

Supporting Information

Infrared spectrum and theoretical calculations of a higher energy isomer of CO-SO₂ complex

Yun Liu, Zening Huang, Cheng Chen, and Chuanxi Duan*

College of Physical Science and Technology, Central China Normal University, Wuhan 430079, China

Table S1 Observed frequencies (in cm^{-1}) for Band I of CO-SO₂.

J'	Ka'	Kc'	J''	Ka''	Kc''	<i>Obs. Freq.</i>	<i>Cal. Freq.</i>	$v_{obs}-v_{cal}$
8	4	4	9	5	4	2147.8643	2147.8663	-0.002
7	4	3	8	5	3	2147.9609	2147.9617	-0.0008
19	2	17	20	3	17	2147.9695	2147.9693	0.0002
12	3	10	13	4	10	2147.9797	2147.9777	0.002
12	3	9	13	4	9	2147.9826	2147.9818	0.0008
6	4	2	7	5	2	2148.0553	2148.0570	-0.0017
11	3	8	12	4	8	2148.0783	2148.0763	0.0019
26	3	24	27	3	25	2148.3204	2148.3202	0.0002
27	0	27	28	0	28	2148.3408	2148.3396	0.0013
26	1	25	27	1	26	2148.3469	2148.3470	-0.0001
8	3	5	9	4	5	2148.3629	2148.3618	0.0011
25	2	23	26	2	24	2148.3650	2148.3655	-0.0005
18	1	17	19	2	17	2148.4027	2148.4023	0.0004
25	4	22	26	4	23	2148.4075	2148.4083	-0.0008
25	5	21	26	5	22	2148.4103	2148.4113	-0.001
25	7	19	26	7	20	2148.4167	2148.4169	-0.0002
25	3	23	26	3	24	2148.4195	2148.4192	0.0003
26	0	26	27	0	27	2148.4366	2148.4343	0.0023
13	2	11	14	3	11	2148.4373	2148.4374	-0.0001
25	1	24	26	1	25	2148.4402	2148.4404	-0.0002
12	2	11	13	3	11	2148.4455	2148.4446	0.0009
7	3	4	8	4	4	2148.4552	2148.4572	-0.002
25	2	24	26	2	25	2148.4634	2148.4619	0.0015
24	2	22	25	2	23	2148.4662	2148.4649	0.0013
24	3	21	25	3	22	2148.4703	2148.4694	0.0009
24	4	20	25	4	21	2148.5042	2148.5015	0.0027
24	4	21	25	4	22	2148.5124	2148.5097	0.0028
12	2	10	13	3	10	2148.5203	2148.5193	0.0011
17	1	16	18	2	16	2148.5258	2148.5247	0.0011
25	0	25	26	0	26	2148.5295	2148.5288	0.0007
11	2	10	12	3	10	2148.5481	2148.5482	-0.0001
6	3	3	7	4	3	2148.5528	2148.5526	0.0002
24	2	23	25	2	24	2148.5575	2148.5579	-0.0004
23	2	21	24	2	22	2148.5635	2148.5647	-0.0013
23	3	20	24	3	21	2148.5756	2148.5749	0.0007
23	4	19	24	4	20	2148.6098	2148.6047	0.0051
23	4	20	24	4	21	2148.6162	2148.6109	0.0053
23	3	21	24	3	22	2148.6220	2148.6176	0.0045
24	0	24	25	0	25	2148.6271	2148.6231	0.004
23	1	22	24	1	23	2148.6288	2148.6273	0.0016
16	1	15	17	2	15	2148.6368	2148.6416	-0.0048

23	2	22	24	2	23	2148.6586	2148.6540	0.0046
23	2	22	24	2	23	2148.6588	2148.6540	0.0048
22	2	20	23	2	21	2148.6691	2148.6652	0.0039
22	3	19	23	3	20	2148.6838	2148.6802	0.0036
10	2	8	11	3	8	2148.6913	2148.6893	0.002
22	1	21	23	1	22	2148.7228	2148.7209	0.0019
22	1	21	23	1	22	2148.7236	2148.7209	0.0027
22	2	21	23	2	22	2148.7534	2148.7501	0.0032
21	2	19	22	2	20	2148.7688	2148.7661	0.0027
21	3	18	22	3	19	2148.7891	2148.7852	0.0039
3	3	0	4	4	0	2148.8377	2148.8380	-0.0002
21	2	20	22	2	21	2148.8501	2148.8463	0.0037
20	2	18	21	2	19	2148.8704	2148.8674	0.003
20	3	17	21	3	18	2148.8938	2148.8898	0.004
21	0	21	22	0	22	2148.9078	2148.9043	0.0035
20	1	19	21	1	20	2148.9116	2148.9091	0.0025
20	5	16	21	5	17	2148.9163	2148.9177	-0.0014
20	6	15	21	6	16	2148.9205	2148.9212	-0.0007
19	2	17	20	2	18	2148.9714	2148.9690	0.0023
19	3	16	20	3	17	2148.9945	2148.9939	0.0006
20	0	20	21	0	21	2148.9974	2148.9975	-0.0002
19	1	18	20	1	19	2149.0033	2149.0039	-0.0006
19	3	17	20	3	18	2149.0158	2149.0148	0.001
19	5	15	20	5	16	2149.0220	2149.0182	0.0038
19	6	14	20	6	15	2149.0275	2149.0216	0.0059
19	2	18	20	2	19	2149.0389	2149.0388	0.0001
6	2	5	7	3	5	2149.0469	2149.0458	0.0011
6	2	4	7	3	4	2149.0524	2149.0517	0.0007
19	0	19	20	0	20	2149.0900	2149.0905	-0.0005
19	1	19	20	1	20	2149.0957	2149.0961	-0.0004
18	1	17	19	1	18	2149.0980	2149.0991	-0.0012
18	3	16	19	3	17	2149.1149	2149.1140	0.0009
18	5	14	19	5	15	2149.1214	2149.1183	0.0031
18	2	17	19	2	18	2149.1357	2149.1352	0.0005
11	1	10	12	2	10	2149.1560	2149.1542	0.0017
17	2	15	18	2	16	2149.1734	2149.1733	0.0001
18	0	18	19	0	19	2149.1832	2149.1832	-0.0001
18	1	18	19	1	19	2149.1897	2149.1899	-0.0003
17	1	16	18	1	17	2149.1942	2149.1949	-0.0007
17	3	14	18	3	15	2149.2000	2149.2001	-0.0001
17	3	15	18	3	16	2149.2137	2149.2132	0.0005
17	5	13	18	5	14	2149.2195	2149.2182	0.0013
17	7	11	18	7	12	2149.2248	2149.2244	0.0003
17	2	16	18	2	17	2149.2295	2149.2315	-0.002

