

Supplementary Materials: High Resolution Infrared Spectroscopy of Monodeutero-oxirane (*c*-C₂H₃DO) and analysis of two fundamentals between 820 and 950 cm⁻¹

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Supplementary Information supplied:

Table A_1: Assigned transitions, ν_{13} fundamental. Wavenumbers are given in cm⁻¹, $\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$ with parameters from Table 6 (model with Coriolis coupling).

Table A_2: Assigned transitions, ν_{12} fundamental. Wavenumbers are given in cm⁻¹, $\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$ with parameters from Table 6 (model with Coriolis coupling).

Table S4_1: Spectroscopic parameters for the ground state of monodeuterooxirane in the MW, GHz and THz ranges resulting from refitting all transitions reported in [17], including results from [14, 43] (values in parenthesis provide statistical 1 σ uncertainties in units of the last specified digits.).

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated transitions E'' with parameters of (WANG) SP from Table 4, $\Delta_{\text{O-C}} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis, including further data of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

Table C1(Corrected version of Table 1 in Albert et al. [14]): Spectroscopic parameters for the ground state of monodeutero-oxirane in the MW and GHz ranges in MHz (values in parenthesis provide statistical 1 σ uncertainties in units of the last specified digits).

Table C2(Corrected version of Table 2 in Albert et al. [14]): Spectroscopic parameters for the ground state of C₂H₃DO in cm⁻¹.

Table CS1(Corrected version of Table S1 in Albert et al. [14]): Observed pure rotational transitions (ν , $\tilde{\nu}$, in MHz and cm⁻¹) of the ground state of monodeutero-oxirane in only MW and GHz regions. J , K_a and K_c are quantum numbers, $\nu_{\text{obs.}}$ and $\tilde{\nu}_{\text{obs.}}$ = observed transition frequencies in MHz and cm⁻¹, and $\tilde{\nu}_{\text{calc.}}$ = wavenumbers using the reported spectroscopic parameters (lower states ", upper states '). Spectroscopic parameters used in fitting are presented in Table C2(2019).

Table CS2 (Corrected version of Table S2 in Albert et al. [14]): Observed pure rotational transitions ($\tilde{\nu}$, in cm⁻¹) of the ground state of monodeutero-oxirane 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 C2 (2019).

Table CS3 (Corrected version of Table S3 in Albert et al. [14]): 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 C2 using transitions listed in Table CS2 (2019).

Figure S_1: A comparison of the THz spectrum of monodeutero-oxirane near 47.7 cm⁻¹(from top to bottom): 1) observed spectrum; 2) simulated spectrum based on the global analysis of this study (Table 4, column 4); 3) simulated spectrum reproduced using data in [14] (Table 4, column 1); 4) simulated spectrum reproduced using data in [17] (Table 4, column 2). Quantum numbers of transitions are arranged in the form of $J'K_a'K_c' - J''K_a''K_c''$.

Figure S_2: A comparison of the THz spectrum of monodeutero-oxirane near 35 cm⁻¹ (from top to bottom): 1) observed spectrum; 2) simulated spectrum based on the global analysis of this study (Table 4, column 4); 3) simulated spectrum reproduced using data in [14] (Table 4, column 1); 4) simulated spectrum reproduced using data in [17] (Table 4, column 2). Quantum numbers of transitions are arranged in the form of $J'K_a'K_c' - J''K_a''K_c''$.

Figure S_3: A comparison of the THz spectrum of monodeutero-oxirane near 47.5 cm⁻¹ (from top to bottom): 1) observed spectrum; 2) simulated spectrum based on the global analysis of this study (Table 4, column 4); 3) simulated spectrum reproduced using data in [14] (Table 4, column 1); 4) simulated spectrum reproduced using data in [17] (Table 4, column 2).

Figure S_4: A comparison of the THz spectrum of monodeutero-oxirane near 49.9 cm⁻¹ (from top to bottom): 1) observed spectrum; 2) simulated spectrum based on the global analysis of this study (Table 4, column 4); 3) simulated spectrum reproduced using data in [14] (Table 4, column 1); 4) simulated spectrum reproduced using data in [17] (Table 4, column 2).

Table Sa: Anharmonic constants as calculated ab initio, see section theory of the main paper.

References: (following the convention of this publication)

[14] S. Albert, Z. Chen, K. Keppler, P. Lerch, M. Quack, V. Schurig and O. Trapp, *Phys. Chem. Chem. Phys.* 2019, **21**, 3669.

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[28] C. Puzzarini, M. Biczysko, J. Bloino and V. Barone, *Astrophys. J.*, 2014, **785**, 107.

[43] C. Hirose, *Bull. Chem. Soc. Jpn.*, 1974, **47**, 1311.

Table A_1: $\nu_{13} \leftarrow$ ground state of $\text{C}_2\text{H}_3\text{DO}$ (Albert, et al., *PCCP*, 2025)

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
6	6	1	7	7	0	826.25990	-0.00232
7	7	1	8	8	0	824.63800	-0.00324
8	8	1	9	9	0	823.01640	-0.00270
9	9	1	10	10	0	821.39470	-0.00161
10	10	1	11	11	0	819.77250	-0.00059
11	11	1	12	12	0	818.14980	0.00023
12	12	1	13	13	0	816.52670	0.00082
13	13	1	14	14	0	814.90350	0.00138
14	14	1	15	15	0	813.27990	0.00151
15	15	1	16	16	0	811.65640	0.00165
16	16	1	17	17	0	810.03260	0.00132
18	18	1	19	19	0	806.78520	0.00025
19	19	1	20	20	0	805.16180	-0.00028
20	20	1	21	21	0	803.53850	-0.00083
21	21	1	22	22	0	801.91540	-0.00121
8	8	1	7	7	0	850.05270	-0.00208
9	9	1	8	8	0	851.66320	-0.00136
10	10	1	9	9	0	853.27230	-0.00054
11	11	1	10	10	0	854.88010	0.00031
12	12	1	11	11	0	856.48640	0.00095
13	13	1	12	12	0	858.09120	0.00134
14	14	1	13	13	0	859.69460	0.00159
15	15	1	14	14	0	861.29640	0.00150
16	16	1	15	15	0	862.89680	0.00131
17	17	1	16	16	0	864.49570	0.00098
18	18	1	17	17	0	866.09290	0.00038
19	19	1	18	18	0	867.68850	-0.00026
20	20	1	19	19	0	869.28230	-0.00099
21	21	1	20	20	0	870.87480	-0.00112
22	22	1	21	21	0	872.46510	-0.00129
23	23	1	22	22	0	874.05410	-0.00030
24	24	1	23	23	0	875.64100	0.00141
6	5	2	7	6	1	826.71580	-0.00574
6	5	1	7	6	2	826.79110	-0.00565
7	6	2	8	7	1	825.12390	-0.00439
7	6	1	8	7	2	825.15010	-0.00455
8	7	2	9	8	1	823.51660	-0.00285
8	7	1	9	8	2	823.52470	-0.00334
9	8	2	10	9	1	821.90270	-0.00178
10	9	2	11	10	1	820.28640	-0.00073
11	10	2	12	11	1	818.66880	0.00003
12	11	2	13	12	1	817.05040	0.00051
13	12	2	14	13	1	815.43170	0.00101
14	13	2	15	14	1	813.81250	0.00122
15	14	2	16	15	1	812.19340	0.00165

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Continuation of Table A_1: ν_{13} ← ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
16	15	2	17	16	1	810.57340	0.00127
17	16	2	18	17	1	808.95290	0.00043
18	17	2	19	18	1	807.33300	0.00021
19	18	2	20	19	1	805.71280	-0.00025
20	19	2	21	20	1	804.09250	-0.00071
21	20	2	22	21	1	802.47190	-0.00127
22	21	2	23	22	1	800.85160	-0.00120
7	6	2	6	5	1	847.97100	-0.00412
7	6	1	6	5	2	848.05020	-0.00401
8	7	2	7	6	1	849.61670	-0.00336
8	7	1	7	6	2	849.64490	-0.00336
9	8	1	8	7	1	851.24780	-0.00071
10	9	1	9	8	2	852.86370	-0.00398
11	10	2	10	9	1	854.47920	0.00026
12	11	2	11	10	1	856.09120	0.00044
13	12	2	12	11	1	857.70180	0.00099
14	13	2	13	12	1	859.31060	0.00135
15	14	2	14	13	1	860.91760	0.00144
16	15	2	15	14	1	862.52270	0.00119
17	16	2	16	15	1	864.12620	0.00093
18	17	2	17	16	1	865.72760	0.00024
19	18	2	18	17	1	867.32740	-0.00028
20	19	2	19	18	1	868.92480	-0.00129
21	20	2	20	19	1	870.52100	-0.00140
22	21	2	21	20	1	872.11500	-0.00139
23	22	2	22	21	1	873.70680	-0.00097
24	23	2	23	22	1	875.29660	0.00040
25	24	2	24	23	1	876.88430	0.00301
21	19	3	22	20	2	803.02510	-0.00043
20	18	3	21	19	2	804.64190	-0.00035
19	17	3	20	18	2	806.25870	0.00006
18	16	3	19	17	2	807.87500	0.00022
17	15	3	18	16	2	809.49140	0.00070
16	14	3	17	15	2	811.10740	0.00096
15	13	3	16	14	2	812.72240	0.00043
14	12	3	15	13	2	814.33810	0.00086
13	11	3	14	12	2	815.95270	0.00057
12	10	3	13	11	2	817.56820	0.00192
11	9	2	12	10	3	819.18390	-0.00193
11	9	3	12	10	2	819.17790	-0.00074
10	8	3	11	9	2	820.78170	-0.00466
10	8	2	11	9	3	820.80540	-0.00248
10	8	3	9	7	2	852.40340	-0.00200
10	8	2	9	7	3	852.46900	-0.00156

Continuation of Table A_1: ν_{13} ← ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
11	9	3	10	8	2	854.04820	-0.00116
12	10	3	11	9	2	855.67700	0.00010
12	10	2	11	9	3	855.68460	-0.00026
13	11	3	12	10	2	857.29950	0.00274
14	12	3	13	11	2	858.91380	0.00120
15	13	3	14	12	2	860.52690	0.00109
16	14	3	15	13	2	862.13780	0.00090
17	15	3	16	14	2	863.74680	0.00076
18	16	3	17	15	2	865.35390	0.00068
19	17	3	18	16	2	866.95850	0.00009
20	18	3	19	17	2	868.56120	-0.00030
21	19	3	20	18	2	870.16220	-0.00013
19	16	4	20	17	3	806.79780	-0.00035
18	15	4	19	16	3	808.40940	-0.00110
17	14	4	18	15	3	810.02170	-0.00087
16	13	4	17	14	3	811.63540	0.00109
15	12	4	16	13	3	813.24760	0.00207
14	11	4	15	12	3	814.85570	0.00016
14	11	3	15	12	4	814.86080	-0.00003
13	10	4	14	11	3	816.46170	-0.00069
13	10	3	14	11	4	816.47820	0.00019
12	9	4	13	10	3	818.06100	0.00005
12	9	3	13	10	4	818.10360	-0.00127
13	10	4	12	9	3	856.84670	-0.00011
13	10	3	12	9	4	856.89420	-0.00050
14	11	4	13	10	3	858.48760	-0.00005
14	11	3	13	10	4	858.50510	0.00013
15	12	4	14	11	3	860.11550	0.00046
15	12	3	14	11	4	860.12170	0.00068
18	15	4	17	14	3	864.96610	0.00000
19	16	4	18	15	3	866.57670	-0.00061
20	17	4	19	16	3	868.18560	-0.00048
21	18	4	20	17	3	869.79220	-0.00016
6	1	6	5	0	5	843.27630	-0.00047
7	1	7	6	0	6	844.27100	0.00124
8	1	8	7	0	7	845.27940	0.00246
9	1	9	8	0	8	846.30060	0.00331
10	1	10	9	0	9	847.33370	0.00384
11	1	11	10	0	10	848.37740	0.00377
12	1	12	11	0	11	849.43040	0.00281
13	1	13	12	0	12	850.49250	0.00184
14	1	14	13	0	13	851.56240	0.00062
15	1	15	14	0	14	852.63920	-0.00070
16	1	16	15	0	15	853.72200	-0.00200

