

Supplementary Materials for:

The Gigahertz and Terahertz spectrum of monodeutero-oxirane

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Table S1: Observed pure rotational transitions ($\tilde{\nu}$, in cm^{-1}) of the ground state of oxirane-D₁ in **only MW and GHz regions**. J , K_a and K_c are quantum numbers, $\tilde{\nu}_{\text{obs.}}$ = observed wavenumbers and $\tilde{\nu}_{\text{calc.}}$ = wavenumbers using the reported spectroscopic parameters (lower states ", upper states '). Spectroscopic parameters used in fitting are presented in Table 2.

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs.}}/\text{cm}^{-1}$	$(\tilde{\nu}_{\text{obs.}} - \tilde{\nu}_{\text{calc.}})/10^{-6} \text{ cm}^{-1}$
1	1	0	1	0	1	0.36442	1.31
2	2	0	2	1	1	0.56113	-0.65
3	2	1	3	1	2	0.70759	-0.55
2	1	1	2	0	2	0.70996	-1.69
4	3	1	4	2	2	0.84870	-0.65
3	3	0	3	2	1	0.91250	0.85
5	3	2	5	2	3	1.05147	-0.23
2	2	1	2	1	2	1.09322	-6.85
6	4	2	6	3	3	1.12667	1.07
4	2	2	4	1	3	1.13045	1.46
5	4	1	5	3	2	1.16908	1.10
1	1	1	0	0	0	1.25354	0.81
3	1	2	3	0	3	1.27390	1.54
3	3	1	3	2	2	1.33885	1.06
4	4	0	4	3	1	1.38978	0.20
7	5	2	7	4	3	1.40271	-2.71
7	4	3	7	3	4	1.40872	2.55
8	5	3	8	4	4	1.40918	-1.49
2	0	2	1	1	1	1.94589	-29.70
4	2	3	4	1	4	1.98017	-24.00
6	4	3	6	3	4	2.09001	-0.28
6	5	2	6	4	3	2.09144	-0.63
2	1	2	1	0	1	2.14265	0.21
11	6	5	11	5	6	2.18473	-0.66
7	6	1	7	5	2	2.19928	-0.20
7	3	4	7	2	5	2.24618	-0.08
12	8	4	12	7	5	2.24647	-0.29
7	5	3	7	4	4	2.25204	-0.40
15	9	6	15	8	7	2.33931	-0.21
14	8	6	14	7	7	2.36387	-0.75
6	2	4	6	1	5	2.41484	0.39
6	6	0	6	5	1	2.41888	0.15
14	9	5	14	8	6	2.42156	-0.11
9	7	2	9	6	3	2.44396	-0.29
7	6	2	7	5	3	2.44997	-0.66
10	5	5	10	4	6	2.46639	-0.62
6	6	1	6	5	2	2.47709	-0.05
8	6	3	8	5	4	2.50195	-0.39
5	1	4	5	0	5	2.50265	0.46

6	3	4	6	2	5	2.50426	0.47
7	4	4	7	3	5	2.50719	-0.08
5	2	4	5	1	5	2.52313	0.60
8	5	4	8	4	5	2.55935	-0.58
16	10	6	16	9	7	2.59901	0.15
13	7	6	13	6	7	2.60678	-1.13
17	10	7	17	9	8	2.61409	0.07
11	8	3	11	7	4	2.65206	-0.26
9	6	4	9	5	5	2.68613	-0.85
16	9	7	16	8	8	2.73280	-1.03
9	4	5	9	3	6	2.73708	-0.14
8	7	1	8	6	2	2.74349	-0.13
18	11	7	18	10	8	2.78661	0.69
13	9	4	13	8	5	2.83021	-0.37
9	7	3	9	6	4	2.83310	-0.71
8	7	2	8	6	3	2.86059	-0.29
2	2	1	1	1	0	2.87146	0.06
10	7	4	10	6	5	2.90178	-1.07
7	7	0	7	6	1	2.90320	0.15
19	11	8	19	10	9	2.91628	1.61
3	0	3	2	1	2	2.91862	0.24
8	3	5	8	2	6	2.92241	0.24
7	7	1	7	6	2	2.92461	0.15
12	6	6	12	5	7	2.93880	-0.94
3	1	3	2	0	2	2.98280	0.62
15	10	5	15	9	6	2.98542	-0.10
20	12	8	20	11	9	2.99139	2.44
9	5	5	9	4	6	2.99653	-0.41
8	4	5	8	3	6	3.01541	0.24
10	6	5	10	5	6	3.02024	-0.60
7	2	5	7	1	6	3.02578	0.60
10	8	2	10	7	3	3.02816	-0.55
15	8	7	15	7	8	3.05047	-1.26
7	3	5	7	2	6	3.05058	0.53
6	1	5	6	0	6	3.07967	1.09
6	2	5	6	1	6	3.08421	0.83
3	1	2	2	2	1	3.09929	0.95
11	7	5	11	6	6	3.11370	-1.00
17	11	6	17	10	7	3.12512	0.07
18	10	8	18	9	9	3.12992	0.08
11	8	4	11	7	5	3.20486	-0.87
2	2	0	1	1	1	3.21701	-0.05
10	8	3	10	7	4	3.22692	-0.24
11	5	6	11	4	7	3.23069	-0.09
9	8	1	9	7	2	3.25416	0.26