8	1	8	9	2	8	2149.2550	2149.2544	0.0006
17	0	17	18	0	18	2149.2743	2149.2757	-0.0014
17	1	17	18	1	18	2149.2845	2149.2837	0.0008
16	1	15	17	1	16	2149.2893	2149.2912	-0.0019
16	3	13	17	3	14	2149.3010	2149.3022	-0.0012
16	4	13	17	4	14	2149.3127	2149.3140	-0.0013
16	5	12	17	5	13	2149.3189	2149.3178	0.0011
16	7	10	17	7	11	2149.3240	2149.3241	-0.0001
16	2	15	17	2	16	2149.3276	2149.3279	-0.0004
3	2	1	4	3	1	2149.3337	2149.3343	-0.0007
16	0	16	17	0	17	2149.3679	2149.3680	-0.0001
16	1	16	17	1	17	2149.3776	2149.3773	0.0004
15	1	14	16	1	15	2149.3881	2149.3880	0.0001
15	3	12	16	3	13	2149.4036	2149.4037	-0.0001
15	3	13	16	3	14	2149.4118	2149.4112	0.0006
15	4	12	16	4	13	2149.4140	2149.4134	0.0006
15	5	11	16	5	12	2149.4187	2149.4170	0.0017
15	2	14	16	2	15	2149.4240	2149.4244	-0.0004
2	2	0	3	3	0	2149.4285	2149.4291	-0.0005
15	0	15	16	0	16	2149.4599	2149.4601	-0.0001
15	1	15	16	1	16	2149.4709	2149.4708	0
14	2	12	15	2	13	2149.4806	2149.4806	0
14	1	13	15	1	14	2149.4853	2149.4851	0.0002
14	3	11	15	3	12	2149.5044	2149.5044	0
14	3	12	15	3	13	2149.5100	2149.5100	0
14	4	11	15	4	12	2149.5123	2149.5124	-0.0001
14	5	10	15	5	11	2149.5164	2149.5160	0.0004
14	2	13	15	2	14	2149.5201	2149.5208	-0.0007
14	8	7	15	8	8	2149.5253	2149.5252	0.0001
14	0	14	15	0	15	2149.5520	2149.5520	-0.0001
14	1	14	15	1	15	2149.5642	2149.5643	-0.0001
13	1	12	14	1	13	2149.5831	2149.5827	0.0004
5	1	5	6	2	5	2149.5991	2149.5992	-0.0001
13	3	10	14	3	11	2149.6052	2149.6046	0.0006
13	3	11	14	3	12	2149.6090	2149.6085	0.0004
13	4	10	14	4	11	2149.6120	2149.6112	0.0008
13	5	9	14	5	10	2149.6160	2149.6146	0.0014
13	2	12	14	2	13	2149.6178	2149.6173	0.0006
13	7	7	14	7	8	2149.6202	2149.6210	-0.0008
13	8	6	14	8	7	2149.6242	2149.6240	0.0003
13	0	13	14	0	14	2149.6442	2149.6440	0.0002
13	1	13	14	1	14	2149.6582	2149.6577	0.0004
5	1	4	6	2	4	2149.6743	2149.6742	0.0001
12	1	11	13	1	12	2149.6814	2149.6806	0.0008