Continuation of Table A_1: ν_{13} ← ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
17	1	17	16	0	16	854.81030	-0.00282
18	1	18	17	0	17	855.90320	-0.00320
19	1	19	18	0	18	857.00010	-0.00296
20	1	20	19	0	19	858.10030	-0.00220
21	1	21	20	0	20	859.20380	-0.00048
22	1	22	21	0	21	860.30940	0.00126
23	1	23	22	0	22	861.41730	0.00319
27	1	27	28	0	28	816.43890	-0.00712
26	1	26	27	0	27	817.09960	0.00031
25	1	25	26	0	26	817.76170	0.00359
24	1	24	25	0	25	818.42530	0.00415
23	1	23	24	0	24	819.09060	0.00315
22	1	22	23	0	23	819.75780	0.00139
21	1	21	22	0	22	820.42710	-0.00065
20	1	20	21	0	21	821.09940	-0.00204
19	1	19	20	0	20	821.77480	-0.00292
18	1	18	19	0	19	822.45390	-0.00311
17	1	17	18	0	18	823.13710	-0.00282
16	1	16	17	0	17	823.82530	-0.00190
15	1	15	16	0	16	824.51900	-0.00071
14	1	14	15	0	15	825.21910	0.00072
13	1	13	14	0	14	825.92610	0.00187
12	1	12	13	0	13	826.64140	0.00310
11	1	11	12	0	12	827.36520	0.00356
10	1	10	11	0	11	828.09900	0.00371
9	1	9	10	0	10	828.84360	0.00332
8	1	8	9	0	9	829.60010	0.00252
7	1	7	8	0	8	830.36950	0.00140
6	1	6	7	0	7	831.15230	-0.00041
5	1	5	6	0	6	831.94960	-0.00271
27	2	26	28	1	27	815.61210	-0.00164
26	2	25	27	1	26	816.27340	0.00217
25	2	24	26	1	25	816.93640	0.00285
24	2	23	25	1	24	817.60200	0.00233
23	2	22	24	1	23	818.26990	0.00101
22	2	21	23	1	22	818.94040	-0.00045
21	2	20	22	1	21	819.61360	-0.00187
20	2	19	21	1	20	820.29020	-0.00272
19	2	18	20	1	19	820.97070	-0.00286
18	2	17	19	1	18	821.65530	-0.00267
17	2	16	18	1	17	822.34500	-0.00183
16	2	15	17	1	16	823.04000	-0.00098
15	2	14	16	1	15	823.74200	0.00067
14	2	13	15	1	14	824.45090	0.00205

Continuation of Table A_1: ν_{13} $\leftarrow$ ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
13	2	12	14	1	13	825.16750	0.00294
8	2	7	7	1	6	845.71540	0.00107
9	2	8	8	1	7	846.72130	0.00225
10	2	9	9	1	8	847.74070	0.00335
11	2	10	10	1	9	848.77110	0.00318
12	2	11	11	1	10	849.81340	0.00371
13	2	12	12	1	11	850.86470	0.00309
14	2	13	13	1	12	851.92450	0.00189
15	2	14	14	1	13	852.99220	0.00057
16	2	15	15	1	14	854.06670	-0.00096
17	2	16	16	1	15	855.14780	-0.00187
18	2	17	17	1	16	856.23420	-0.00255
19	2	18	18	1	17	857.32510	-0.00297
20	2	19	19	1	18	858.42030	-0.00260
21	2	20	20	1	19	859.51890	-0.00177
22	2	21	21	1	20	860.62050	-0.00049
23	2	22	22	1	21	861.72490	0.00121
24	2	23	23	1	22	862.83140	0.00256
25	2	24	24	1	23	863.93980	0.00302
26	2	25	25	1	24	865.05040	0.00221
27	2	26	26	1	25	866.16230	-0.00180
28	3	26	29	2	27	814.12810	-0.00286
27	3	25	28	2	26	814.78740	0.00100
26	3	24	27	2	25	815.45000	0.00263
25	3	23	26	2	24	816.11520	0.00247
24	3	22	25	2	23	816.78300	0.00129
23	3	21	24	2	22	817.45370	-0.00016
22	3	20	23	2	21	818.12750	-0.00153
21	3	19	22	2	20	818.80490	-0.00241
20	3	18	21	2	19	819.48630	-0.00272
19	3	17	20	2	18	820.17240	-0.00226
18	3	16	19	2	17	820.86310	-0.00179
16	3	14	17	2	15	822.26280	0.00050
15	3	13	16	2	14	822.97310	0.00179
10	3	8	9	2	7	848.16350	0.00192
11	3	9	10	2	8	849.17980	0.00304
12	3	10	11	2	9	850.20810	0.00323
13	3	11	12	2	10	851.24780	0.00343
14	3	12	13	2	11	852.29680	0.00272
15	3	13	14	2	12	853.35480	0.00189
16	3	14	15	2	13	854.42040	0.00061
18	3	16	17	2	15	856.57170	-0.00197
19	3	17	18	2	16	857.65630	-0.00249
20	3	18	19	2	17	858.74570	-0.00258

Continuation of Table A_1: ν_{13} ← ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
21	3	19	20	2	18	859.83890	-0.00254
22	3	20	21	2	19	860.93630	-0.00147
23	3	21	22	2	20	862.03660	-0.00033
24	3	22	23	2	21	863.13980	0.00099
25	3	23	24	2	22	864.24550	0.00195
29	4	26	30	3	27	812.64760	-0.00333
28	4	25	29	3	26	813.30480	0.00125
27	4	24	28	3	25	813.96530	0.00280
26	4	23	27	3	24	814.62880	0.00228
24	4	21	25	3	22	815.96640	-0.00022
23	4	20	24	3	21	816.64080	-0.00112
22	4	19	23	3	20	817.31830	-0.00237
21	4	18	22	3	19	818.00030	-0.00282
20	4	17	21	3	18	818.68730	-0.00240
19	4	16	20	3	17	819.37920	-0.00181
18	4	15	19	3	16	820.07890	0.00112
17	4	14	18	3	15	820.78170	0.00087
16	4	13	17	3	14	821.49280	0.00175
15	4	12	16	3	13	822.21160	0.00223
14	4	11	15	3	12	822.94020	0.00347
13	4	10	14	3	11	823.67730	0.00322
12	4	9	11	3	8	850.62000	0.00278
13	4	10	12	3	9	851.64480	0.00316
14	4	11	13	3	10	852.68140	0.00312
15	4	12	14	3	11	853.72750	0.00205
16	4	13	15	3	12	854.78340	0.00150
17	4	14	16	3	13	855.84740	0.00090
18	4	15	17	3	14	856.91930	0.00105
19	4	16	18	3	15	857.99430	-0.00187
20	4	17	19	3	16	859.07690	-0.00249
21	4	18	20	3	17	860.16470	-0.00244
22	4	19	21	3	18	861.25670	-0.00210
23	4	20	22	3	19	862.35250	-0.00141
24	4	21	23	3	20	863.45270	0.00052
25	4	22	24	3	21	864.55540	0.00181
26	4	23	25	3	22	865.66060	0.00226
27	4	24	26	3	23	866.76950	0.00254
28	4	25	27	3	24	867.88090	0.00059
29	4	26	28	3	25	868.99650	-0.00311
30	5	26	31	4	27	811.17000	-0.00353
29	5	25	30	4	26	811.82380	0.00122
28	5	24	29	4	25	812.48200	0.00319
27	5	23	28	4	24	813.14370	0.00284
25	5	21	26	4	22	814.47950	0.00063

Continuation of Table A_1: ν_{13} ← ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
24	5	20	25	4	21	815.15320	-0.00067
23	5	19	24	4	20	815.83120	-0.00149
22	5	18	23	4	19	816.51340	-0.00211
21	5	17	22	4	18	817.20040	-0.00229
20	5	16	21	4	17	817.89270	-0.00206
19	5	15	20	4	16	818.59320	0.00082
18	5	14	19	4	15	819.29710	0.00080
17	5	13	18	4	14	820.00860	0.00124
16	5	12	17	4	13	820.72720	0.00080
14	5	10	13	4	9	853.08240	0.00258
15	5	11	14	4	10	854.11520	0.00289
16	5	12	15	4	11	855.15660	0.00030
17	5	13	16	4	12	856.21140	0.00142
18	5	14	17	4	13	857.27270	0.00061
19	5	15	18	4	14	858.34240	0.00087
20	5	16	19	4	15	859.41490	-0.00244
21	5	17	20	4	16	860.49640	-0.00227
22	5	18	21	4	17	861.58240	-0.00237
24	5	20	23	4	19	863.76840	-0.00075
25	5	21	24	4	20	864.86750	0.00070
26	5	22	25	4	21	865.97010	0.00204
27	5	23	26	4	22	867.07620	0.00296
15	6	10	16	5	11	820.70600	0.00237
16	6	11	17	5	12	819.96960	0.00330
17	6	12	18	5	13	819.23670	-0.00187
18	6	13	19	5	14	818.52010	0.00070
19	6	14	20	5	15	817.80880	0.00078
21	6	16	22	5	17	816.40250	-0.00309
22	6	17	23	5	18	815.71100	-0.00215
23	6	18	24	5	19	815.02400	-0.00177
24	6	19	25	5	20	814.33810	-0.00489
25	6	20	26	5	21	813.66470	0.00016
26	6	21	27	5	22	812.99170	0.00138
27	6	22	28	5	23	812.32340	0.00291
29	6	24	30	5	25	810.99910	0.00306
30	6	25	31	5	26	810.34410	0.00086
31	6	26	32	5	27	809.69380	-0.00477
18	6	13	17	5	12	857.63850	0.00082
19	6	14	18	5	13	858.69740	0.00050
20	6	15	19	5	14	859.76510	0.00129
21	6	16	20	5	15	860.83440	-0.00299
22	6	17	21	5	16	861.91500	-0.00177
23	6	18	22	5	17	862.99940	-0.00185
24	6	19	23	5	18	864.08950	-0.00079

Continuation of Table A_1: ν_{13} $\leftarrow$ ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
25	6	20	24	5	19	865.18350	-0.00002
26	6	21	25	5	20	866.28230	0.00150
32	7	26	33	6	27	808.21950	-0.00627
31	7	25	32	6	26	808.86590	0.00066
30	7	24	31	6	25	809.51720	0.00332
29	7	23	30	6	24	810.17370	0.00365
28	7	22	29	6	23	810.83640	0.00384
27	7	21	28	6	22	811.50270	0.00215
25	7	19	26	6	20	812.85090	-0.00019
24	7	18	25	6	19	813.53180	-0.00157
23	7	17	24	6	18	814.21880	-0.00171
20	7	14	21	6	15	816.31610	0.00101
19	7	13	20	6	14	817.02600	-0.00015
18	7	12	19	6	13	817.74090	-0.00379

Table A_2: $\nu_{12} \leftarrow$ ground state of $\text{C}_2\text{H}_3\text{DO}$ (Albert, et al., *PCCP* 2025)

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
9	9	1	8	8	0	910.21050	-0.00012
10	10	1	9	9	0	911.79310	-0.00009
11	11	1	10	10	0	913.37180	0.00011
12	12	1	11	11	0	914.94620	0.00005
13	13	1	12	12	0	916.51650	-0.00004
14	14	1	13	13	0	918.08280	-0.00004
15	15	1	14	14	0	919.64500	-0.00005
16	16	1	15	15	0	921.20320	0.00007
17	17	1	16	16	0	922.75720	0.00013
18	18	1	17	17	0	924.30690	0.00004
19	19	1	18	18	0	925.85260	0.00013
20	20	1	19	19	0	927.39400	0.00010
21	21	1	20	20	0	928.93120	0.00007
22	22	1	21	21	0	930.46420	0.00006
23	23	1	22	22	0	931.99290	-0.00003
24	24	1	23	23	0	933.51740	-0.00008
25	25	1	24	24	0	935.03780	0.00000
26	26	1	25	25	0	936.55380	-0.00006
27	27	1	26	26	0	938.06580	0.00013
28	28	1	27	27	0	939.57290	-0.00031
29	29	1	28	28	0	941.07620	-0.00028
30	30	1	29	29	0	942.57510	-0.00038
31	31	1	30	30	0	944.07010	-0.00010
32	32	1	31	31	0	945.56040	-0.00023
33	33	1	32	32	0	947.04650	-0.00027
34	34	1	33	33	0	948.52880	0.00018
35	35	1	34	34	0	950.00630	0.00013
36	36	1	35	35	0	951.47980	0.00038
28	28	1	29	29	0	848.16820	-0.00032
29	29	1	30	30	0	846.47540	0.00010
27	27	1	28	28	0	849.86030	0.00014
26	26	1	27	27	0	851.54990	-0.00023
25	25	1	26	26	0	853.23830	-0.00003
24	24	1	25	25	0	854.92440	-0.00029
23	23	1	24	24	0	856.60910	-0.00001
22	22	1	23	23	0	858.29160	0.00008
21	21	1	22	22	0	859.97190	0.00008
20	20	1	21	21	0	861.64990	-0.00004
19	19	1	20	20	0	863.32560	-0.00019
18	18	1	19	19	0	864.99920	-0.00009
17	17	1	18	18	0	866.67030	-0.00006
15	15	1	16	16	0	870.00480	-0.00010
14	14	1	15	15	0	871.66820	-0.00002
13	13	1	14	14	0	873.32890	0.00010
11	11	1	12	12	0	876.64140	-0.00008