19	12	7	19	11	8	3.25710	0.26
12	9	3	12	8	4	3.27497	-0.04
12	8	5	12	7	6	3.29544	-1.03
9	8	2	9	7	3	3.30177	0.42
8	8	0	8	7	1	3.37384	1.19
8	8	1	8	7	2	3.38109	1.11
21	13	8	21	12	9	3.38925	1.06
14	7	7	14	6	8	3.42155	-1.21
10	4	6	10	3	7	3.42670	0.43
12	7	6	12	6	7	3.47655	-0.49
11	6	6	11	5	7	3.47914	0.03
14	10	4	14	9	5	3.48614	-0.36
17	9	8	17	8	9	3.51340	-0.96
10	5	6	10	4	7	3.51799	0.42
23	14	9	23	13	10	3.52934	2.91
13	8	6	13	7	7	3.53821	-1.23
9	3	6	9	2	7	3.54179	0.91
20	11	9	20	10	10	3.55446	2.35
9	4	6	9	3	7	3.56831	0.62
13	9	5	13	8	6	3.56916	-1.35
11	9	2	11	8	3	3.57313	0.25
12	9	4	12	8	5	3.58006	-0.90
8	2	6	8	1	7	3.60852	1.80
8	3	6	8	2	7	3.61440	1.45
7	1	6	7	0	7	3.64896	1.95
7	2	6	7	1	7	3.64987	1.83
11	9	3	11	8	4	3.66086	0.05
16	11	5	16	10	6	3.66451	-0.95
14	9	6	14	8	7	3.68619	-1.04
13	6	7	13	5	8	3.72598	-0.28
10	9	1	10	8	2	3.73995	1.30
10	9	2	10	8	3	3.75757	1.06
3	2	2	2	1	1	3.76053	0.81
18	12	6	18	11	7	3.81382	-1.39
4	0	4	3	1	3	3.83251	1.10
9	9	0	9	8	1	3.83828	2.57
9	9	1	9	8	2	3.84059	2.23
4	1	4	3	0	3	3.84742	1.47
13	10	3	13	9	4	3.86027	-0.32
16	8	8	16	7	9	3.91199	-0.97
14	10	5	14	9	6	3.92339	-1.47
12	5	7	12	4	8	3.92828	0.49
15	10	6	15	9	7	3.92909	-1.47
14	8	7	14	7	8	3.93067	-0.30
20	13	7	20	12	8	3.93891	-2.09

13	7	7	13	6	8	3.95757	0.20
15	9	7	15	8	8	3.96202	-0.71
19	10	9	19	9	10	3.99237	0.45

Table S2: Observed pure rotational transitions ($\tilde{\nu}$, in cm^{-1}) of the ground state of oxirane- D_1 in **MW, GHz and THz** ranges. J , K_a and K_c are quantum numbers, $\tilde{\nu}_{\text{obs.}}$ = observed wavenumbers and $\tilde{\nu}_{\text{calc.}}$ = wavenumbers using the reported spectroscopic parameters (lower states ", upper states '). Spectroscopic parameters used in fitting are presented in Table 2.

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs.}}/\text{cm}^{-1}$	$(\tilde{\nu}_{\text{obs.}} - \tilde{\nu}_{\text{calc.}})/10^{-6} \text{ cm}^{-1}$
1	1	0	1	0	1	0.36442	1.31
2	2	0	2	1	1	0.56113	-0.66
3	2	1	3	1	2	0.70759	-0.53
2	1	1	2	0	2	0.70996	-1.68
4	3	1	4	2	2	0.84870	-0.63
3	3	0	3	2	1	0.91250	0.81
5	3	2	5	2	3	1.05147	-0.13
2	2	1	2	1	2	1.09322	-6.86
6	4	2	6	3	3	1.12667	1.17
4	2	2	4	1	3	1.13045	1.50
5	4	1	5	3	2	1.16908	1.08
1	1	1	0	0	0	1.25354	0.80
3	1	2	3	0	3	1.27390	1.51
3	3	1	3	2	2	1.33885	1.04
4	4	0	4	3	1	1.38978	0.10
7	5	2	7	4	3	1.40271	-2.68
7	4	3	7	3	4	1.40872	2.81
8	5	3	8	4	4	1.40918	-1.25
2	0	2	1	1	1	1.94589	-29.80
4	2	3	4	1	4	1.98017	-24.10
6	4	3	6	3	4	2.09001	-0.21
6	5	2	6	4	3	2.09144	-0.59
2	1	2	1	0	1	2.14265	0.14
11	6	5	11	5	6	2.18473	0.13
7	6	1	7	5	2	2.19928	-0.41
7	3	4	7	2	5	2.24618	-0.01
12	8	4	12	7	5	2.24647	-0.25
7	5	3	7	4	4	2.25204	-0.24
15	9	6	15	8	7	2.33931	-0.01
14	8	6	14	7	7	2.36387	0.02
6	2	4	6	1	5	2.41484	0.18
6	6	0	6	5	1	2.41888	-0.21
14	9	5	14	8	6	2.42156	-0.07
9	7	2	9	6	3	2.44396	-0.43
7	6	2	7	5	3	2.44997	-0.68
10	5	5	10	4	6	2.46639	-0.01
6	6	1	6	5	2	2.47709	-0.35
8	6	3	8	5	4	2.50195	-0.18
5	1	4	5	0	5	2.50265	0.03