12	2	10	13	2	11	2149.6859	2149.6850	0.0008
8	2	7	8	3	5	2149.6988	2149.6982	0.0006
12	3	9	13	3	10	2149.7049	2149.7041	0.0007
12	3	10	13	3	11	2149.7076	2149.7068	0.0007
12	4	9	13	4	10	2149.7104	2149.7096	0.0007
12	2	11	13	2	12	2149.7142	2149.7137	0.0006
12	6	7	13	6	8	2149.7179	2149.7162	0.0017
12	7	6	13	7	7	2149.7220	2149.7194	0.0026
12	8	5	13	8	6	2149.7266	2149.7224	0.0042
10	2	8	10	3	8	2149.7300	2149.7292	0.0008
12	0	12	13	0	13	2149.7364	2149.7360	0.0004
12	1	12	13	1	13	2149.7513	2149.7510	0.0003
11	1	10	12	1	11	2149.7789	2149.7787	0.0002
11	2	9	12	2	10	2149.7872	2149.7867	0.0005
11	3	8	12	3	9	2149.8030	2149.8031	-0.0001
11	3	9	12	3	10	2149.8048	2149.8049	-0.0001
11	4	8	12	4	9	2149.8074	2149.8078	-0.0003
11	2	10	12	2	11	2149.8107	2149.8101	0.0006
11	6	6	12	6	7	2149.8143	2149.8142	0.0001
11	8	4	12	8	5	2149.8187	2149.8205	-0.0017
13	1	13	13	2	11	2149.8211	2149.8215	-0.0004
11	0	11	12	0	12	2149.8283	2149.8282	0.0002
7	0	7	8	1	7	2149.8405	2149.8396	0.0009
11	1	11	12	1	12	2149.8446	2149.8443	0.0003
10	1	9	11	1	10	2149.8774	2149.8770	0.0004
10	2	8	11	2	9	2149.8881	2149.8879	0.0003
10	3	7	11	3	8	2149.9021	2149.9016	0.0006
10	2	9	11	2	10	2149.9058	2149.9064	-0.0006
10	5	6	11	5	7	2149.9085	2149.9087	-0.0002
10	6	5	11	6	6	2149.9118	2149.9118	-0.0001
10	7	4	11	7	5	2149.9156	2149.9151	0.0006
2	1	2	3	2	2	2149.9180	2149.9174	0.0006
10	0	10	11	0	11	2149.9207	2149.9206	0.0001
16	2	14	17	1	16	2149.9252	2149.9253	-0.0001
2	1	1	3	2	1	2149.9325	2149.9332	-0.0007
10	1	10	11	1	11	2149.9376	2149.9375	0
9	1	8	10	1	9	2149.9757	2149.9754	0.0003
9	2	7	10	2	8	2149.9882	2149.9884	-0.0002
9	3	7	10	3	8	2149.9993	2150.0003	-0.0009
9	2	8	10	2	9	2150.0021	2150.0026	-0.0005
9	5	5	10	5	6	2150.0049	2150.0060	-0.0012
9	6	4	10	6	5	2150.0082	2150.0092	-0.001
9	0	9	10	0	10	2150.0129	2150.0133	-0.0004
1	1	1	2	2	1	2150.0164	2150.0176	-0.0012

9	1	9	10	1	10	2150.0299	2150.0307	-0.0007
8	1	7	9	1	8	2150.0732	2150.0739	-0.0007
5	0	5	6	1	5	2150.0767	2150.0774	-0.0007
8	2	6	9	2	7	2150.0874	2150.0883	-0.0009
8	3	6	9	3	7	2150.0963	2150.0975	-0.0012
8	2	7	9	2	8	2150.0985	2150.0988	-0.0003
8	5	4	9	5	5	2150.1016	2150.1030	-0.0014
8	0	8	9	0	9	2150.1063	2150.1064	-0.0001
7	1	7	7	2	5	2150.1128	2150.1139	-0.0011
8	1	8	9	1	9	2150.1239	2150.1237	0.0002
5	1	5	5	2	3	2150.1640	2150.1611	0.0028
7	1	6	8	1	7	2150.1726	2150.1724	0.0003
7	2	5	8	2	6	2150.1868	2150.1874	-0.0006
4	0	4	5	1	4	2150.1905	2150.1904	0.0001
7	2	6	8	2	7	2150.1940	2150.1948	-0.0008
7	4	4	8	4	5	2150.1959	2150.1969	-0.0011
7	0	7	8	0	8	2150.1997	2150.1999	-0.0001
7	7	1	8	7	2	2150.2042	2150.2060	-0.0017
7	1	7	8	1	8	2150.2160	2150.2167	-0.0007
12	1	11	13	0	13	2150.2547	2150.2534	0.0013
6	1	5	6	2	5	2150.2613	2150.2597	0.0015
6	1	5	7	1	6	2150.2700	2150.2708	-0.0008
7	1	6	7	2	6	2150.2761	2150.2763	-0.0001
6	2	4	7	2	5	2150.2858	2150.2857	0.0001
6	2	5	7	2	6	2150.2907	2150.2907	0
6	0	6	7	0	7	2150.2944	2150.2937	0.0007
6	6	1	7	6	2	2150.2978	2150.2991	-0.0013
6	1	6	7	1	7	2150.3097	2150.3096	0.0001
5	1	4	6	1	5	2150.3689	2150.3692	-0.0002
5	2	3	6	2	4	2150.3833	2150.3833	0
5	2	4	6	2	5	2150.3868	2150.3864	0.0003
5	0	5	6	0	6	2150.3885	2150.3879	0.0007
5	5	1	6	5	2	2150.3912	2150.3922	-0.0009
5	1	5	6	1	6	2150.4036	2150.4024	0.0012
2	0	2	3	1	2	2150.4072	2150.4061	0.0011
4	1	3	5	1	4	2150.4670	2150.4674	-0.0003
15	1	14	15	2	14	2150.4736	2150.4743	-0.0006
4	2	2	5	2	3	2150.4798	2150.4802	-0.0003
4	0	4	5	0	5	2150.4821	2150.4823	-0.0002
4	4	1	5	4	2	2150.4838	2150.4853	-0.0015
4	1	4	5	1	5	2150.4953	2150.4950	0.0003
3	1	2	4	1	3	2150.5647	2150.5654	-0.0008
3	0	3	4	0	4	2150.5765	2150.5768	-0.0003
3	1	3	4	1	4	2150.5868	2150.5875	-0.0007