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of $\text{C}_2\text{H}_3\text{DO}$

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
10	10	1	11	11	0	878.29320	-0.00023
9	9	1	10	10	0	879.94210	-0.00026
8	8	1	9	9	0	881.58800	-0.00018
7	7	1	8	8	0	883.23080	0.00009
6	6	1	7	7	0	884.86950	0.00001
4	4	1	5	5	0	888.12750	-0.00041
5	5	0	6	6	1	886.51040	-0.00056
4	4	0	5	5	1	888.15200	-0.00078
9	8	2	8	7	1	909.78400	0.00010
7	6	2	8	7	1	883.71030	-0.00018
8	7	2	9	8	1	882.08020	-0.00033
11	10	2	10	9	1	912.96150	0.00048
12	11	2	11	10	1	914.54140	0.00005
13	12	2	12	11	1	916.11730	0.00003
14	13	2	13	12	1	917.68910	0.00014
15	14	2	14	13	1	919.25640	-0.00007
16	15	2	15	14	1	920.81970	-0.00010
17	16	2	16	15	1	922.37900	0.00006
18	17	2	17	16	1	923.93390	0.00000
19	18	2	18	17	1	925.48490	0.00025
20	19	2	19	18	1	927.03120	0.00002
21	20	2	20	19	1	928.57370	0.00022
22	21	2	21	20	1	930.11160	0.00007
23	22	2	22	21	1	931.64530	-0.00003
24	23	2	23	22	1	933.17480	-0.00007
25	24	2	24	23	1	934.70020	0.00006
26	25	2	25	24	1	936.22110	-0.00002
27	26	2	26	25	1	937.73800	0.00018
28	27	2	27	26	1	939.25020	-0.00002
29	28	2	28	27	1	940.75800	-0.00032
30	29	2	29	28	1	942.26210	-0.00001
31	30	2	30	29	1	943.76150	-0.00010
32	31	2	31	30	1	945.25670	-0.00006
33	32	2	32	31	1	946.74790	0.00029
35	34	2	34	33	1	949.71690	0.00058
36	35	2	35	34	1	951.19440	0.00022
37	36	2	36	35	1	952.66700	-0.00071
38	37	2	37	36	1	954.13650	-0.00039
33	32	2	34	33	1	840.28470	0.00041
32	31	2	33	32	1	841.98010	0.00037
31	30	2	32	31	1	843.67370	-0.00016
30	29	2	31	30	1	845.36700	0.00039
29	28	2	30	29	1	847.05770	-0.00017
28	27	2	29	28	1	848.74740	-0.00017

Continuation of Table A_2: ν_{12} ← ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
27	26	2	28	27	1	850.43590	0.00029
26	25	2	27	26	1	852.12190	-0.00001
24	23	2	25	24	1	855.48880	-0.00013
23	22	2	24	23	1	857.16930	-0.00018
22	21	2	23	22	1	858.84810	0.00016
20	19	2	21	20	1	862.19840	0.00011
19	18	2	20	19	1	863.86990	-0.00011
18	17	2	19	18	1	865.53940	0.00007
17	16	2	18	17	1	867.20610	-0.00005
16	15	2	17	16	1	868.87030	-0.00012
15	14	2	16	15	1	870.53210	0.00004
14	13	2	15	14	1	872.19090	-0.00009
12	11	2	13	12	1	875.50040	-0.00007
11	10	2	12	11	1	877.15090	0.00004
8	7	1	9	8	2	882.08940	-0.00011
7	6	1	8	7	2	883.73760	-0.00026
11	9	3	12	10	2	877.65260	-0.00046
14	12	3	13	11	2	917.28380	0.00027
15	13	3	14	12	2	918.85720	-0.00009
16	14	3	15	13	2	920.42640	-0.00007
17	15	3	16	14	2	921.99120	-0.00004
18	16	3	17	15	2	923.55150	-0.00020
19	17	3	18	16	2	925.10800	0.00015
20	18	3	19	17	2	926.65970	0.00000
21	19	3	20	18	2	928.20730	0.00004
22	20	3	21	19	2	929.75060	0.00007
23	21	3	22	20	2	931.28950	0.00001
24	22	3	23	21	2	932.82420	0.00006
25	23	3	24	22	2	934.35450	0.00002
26	24	3	25	23	2	935.88070	0.00020
27	25	3	26	24	2	937.40230	0.00011
28	26	3	27	25	2	938.91990	0.00035
29	27	3	28	26	2	940.43280	0.00023
30	28	3	29	27	2	941.94120	-0.00005
31	29	3	30	28	2	943.44550	-0.00008
32	30	3	31	29	2	944.94560	0.00004
33	31	3	32	30	2	946.44130	0.00010
34	32	3	33	31	2	947.93260	0.00013
35	33	3	34	32	2	949.41940	0.00001
27	25	3	28	26	2	851.00470	-0.00028
25	23	3	26	24	2	854.36830	0.00003
24	22	3	25	23	2	856.04690	-0.00009
23	21	3	24	22	2	857.72380	0.00015
22	20	3	23	21	2	859.39820	0.00004

Continuation of Table A_2: ν_{12} ← ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
21	19	3	22	20	2	861.07050	0.00004
20	18	3	21	19	2	862.74050	0.00005
19	17	3	20	18	2	864.40800	-0.00007
18	16	3	19	17	2	866.07320	-0.00005
17	15	3	18	16	2	867.73600	0.00009
16	14	3	17	15	2	869.39600	0.00000
15	13	3	16	14	2	871.05340	-0.00005
14	12	3	15	13	2	872.70820	0.00002
13	11	3	14	12	2	874.36050	0.00045
16	13	4	15	12	3	920.01880	0.00066
17	14	4	16	13	3	921.59060	0.00023
18	15	4	17	14	3	923.15740	-0.00001
19	16	4	18	15	3	924.71980	0.00009
20	17	4	19	16	3	926.27750	0.00004
21	18	4	20	17	3	927.83080	0.00006
22	19	4	21	18	3	929.37970	0.00012
23	20	4	22	19	3	930.92410	0.00008
24	21	4	23	20	3	932.46410	0.00005
25	22	4	24	21	3	933.99970	0.00000
26	23	4	25	22	3	935.53110	0.00015
27	24	4	26	23	3	937.05790	0.00008
28	25	4	27	24	3	938.58040	0.00010
29	26	4	28	25	3	940.09830	-0.00010
30	27	4	29	26	3	941.61150	-0.00060
31	28	4	30	27	3	943.12240	0.00098
32	29	4	31	28	3	944.62640	0.00005
33	30	4	32	29	3	946.12730	0.00042
34	31	4	33	30	3	947.62290	-0.00012
35	32	4	34	31	3	949.11480	0.00003
36	33	4	35	32	3	950.60260	0.00048
26	23	4	27	24	3	853.24720	0.00002
24	21	4	25	22	3	856.59900	-0.00001
23	20	4	24	21	3	858.27200	0.00019
22	19	4	23	20	3	859.94220	-0.00023
21	18	4	22	19	3	861.61080	-0.00001
20	17	4	21	18	3	863.27700	0.00014
19	16	4	20	17	3	864.94060	0.00005
18	15	4	19	16	3	866.60180	-0.00001
17	14	4	18	15	3	868.26060	0.00002
16	13	4	17	14	3	869.91700	0.00024
14	11	4	15	12	3	873.21950	-0.00041
13	10	4	14	11	3	874.86390	-0.00022
19	15	5	18	14	4	924.31580	0.00044
21	17	5	20	16	4	927.44080	-0.00012

Continuation of Table A_2: ν_{12} ← ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
22	18	5	21	17	4	928.99620	0.00001
23	19	5	22	18	4	930.54690	0.00014
24	20	5	23	19	4	932.09250	-0.00023
25	21	5	24	20	4	933.63390	-0.00023
26	22	5	25	21	4	935.17110	0.00009
27	23	5	26	22	4	936.70330	-0.00008
28	24	5	27	23	4	938.23120	-0.00008
29	25	5	28	24	4	939.75470	0.00000
30	26	5	29	25	4	941.27330	-0.00036
31	27	5	30	26	4	942.78820	0.00004
32	28	5	31	27	4	944.29810	-0.00012
33	29	5	32	28	4	945.80390	0.00008
34	30	5	33	29	4	947.30420	-0.00079
35	31	5	34	30	4	948.80170	-0.00001
36	32	5	35	31	4	950.29360	-0.00040
37	33	5	36	32	4	951.78140	-0.00045
25	21	5	26	22	4	855.47420	0.00004
24	20	5	25	21	4	857.14580	0.00044
23	19	5	24	20	4	858.81440	-0.00004
22	18	5	23	19	4	860.48150	0.00014
21	17	5	22	18	4	862.14600	-0.00007
20	16	5	21	17	4	863.80840	-0.00012
19	15	5	20	16	4	865.46870	0.00006
18	14	5	19	15	4	867.12670	0.00042
17	13	5	18	14	4	868.78050	-0.00049
23	18	6	22	17	5	930.15410	0.00008
24	19	6	23	18	5	931.70700	-0.00010
25	20	6	24	19	5	933.25510	-0.00007
26	21	6	25	20	5	934.79830	-0.00011
27	22	6	26	21	5	936.33640	-0.00050
28	23	6	27	22	5	937.87080	0.00008
29	24	6	28	23	5	939.39980	-0.00011
30	25	6	29	24	5	940.92420	-0.00030
31	26	6	30	25	5	942.44400	-0.00052
32	27	6	31	26	5	943.95990	-0.00010
33	28	6	32	27	5	945.47070	-0.00024
34	29	6	33	28	5	946.97750	0.00014
36	31	6	35	30	5	949.97680	0.00011
37	32	6	36	31	5	951.47040	0.00078
11	9	2	12	10	3	877.66070	0.00005
10	8	3	11	9	2	879.28980	-0.00041
10	8	2	11	9	3	879.31260	-0.00019
14	11	4	15	12	3	873.21950	-0.00041
14	11	3	15	12	4	873.22530	-0.00026

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of $\text{C}_2\text{H}_3\text{DO}$

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
13	10	4	14	11	3	874.86390	-0.00022
13	10	3	14	11	4	874.88050	-0.00016
9	8	1	8	7	2	909.79340	0.00002
8	7	2	7	6	1	908.18120	0.00006
8	7	1	7	6	2	908.20960	-0.00013
12	10	3	11	9	2	914.11990	0.00059
12	10	2	11	9	3	914.12740	-0.00002
11	9	3	10	8	2	912.52340	-0.00038
11	9	2	10	8	3	912.54760	-0.00003
15	12	4	14	11	3	918.43940	-0.00023
15	12	3	14	11	4	918.44540	-0.00033
14	11	4	13	10	3	916.85190	-0.00011
14	11	3	13	10	4	916.86980	0.00011
18	14	5	17	13	4	922.74370	-0.00015
18	14	4	17	13	5	922.74810	-0.00004
17	13	5	16	12	4	921.16420	0.00001
17	13	4	16	12	5	921.17640	-0.00008
16	12	5	15	11	4	919.57100	-0.00049
16	12	4	15	11	5	919.60560	0.00032
25	20	6	26	21	5	856.01920	0.00017
23	18	6	24	19	5	859.35240	-0.00011
22	17	6	23	18	5	861.01620	0.00006
21	16	6	22	17	5	862.67770	0.00009
24	18	7	23	17	6	931.30130	0.00013
25	19	7	24	18	6	932.85870	0.00042
26	20	7	25	19	6	934.40950	0.00002
27	21	7	26	20	6	935.95510	-0.00020
28	22	7	27	21	6	937.49590	-0.00009
29	23	7	28	22	6	939.03220	0.00048
30	24	7	29	23	6	940.56200	-0.00060
31	25	7	30	24	6	942.08840	-0.00029
32	26	7	31	25	6	943.60990	-0.00017
27	20	8	26	19	7	935.55320	0.00020
28	21	8	27	20	7	937.10320	0.00050
29	22	8	28	21	7	938.64600	-0.00052
30	23	8	29	22	7	940.18410	-0.00078
31	24	8	30	23	7	941.71790	-0.00012
32	25	8	31	24	7	943.24640	0.00031
33	26	8	32	25	7	944.76930	0.00008
34	27	8	33	26	7	946.28760	0.00013
35	28	8	34	27	7	947.80110	0.00018
30	22	9	29	21	8	939.78690	0.00075
31	23	9	30	22	8	941.32890	0.00061
32	24	9	31	23	8	942.86460	0.00005