6	3	4	6	2	5	2.50426	0.25
7	4	4	7	3	5	2.50719	-0.10
5	2	4	5	1	5	2.52313	0.17
8	5	4	8	4	5	2.55935	-0.40
16	10	6	16	9	7	2.59901	-0.02
13	7	6	13	6	7	2.60678	-0.07
17	10	7	17	9	8	2.61409	-0.27
11	8	3	11	7	4	2.65206	-0.29
9	6	4	9	5	5	2.68613	-0.51
16	9	7	16	8	8	2.73280	-0.45
9	4	5	9	3	6	2.73708	0.08
8	7	1	8	6	2	2.74349	-0.45
18	11	7	18	10	8	2.78661	-0.14
13	9	4	13	8	5	2.83021	-0.24
9	7	3	9	6	4	2.83310	-0.50
8	7	2	8	6	3	2.86059	-0.45
2	2	1	1	1	0	2.87146	-0.02
10	7	4	10	6	5	2.90178	-0.60
7	7	0	7	6	1	2.90320	-0.50
19	11	8	19	10	9	2.91628	-0.05
3	0	3	2	1	2	2.91862	0.02
8	3	5	8	2	6	2.92241	0.05
7	7	1	7	6	2	2.92461	-0.47
12	6	6	12	5	7	2.93880	-0.03
3	1	3	2	0	2	2.98280	0.40
15	10	5	15	9	6	2.98542	0.17
20	12	8	20	11	9	2.99139	0.09
9	5	5	9	4	6	2.99653	-0.35
8	4	5	8	3	6	3.01541	0.00
10	6	5	10	5	6	3.02024	-0.27
7	2	5	7	1	6	3.02578	0.05
10	8	2	10	7	3	3.02816	-0.69
15	8	7	15	7	8	3.05047	-0.08
7	3	5	7	2	6	3.05058	-0.03
6	1	5	6	0	6	3.07967	0.23
6	2	5	6	1	6	3.08421	-0.02
3	1	2	2	2	1	3.09929	0.72
11	7	5	11	6	6	3.11370	-0.45
17	11	6	17	10	7	3.12512	0.35
18	10	8	18	9	9	3.12992	-0.13
11	8	4	11	7	5	3.20486	-0.30
2	2	0	1	1	1	3.21701	-0.11
10	8	3	10	7	4	3.22692	-0.07
11	5	6	11	4	7	3.23069	0.34
9	8	1	9	7	2	3.25416	-0.27

19	12	7	19	11	8	3.25710	0.21
12	9	3	12	8	4	3.27497	0.15
12	8	5	12	7	6	3.29544	-0.28
9	8	2	9	7	3	3.30177	-0.01
8	8	0	8	7	1	3.37384	-0.02
8	8	1	8	7	2	3.38109	-0.08
21	13	8	21	12	9	3.38925	0.00
14	7	7	14	6	8	3.42155	-0.08
10	4	6	10	3	7	3.42670	0.32
12	7	6	12	6	7	3.47655	-0.03
11	6	6	11	5	7	3.47914	0.18
14	10	4	14	9	5	3.48614	0.30
17	9	8	17	8	9	3.51340	-0.05
10	5	6	10	4	7	3.51799	0.19
23	14	9	23	13	10	3.52934	-0.44
13	8	6	13	7	7	3.53821	-0.53
9	3	6	9	2	7	3.54179	0.30
20	11	9	20	10	10	3.55446	0.35
9	4	6	9	3	7	3.56831	-0.03
13	9	5	13	8	6	3.56916	-0.35
11	9	2	11	8	3	3.57313	0.08
12	9	4	12	8	5	3.58006	-0.21
8	2	6	8	1	7	3.60852	0.73
8	3	6	8	2	7	3.61440	0.38
7	1	6	7	0	7	3.64896	0.46
7	2	6	7	1	7	3.64987	0.34
11	9	3	11	8	4	3.66086	0.09
16	11	5	16	10	6	3.66451	0.30
14	9	6	14	8	7	3.68619	-0.08
13	6	7	13	5	8	3.72598	0.35
10	9	1	10	8	2	3.73995	0.32
10	9	2	10	8	3	3.75757	0.13
3	2	2	2	1	1	3.76053	0.54
18	12	6	18	11	7	3.81382	0.52
4	0	4	3	1	3	3.83251	0.63
9	9	0	9	8	1	3.83828	0.41
9	9	1	9	8	2	3.84059	0.08
4	1	4	3	0	3	3.84742	1.00
13	10	3	13	9	4	3.86027	0.19
16	8	8	16	7	9	3.91199	0.18
14	10	5	14	9	6	3.92339	-0.10
12	5	7	12	4	8	3.92828	0.48
15	10	6	15	9	7	3.92909	-0.10
14	8	7	14	7	8	3.93067	0.16
20	13	7	20	12	8	3.93891	0.44