2	1	1	3	1	2	2150.6633	2150.6633	0
2	0	2	3	0	3	2150.6718	2150.6715	0.0003
2	1	2	3	1	3	2150.6798	2150.6798	0.0001
2	0	2	2	1	2	2150.7135	2150.7136	0
4	0	4	4	1	4	2150.7293	2150.7296	-0.0003
6	0	6	6	1	6	2150.7545	2150.7526	0.0019
1	1	0	2	1	1	2150.7618	2150.7609	0.0009
1	0	1	2	0	2	2150.7665	2150.7662	0.0003
1	1	1	2	1	2	2150.7719	2150.7718	0.0001
8	0	8	8	1	8	2150.7802	2150.7798	0.0003
9	0	9	9	1	9	2150.7926	2150.7939	-0.0013
10	0	10	10	1	10	2150.8079	2150.8077	0.0002
11	0	11	11	1	11	2150.8216	2150.8208	0.0007
12	0	12	12	1	12	2150.8339	2150.8329	0.001
21	1	21	21	0	21	2150.9086	2150.9083	0.0004
9	2	8	9	2	7	2150.9159	2150.9137	0.0023
3	3	0	3	3	1	2150.9556	2150.9556	0
15	1	15	15	0	15	2150.9835	2150.9821	0.0014
4	1	3	4	1	4	2151.0073	2151.0066	0.0007
13	1	13	13	0	13	2151.0163	2151.0149	0.0014
12	1	12	12	0	12	2151.0334	2151.0329	0.0005
1	0	1	0	0	0	2151.0498	2151.0490	0.0007
11	1	11	11	0	11	2151.0521	2151.0517	0.0004
6	1	5	6	1	6	2151.0632	2151.0629	0.0003
14	2	12	14	2	13	2151.0662	2151.0656	0.0006
10	1	10	10	0	10	2151.0715	2151.0710	0.0005
5	2	3	6	1	5	2151.0776	2151.0783	-0.0007
9	1	9	9	0	9	2151.0914	2151.0904	0.001
7	1	6	7	1	7	2151.0988	2151.0986	0.0001
8	1	8	8	0	8	2151.1096	2151.1096	0
7	1	7	7	0	7	2151.1277	2151.1281	-0.0004
2	1	2	1	1	1	2151.1375	2151.1376	-0.0001
2	0	2	1	0	1	2151.1427	2151.1427	0.0001
2	1	1	1	1	0	2151.1483	2151.1484	-0.0001
5	1	5	5	0	5	2151.1604	2151.1612	-0.0008
4	1	4	4	0	4	2151.1743	2151.1749	-0.0005
3	1	3	3	0	3	2151.1875	2151.1862	0.0012
2	1	2	2	0	2	2151.1950	2151.1950	0
1	1	1	1	0	1	2151.2006	2151.2010	-0.0004
6	0	6	5	1	4	2151.2201	2151.2196	0.0006
3	1	3	2	1	2	2151.2288	2151.2283	0.0005
3	0	3	2	0	2	2151.2366	2151.2358	0.0008
3	1	2	2	1	1	2151.2448	2151.2444	0.0004
17	2	16	17	1	16	2151.2845	2151.2841	0.0004

7	0	7	6	1	5	2151.2913	2151.2913	0.0001
1	1	0	0	0	0	2151.3005	2151.3007	-0.0002
4	1	4	3	1	3	2151.3178	2151.3186	-0.0008
16	2	15	16	1	15	2151.3227	2151.3240	-0.0013
4	0	4	3	0	3	2151.3278	2151.3284	-0.0006
4	2	3	3	2	2	2151.3292	2151.3300	-0.0008
4	1	3	3	1	2	2151.3388	2151.3400	-0.0012
8	0	8	7	1	6	2151.3580	2151.3581	-0.0001
15	2	14	15	1	14	2151.3620	2151.3633	-0.0013
2	1	1	1	0	1	2151.3988	2151.3998	-0.001
5	1	5	4	1	4	2151.4081	2151.4085	-0.0004
5	0	5	4	0	4	2151.4199	2151.4203	-0.0004
5	2	3	4	2	2	2151.4227	2151.4243	-0.0015
5	1	4	4	1	3	2151.4347	2151.4351	-0.0004
12	2	11	12	1	11	2151.4734	2151.4739	-0.0006
6	1	6	5	1	5	2151.4981	2151.4980	0.0001
3	1	2	2	0	2	2151.5016	2151.5013	0.0003
11	2	10	11	1	10	2151.5081	2151.5073	0.0008
6	0	6	5	0	5	2151.5114	2151.5114	0
6	2	4	5	2	3	2151.5158	2151.5177	-0.0019
6	1	5	5	1	4	2151.5297	2151.5298	-0.0001
7	1	7	6	1	6	2151.5848	2151.5871	-0.0022
8	2	7	8	1	7	2151.5924	2151.5938	-0.0014
7	0	7	6	0	6	2151.6006	2151.6018	-0.0011
7	2	6	6	2	5	2151.6052	2151.6064	-0.0012
7	3	5	6	3	4	2151.6071	2151.6084	-0.0013
7	2	5	6	2	4	2151.6103	2151.6112	-0.0009
7	1	6	6	1	5	2151.6241	2151.6240	0.0001
8	1	8	7	1	7	2151.6758	2151.6757	0.0001
3	2	2	3	1	2	2151.6847	2151.6839	0.0008
8	0	8	7	0	7	2151.6910	2151.6912	-0.0002
8	2	7	7	2	6	2151.6969	2151.6977	-0.0008
8	3	6	7	3	5	2151.6995	2151.7002	-0.0006
8	2	6	7	2	5	2151.7045	2151.7047	-0.0002
8	1	7	7	1	6	2151.7180	2151.7177	0.0003
9	1	9	8	1	8	2151.7648	2151.7639	0.0009
9	0	9	8	0	8	2151.7808	2151.7798	0.001
9	2	8	8	2	7	2151.7893	2151.7885	0.0007
9	3	7	8	3	6	2151.7921	2151.7916	0.0004
9	2	7	8	2	6	2151.7993	2151.7984	0.0009
9	1	8	8	1	7	2151.8118	2151.8108	0.001
9	2	7	9	1	9	2151.8416	2151.8398	0.0017
10	1	10	9	1	9	2151.8523	2151.8516	0.0007
10	0	10	9	0	9	2151.8683	2151.8675	0.0008