Continuation of Table A_2: $\nu_{12} \leftarrow$ ground state of $\text{C}_2\text{H}_3\text{DO}$

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
34	26	9	33	25	8	945.92060	-0.00012
35	27	9	34	26	8	947.44100	-0.00001
36	28	9	35	27	8	948.95610	-0.00017
4	0	4	3	1	3	899.92630	0.00007
4	1	4	3	0	3	899.94110	-0.00017
8	1	8	7	0	7	903.70720	0.00008
9	1	9	8	0	8	904.67340	0.00005
10	1	10	9	0	9	905.64880	0.00030
11	1	11	10	0	10	906.63280	0.00034
12	1	12	11	0	11	907.62550	0.00041
13	1	13	12	0	12	908.62650	0.00023
14	1	14	13	0	13	909.63630	0.00045
15	1	15	14	0	14	910.65410	0.00042
16	1	16	15	0	15	911.68010	0.00051
17	1	17	16	0	16	912.71390	0.00048
18	1	18	17	0	17	913.75530	0.00031
19	1	19	18	0	18	914.80450	0.00038
20	1	20	19	0	19	915.86070	0.00009
21	1	21	20	0	20	916.92440	0.00013
22	1	22	21	0	21	917.99490	0.00000
23	1	23	22	0	22	919.07220	-0.00008
24	1	24	23	0	23	920.15600	-0.00021
25	1	25	24	0	24	921.24620	-0.00027
26	1	26	25	0	25	922.34240	-0.00045
27	1	27	26	0	26	923.44460	-0.00051
28	1	28	27	0	27	924.55250	-0.00054
29	1	29	28	0	28	925.66580	-0.00062
30	1	30	29	0	29	926.78450	-0.00053
31	1	31	30	0	30	927.90810	-0.00053
32	1	32	31	0	31	929.03680	-0.00022
33	1	33	32	0	32	930.17000	0.00003
34	1	34	33	0	33	931.30730	0.00003
35	1	35	34	0	34	932.44880	0.00008
36	1	36	35	0	35	933.59430	0.00019
37	1	37	36	0	36	934.74360	0.00036
38	1	38	37	0	37	935.89630	0.00037
39	1	39	38	0	38	937.05280	0.00080
40	1	40	39	0	39	938.21160	0.00031
42	1	42	41	0	41	940.53910	0.00023
43	1	43	42	0	42	941.70700	0.00011
44	1	44	43	0	43	942.87630	-0.00127
9	2	8	8	1	7	905.13190	-0.00017
10	2	9	9	1	8	906.09460	0.00009
11	2	10	10	1	9	907.06630	0.00029

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of $\text{C}_2\text{H}_3\text{DO}$

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
12	2	11	11	1	10	908.04660	0.00026
13	2	12	12	1	11	909.03570	0.00035
14	2	13	13	1	12	910.03340	0.00051
15	2	14	14	1	13	911.03920	0.00038
16	2	15	15	1	14	912.05340	0.00042
17	2	16	16	1	15	913.07560	0.00041
18	2	17	17	1	16	914.10570	0.00040
19	2	18	18	1	17	915.14350	0.00039
20	2	19	19	1	18	916.18870	0.00024
21	2	20	20	1	19	917.24150	0.00037
22	2	21	21	1	20	918.30100	0.00006
23	2	22	22	1	21	919.36770	0.00002
24	2	23	23	1	22	920.44100	-0.00015
25	2	24	24	1	23	921.52090	-0.00022
26	2	25	25	1	24	922.60720	-0.00019
27	2	26	26	1	25	923.69950	-0.00024
28	2	27	27	1	26	924.79760	-0.00034
29	2	28	28	1	27	925.90140	-0.00038
30	2	29	29	1	28	927.01050	-0.00052
31	2	30	30	1	29	928.12490	-0.00056
32	2	31	31	1	30	929.24440	-0.00046
33	2	32	32	1	31	930.36860	-0.00041
34	2	33	33	1	32	931.49760	-0.00009
35	2	34	34	1	33	932.63060	-0.00010
36	2	35	35	1	34	933.76800	0.00018
38	2	37	37	1	36	936.05420	0.00060
39	2	38	38	1	37	937.20280	0.00092
40	2	39	39	1	38	938.35420	0.00068
41	2	40	40	1	39	939.50940	0.00105
42	2	41	41	1	40	940.66670	0.00049
43	2	42	42	1	41	941.82600	-0.00097
44	2	43	43	1	42	942.98940	-0.00109
43	1	43	44	0	44	863.95760	-0.00085
41	1	41	42	0	42	865.15990	0.00049
40	1	40	41	0	41	865.76570	0.00074
39	1	39	40	0	40	866.37480	0.00075
38	1	38	39	0	39	866.98730	0.00047
37	1	37	38	0	38	867.60390	0.00043
36	1	36	37	0	37	868.22440	0.00029
35	1	35	36	0	36	868.84910	0.00015
34	1	34	35	0	35	869.47810	-0.00007
33	1	33	34	0	34	870.11160	-0.00035
32	1	32	33	0	33	870.75010	-0.00039
31	1	31	32	0	32	871.39360	-0.00039

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of $\text{C}_2\text{H}_3\text{DO}$

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
30	1	30	31	0	31	872.04190	-0.00077
29	1	29	30	0	30	872.69620	-0.00051
28	1	28	29	0	29	873.35580	-0.00054
27	1	27	28	0	28	874.02130	-0.00047
26	1	26	27	0	27	874.69280	-0.00040
25	1	25	26	0	26	875.37050	-0.00035
24	1	24	25	0	25	876.05470	-0.00022
23	1	23	24	0	24	876.74550	-0.00013
22	1	22	23	0	23	877.44320	0.00003
21	1	21	22	0	22	878.14790	0.00016
20	1	20	21	0	21	878.85980	0.00025
19	1	19	20	0	20	879.57910	0.00033
18	1	18	19	0	19	880.30590	0.00030
17	1	17	18	0	18	881.04060	0.00038
16	1	16	17	0	17	881.78320	0.00041
15	1	15	16	0	16	882.53390	0.00042
14	1	14	15	0	15	883.29290	0.00045
13	1	13	14	0	14	884.06030	0.00045
12	1	12	13	0	13	884.83620	0.00039
11	1	11	12	0	12	885.62080	0.00034
10	1	10	11	0	11	886.41420	0.00026
9	1	9	10	0	10	887.21640	0.00007
8	1	8	9	0	9	888.02780	0.00004
7	1	7	8	0	8	888.84830	0.00000
6	1	6	7	0	7	889.67800	-0.00006
3	0	3	4	1	4	892.21420	-0.00067
3	1	3	4	0	4	892.23000	-0.00016
40	2	39	41	1	40	864.78550	0.00069
38	2	37	39	1	38	866.02180	0.00050
36	2	35	37	1	36	867.27410	0.00025
35	2	34	36	1	35	867.90650	-0.00008
34	2	33	35	1	34	868.54370	-0.00017
33	2	32	34	1	33	869.18570	-0.00022
32	2	31	33	1	32	869.83250	-0.00041
31	2	30	32	1	31	870.48460	-0.00046
30	2	29	31	1	30	871.14230	-0.00027
29	2	28	30	1	29	871.80520	-0.00045
28	2	27	29	1	28	872.47410	-0.00042
27	2	26	28	1	27	873.14890	-0.00047
26	2	25	27	1	26	873.83020	-0.00023
25	2	24	26	1	25	874.51780	-0.00009
24	2	23	25	1	24	875.21200	0.00002
23	2	22	24	1	23	875.91290	0.00002
22	2	21	23	1	22	876.62090	0.00010

Continuation of Table A_2: ν_{12} ← ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
21	2	20	22	1	21	877.33620	0.00027
20	2	19	21	1	20	878.05870	0.00022
9	2	7	8	3	6	905.60240	-0.00039
9	3	7	8	2	6	905.61010	-0.00016
8	2	6	7	3	5	904.65240	-0.00003
8	3	6	7	2	5	904.68450	-0.00021
7	3	5	6	2	4	903.80250	-0.00057
7	2	5	6	3	4	903.68220	0.00055
10	3	8	9	2	7	906.55540	-0.00047
11	3	9	10	2	8	907.51330	-0.00017
12	3	10	11	2	9	908.48120	0.00038
13	3	11	12	2	10	909.45760	0.00036
14	3	12	13	2	11	910.44270	0.00027
15	3	13	14	2	12	911.43660	0.00041
16	3	14	15	2	13	912.43880	0.00045
17	3	15	16	2	14	913.44920	0.00046
18	3	16	17	2	15	914.46760	0.00041
19	3	17	18	2	16	915.49400	0.00049
20	3	18	19	2	17	916.52790	0.00038
21	3	19	20	2	18	917.56920	0.00017
22	3	20	21	2	19	918.61810	0.00025
23	3	21	22	2	20	919.67400	0.00022
24	3	22	23	2	21	920.73660	-0.00001
25	3	23	24	2	22	921.80610	-0.00004
26	3	24	25	2	23	922.88200	-0.00014
27	3	25	26	2	24	923.96430	-0.00011
28	3	26	27	2	25	925.05230	-0.00042
29	3	27	28	2	26	926.14660	-0.00026
30	3	28	29	2	27	927.24630	-0.00030
31	3	29	30	2	28	928.35130	-0.00042
32	3	30	31	2	29	929.46180	-0.00020
33	3	31	32	2	30	930.57700	-0.00021
34	3	32	33	2	31	931.69700	-0.00015
36	3	34	35	2	33	933.95070	0.00038
37	3	35	36	2	34	935.08370	0.00055
40	3	38	39	2	37	938.50490	0.00070
41	3	39	40	2	38	939.65230	0.00083
42	3	40	41	2	39	940.80220	0.00029
43	3	41	42	2	40	941.95600	0.00063
44	3	42	43	2	41	943.11140	-0.00033
45	3	43	44	2	42	944.26980	-0.00103
38	3	36	39	2	37	865.06410	-0.00074
37	3	35	38	2	36	865.69700	0.00037
36	3	34	37	2	35	866.33310	0.00031