13	7	7	13	6	8	3.95757	0.39
15	9	7	15	8	8	3.96202	-0.05
19	10	9	19	9	10	3.99237	0.39
16	15	1	15	14	2	25.16907	462.00
23	8	15	22	9	14	25.26925	119.00
24	7	17	23	8	16	25.57088	-196.00
28	1	27	27	2	26	25.71829	-121.00
24	8	16	23	9	15	26.14916	38.00
26	5	21	25	6	20	26.20216	-148.00
25	7	18	24	8	17	26.45447	-196.00
27	4	23	26	5	22	26.52302	-105.00
29	1	28	28	2	27	26.60477	-80.60
26	6	20	25	7	19	26.76907	-88.90
17	16	1	16	15	2	26.78081	106.00
30	0	30	29	1	29	26.92788	-100.00
25	8	17	24	9	16	27.03017	-11.00
27	5	22	26	6	21	27.08788	-114.00
29	2	27	28	3	26	27.16790	-139.00
26	7	19	25	8	18	27.33846	-82.30
28	4	24	27	5	23	27.40891	-167.00
30	1	29	29	2	28	27.49102	-77.40
25	9	16	24	10	15	27.61405	263.00
27	6	21	26	7	20	27.65415	-56.80
31	0	31	30	1	30	27.81414	-63.30
26	8	18	25	9	17	27.91200	-8.00
28	5	23	27	6	22	27.97348	-88.00
30	2	28	29	3	27	28.05400	-117.00
27	7	20	26	8	19	28.22246	-113.00
29	4	25	28	5	24	28.29476	-99.50
31	1	30	30	2	29	28.37709	-67.00
18	17	1	17	16	2	28.39178	-231.00
26	9	17	25	10	16	28.49202	-52.40
28	6	22	27	7	21	28.53914	-61.60
30	3	27	29	4	26	28.61724	66.90
32	0	32	31	1	31	28.70016	-80.50
27	8	19	26	9	18	28.79429	-74.00
18	18	0	17	17	1	28.84857	-163.00
29	5	24	28	6	23	28.85881	-174.00
31	2	29	30	3	28	28.93996	-35.00
28	7	21	27	8	20	29.10664	-55.00
30	4	26	29	5	25	29.18037	-90.10
32	1	31	31	2	30	29.26296	-69.30
27	9	18	26	10	17	29.37154	-47.90
29	6	23	28	7	22	29.42402	-84.70
31	3	28	30	4	27	29.50274	-101.00

33	0	33	32	1	32	29.58613	55.00
28	8	20	27	9	19	29.67700	-78.30
30	5	25	29	6	24	29.74419	-52.50
32	2	30	31	3	29	29.82559	-90.00
27	10	17	26	11	16	29.95764	137.00
29	7	22	28	8	21	29.99077	-59.90
19	18	1	18	17	2	30.00236	-110.00
31	4	27	30	5	26	30.06582	-57.40
33	1	32	32	2	31	30.14861	-89.30
28	9	19	27	10	18	30.25194	-48.10
30	6	24	29	7	23	30.30886	-36.80
32	3	29	31	4	28	30.38824	-75.00
19	19	0	18	18	1	30.45915	412.00
34	0	34	33	1	33	30.47168	-36.70
31	5	26	30	6	25	30.62927	-63.00
33	2	31	32	3	30	30.71113	-34.00
28	10	18	27	11	17	30.83398	-50.40
30	7	23	29	8	22	30.87487	-57.80
32	4	28	31	5	27	30.95106	-37.00
34	1	33	33	2	32	31.03413	-28.90
29	9	20	28	10	19	31.13296	-65.60
31	6	25	30	7	24	31.19346	-80.10
33	3	30	32	4	29	31.27356	-24.30
35	0	35	34	1	34	31.35712	-30.70
32	5	27	31	6	26	31.51419	-50.50
34	2	32	33	3	31	31.59654	104.00
20	19	1	19	18	2	31.61191	-142.00
29	10	19	28	11	18	31.71189	-36.10
31	7	24	30	8	23	31.75889	-67.20
33	4	29	32	5	28	31.83607	-45.00
35	1	34	34	2	33	31.91938	-31.30
30	9	21	29	10	20	32.01427	-231.00
20	20	0	19	19	1	32.06770	-139.00
32	6	26	31	7	25	32.07800	-35.20
34	3	31	33	4	30	32.15862	-26.20
36	0	36	35	1	35	32.24233	-40.00
29	11	18	28	12	17	32.30018	125.00
31	8	23	30	9	22	32.32624	16.90
33	5	28	32	6	27	32.39889	-62.50
35	2	33	34	3	32	32.48146	-30.40
30	10	20	29	11	19	32.59086	20.40
32	7	25	31	8	24	32.64284	-37.30
34	4	30	33	5	29	32.72085	-72.80
36	1	35	35	2	34	32.80444	-7.29
31	9	22	30	10	21	32.89623	-28.90

33	6	27	32	7	26	32.96238	25.00
22	17	5	21	16	6	32.98443	-83.10
35	3	32	34	4	31	33.04348	-2.32
37	0	37	36	1	36	33.12734	-24.70
30	11	19	29	12	18	33.17480	22.60
32	8	24	31	9	23	33.20927	-65.20
21	20	1	20	19	2	33.22122	515.00
34	5	29	33	6	28	33.28345	-6.22
36	2	34	35	3	33	33.36636	35.40
31	10	21	30	11	20	33.47045	-26.20
33	7	26	32	8	25	33.52663	-42.70
35	4	31	34	5	30	33.60553	18.00
37	1	36	36	2	35	33.68926	5.95
32	9	23	31	10	22	33.77823	28.40
34	6	28	33	7	27	33.84644	-47.70
36	3	33	35	4	32	33.92808	-13.20
38	0	38	37	1	37	34.01210	-34.90
31	11	20	30	12	19	34.05087	-142.00
35	5	30	34	6	29	34.16774	-8.57
37	2	35	36	3	34	34.25091	-16.30
32	10	22	31	11	21	34.35062	-10.70
34	7	27	33	8	26	34.41031	-1.24
36	4	32	35	5	31	34.48983	-40.60
38	1	37	37	2	36	34.57381	-18.60
23	18	5	22	17	6	34.59551	-351.00
33	9	24	32	10	23	34.66024	6.17
35	6	29	34	7	28	34.73040	-9.56
37	3	34	36	4	33	34.81249	12.30
22	21	1	21	20	2	34.82829	-98.40
39	0	39	38	1	38	34.89669	14.60
32	11	21	31	12	20	34.92833	-28.40
34	8	26	33	9	25	34.97538	-8.15
36	5	31	35	6	30	35.05179	-35.00
23	19	4	22	18	5	35.06189	-140.00
38	2	36	37	3	35	35.13526	-38.60
35	7	28	34	8	27	35.29384	58.10
37	4	33	36	5	32	35.37398	-22.70
39	1	38	38	2	37	35.45818	11.10
34	9	25	33	10	24	35.54230	20.30
36	6	30	35	7	29	35.61415	20.60
38	3	35	37	4	34	35.69661	-8.32
40	0	40	39	1	39	35.78097	-9.57
33	11	22	32	12	21	35.80653	-2.57
35	8	27	34	9	26	35.85825	11.80
37	5	32	36	6	31	35.93574	79.40