10	2	9	9	2	8	2151.8796	2151.8789	0.0007
10	3	8	9	3	7	2151.8829	2151.8828	0.0001
2	2	0	1	1	0	2151.8872	2151.8872	0
10	2	8	9	2	7	2151.8929	2151.8921	0.0008
10	1	9	9	1	8	2151.9043	2151.9033	0.0011
11	2	9	11	1	11	2151.9239	2151.9232	0.0008
7	1	6	6	0	6	2151.9367	2151.9345	0.0022
11	1	11	10	1	10	2151.9400	2151.9388	0.0012
11	0	11	10	0	10	2151.9557	2151.9543	0.0014
11	2	10	10	2	9	2151.9700	2151.9688	0.0013
11	3	9	10	3	8	2151.9738	2151.9737	0.0002
11	3	8	10	3	7	2151.9756	2151.9747	0.0008
11	2	9	10	2	8	2151.9871	2151.9858	0.0013
3	2	2	2	1	2	2151.9903	2151.9913	-0.001
11	1	10	10	1	9	2151.9964	2151.9951	0.0013
12	1	12	11	1	11	2152.0261	2152.0255	0.0006
12	0	12	11	0	11	2152.0409	2152.0402	0.0006
8	1	7	7	0	7	2152.0514	2152.0508	0.0006
12	2	11	11	2	10	2152.0583	2152.0581	0.0001
12	3	10	11	3	9	2152.0631	2152.0642	-0.0011
12	3	9	11	3	8	2152.0657	2152.0658	-0.0001
12	2	10	11	2	9	2152.0792	2152.0795	-0.0003
12	1	11	11	1	10	2152.0858	2152.0862	-0.0004
13	1	13	12	1	12	2152.1112	2152.1118	-0.0006
13	0	13	12	0	12	2152.1252	2152.1255	-0.0003
13	2	12	12	2	11	2152.1473	2152.1470	0.0004
13	5	9	12	5	8	2152.1522	2152.1515	0.0007
13	3	11	12	3	10	2152.1543	2152.1543	0
13	3	10	12	3	9	2152.1575	2152.1568	0.0008
9	3	7	9	2	7	2152.1618	2152.1632	-0.0014
13	2	11	12	2	10	2152.1745	2152.1731	0.0014
13	1	12	12	1	11	2152.1781	2152.1766	0.0014
7	3	5	7	2	5	2152.1833	2152.1823	0.0009
8	3	5	8	2	7	2152.1939	2152.1928	0.0011
5	2	4	4	1	4	2152.1963	2152.1957	0.0006
14	1	14	13	1	13	2152.1989	2152.1976	0.0013
14	0	14	13	0	13	2152.2109	2152.2100	0.0009
14	2	13	13	2	12	2152.2349	2152.2353	-0.0004
14	5	10	13	5	9	2152.2403	2152.2406	-0.0003
14	3	12	13	3	11	2152.2424	2152.2441	-0.0017
14	3	11	13	3	10	2152.2467	2152.2476	-0.0009
14	1	13	13	1	12	2152.2653	2152.2663	-0.001
15	1	15	14	1	14	2152.2816	2152.2828	-0.0012
15	0	15	14	0	14	2152.2926	2152.2939	-0.0013

6	2	5	5	1	5	2152.2999	2152.3015	-0.0016
7	2	5	6	1	5	2152.3041	2152.3062	-0.0021
15	2	14	14	2	13	2152.3217	2152.3231	-0.0013
15	5	11	14	5	10	2152.3291	2152.3293	-0.0002
15	3	13	14	3	12	2152.3318	2152.3335	-0.0017
15	3	12	14	3	11	2152.3375	2152.3384	-0.0009
15	1	14	14	1	13	2152.3539	2152.3550	-0.0011
15	2	13	14	2	12	2152.3584	2152.3593	-0.0009
16	1	16	15	1	15	2152.3668	2152.3676	-0.0008
16	0	16	15	0	15	2152.3766	2152.3773	-0.0008
8	2	6	7	1	6	2152.3830	2152.3859	-0.0028
16	2	15	15	2	14	2152.4102	2152.4103	-0.0001
16	5	12	15	5	11	2152.4180	2152.4177	0.0003
16	3	14	15	3	13	2152.4224	2152.4225	-0.0001
16	3	13	15	3	12	2152.4299	2152.4292	0.0007
16	1	15	15	1	14	2152.4433	2152.4429	0.0004
17	1	17	16	1	16	2152.4526	2152.4519	0.0007
17	0	17	16	0	16	2152.4611	2152.4603	0.0008
3	3	0	2	2	0	2152.4819	2152.4817	0.0002
17	2	16	16	2	15	2152.4980	2152.4969	0.0011
17	6	12	16	6	11	2152.5030	2152.5017	0.0013
17	5	13	16	5	12	2152.5070	2152.5056	0.0013
17	3	15	16	3	14	2152.5122	2152.5111	0.0012
17	3	14	16	3	13	2152.5214	2152.5199	0.0015
17	1	16	16	1	15	2152.5305	2152.5299	0.0007
18	1	18	17	1	17	2152.5366	2152.5357	0.0009
18	0	18	17	0	17	2152.5438	2152.5429	0.0009
4	3	1	3	2	1	2152.5734	2152.5742	-0.0008
18	2	17	17	2	16	2152.5824	2152.5830	-0.0006
18	6	13	17	6	12	2152.5882	2152.5887	-0.0005
18	5	14	17	5	13	2152.5927	2152.5933	-0.0006
18	3	16	17	3	15	2152.5985	2152.5992	-0.0007
18	3	15	17	3	14	2152.6101	2152.6107	-0.0006
18	1	17	17	1	16	2152.6143	2152.6158	-0.0015
19	1	19	18	1	18	2152.6181	2152.6191	-0.001
19	0	19	18	0	18	2152.6240	2152.6251	-0.0011
18	2	16	17	2	15	2152.6338	2152.6350	-0.0012
16	4	12	16	3	14	2152.6395	2152.6388	0.0006
13	4	10	13	3	10	2152.6519	2152.6514	0.0005
19	9	11	18	9	10	2152.6548	2152.6543	0.0006
12	4	9	12	3	9	2152.6586	2152.6602	-0.0016
19	2	18	18	2	17	2152.6680	2152.6685	-0.0005
11	4	7	11	3	9	2152.6699	2152.6704	-0.0006
19	6	14	18	6	13	2152.6756	2152.6753	0.0003

