0	0	4483.177	-0.002
						1	1	1	1	4483.836	-0.002
						1	1	2	2	4483.836	-0.002
						1	1	0	0	4483.836	-0.002
						2	3	2	2	4484.073	0.002
						1	2	1	1	4484.308	0.001
						1	2	2	2	4484.308	0.001
						2	2	1	1	4484.790	-0.000
						1	0	1	1	4485.028	0.001
2	1	2	1	0	1	2	4	2	3	6361.076	0.002
						0	2	2	1	6361.398	0.000

						1	3	1	2	6361.520	-0.002
						2	3	2	2	6361.720	-0.001
						2	2	0	1	6362.282	-0.001
						2	3	2	3	6362.478	0.004
						1	1	1	1	6362.606	-0.002
3	1	3	2	0	2	1	3	1	2	8083.396	0.003
						0	3	0	2	8083.416	-0.000
						2	5	2	4	8083.492	-0.001
						1	4	1	3	8084.010	0.001
						2	4	2	3	8084.213	-0.001
						2	3	2	2	8084.736	-0.002