34	10	24	33	11	23	36.11192	74.60
36	7	29	35	8	28	36.17710	32.80
24	19	5	23	18	6	36.20568	-154.00
38	4	34	37	5	33	36.25789	-1.50
40	1	39	39	2	38	36.34225	-22.10
35	9	26	34	10	25	36.42435	36.30
23	22	1	22	21	2	36.43495	-95.30
37	6	31	36	7	30	36.49763	-0.97
39	3	36	38	4	35	36.58054	26.00
41	0	41	40	1	40	36.66505	14.70
24	20	4	23	19	5	36.67008	-60.50
34	11	23	33	12	22	36.68530	21.80
36	8	28	35	9	27	36.74097	13.00
38	5	33	37	6	32	36.81929	20.60
40	2	38	39	3	37	36.90332	17.30
35	10	25	34	11	24	36.99276	57.80
37	7	30	36	8	29	37.06007	-66.50
39	4	35	38	5	34	37.14166	116.00
41	1	40	40	2	39	37.22611	-13.20
36	9	27	35	10	26	37.30623	-32.50
38	6	32	37	7	31	37.38093	25.50
40	3	37	39	4	36	37.46415	-14.60
42	0	42	41	1	41	37.54886	11.30
35	11	24	34	12	23	37.56446	19.90
37	8	29	36	9	28	37.62351	14.70
39	5	34	38	6	33	37.70262	-3.17
41	2	39	40	3	38	37.78695	10.50
25	20	5	24	19	6	37.81434	-61.20
36	10	26	35	11	25	37.87361	-2.30
38	7	31	37	8	30	37.94304	35.10
40	4	36	39	5	35	38.02493	-7.04
24	23	1	23	22	2	38.04058	-54.90
42	1	41	41	2	40	38.10972	6.73
37	9	28	36	10	27	38.18811	-0.26
39	6	33	38	7	32	38.26380	-132.00
25	21	4	24	20	5	38.27699	-51.20
41	3	38	40	4	37	38.34759	36.00
43	0	43	42	1	42	38.43241	2.15
36	11	25	35	12	24	38.44379	-79.00
24	24	0	23	23	1	38.49428	-57.00
38	8	30	37	9	29	38.50588	22.10
40	5	35	39	6	34	38.58578	48.40
42	2	40	41	3	39	38.67034	32.10
37	10	27	36	11	26	38.75454	26.50
39	7	32	38	8	31	38.82573	89.50

41	4	37	40	5	36	38.90807	-1.87
43	1	42	42	2	41	38.99307	14.50
38	9	29	37	10	28	39.06978	-34.10
42	3	39	41	4	38	39.23069	0.85
44	0	44	43	1	43	39.31573	34.10
37	11	26	36	12	25	39.32347	-5.37
39	8	31	38	9	30	39.38803	22.00
26	21	5	25	20	6	39.42152	-47.60
41	5	36	40	6	35	39.46855	-34.70
43	2	41	42	3	40	39.55345	35.10
38	10	28	37	11	27	39.63538	10.10
25	24	1	24	23	2	39.64504	-71.70
40	7	33	39	8	32	39.70816	130.00
42	4	38	41	5	37	39.79100	60.40
44	1	43	43	2	42	39.87613	7.18
26	22	4	25	21	5	39.88269	-32.10
39	9	30	38	10	29	39.95123	-125.00
41	6	35	40	7	34	40.02927	36.40
25	25	0	24	24	1	40.09821	-41.40
43	3	40	42	4	39	40.11358	29.10
45	0	45	44	1	44	40.19874	11.10
38	11	27	37	12	26	40.20324	71.80
40	8	32	39	9	31	40.26994	7.21
42	5	37	41	6	36	40.35119	29.30
44	2	42	43	3	41	40.43627	15.30
39	10	29	38	11	28	40.51618	60.10
43	4	39	42	5	38	40.67354	9.03
45	1	44	44	2	43	40.75886	-62.50
40	9	31	39	10	30	40.83273	18.70
42	6	36	41	7	35	40.91171	221.00
44	3	41	43	4	40	40.99627	138.00
27	22	5	26	21	6	41.02732	-31.50
46	0	46	45	1	45	41.08148	3.10
39	11	28	38	12	27	41.08285	-21.80
41	8	33	40	9	32	41.15166	29.30
26	25	1	25	24	2	41.24838	-54.40
45	2	43	44	3	42	41.31883	16.80
40	10	30	39	11	29	41.39681	59.40
42	7	35	41	8	34	41.47211	41.40
27	23	4	26	22	5	41.48710	-44.40
44	4	40	43	5	39	41.55586	10.20
46	1	45	45	2	44	41.64146	16.50
26	26	0	25	25	1	41.70097	-17.70
41	9	32	40	10	31	41.71395	77.30
43	6	37	42	7	36	41.79351	34.00