19	5	15	18	5	14	2152.6809	2152.6806	0.0004
19	3	17	18	3	16	2152.6840	2152.6868	-0.0028
19	1	18	18	1	17	2152.7002	2152.7008	-0.0006
20	1	20	19	1	19	2152.7020	2152.7019	0.0001
20	0	20	19	0	19	2152.7071	2152.7070	0.0001
12	2	10	11	1	10	2152.7117	2152.7113	0.0004
19	2	17	18	2	16	2152.7243	2152.7255	-0.0013
20	2	19	19	2	18	2152.7503	2152.7533	-0.003
20	7	14	19	7	13	2152.7527	2152.7549	-0.0022
6	3	3	5	2	3	2152.7556	2152.7568	-0.0012
6	3	4	5	2	4	2152.7610	2152.7599	0.0011
20	5	16	19	5	15	2152.7645	2152.7675	-0.0029
20	3	18	19	3	17	2152.7712	2152.7739	-0.0027
20	1	19	19	1	18	2152.7804	2152.7848	-0.0044
21	0	21	20	0	20	2152.7845	2152.7885	-0.004
20	3	17	19	3	16	2152.7885	2152.7923	-0.0038
20	2	18	19	2	17	2152.8102	2152.8153	-0.0052
21	2	20	20	2	19	2152.8333	2152.8376	-0.0043
14	1	13	13	0	13	2152.8402	2152.8391	0.001
7	3	4	6	2	4	2152.8474	2152.8464	0.001
7	3	5	6	2	5	2152.8509	2152.8524	-0.0015
21	3	19	20	3	18	2152.8583	2152.8606	-0.0023
21	4	17	20	4	16	2152.8610	2152.8625	-0.0014
21	1	20	20	1	19	2152.8636	2152.8678	-0.0042
22	0	22	21	0	21	2152.8667	2152.8696	-0.0029
21	3	18	20	3	17	2152.8805	2152.8831	-0.0026
21	2	19	20	2	18	2152.8996	2152.9043	-0.0047
22	2	21	21	2	20	2152.9150	2152.9213	-0.0063
22	7	16	21	7	15	2152.9217	2152.9245	-0.0028
22	6	17	21	6	16	2152.9287	2152.9327	-0.004
8	3	5	7	2	5	2152.9326	2152.9344	-0.0018
22	5	18	21	5	17	2152.9375	2152.9402	-0.0027
23	0	23	22	0	22	2152.9461	2152.9505	-0.0044
22	3	19	21	3	18	2152.9735	2152.9738	-0.0002
15	2	13	14	1	13	2152.9797	2152.9800	-0.0003
22	2	20	21	2	19	2152.9886	2152.9924	-0.0037
23	2	22	22	2	21	2153.0007	2153.0044	-0.0037
23	7	17	22	7	16	2153.0053	2153.0087	-0.0034
23	6	18	22	6	17	2153.0147	2153.0177	-0.003
9	3	6	8	2	6	2153.0195	2153.0205	-0.001
24	0	24	23	0	23	2153.0271	2153.0309	-0.0038
23	4	19	22	4	18	2153.0339	2153.0376	-0.0036
9	3	7	8	2	7	2153.0370	2153.0381	-0.001
23	3	20	22	3	19	2153.0641	2153.0643	-0.0003

23	2	21	22	2	20	2153.0801	2153.0796	0.0006
24	2	23	23	2	22	2153.0866	2153.0869	-0.0003
25	1	25	24	1	24	2153.1092	2153.1091	0.0001
25	0	25	24	0	24	2153.1109	2153.1109	0
24	3	22	23	3	21	2153.1161	2153.1171	-0.0011
24	4	21	23	4	20	2153.1205	2153.1195	0.001
14	5	9	14	4	11	2153.1469	2153.1485	-0.0017
24	3	21	23	3	20	2153.1518	2153.1546	-0.0028
24	2	22	23	2	21	2153.1615	2153.1658	-0.0044
5	4	1	4	3	1	2153.1659	2153.1656	0.0004
8	5	3	8	4	5	2153.1847	2153.1841	0.0005
25	1	24	24	1	23	2153.1886	2153.1909	-0.0023
25	5	21	24	5	20	2153.1958	2153.1966	-0.0009
25	3	23	24	3	22	2153.2016	2153.2015	0.0001
25	4	22	24	4	21	2153.2072	2153.2051	0.0021
25	4	21	24	4	20	2153.2146	2153.2122	0.0024
25	3	22	24	3	21	2153.2444	2153.2445	-0.0002
25	2	23	24	2	22	2153.2497	2153.2511	-0.0014
12	3	9	11	2	9	2153.2644	2153.2644	0
27	0	27	26	0	26	2153.2710	2153.2698	0.0011
26	5	22	25	5	21	2153.2822	2153.2814	0.0008
26	3	24	25	3	23	2153.2866	2153.2852	0.0014
26	4	23	25	4	22	2153.2890	2153.2903	-0.0013
17	1	16	16	0	16	2153.2936	2153.2949	-0.0013
26	4	22	25	4	21	2153.3024	2153.2994	0.003
12	3	10	11	2	10	2153.3219	2153.3204	0.0015
27	2	26	26	2	25	2153.3308	2153.3306	0.0002
26	3	23	25	3	22	2153.3334	2153.3340	-0.0005
13	3	10	12	2	10	2153.3411	2153.3403	0.0008
7	4	3	6	3	3	2153.3481	2153.3482	-0.0001
27	6	22	26	6	21	2153.3540	2153.3538	0.0002
15	2	14	14	1	14	2153.3605	2153.3600	0.0004
27	3	25	26	3	24	2153.3686	2153.3683	0.0003
27	4	24	26	4	23	2153.3733	2153.3750	-0.0017
27	4	23	26	4	22	2153.3896	2153.3866	0.003
14	3	11	13	2	11	2153.4112	2153.4134	-0.0023
13	3	11	12	2	11	2153.4161	2153.4162	-0.0001
27	3	24	26	3	23	2153.4219	2153.4228	-0.0009
29	0	29	28	0	28	2153.4256	2153.4270	-0.0014
28	3	26	27	3	25	2153.4509	2153.4508	0.0001
28	4	25	27	4	24	2153.4582	2153.4592	-0.001
28	4	24	27	4	23	2153.4768	2153.4738	0.003
15	3	12	14	2	12	2153.4862	2153.4840	0.0022
16	2	15	15	1	15	2153.4909	2153.4893	0.0016