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
35	3	33	36	2	34	866.97340	-0.00011
31	3	29	32	2	30	869.58520	-0.00062
30	3	28	31	2	29	870.25200	-0.00028
29	3	27	30	2	28	870.92410	-0.00041
28	3	26	29	2	27	871.60250	-0.00022
27	3	25	28	2	26	872.28690	-0.00022
26	3	24	27	2	25	872.97770	-0.00022
25	3	23	26	2	24	873.67520	-0.00011
24	3	22	25	2	23	874.37950	-0.00001
23	3	21	24	2	22	875.09080	0.00009
22	3	20	23	2	21	875.80940	0.00029
21	3	19	22	2	20	876.53510	0.00020
20	3	18	21	2	19	877.26860	0.00034
19	3	17	20	2	18	878.00970	0.00032
18	3	16	19	2	17	878.75880	0.00039
17	3	15	18	2	16	879.51590	0.00038
16	3	14	17	2	15	880.28120	0.00033
15	3	13	16	2	14	881.05510	0.00051
14	3	12	15	2	13	881.83710	0.00028
13	3	11	14	2	12	882.62800	0.00033
12	3	10	13	2	11	883.42740	0.00017
11	3	9	12	2	10	884.23560	0.00001
10	3	8	11	2	9	885.05270	-0.00016
9	3	7	10	2	8	885.87830	-0.00106
8	2	6	9	3	7	886.70900	0.00015
8	3	6	9	2	7	886.71660	-0.00011
7	2	5	8	3	6	887.53780	-0.00015
7	3	5	8	2	6	887.57120	-0.00019
6	2	4	7	3	5	888.34110	-0.00021
6	3	4	7	2	5	888.46440	-0.00074
9	3	6	8	4	5	906.04370	-0.00016
9	4	6	8	3	5	906.17260	-0.00039
12	4	9	11	3	8	908.93140	-0.00064
13	4	10	12	3	9	909.89390	-0.00009
14	4	11	13	3	10	910.86610	0.00022
15	4	12	14	3	11	911.84720	0.00033
16	4	13	15	3	12	912.83690	0.00031
17	4	14	16	3	13	913.83510	0.00031
18	4	15	17	3	14	914.84170	0.00043
19	4	16	18	3	15	915.85630	0.00048
20	4	17	19	3	16	916.87860	0.00035
21	4	18	20	3	17	917.90870	0.00032
22	4	19	21	3	18	918.94630	0.00030
23	4	20	22	3	19	919.99100	0.00009

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of $\text{C}_2\text{H}_3\text{DO}$

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
24	4	21	23	3	20	921.04290	-0.00001
25	4	22	24	3	21	922.10180	0.00001
26	4	23	25	3	22	923.16720	-0.00015
27	4	24	26	3	23	924.23910	-0.00025
28	4	25	27	3	24	925.31740	-0.00020
29	4	26	28	3	25	926.40160	-0.00027
30	4	27	29	3	26	927.49180	-0.00013
31	4	28	30	3	27	928.58720	-0.00037
32	4	29	31	3	28	929.68820	-0.00037
33	4	30	32	3	29	930.79430	-0.00040
34	4	31	33	3	30	931.90560	-0.00014
35	4	32	34	3	31	933.02170	0.00022
36	4	33	35	3	32	934.14190	0.00020
37	4	34	36	3	33	935.26630	0.00010
38	4	35	37	3	34	936.39470	-0.00006
39	4	36	38	3	35	937.52670	-0.00051
40	4	37	39	3	36	938.66360	0.00027
41	4	38	40	3	37	939.80360	0.00065
42	4	39	41	3	38	940.94630	0.00039
44	4	41	43	3	40	943.24160	0.00043
45	4	42	44	3	41	944.39260	-0.00060
46	4	43	45	3	42	945.54710	-0.00089
32	4	29	33	3	30	868.02610	-0.00032
31	4	28	32	3	29	868.69580	-0.00038
30	4	27	31	3	28	869.37140	-0.00030
29	4	26	30	3	27	870.05300	-0.00019
28	4	25	29	3	26	870.74060	-0.00025
27	4	24	28	3	25	871.43480	-0.00009
26	4	23	27	3	24	872.13540	-0.00012
25	4	22	26	3	23	872.84290	-0.00004
24	4	21	25	3	22	873.55750	0.00016
23	4	20	24	3	21	874.27930	0.00038
22	4	19	23	3	20	875.00820	0.00033
21	4	18	22	3	19	875.74470	0.00034
20	4	17	21	3	18	876.48880	0.00023
19	4	16	20	3	17	877.24110	0.00044
18	4	15	19	3	16	878.00120	0.00040
17	4	14	18	3	15	878.76940	0.00028
16	4	13	17	3	14	879.54590	0.00016
11	3	8	10	4	7	907.97470	0.00062
11	4	8	10	3	7	907.98260	-0.00004
10	3	7	9	4	6	907.01890	-0.00023
10	4	7	9	3	6	907.05430	-0.00018
42	5	38	43	4	39	860.63360	0.00022

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of $\text{C}_2\text{H}_3\text{DO}$

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
41	5	37	42	4	38	861.26340	-0.00007
39	5	35	40	4	36	862.53640	0.00048
38	5	34	39	4	35	863.17940	0.00078
36	5	32	37	4	33	864.47790	0.00002
35	5	31	36	4	32	865.13470	-0.00013
34	5	30	35	4	31	865.79690	-0.00001
33	5	29	34	4	30	866.46450	0.00017
32	5	28	33	4	29	867.13720	-0.00010
31	5	27	32	4	28	867.81590	-0.00012
30	5	26	31	4	27	868.50030	-0.00039
29	5	25	30	4	26	869.19130	-0.00023
28	5	24	29	4	25	869.88860	-0.00013
27	5	23	28	4	24	870.59250	0.00000
26	5	22	27	4	23	871.30310	0.00007
25	5	21	26	4	22	872.02060	0.00007
24	5	20	25	4	21	872.74540	0.00023
23	5	19	24	4	20	873.47730	0.00015
22	5	18	23	4	19	874.21700	0.00036
21	5	17	22	4	18	874.96410	0.00030
20	5	16	21	4	17	875.71900	0.00021
19	5	15	20	4	16	876.48210	0.00036
18	5	14	19	4	15	877.25310	0.00032
17	5	13	18	4	14	878.03230	0.00029
16	5	12	17	4	13	878.81970	0.00020
15	5	11	16	4	12	879.61530	0.00004
14	5	10	15	4	11	880.41930	-0.00005
12	4	8	13	5	9	882.04530	0.00009
12	5	8	13	4	9	882.05480	-0.00004
11	4	7	12	5	8	882.85590	-0.00026
11	5	7	12	4	8	882.89390	-0.00015
10	4	6	11	5	7	883.63600	-0.00082
10	5	6	11	4	7	883.77040	0.00005
9	4	5	10	5	6	884.33770	0.00022
9	5	5	10	4	6	884.73730	-0.00002
10	4	6	9	5	5	907.36030	0.00013
10	5	6	9	4	5	907.75250	-0.00044
11	4	7	10	5	6	908.40970	0.00016
11	5	7	10	4	6	908.53850	0.00006
12	4	8	11	5	7	909.38650	-0.00018
12	5	8	11	4	7	909.42270	0.00002
13	4	9	12	5	8	910.34510	-0.00002
13	5	9	12	4	8	910.35430	0.00017
15	5	11	14	4	10	912.27340	0.00012
16	5	12	15	4	11	913.24950	0.00011

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
17	5	13	16	4	12	914.23500	0.00036
18	5	14	17	4	13	915.22870	0.00013
19	5	15	18	4	14	916.23120	0.00030
21	5	17	20	4	16	918.26010	0.00032
22	5	18	21	4	17	919.28620	0.00030
23	5	19	22	4	18	920.31970	0.00018
24	5	20	23	4	19	921.36060	0.00015
25	5	21	24	4	20	922.40870	0.00025
26	5	22	25	4	21	923.46330	-0.00004
27	5	23	26	4	22	924.52480	-0.00008
28	5	24	27	4	23	925.59260	-0.00025
29	5	25	28	4	24	926.66690	-0.00016
30	5	26	29	4	25	927.74690	-0.00036
31	5	27	30	4	26	928.83290	-0.00034
32	5	28	31	4	27	929.92420	-0.00057
33	5	29	32	4	28	931.02160	-0.00004
34	5	30	33	4	29	932.12360	-0.00003
35	5	31	34	4	30	933.23030	-0.00021
36	5	32	35	4	31	934.34190	-0.00017
37	5	33	36	4	32	935.45800	-0.00009
38	5	34	37	4	33	936.57860	0.00022
39	5	35	38	4	34	937.70300	0.00027
11	5	6	10	6	5	908.52440	-0.00029
11	6	6	10	5	5	909.47120	-0.00005
12	5	7	11	6	6	909.73260	0.00015
12	6	7	11	5	6	910.11050	-0.00043
13	5	8	12	6	7	910.77620	-0.00036
13	6	8	12	5	7	910.90010	-0.00005
14	5	9	13	6	8	911.75410	0.00002
15	6	10	14	5	9	912.72450	0.00021
17	6	12	16	5	11	914.65100	0.00004
18	6	13	17	5	12	915.63130	0.00030
19	6	14	18	5	13	916.62040	0.00021
20	6	15	19	5	14	917.61840	0.00037
21	6	16	20	5	15	918.62440	0.00022
22	6	17	21	5	16	919.63860	0.00025
23	6	18	22	5	17	920.66060	0.00029
24	6	19	23	5	18	921.69000	0.00019
25	6	20	24	5	19	922.72680	0.00016
26	6	21	25	5	20	923.77040	-0.00017
27	6	22	26	5	21	924.82140	0.00002
29	6	24	28	5	23	926.94270	-0.00005
30	6	25	29	5	24	928.01270	-0.00017
31	6	26	30	5	25	929.08890	-0.00007

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
33	6	28	32	5	27	931.25810	-0.00017
34	6	29	33	5	28	932.35100	-0.00001
36	6	31	35	5	30	934.55210	0.00052
37	6	32	36	5	31	935.65910	0.00013
38	6	33	37	5	32	936.77150	0.00067
39	6	34	38	5	33	937.88720	0.00026
40	6	35	39	5	34	939.00730	0.00020
40	6	35	41	5	36	860.95270	0.00027
39	6	34	40	5	35	861.59810	-0.00013
38	6	33	39	5	34	862.24870	0.00010
37	6	32	38	5	33	862.90390	0.00019
36	6	31	37	5	32	863.56350	-0.00027
35	6	30	36	5	31	864.22880	-0.00017
34	6	29	35	5	30	864.89920	-0.00031
33	6	28	34	5	29	865.57550	-0.00008
32	6	27	33	5	28	866.25710	-0.00029
31	6	26	32	5	27	866.94480	-0.00035
30	6	25	31	5	26	867.63880	-0.00025
29	6	24	30	5	25	868.33900	-0.00030
28	6	23	29	5	24	869.04610	0.00001
27	6	22	28	5	23	869.75960	-0.00003
26	6	21	27	5	22	870.48020	0.00011
25	6	20	26	5	21	871.20790	0.00024
24	6	19	25	5	20	871.94260	0.00008
23	6	18	24	5	19	872.68490	0.00008
22	6	17	23	5	18	873.43500	0.00027
21	6	16	22	5	17	874.19270	0.00032
20	6	15	21	5	16	874.95810	0.00023
19	6	14	20	5	15	875.73160	0.00030
18	6	13	19	5	14	876.51290	0.00018
17	6	12	18	5	13	877.30220	0.00009
16	6	11	17	5	12	878.09920	-0.00028
14	5	9	15	6	10	879.71060	0.00016
14	6	9	15	5	10	879.72020	0.00008
13	5	8	14	6	9	880.51330	-0.00005
13	6	8	14	5	9	880.55060	0.00009
12	5	7	13	6	8	881.28600	-0.00028
12	6	7	13	5	8	881.41480	-0.00051
11	6	6	12	5	7	882.36440	-0.00057
35	7	29	36	6	30	863.33160	-0.00028
34	7	28	35	6	29	864.01090	-0.00004
33	7	27	34	6	28	864.69570	-0.00003
32	7	26	33	6	27	865.38610	-0.00035
31	7	25	32	6	26	866.08340	0.00010

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of $\text{C}_2\text{H}_3\text{DO}$