45	3	42	44	4	41	41.87866	219.00
40	11	29	39	12	28	41.96263	85.30
47	0	47	46	1	46	41.96396	2.87
42	8	34	41	9	33	42.03312	34.40
44	5	39	43	6	38	42.11554	45.50
46	2	44	45	3	43	42.20112	28.50
41	10	31	40	11	30	42.27728	57.80
43	7	36	42	8	35	42.35372	35.40
45	4	41	44	5	40	42.43796	75.10
47	1	46	46	2	45	42.52359	-98.00
42	9	33	41	10	32	42.59478	-19.60
28	23	5	27	22	6	42.63175	0.29
44	6	38	43	7	37	42.67513	-47.20
46	3	43	45	4	42	42.76050	40.70
29	21	9	28	20	8	42.82440	0.15
41	11	30	40	12	29	42.84227	129.00
48	0	48	47	1	47	42.84622	73.30
27	26	1	26	25	2	42.85052	-32.20
43	8	35	42	9	34	42.91430	13.80
45	5	40	44	6	39	42.99728	38.60
47	2	45	46	3	44	43.08311	28.10
28	24	4	27	23	5	43.09027	-25.60
42	10	32	41	11	31	43.15753	18.10
44	7	37	43	8	36	43.23512	83.70
27	27	0	26	26	1	43.30249	-11.10
46	4	42	45	5	41	43.31964	5.81
48	1	47	47	2	46	43.40566	22.80
43	9	34	42	10	33	43.47552	30.10
45	6	39	44	7	38	43.55665	52.80
47	3	44	46	4	43	43.64220	6.08
42	11	31	41	12	30	43.72166	40.50
49	0	49	48	1	48	43.72807	20.40
46	5	41	45	6	40	43.87873	34.00
48	2	46	47	3	45	43.96480	20.60
43	10	33	42	11	32	44.03765	53.90
45	7	38	44	8	37	44.11607	-23.40
47	4	43	46	5	42	44.20112	31.40
29	24	5	28	23	6	44.23470	-55.30
49	1	48	48	2	47	44.28744	149.00
44	9	35	43	10	34	44.35598	36.10
46	6	40	45	7	39	44.43772	-12.30
28	27	1	27	26	2	44.45141	-2.68
48	3	45	47	4	44	44.52364	17.70
43	11	32	42	12	31	44.60099	42.70
50	0	50	49	1	49	44.60965	5.80

45	8	37	44	9	36	44.67591	34.40
47	5	42	46	6	41	44.75964	-207.00
49	2	47	48	3	46	44.84620	22.00
28	28	0	27	27	1	44.90275	7.16
44	10	34	43	11	33	44.91751	57.00
46	7	39	45	8	38	44.99692	49.70
48	4	44	47	5	43	45.08226	24.90
50	1	49	49	2	48	45.16867	24.90
45	9	36	44	10	35	45.23619	65.90
47	6	41	46	7	40	45.31862	61.50
49	3	46	48	4	45	45.40482	72.30
44	11	33	43	12	32	45.48013	36.20
51	0	51	50	1	50	45.49100	52.50
48	5	43	47	6	42	45.64073	34.80
50	2	48	49	3	47	45.72728	17.90
45	10	35	44	11	34	45.79711	31.40
30	25	5	29	24	6	45.83637	3.49
47	7	40	46	8	39	45.87736	24.40
49	4	45	48	5	44	45.96310	25.30
31	23	9	30	22	8	46.04222	160.00
51	1	50	50	2	49	46.04979	103.00
29	28	1	28	27	2	46.05093	-45.30
46	9	37	45	10	36	46.11607	43.80
48	6	42	47	7	41	46.19911	25.60
50	3	47	49	4	46	46.28553	-36.10
45	11	34	44	12	33	46.35907	31.00
52	0	52	51	1	51	46.37197	21.30
47	8	39	46	9	38	46.43630	-17.30
29	29	0	28	28	1	46.50167	0.74
49	5	44	48	6	43	46.52123	0.60
51	2	49	50	3	48	46.60806	14.30
48	7	41	47	8	40	46.75747	-32.90
50	4	46	49	5	45	46.84372	113.00
52	1	51	51	2	50	46.93042	-1.35
47	9	38	46	10	37	46.99569	33.60
49	6	43	48	7	42	47.07928	-7.35
51	3	48	50	4	47	47.16640	337.00
46	11	35	45	12	34	47.23784	70.20
53	0	53	52	1	52	47.25256	-63.00
50	5	45	49	6	44	47.40143	-15.50
31	26	5	30	25	6	47.43653	-7.68
52	2	50	51	3	49	47.48853	22.10
49	7	42	48	8	41	47.63735	-12.10
32	24	9	31	23	8	47.64707	79.40
30	29	1	29	28	2	47.64917	-30.40