28	2	26	27	2	25	2153.4979	2153.5006	-0.0028
30	0	30	29	0	29	2153.5038	2153.5049	-0.0011
14	3	12	13	2	12	2153.5088	2153.5132	-0.0044
9	4	5	8	3	5	2153.5296	2153.5286	0.0011
29	3	27	28	3	26	2153.5336	2153.5326	0.001
29	4	26	28	4	25	2153.5428	2153.5429	-0.0001
16	3	13	15	2	13	2153.5549	2153.5524	0.0025

Table S2 Observed frequencies (in cm^{-1}) for Band II of CO-SO₂.

J'	Ka'	Kc'	J''	Ka''	Kc''	<i>Obs. Freq.</i>	<i>Cal. Freq.</i>	$v_{obs-v_{cal}}$
20	0	20	21	0	21	2145.8434	2145.8422	0.0013
19	2	18	20	2	19	2145.8694	2145.8730	-0.0036
18	2	16	19	2	17	2145.8752	2145.8728	0.0024
18	2	17	19	2	18	2145.9883	2145.9917	-0.0034
17	2	15	18	2	16	2146.0040	2146.0016	0.0024
18	0	18	19	0	19	2146.0706	2146.0684	0.0022
17	6	12	18	6	13	2146.0945	2146.0919	0.0026
17	2	16	18	2	17	2146.1081	2146.1105	-0.0023
16	2	14	17	2	15	2146.1323	2146.1314	0.0008
17	0	17	18	0	18	2146.1834	2146.1813	0.0021
16	4	13	17	4	14	2146.1987	2146.1914	0.0073
16	6	11	17	6	12	2146.2165	2146.2190	-0.0025
16	2	15	17	2	16	2146.2251	2146.2293	-0.0043
15	2	13	16	2	14	2146.2596	2146.2618	-0.0021
16	0	16	17	0	17	2146.2946	2146.2941	0.0005
15	4	12	16	4	13	2146.3214	2146.3196	0.0018
15	4	11	16	4	12	2146.3214	2146.3149	0.0064
15	6	10	16	6	11	2146.3387	2146.3442	-0.0055
15	2	14	16	2	15	2146.3433	2146.3483	-0.0049
14	2	12	15	2	13	2146.3885	2146.3921	-0.0036
15	0	15	16	0	16	2146.4070	2146.4067	0.0003
14	4	10	15	4	11	2146.4455	2146.4435	0.0020
14	4	11	15	4	12	2146.4455	2146.4461	-0.0006
14	2	13	15	2	14	2146.4621	2146.4672	-0.0052
14	8	7	15	8	8	2146.4925	2146.4937	-0.0012
13	2	11	14	2	12	2146.5195	2146.5220	-0.0025
14	0	14	15	0	15	2146.5195	2146.5193	0.0003
13	4	9	14	4	10	2146.5716	2146.5697	0.0020
13	4	10	14	4	11	2146.5717	2146.5711	0.0006
13	2	12	14	2	13	2146.5841	2146.5862	-0.0021
13	6	8	14	6	9	2146.5934	2146.5900	0.0034
13	0	13	14	0	14	2146.6341	2146.6317	0.0024
12	2	10	13	2	11	2146.6498	2146.6513	-0.0015
12	4	9	13	4	10	2146.6956	2146.6948	0.0008
12	2	11	13	2	12	2146.7043	2146.7051	-0.0008
12	6	7	13	6	8	2146.7100	2146.7112	-0.0012
12	8	5	13	8	6	2146.7267	2146.7312	-0.0045
12	0	12	13	0	13	2146.7467	2146.7441	0.0027
11	2	9	12	2	10	2146.7797	2146.7799	-0.0002
11	4	8	12	4	9	2146.8189	2146.8173	0.0016
11	2	10	12	2	11	2146.8245	2146.8240	0.0005