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
30	7	24	31	6	25	866.78640	-0.00007
29	7	23	30	6	24	867.49630	0.00015
28	7	22	29	6	23	868.21260	0.00006
27	7	21	28	6	22	868.93590	0.00009
26	7	20	27	6	21	869.66610	-0.00004
25	7	19	26	6	20	870.40390	0.00022
24	7	18	25	6	19	871.14880	0.00022
23	7	17	24	6	18	871.90130	0.00032
22	7	16	23	6	17	872.66120	0.00022
21	7	15	22	6	16	873.42890	0.00026
20	7	14	21	6	15	874.20390	-0.00010
16	6	10	17	7	11	877.37380	-0.00011
16	7	10	17	6	11	877.38340	0.00011
15	7	9	16	6	10	878.20440	-0.00016
14	6	8	15	7	9	878.93550	-0.00042
14	7	8	15	6	9	879.05620	-0.00093
13	7	7	14	6	8	879.98740	-0.00013
12	6	6	13	7	7	880.16820	0.00016
12	7	6	13	6	7	881.09040	-0.00059
14	6	8	13	7	7	912.10630	-0.00021
14	7	8	13	6	7	912.46090	-0.00017
15	6	9	14	7	8	913.14340	0.00000
15	7	9	14	6	8	913.25830	-0.00031
16	7	10	15	6	9	914.15340	-0.00008
17	6	11	16	7	10	915.08400	-0.00007
17	7	11	16	6	10	915.09290	0.00019
22	7	16	21	6	15	920.00490	0.00027
23	7	17	22	6	16	921.01430	0.00000
24	7	18	23	6	17	922.03210	0.00022
25	7	19	24	6	18	923.05740	0.00031
26	7	20	25	6	19	924.08980	0.00012
27	7	21	26	6	20	925.12970	0.00028
28	7	22	27	6	21	926.17590	-0.00017
30	7	24	29	6	23	928.28900	-0.00015
31	7	25	30	6	24	929.35510	-0.00004
32	7	26	31	6	25	930.42700	-0.00011
33	7	27	32	6	26	931.50460	-0.00025
34	7	28	33	6	27	932.58800	-0.00014
35	7	29	34	6	28	933.67630	-0.00044
36	7	30	35	6	29	934.77030	-0.00014
37	7	31	36	6	30	935.86850	-0.00052
38	7	32	37	6	31	936.97230	0.00003
39	7	33	38	6	32	938.08010	0.00013
40	7	34	39	6	33	939.19210	0.00018

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of $\text{C}_2\text{H}_3\text{DO}$

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
41	7	35	40	6	34	940.30880	0.00087
43	7	37	42	6	36	942.55190	0.00055
45	7	39	44	6	38	944.80800	-0.00082
22	8	15	21	7	14	920.38690	-0.00003
23	8	16	22	7	15	921.38330	0.00010
25	8	18	24	7	17	923.40110	0.00018
26	8	19	25	7	18	924.42170	0.00008
27	8	20	26	7	19	925.44980	0.00000
28	8	21	27	7	20	926.48520	0.00000
29	8	22	28	7	21	927.52790	0.00034
31	8	24	30	7	23	929.63210	-0.00009
32	8	25	31	7	24	930.69390	-0.00008
33	8	26	32	7	25	931.76150	-0.00028
32	8	25	33	7	26	864.52400	-0.00015
31	8	24	32	7	25	865.22990	-0.00019
30	8	23	31	7	24	865.94230	-0.00020
27	8	20	28	7	21	868.12060	0.00027
26	8	19	27	7	20	868.86040	0.00009
25	8	18	26	7	19	869.60770	0.00017
24	8	17	25	7	18	870.36240	0.00031
22	8	15	23	7	16	871.89360	0.00021
18	7	11	19	8	12	875.03560	-0.00015
18	8	11	19	7	12	875.04430	-0.00030
17	7	10	18	8	11	875.82350	-0.00041
17	8	10	18	7	11	875.85670	0.00002
16	7	9	17	8	10	876.58460	-0.00063
16	8	9	17	7	10	876.69650	-0.00028
15	8	8	16	7	9	877.60700	-0.00010
16	7	9	15	8	8	914.47970	-0.00040
17	7	10	16	8	9	915.50930	0.00040
17	8	10	16	7	9	915.61410	-0.00001
18	7	11	17	8	10	916.48570	0.00051
25	9	17	24	8	16	923.75960	-0.00032
26	9	18	25	8	17	924.76800	0.00020
27	9	19	26	8	18	925.78370	0.00000
30	9	22	29	8	21	928.87610	0.00004
32	9	24	31	8	23	930.97210	0.00009
33	9	25	32	8	24	932.02980	0.00027
34	9	26	33	8	25	933.09300	-0.00008
35	9	27	34	8	26	934.16230	-0.00014
38	9	30	39	8	31	859.50890	0.00010
37	9	29	38	8	30	860.18770	-0.00023
36	9	28	37	8	29	860.87260	0.00003
34	9	26	35	8	27	862.25890	-0.00024

Continuation of Table A_2: ν_{12} ← ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
33	9	25	34	8	26	862.96110	-0.00034
32	9	24	33	8	25	863.66960	-0.00038
31	9	23	32	8	24	864.38510	0.00016
30	9	22	31	8	23	865.10670	0.00022
29	9	21	30	8	22	865.83480	0.00004
28	9	20	29	8	21	866.57010	0.00019
27	9	19	28	8	20	867.31200	-0.00004
26	9	18	27	8	19	868.06150	0.00027
25	9	17	26	8	18	868.81760	0.00007
24	9	16	25	8	17	869.58110	0.00018
23	9	15	24	8	16	870.35120	-0.00012
22	9	14	23	8	15	871.12860	0.00003
20	9	12	21	8	13	872.70440	0.00014
19	9	11	20	8	12	873.50700	-0.00021
18	8	10	19	9	11	874.23310	-0.00080
18	9	10	19	8	11	874.33440	-0.00051
18	9	10	17	8	9	917.14510	0.00009
19	8	11	18	9	10	917.87160	-0.00062
19	9	11	18	8	10	917.96690	0.00014
20	8	12	19	9	11	918.84770	0.00008
20	9	12	19	8	11	918.87520	0.00007
21	8	13	20	9	12	919.81520	-0.00006
21	9	13	20	8	12	919.82280	0.00012
27	10	18	26	9	17	926.13270	-0.00027
28	10	19	27	9	18	927.14370	0.00002
29	10	20	28	9	19	928.16250	0.00020
30	10	21	29	9	20	929.18850	0.00007
33	10	24	32	9	23	932.30870	-0.00006
34	10	25	33	9	24	933.36190	-0.00001
35	10	26	34	9	25	934.42090	-0.00025
20	9	11	19	10	10	919.22020	0.00028
20	10	11	19	9	10	919.48160	0.00045
21	9	12	20	10	11	920.23240	-0.00026
22	10	13	21	9	12	921.23170	-0.00012
23	10	14	22	9	13	922.18290	-0.00057
38	10	29	39	9	30	858.61100	-0.00043
37	10	28	38	9	29	859.29890	0.00027
36	10	27	37	9	28	859.99180	0.00029
35	10	26	36	9	27	860.69030	0.00006
34	10	25	35	9	26	861.39540	0.00041
33	10	24	34	9	25	862.10580	-0.00014
31	10	22	32	9	23	863.54700	0.00000
30	10	21	31	9	22	864.27740	0.00000
29	10	20	30	9	21	865.01460	0.00008

Continuation of Table A_2: ν_{12} $\leftarrow$ ground state of C₂H₃DO

J'	K_a'	K_c'	J''	K_a''	K_c''	$\tilde{\nu}_{\text{obs}}$	$\tilde{\nu}_{\text{obs}} - \tilde{\nu}_{\text{calc}}$
28	10	19	29	9	20	865.75860	0.00018
26	10	17	27	9	18	867.26660	-0.00005
25	10	16	26	9	17	868.03080	-0.00003
34	11	24	35	10	25	860.53850	0.00077
33	11	23	34	10	24	861.25670	-0.00040
32	11	22	33	10	23	861.98280	-0.00002
31	11	21	32	10	22	862.71480	-0.00021
29	11	19	30	10	20	864.19880	-0.00014
28	11	18	29	10	19	864.95040	-0.00025
27	11	17	28	10	18	865.70860	-0.00010
26	11	16	27	10	17	866.47260	-0.00028
27	24	3	28	25	3	851.56860	0.00030
25	21	4	26	22	4	855.47420	0.00004
28	24	4	29	25	4	850.44860	0.00001
30	26	4	31	27	4	847.08880	-0.00017
31	27	4	32	28	4	845.40660	-0.00003
14	10	5	15	11	4	873.70010	-0.00042
15	11	4	16	12	5	872.10530	-0.00044
15	11	5	16	12	4	872.07380	-0.00036
16	11	5	17	12	6	871.03640	0.00014
16	11	6	17	12	5	870.89720	0.00014
16	12	4	17	13	5	870.44250	-0.00031
16	12	5	17	13	4	870.43120	-0.00025
17	12	5	18	13	6	869.33730	0.00013
18	13	5	19	14	6	867.66360	0.00008
19	14	5	20	15	6	866.00000	0.00008
19	14	6	20	15	5	865.99250	0.00007
5	2	4	4	1	3	901.42730	-0.00038
6	1	5	5	2	4	902.28770	-0.00005
6	2	5	5	1	4	902.31340	-0.00019
7	1	6	6	2	5	903.23220	0.00036
7	2	6	6	1	5	903.23700	-0.00045

Table S4_1: Spectroscopic parameters for the ground state of monodeutero-oxirane in the MW, GHz and THz ranges resulting from refitting all transitions reported in Müller et al. [d] (which included data from Albert et al. [a,b,c])

	MNRAS [d] published I ^r	I ^r (all lines in MHz [c])	MNRAS [d] published III ^l	III ^l (all lines in MHz [c])	
A /MHz	24252.647815(44)	24252.647869(44)	24252.670221(39)	24252.670290(39)	A /MHz
B /MHz	19905.523291(40)	19905.523395(40)	19905.493836(40)	19905.493942(40)	B /MHz
C /MHz	13327.583649 (53)	13327.583788(53)	13327.592078(53)	13327.592212(53)	C /MHz
Δ_J /kHz	17.04198 (11)	17.04234(11)	18.028074(55)	18.028010(55)	Δ_J /kHz
Δ_K /kHz	25.46266 (18)	25.46255(18)	-52.12684(11)	-52.12666(11)	Δ_K /kHz
Δ_{JK} /kHz	17.25673 (12)	17.25657(12)	41.656664(99)	41.656922(99)	Δ_{JK} /kHz
δ_j /kHz	4.742161 (17)	4.742146(17)	-0.7437580(78)	-0.7437574(78)	d_2 /kHz
δ_k /kHz	13.231691 (56)	13.231618(56)	8.308952(26)	8.308916(26)	d_1 /kHz
ϕ_J /mHz	12.36(10)	12.73(10)	21.586(95)	21.994(11)	ϕ_J /mHz
ϕ_{JK} /mHz	141.97(15)	141.84(15)	-123.99(12)	-123.80(12)	ϕ_{JK} /mHz
ϕ_{KJ} /mHz	-835.25(36)	-835.55(36)	220.07(11)	218.60(95)	ϕ_{KJ} /mHz
ϕ_K /mHz	808.08(30)	808.18(30)	-114.912(41)	-114.879(41)	ϕ_K /mHz
η_J /mHz	4.797(13)	4.789(13)	-15.0709(32)	-15.0724(32)	h_3 /mHz
η_{JK} /mHz	62.667(69)	62.589(69)	26.227(12)	26.227(12)	h_2 /mHz
η_K /mHz	30.21(10)	30.14(10)	10.979(26)	10.939(26)	h_1 /mHz
L_K /Hz	-9.13 (24)	-9.20(24)	-1.577(11)	-1.575(11)	L_K /Hz
L_{KKJ} /Hz	6.51 (27)	6.54(27)	4.280(37)	4.261(37)	L_{KKJ} /Hz
L_{JK} /Hz	1.55 (19)	1.70(19)	-4.424(53)	-4.375(53)	L_{JK} /Hz
L_{JJK} /Hz	-2.099 (64)	-2.063(64)	2.546(39)	2.491(39)	L_{JJK} /Hz
L_J /Hz	-0.169 (30)	-0.284(30)	-0.921(27)	-1.008(27)	L_J /Hz
l_K /Hz	-4.571 (60)	-4.613(60)	399.2(74)	387.2(74)	l_1 / 10 ⁻³ Hz
l_{KJ} /Hz	2.243 (41)	2.288(41)	-209.4(47)	-210.0(47)	l_2 / 10 ⁻³ Hz
l_{JK} /Hz	-1.191 (24)	-1.170(24)	177.5(18)	177.8(18)	l_3 / 10 ⁻³ Hz
l_J / 10 ⁻³ Hz	-34.7 (36)	-34.2(36)	26.71(31)	26.86(31)	l_4 / 10 ⁻³ Hz
P_K / 10 ⁻³ Hz	1.30 (10)	1.22(10)			
P_{KKJ} / 10 ⁻³ Hz	-1.94 (17)	-1.75(17)			
P_{KJ} / 10 ⁻³ Hz	0.851 (99)	0.716(99)			
		2.405	-1.948 (133)	-1.827 (133)	p_5 / 10 ⁻⁶ Hz
d_{rms} / kHz	10.455 ^e	2404.659	10.402 ^e	2405.024	d_{rms} / kHz
n	2418	2418	2418	2418	

[a] Based on data published in Albert et al., *Phys.Chem.Chem.Phys.* 2019, **21**, 3669. [b] Values in parenthesis indicate uncertainties as 1 σ in units of the last digits given. Rotational constants without parenthesis were held fixed to the respective values of the ground state obtained by fitting only transitions in the GHz region of this study.