51	4	47	50	5	46	47.72379	-18.20
53	1	52	52	2	51	47.81086	20.00
48	9	39	47	10	38	47.87500	21.30
31	27	4	30	26	5	47.89174	-26.60
50	6	44	49	7	43	47.95919	14.00
52	3	49	51	4	48	48.04630	57.50
30	30	0	29	29	1	48.09922	-5.77
47	11	36	46	12	35	48.11603	-223.00
51	5	46	50	6	45	48.28128	-60.30
53	2	51	52	3	50	48.36868	33.90
50	7	43	49	8	42	48.51681	-78.40
52	4	48	51	5	47	48.60368	-5.37
54	1	53	53	2	52	48.69098	57.60
49	9	40	48	10	39	48.75400	-3.69
51	6	45	50	7	44	48.83854	-207.00
53	3	50	52	4	49	48.92614	46.20
48	11	37	47	12	36	48.99417	-304.00
55	0	55	54	1	54	49.01300	-14.40
32	27	5	31	26	6	49.03527	-2.76
52	5	47	51	6	46	49.16080	-108.00
31	30	1	30	29	2	49.24605	31.40
51	7	44	50	8	43	49.39607	-23.10
53	4	49	52	5	48	49.48325	13.20
32	28	4	31	27	5	49.48949	10.30
50	9	41	49	10	40	49.63279	72.50
31	31	0	30	30	1	49.69539	20.10
52	6	46	51	7	45	49.71804	62.90
54	3	51	53	4	50	49.80559	-18.70
49	11	38	48	12	37	49.87242	-9.38
56	0	56	55	1	55	49.89241	-304.00
53	5	48	52	6	47	50.04009	-49.30
52	7	45	51	8	44	50.27491	-58.40
54	4	50	53	5	49	50.36239	-60.80
56	1	55	55	2	54	50.45003	-77.70
53	6	47	52	7	46	50.59654	-331.00
33	28	5	32	27	6	50.63252	2.29
55	3	52	54	4	51	50.68470	-91.50
50	11	39	49	12	38	50.75017	70.40
57	0	57	56	1	56	50.77191	-176.00
32	31	1	31	30	2	50.84142	8.55
34	26	9	33	25	8	50.85059	39.40
33	29	4	32	28	5	51.08573	-0.23
32	32	0	31	31	1	51.29009	31.80
57	1	56	56	2	55	51.32923	38.90
56	3	53	55	4	52	51.56359	-30.30

58	0	58	57	1	57	51.65130	196.00
34	29	5	33	28	6	52.22830	52.60
33	32	1	32	31	2	52.43534	27.40
35	27	9	34	26	8	52.44942	26.90
34	30	4	33	29	5	52.68045	-24.70
33	33	0	32	32	1	52.88329	47.50
35	30	5	34	29	6	53.82243	7.71
34	33	1	33	32	2	54.02771	24.20
36	28	9	35	27	8	54.04640	36.10
35	31	4	34	30	5	54.27368	-5.48
34	34	0	33	33	1	54.47491	34.50
35	34	1	34	33	2	55.61853	53.20
37	29	9	36	28	8	55.64152	50.10
36	32	4	35	31	5	55.86537	61.40
35	35	0	34	34	1	56.06495	30.80
37	32	5	36	31	6	57.00597	24.90
36	35	1	35	34	2	57.20767	16.60
38	30	9	37	29	8	57.23477	42.10
37	33	4	36	32	5	57.45533	15.80
36	36	0	35	35	1	57.65333	18.40
38	33	5	37	32	6	58.59524	10.60
37	36	1	36	35	2	58.79514	-17.80
38	34	4	37	33	5	59.04364	1.54
37	37	0	36	36	1	59.24004	18.10
39	34	5	38	33	6	60.18279	-3.34
38	37	1	37	36	2	60.38094	4.05
40	32	9	39	31	8	60.41570	37.30
39	35	4	38	34	5	60.63024	-1.88
38	38	0	37	37	1	60.82502	29.70
40	35	5	39	34	6	61.76859	-0.41
39	38	1	38	37	2	61.96497	-1.08
40	36	4	39	35	5	62.21509	1.08
39	39	0	38	38	1	62.40822	36.80
41	36	5	40	35	6	63.35259	-14.70
40	39	1	39	38	2	63.54719	2.50
41	37	4	40	36	5	63.79823	103.00
42	37	5	41	36	6	64.93474	-28.80
41	40	1	40	39	2	65.12749	-65.60
43	38	5	42	37	6	66.51496	-78.90
44	39	5	43	38	6	68.09330	-82.20
45	40	5	44	39	6	69.66964	-115.00

Table S3: Predicted frequencies of most promising transitions (in MHz) to be found in the range of 300-400 GHz at 100 K based on the spectroscopic parameters reported in Table 2 using transitions listed in Table S2.

J'	K_a'	K_c'	J''	K_a''	K_c''	<i>Predicted Frequency / MHz</i>
11	1	11	10	0	10	301599.4289
11	0	11	10	1	10	301599.4275
9	4	6	8	3	5	301889.1625
9	4	5	8	5	4	303433.5057
10	3	8	9	2	7	309016.9997
10	2	8	9	3	7	308970.7247
8	5	4	7	4	3	313907.7486
7	5	2	6	4	3	316595.2000
7	6	2	6	5	1	317359.3685
11	2	10	10	1	9	318568.7666
11	1	10	10	2	9	318568.5921
7	6	1	6	5	2	319822.0689
10	3	7	9	4	6	325814.5753
10	4	7	9	3	6	326851.5739
12	1	12	11	0	11	328228.5634
12	0	12	11	1	11	328228.5632
9	5	5	8	4	4	331561.4189
7	7	0	6	6	1	332594.6007
7	7	1	6	6	0	332520.5467
11	3	9	10	2	8	335598.6183
11	2	9	10	3	8	335589.5087
10	4	6	9	5	5	338724.1458
12	2	11	11	1	10	345194.4414
12	1	11	11	2	10	345194.4130
8	6	3	7	5	2	346865.6242
10	5	6	9	4	5	350262.8153
11	4	8	10	3	7	352925.9235
11	3	8	10	4	7	352675.5220
13	1	13	12	0	12	354853.0948
13	0	13	12	1	12	354853.0947
8	6	2	7	5	3	358780.9525
12	3	10	11	2	9	362202.4977
12	2	10	11	3	9	362200.7942
8	7	2	7	6	1	366693.3006
8	7	1	7	6	2	367574.4813
11	4	7	10	5	6	368706.3132
9	6	4	8	5	3	369846.0542
7	3	4	6	2	5	370049.1985
13	2	12	12	1	11	371816.5348
13	1	12	12	2	11	371816.5303