11	6	6	12	6	7	2146.8319	2146.8314	0.0005
11	0	11	12	0	12	2146.8571	2146.8564	0.0006
10	2	8	11	2	9	2146.9083	2146.9076	0.0007
10	4	7	11	4	8	2146.9401	2146.9388	0.0013
10	2	9	11	2	10	2146.9436	2146.9427	0.0009
10	6	5	11	6	6	2146.9525	2146.9509	0.0015
10	0	10	11	0	11	2146.9702	2146.9690	0.0013
9	2	7	10	2	8	2147.0339	2147.0342	-0.0002
9	2	8	10	2	9	2147.0616	2147.0614	0.0002
9	6	4	10	6	5	2147.0719	2147.0698	0.0020
8	2	6	9	2	7	2147.1597	2147.1596	0.0001
8	2	7	9	2	8	2147.1814	2147.1799	0.0015
8	6	3	9	6	4	2147.1928	2147.1883	0.0045
8	0	8	9	0	9	2147.1968	2147.1951	0.0017
7	2	5	8	2	6	2147.2823	2147.2839	-0.0016
7	2	6	8	2	7	2147.2971	2147.2983	-0.0012
7	4	4	8	4	5	2147.2994	2147.2989	0.0004
7	0	7	8	0	8	2147.3079	2147.3091	-0.0011
6	2	4	7	2	5	2147.4052	2147.4068	-0.0017
6	2	5	7	2	6	2147.4149	2147.4166	-0.0017
6	4	3	7	4	4	2147.4180	2147.4179	0.0001
6	0	6	7	0	7	2147.4216	2147.4237	-0.0021
5	2	3	6	2	4	2147.5270	2147.5286	-0.0016
5	2	4	6	2	5	2147.5336	2147.5348	-0.0012
5	0	5	6	0	6	2147.5376	2147.5391	-0.0015
4	2	2	5	2	3	2147.6480	2147.6493	-0.0013
4	2	3	5	2	4	2147.6518	2147.6529	-0.0011
4	0	4	5	0	5	2147.6531	2147.6551	-0.0020
4	4	1	5	4	2	2147.6557	2147.6549	0.0008
3	2	1	4	2	2	2147.7700	2147.7691	0.0010
3	0	3	4	0	4	2147.7721	2147.7717	0.0003
2	0	2	3	0	3	2147.8900	2147.8888	0.0013
1	0	1	2	0	2	2148.0053	2148.0061	-0.0008
0	0	0	1	0	1	2148.1292	2148.1235	0.0057
9	2	8	9	2	7	2148.1560	2148.1536	0.0024
13	4	9	13	4	10	2148.2133	2148.2131	0.0002
6	2	5	6	2	4	2148.2190	2148.2205	-0.0015
13	6	8	13	6	7	2148.2255	2148.2259	-0.0004
9	4	6	9	4	5	2148.2303	2148.2316	-0.0013
8	4	5	8	4	4	2148.2341	2148.2347	-0.0006
4	4	1	4	4	0	2148.2456	2148.2418	0.0038
6	6	1	6	6	0	2148.2456	2148.2457	-0.0001
9	2	7	9	2	8	2148.3015	2148.3017	-0.0002
13	12	1	13	12	2	2148.3149	2148.3147	0.0002

1	0	1	0	0	0	2148.3577	2148.3578	-0.0002
2	0	2	1	0	1	2148.4741	2148.4743	-0.0002
3	0	3	2	0	2	2148.5891	2148.5899	-0.0008
3	2	2	2	2	1	2148.5911	2148.5918	-0.0007
4	0	4	3	0	3	2148.7058	2148.7042	0.0016
4	2	3	3	2	2	2148.7066	2148.7076	-0.0010
4	2	2	3	2	1	2148.7086	2148.7100	-0.0014
5	0	5	4	0	4	2148.8173	2148.8168	0.0005
5	2	4	4	2	3	2148.8208	2148.8226	-0.0018
5	2	3	4	2	2	2148.8246	2148.8276	-0.0030
6	0	6	5	0	5	2148.9290	2148.9272	0.0017
6	2	5	5	2	4	2148.9346	2148.9367	-0.0021
6	4	3	5	4	2	2148.9403	2148.9432	-0.0028
6	2	4	5	2	3	2148.9461	2148.9459	0.0002
7	0	7	6	0	6	2149.0350	2149.0349	0.0001
7	2	6	6	2	5	2149.0468	2149.0498	-0.0030
7	2	5	6	2	4	2149.0700	2149.0651	0.0049
8	0	8	7	0	7	2149.1438	2149.1394	0.0044
8	2	7	7	2	6	2149.1604	2149.1615	-0.0010
8	4	5	7	4	4	2149.1709	2149.1730	-0.0020
8	6	3	7	6	2	2149.1790	2149.1815	-0.0025
8	2	6	7	2	5	2149.1861	2149.1851	0.0010
9	0	9	8	0	8	2149.2440	2149.2405	0.0035
9	2	8	8	2	7	2149.2710	2149.2715	-0.0005
9	2	7	8	2	6	2149.3061	2149.3059	0.0001
10	2	8	9	2	7	2149.4285	2149.4273	0.0012
11	0	11	10	0	10	2149.4333	2149.4313	0.0020
11	2	10	10	2	9	2149.4854	2149.4855	-0.0001
12	0	12	11	0	11	2149.5201	2149.5212	-0.0011
12	6	7	11	6	6	2149.6367	2149.6352	0.0014
14	0	14	13	0	13	2149.6911	2149.6903	0.0008
15	0	15	14	0	14	2149.7655	2149.7694	-0.0039
16	2	15	15	2	14	2149.9649	2149.9662	-0.0014
18	0	18	17	0	17	2149.9839	2149.9832	0.0007
17	2	16	16	2	15	2150.0465	2150.0497	-0.0032
16	4	12	15	4	11	2150.0639	2150.0629	0.0010
16	2	14	15	2	13	2150.1292	2150.1263	0.0029
21	0	21	20	0	20	2150.1564	2150.1552	0.0012
17	2	15	16	2	14	2150.2310	2150.2292	0.0018
18	2	16	17	2	15	2150.3219	2150.3252	-0.0032
19	6	14	18	6	13	2150.3762	2150.3752	0.0010
20	4	17	19	4	16	2150.4481	2150.4484	-0.0003