[c] All FT-THz transitions were converted to MHz. [d] Reproduced from data reported in Müller et al., *MNRAS* 2023, **518**, 185. [e] Müller et al. stated 9.13 kHz for sub-mm data alone and 2.1 MHz for FIR alone, similar for the d_{rms} value of MNRAS published III^l.

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
1	1	1	0	0	0	37580.170	0.023	0.021	0.00	a
1	1	0	1	0	1	10925.000	0.044	0.041	33233.0378	a
2	0	2	1	1	1	58337.180	0.095	0.095	37580.1463	a
2	1	2	1	0	1	64234.970	-0.003	-0.005	33233.0378	b
2	2	1	1	1	0	86084.260	0.001	-0.006	44157.9943	b
2	2	0	1	1	1	96443.580	-0.001	-0.008	37580.1463	b
2	1	1	2	0	2	21284.050	-0.046	-0.048	95917.2311	a
2	2	0	2	1	1	16822.390	-0.010	-0.015	117201.3267	a
3	0	3	2	1	2	87497.970	-0.017	-0.018	97468.0101	b
3	1	3	2	0	2	89421.945	-0.003	-0.005	95917.2311	b
3	1	2	2	2	1	92914.360	-0.003	-0.001	130242.2531	b
3	2	2	2	1	1	112738.000	0.009	0.003	117201.3267	b
3	1	2	3	0	3	38190.670	0.051	0.047	184965.9963	a
3	2	1	3	1	2	21212.880	-0.009	-0.012	223156.6148	a
3	3	0	3	2	1	27356.030	0.041	0.033	244369.5034	a
3	3	1	3	2	2	40137.710	0.049	0.040	229939.3169	a
4	0	4	3	1	3	114895.670	-0.009	-0.009	185339.1786	b
4	1	4	3	0	3	115342.600	0.003	0.002	184965.9963	b
4	2	2	4	1	3	33890.100	0.050	0.047	357278.9365	a
4	3	1	4	2	2	25443.480	-0.006	-0.012	391168.9863	a
4	4	0	4	3	1	41664.470	0.027	0.015	416612.4718	a
5	3	2	5	2	3	31522.220	0.004	0.000	569776.1013	a
5	4	1	5	3	2	35048.150	0.054	0.043	601298.3165	a
5	1	4	5	0	5	75027.590	0.010	0.000	442025.8221	b
5	2	4	5	1	5	75641.550	0.015	0.005	442038.9428	b
6	4	2	6	3	3	33776.670	0.050	0.043	821971.3061	a
6	4	3	6	3	4	62656.825	0.012	0.001	777979.0908	b
6	5	2	6	4	3	62699.865	0.008	-0.006	840635.9031	b
6	2	4	6	1	5	72394.960	0.012	0.004	702765.0847	b
6	6	0	6	5	1	72516.095	0.022	0.005	905138.4233	b
6	6	1	6	5	2	74261.270	0.017	0.001	903335.7599	b
6	3	4	6	2	5	75075.845	0.019	0.009	702903.2653	b
6	1	5	6	0	6	92326.200	0.012	0.000	610438.8974	b
6	2	5	6	1	6	92462.185	0.005	-0.008	610441.0859	b
8	0	8	6	0	6	416756.485	-4.660	-4.656	610438.8974	e
8	8	0	6	6	0	713569.006	9.180	9.148	977654.4955	e
7	4	3	7	3	4	42232.500	0.092	0.088	1072938.1005	a
7	5	2	7	4	3	42052.250	-0.056	-0.069	1115170.5077	a
7	6	1	7	5	2	65932.715	0.019	0.001	1157222.8134	b
7	3	4	7	2	5	67338.650	0.003	-0.002	1005599.4546	b
7	5	3	7	4	4	67514.320	0.016	0.003	1081534.3408	b
7	6	2	7	5	3	73448.350	0.007	-0.009	1149048.6444	b
7	4	4	7	3	5	75163.800	0.012	0.001	1006370.5529	b
7	7	0	7	6	1	87035.740	0.010	-0.007	1223155.5092	b
7	7	1	7	6	2	87677.750	0.011	-0.006	1222496.9862	b

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(\text{SP})$ / MHz	$\Delta_{O-C}(\text{LP})$ / MHz	E''/h (MHz)	Source
7	2	5	7	1	6	90710.475	0.006	-0.005	914888.9865	b
7	3	5	7	2	6	91454.150	0.006	-0.006	914916.4094	b
7	1	6	7	0	7	109393.200	0.011	-0.004	805495.7982	b
7	2	6	7	1	7	109420.270	0.007	-0.007	805496.1474	b
8	6	2	7	3	5	501450.893	0.027	-0.013	1006370.5529	c
8	7	1	7	4	4	508534.767	0.044	-0.004	1081534.3408	c
9	0	9	7	0	7	470053.589	-1.870	-1.874	805495.7982	e
9	0	9	7	0	7	470056.587	1.120	1.124	805495.7982	e
9	1	8	7	1	6	504026.070	-6.500	-6.499	914888.9865	e
8	5	3	8	4	4	42246.240	-0.021	-0.029	1409545.7613	b
8	6	3	8	5	4	75006.560	0.021	0.006	1429082.3274	b
8	5	4	8	4	5	76727.350	0.007	-0.005	1352354.9848	b
8	7	1	8	6	2	82247.660	0.015	-0.004	1507821.4144	b
8	7	2	8	6	3	85758.420	0.013	-0.004	1504088.8657	b
8	3	5	8	2	6	87611.670	0.005	-0.003	1261773.7141	b
8	4	5	8	3	6	90399.850	0.009	-0.002	1261955.1446	b
8	8	0	8	7	1	101145.270	0.018	0.001	1590069.0588	b
8	8	1	8	7	2	101362.465	0.016	-0.001	1589847.2714	b
8	2	6	8	1	7	108180.625	0.020	0.007	1153593.1098	b
8	3	6	8	2	7	108356.975	0.010	-0.003	1153598.1805	b
9	3	6	8	2	7	496848.815	0.024	-0.002	1153598.1805	c
9	7	3	8	4	4	497031.243	0.048	0.003	1409545.7613	c
9	4	6	8	1	7	497687.704	0.028	0.000	1153593.1098	c
9	3	7	8	0	8	517105.414	0.032	0.001	1027200.0351	c
9	8	1	8	6	2	497810.690	0.036	-0.001	1507821.4144	c
9	8	2	8	6	3	501472.651	0.043	0.007	1504088.8657	c
9	9	1	8	7	2	530852.182	0.052	0.017	1589847.2714	c
9	8	2	8	5	3	553769.512	0.060	0.005	1451792.0219	c
9	6	3	8	3	6	572851.626	0.028	-0.007	1261955.1446	c
9	9	1	8	6	2	612878.040	0.052	-0.002	1507821.4144	c
10	0	10	8	0	8	523347.694	-0.430	-0.429	1027200.0351	e
10	0	10	8	0	8	523347.694	-0.430	-0.429	1027200.0351	e
10	1	9	8	1	7	557284.200	-7.580	-7.585	1153593.1098	e
10	10	0	8	8	0	907423.804	4.410	4.376	1691214.3094	e
10	10	0	8	8	0	907426.801	7.410	7.374	1691214.3094	e
9	7	2	9	6	3	73267.970	0.018	-0.002	1834806.7367	b
9	6	4	9	5	5	80528.270	0.008	-0.006	1741114.5629	b
9	4	5	9	3	6	82055.520	0.004	-0.001	1650446.9666	b
9	7	3	9	6	4	84934.140	0.012	-0.004	1821642.8244	b
9	5	5	9	4	6	89833.785	0.002	-0.009	1651280.7809	b
9	8	1	9	7	2	97557.390	0.014	-0.004	1908074.6881	b
9	8	2	9	7	3	98984.540	0.022	0.004	1906576.9510	b
9	3	6	9	2	7	106180.250	0.008	-0.004	1544266.7254	b
9	4	6	9	3	7	106975.370	0.000	-0.012	1544305.4118	b
9	9	0	9	8	1	115068.600	0.021	0.005	2005632.0633	b