11	5	7	10	4	6	372480.5723
12	4	9	11	3	8	379361.0166
12	3	9	11	4	8	379305.5494
8	8	0	7	7	1	381039.9932
8	8	1	7	7	0	381018.8640
14	1	14	13	0	13	381472.6101
14	0	14	13	1	13	381472.6101
10	6	5	9	5	4	387276.3173
13	3	11	12	2	10	388811.4562
13	2	11	12	3	10	388811.1503
12	4	8	11	5	7	396299.5358
12	5	8	11	4	7	397350.0963
14	2	13	13	1	12	398434.2627
14	1	13	13	2	12	398434.2620
9	7	3	8	6	2	398756.9322

Figure S1: Simulated spectrum of oxirane-D₁ in the range of 300-400 GHz at T = 100 K based on spectroscopic parameters reported in Table 2 using transitions reported in Table S2.

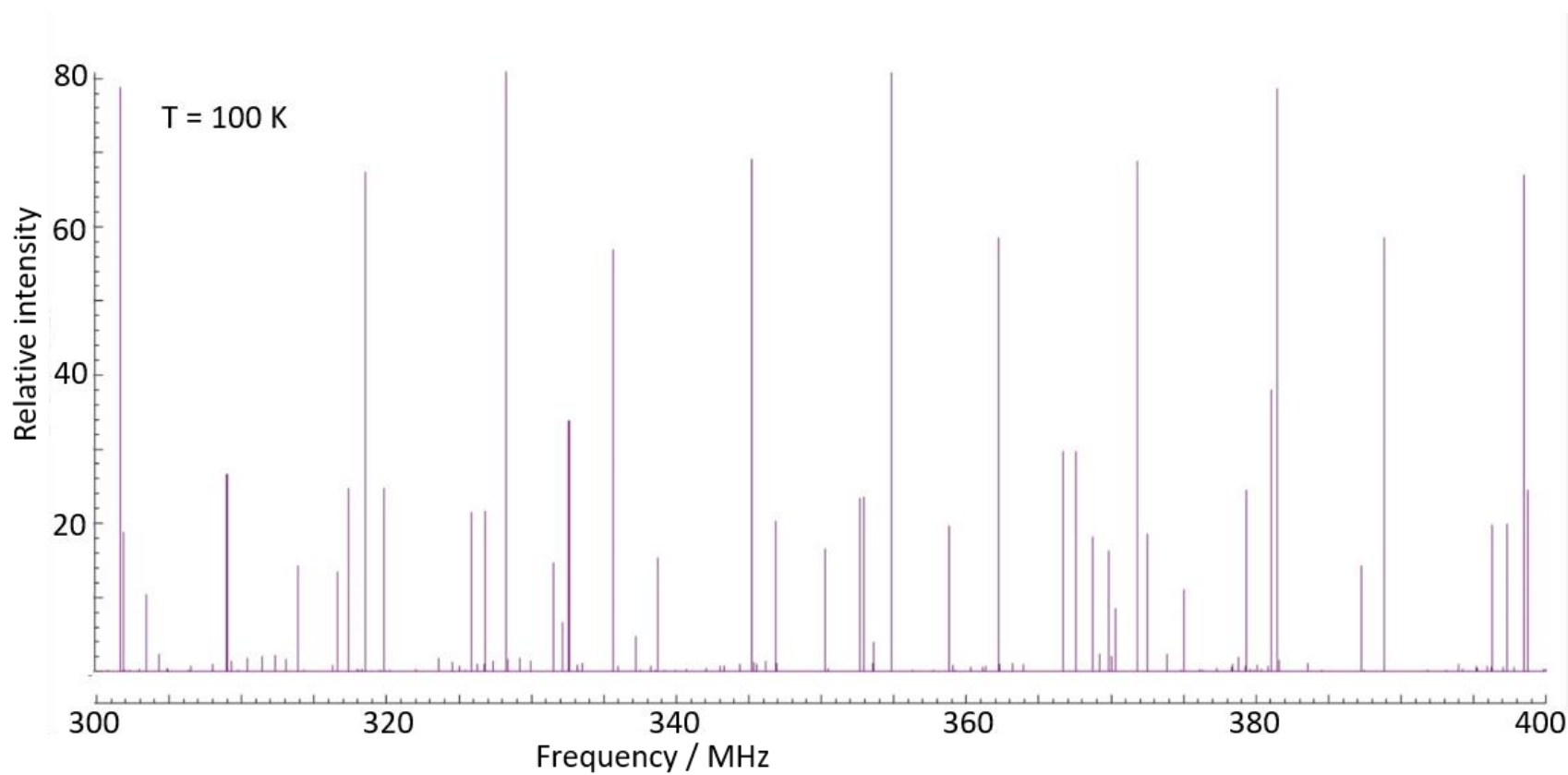


Figure S2: Simulated spectrum of oxirane-D₁ in the range of 300-400 GHz at T = 200 K based on spectroscopic parameters reported in Table 2 using transitions reported in Table S2.