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
9	9	1	9	8	2	115137.940	0.011	-0.005	2005561.4688	b
10	5	5	9	4	6	502492.137	0.011	-0.002	1651280.7809	c
10	6	5	9	3	6	522871.910	0.031	0.004	1650446.9666	c
10	7	4	9	4	5	527809.524	0.034	-0.003	1732502.4822	c
10	4	6	9	3	7	535527.162	0.030	0.006	1544305.4118	c
10	5	6	9	2	7	538507.544	0.029	0.002	1544266.7254	c
10	5	5	9	3	6	503325.971	0.031	0.017	1650446.9666	c
10	6	5	9	4	6	522038.085	0.020	-0.006	1651280.7809	c
10	8	2	9	6	3	522795.489	0.012	-0.027	1834806.7367	c
10	8	3	9	6	4	535409.636	0.032	-0.003	1821642.8244	c
10	5	6	9	3	7	538468.857	0.028	0.002	1544305.4118	c
10	3	7	9	2	8	558180.159	0.030	0.001	1418922.4395	c
10	4	7	9	1	8	558386.073	0.020	-0.010	1418921.5489	c
10	9	1	9	7	2	561648.253	0.010	-0.025	1908074.6881	c
10	9	2	9	7	3	563124.495	0.065	0.031	1906576.9510	c
10	2	8	9	1	9	577739.984	0.034	0.001	1275551.2656	c
10	7	3	9	4	6	615539.620	0.050	0.011	1651280.7809	c
10	8	2	9	5	5	616487.708	0.056	0.008	1741114.5629	c
10	10	1	9	7	2	690558.743	0.060	0.010	1908074.6881	c
11	0	11	9	0	9	576638.801	1.030	1.029	1275551.2575	e
11	0	11	9	0	9	576641.799	4.020	4.027	1275551.2575	e
11	1	10	9	1	8	610563.316	-0.381	-0.381	1418921.5489	e
11	2	9	9	2	7	644634.729	-9.280	-9.285	1544266.7254	e
11	10	1	9	8	1	976642.884	-9.460	-9.495	2005632.0633	e
11	11	0	9	9	0	1004298.738	1.290	1.266	2120700.6416	e
11	11	0	9	9	0	1004301.736	4.290	4.264	2120700.6416	e
10	5	5	10	4	6	73940.365	0.002	-0.001	2079832.5389	b
10	7	4	10	6	5	86993.135	0.008	-0.008	2173318.8405	b
10	6	5	10	5	6	90544.615	0.009	-0.003	2082774.2353	b
10	8	2	10	7	3	90781.870	0.005	-0.015	2266820.3442	b
10	8	3	10	7	4	96740.480	0.022	0.005	2260311.9666	b
10	4	6	10	3	7	102729.985	0.008	-0.001	1977102.5629	b
10	5	6	10	4	7	105466.650	0.010	-0.002	1977307.5960	b
10	9	1	10	8	2	112120.740	0.022	0.005	2357602.2085	b
10	9	2	10	8	3	112648.970	0.017	0.000	2357052.4236	b
11	11	1	10	10	0	526364.514	0.213	0.202	2598633.6961	c
11	11	0	10	10	1	526364.514	-0.205	-0.216	2598633.3649	c
11	7	4	10	6	5	496044.243	0.007	-0.003	2173318.8405	c
11	9	3	10	8	2	498197.879	0.016	-0.001	2357602.2085	c
11	9	2	10	8	3	498937.160	0.018	0.001	2357052.4236	c
11	10	2	10	9	1	512555.123	0.010	-0.005	2469722.9254	c
11	10	1	10	9	2	512583.043	0.011	-0.003	2469701.3757	c
11	6	5	10	5	6	531058.465	0.014	0.006	2082774.2353	c
11	7	5	10	4	6	570138.586	0.029	-0.002	2079832.5389	c
11	5	6	10	4	7	571028.417	0.009	-0.008	1977307.5960	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
11	6	6	10	3	7	579522.185	0.023	-0.002	1977102.5629	c
11	8	4	10	5	5	592277.541	0.039	-0.007	2153772.9016	c
11	4	7	10	3	8	598183.525	0.025	0.000	1853298.8988	c
11	5	7	10	2	8	599031.629	0.039	0.012	1853291.2103	c
11	3	8	10	2	9	619111.446	0.024	-0.006	1710885.0395	c
11	4	8	10	1	9	619157.616	0.027	-0.003	1710884.8893	c
11	7	4	10	5	5	515590.210	0.034	0.011	2153772.9016	c
11	8	3	10	6	4	543965.693	0.039	0.001	2204904.1122	c
11	7	5	10	5	6	567196.881	0.021	-0.007	2082774.2353	c
11	5	6	10	3	7	571233.473	0.032	0.014	1977102.5629	c
11	8	4	10	6	5	572731.591	0.028	-0.005	2173318.8405	c
11	6	6	10	4	7	579317.160	0.031	0.006	1977307.5960	c
11	9	2	10	7	3	589169.252	0.030	-0.007	2266820.3442	c
11	9	3	10	6	4	650896.017	0.056	0.000	2204904.1122	c
11	10	1	10	9	1	512561.512	0.030	0.016	2469722.9254	c
11	10	2	10	9	2	512576.699	0.036	0.021	2469701.3757	c
11	8	3	10	5	6	666095.571	0.039	-0.005	2082774.2353	c
11	9	2	10	6	5	682670.789	0.062	0.012	2173318.8405	c
11	10	1	10	7	4	721972.480	0.038	-0.011	2260311.9666	c
12	0	12	10	0	10	629923.913	0.145	0.148	1550548.1541	e
12	1	11	10	1	9	663842.431	5.070	5.070	1710884.8893	e
12	2	10	10	2	8	697847.890	-5.300	-5.302	1853291.2103	e
12	11	1	10	9	1	1073568.784	7.060	7.034	2469722.9254	e
12	11	1	10	9	1	1073574.780	13.100	13.030	2469722.9254	e
12	12	0	10	10	0	1101146.692	2.580	2.558	2598633.6961	e
12	12	0	10	10	0	1101149.690	5.570	5.556	2598633.6961	e
11	6	5	11	5	6	65496.695	0.011	0.009	2548335.9982	b
11	8	3	11	7	4	79506.710	0.020	-0.002	2669363.0721	b
11	7	5	11	6	6	93346.380	0.008	-0.006	2556624.7191	b
11	8	4	11	7	5	96079.325	0.017	-0.001	2649971.0902	b
11	5	6	11	4	7	96853.615	0.009	0.004	2451482.3927	b
11	6	6	11	5	7	104301.940	0.014	0.002	2452322.7943	b
11	9	2	11	8	3	107119.820	0.019	0.001	2748869.7612	b
11	9	3	11	8	4	109749.690	0.020	0.003	2746050.3975	b
12	12	1	11	11	0	574779.771	0.065	0.058	3124998.0783	c
12	12	0	11	11	1	574779.771	-0.044	-0.051	3124997.9917	c
12	8	5	11	7	4	502856.788	0.021	-0.001	2669363.0721	c
12	9	4	11	8	3	530677.573	0.020	0.003	2748869.7612	c
12	8	4	11	7	5	532505.535	0.018	0.007	2649971.0902	c
12	9	3	11	8	4	534607.315	0.012	-0.003	2746050.3975	c
12	10	3	11	9	2	546948.210	0.013	0.000	2855989.5610	c
12	10	2	11	9	3	547200.005	0.014	0.001	2855800.0667	c
12	7	5	11	6	6	558504.323	0.004	-0.002	2556624.7191	c
12	11	2	11	10	1	560998.414	0.005	-0.005	2982284.4021	c
12	11	1	11	10	2	561006.625	0.013	0.003	2982278.0336	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
12	6	6	11	5	7	602178.950	0.006	-0.005	2452322.7943	c
12	7	6	11	4	7	621942.669	0.024	-0.002	2451482.3927	c
12	8	5	11	5	6	623883.885	0.043	0.005	2548335.9982	c
12	5	7	11	4	8	636356.432	0.025	0.004	2330042.4722	c
12	6	7	11	3	8	639204.275	0.019	-0.006	2329996.4552	c
12	9	4	11	6	5	665714.680	0.046	-0.007	2613832.6812	c
12	3	9	11	2	10	679883.610	0.034	0.002	2029485.2646	c
12	4	9	11	1	10	679893.274	0.023	-0.008	2029485.2397	c
12	7	5	11	5	6	566793.062	0.022	0.008	2548335.9982	c
12	8	4	11	6	5	568643.959	0.033	0.002	2613832.6812	c
12	6	6	11	4	7	603019.363	0.017	0.005	2451482.3927	c
12	8	5	11	6	6	615595.141	0.020	-0.010	2556624.7191	c
12	7	6	11	5	7	621102.270	0.027	0.002	2452322.7943	c
12	9	4	11	7	5	629576.266	0.041	0.008	2649971.0902	c
12	6	7	11	4	8	639158.251	0.012	-0.013	2330042.4722	c
12	10	2	11	8	3	654130.323	0.026	-0.006	2748869.7612	c
12	6	6	11	5	6	506165.762	0.022	0.015	2548335.9982	c
12	8	4	11	7	4	513113.555	0.020	0.003	2669363.0721	c
12	5	7	11	4	7	514916.500	0.015	0.004	2451482.3927	c
12	7	6	11	6	6	516800.343	0.026	0.013	2556624.7191	c
12	6	7	11	5	7	516877.920	0.004	-0.008	2452322.7943	c
12	4	8	11	3	8	518635.469	0.004	-0.009	2329996.4552	c
12	5	8	11	4	8	518802.779	-0.004	-0.017	2330042.4722	c
12	3	9	11	2	9	520458.113	0.004	-0.010	2188910.7305	c
12	4	9	11	3	9	520466.346	0.036	0.022	2188912.1794	c
12	2	10	11	1	10	521659.309	0.148	0.132	2029485.2397	c
12	3	10	11	2	10	521659.309	-0.090	-0.105	2029485.2646	c
12	8	5	11	7	5	522248.763	0.013	-0.002	2649971.0902	c
12	1	11	11	0	11	522533.230	0.005	-0.013	1852189.0263	c
12	2	11	11	1	11	522533.230	0.001	-0.017	1852189.0263	c
12	9	3	11	8	3	531787.957	0.018	0.001	2748869.7612	c
12	9	4	11	8	4	533496.936	0.019	0.004	2746050.3975	c
12	10	2	11	9	2	547010.514	0.018	0.004	2855989.5610	c
12	11	2	11	9	3	687482.772	0.026	0.002	2855800.0667	c
12	9	3	11	6	6	724033.037	0.053	0.007	2556624.7191	c
13	0	13	11	0	11	683206.026	0.399	0.403	1852189.0263	e
13	1	12	11	1	10	717103.560	-5.770	-5.769	2029485.2397	e
13	2	11	11	2	9	751094.028	6.340	6.347	2188910.7305	e
13	3	10	11	3	8	785285.358	-17.300	-17.287	2329996.4552	e
13	12	1	11	10	1	1170413.739	-2.300	-2.317	2982284.4021	e
13	12	1	11	10	1	1170419.735	3.690	3.679	2982284.4021	e
13	13	0	11	11	0	1197955.673	-2.000	-2.008	3124998.0783	e
13	13	0	11	11	0	1197961.668	3.990	3.988	3124998.0783	e
12	8	4	12	7	5	67347.590	0.021	0.001	3115129.0329	b
12	6	6	12	5	7	88102.860	-0.001	-0.002	2966398.8728	b

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
12	9	3	12	8	4	98181.120	0.025	0.004	3182476.6019	b
12	8	5	12	7	6	98794.820	0.016	0.000	3073425.0312	b
12	7	6	12	6	7	104224.340	0.013	0.001	2969200.7052	b
12	9	4	12	8	5	107327.490	0.015	-0.003	3172219.8346	b
12	5	7	12	4	8	117766.965	0.006	-0.002	2848631.9154	b
13	13	1	12	12	0	623177.970	0.031	0.030	3699777.8012	c
13	13	0	12	12	1	623177.970	0.003	0.002	3699777.7787	c
13	8	6	12	7	5	519008.422	0.016	-0.005	3115129.0329	c
13	9	5	12	8	4	558661.442	0.017	-0.001	3182476.6019	c
13	9	4	12	8	5	573665.455	0.009	-0.003	3172219.8346	c
13	10	4	12	9	3	580546.963	0.018	0.004	3280657.6956	c
13	10	3	12	9	4	582065.904	0.009	-0.004	3279547.3090	c
13	8	5	12	7	6	587612.667	0.004	-0.001	3073425.0312	c
13	11	3	12	10	2	595497.478	0.011	0.002	3403000.0520	c
13	11	2	12	10	3	595579.509	0.007	-0.003	3402937.7527	c
13	12	2	12	11	1	609415.281	0.001	-0.004	3543284.6398	c
13	12	1	12	11	2	609417.631	0.000	-0.006	3543282.8060	c
13	7	6	12	6	7	629259.892	0.005	0.000	2969200.7052	c
13	8	6	12	5	7	667738.592	0.025	-0.005	2966398.8728	c
13	6	7	12	5	8	671466.164	0.026	0.011	2848845.2498	c
13	7	7	12	4	8	679432.589	0.020	-0.004	2848631.9154	c
13	6	8	12	3	9	700050.690	0.025	0.000	2709368.8344	c
13	9	4	12	7	5	630756.295	0.047	0.010	3115129.0329	c
13	7	6	12	5	7	632061.737	0.018	0.010	2966398.8728	c
13	7	6	12	6	6	543958.876	0.017	0.010	3054501.7329	c
13	8	5	12	7	5	545908.672	0.012	-0.002	3115129.0329	c
13	7	7	12	6	7	558863.807	0.029	0.018	2969200.7052	c
13	5	8	12	4	8	559977.310	0.013	0.003	2848631.9154	c
13	6	8	12	5	8	560574.237	-0.012	-0.023	2848845.2498	c
13	8	6	12	7	6	560712.417	0.009	-0.004	3073425.0312	c
13	4	9	12	3	9	562580.727	-0.002	-0.015	2709368.8344	c
13	5	9	12	4	9	562620.856	0.015	0.002	2709378.4841	c
13	9	4	12	8	4	563408.696	0.017	0.001	3182476.6019	c
13	3	10	12	2	10	564154.721	0.018	0.004	2551144.3961	c
13	4	10	12	3	10	564156.359	-0.001	-0.015	2551144.6578	c
13	2	11	12	1	11	565276.223	0.057	0.040	2374722.2465	c
13	3	11	12	2	11	565276.223	0.015	-0.001	2374722.2504	c
13	10	3	12	9	3	580955.509	0.000	-0.013	3280657.6956	c
13	10	4	12	9	4	581657.362	0.030	0.017	3279547.3090	c
13	11	3	12	10	3	595559.780	0.014	0.004	3402937.7527	c
13	9	5	12	7	6	667713.028	0.032	0.002	3073425.0312	c
13	6	7	12	4	8	671679.481	0.008	-0.007	2848631.9154	c
13	10	3	12	8	4	679136.631	0.028	-0.007	3182476.6019	c
13	7	7	12	5	8	679219.256	0.022	-0.001	2848845.2498	c
13	10	4	12	8	5	688984.843	0.036	0.006	3172219.8346	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
13	5	8	12	4	9	699230.759	0.029	0.006	2709378.4841	c
13	6	8	12	4	9	700041.033	0.017	-0.008	2709378.4841	c
13	4	9	12	3	10	720804.941	0.034	0.005	2551144.6578	c
13	5	9	12	2	10	720854.963	0.032	0.004	2551144.3961	c
14	0	14	12	0	12	736476.148	-6.780	-6.775	2180471.9164	e
14	0	14	12	0	12	736482.144	-0.784	-0.779	2180471.9164	e
14	1	13	12	1	11	770379.677	1.630	1.630	2374722.2465	e
14	1	13	12	1	11	770382.675	4.620	4.628	2374722.2465	e
14	2	12	12	2	10	804331.173	0.969	0.973	2551144.3961	e
14	3	11	12	3	9	838441.559	-4.800	-4.794	2709368.8344	e
14	3	11	12	3	9	838444.557	-1.800	-1.796	2709368.8344	e
14	11	3	12	9	3	1210711.842	17.500	17.517	3280657.6956	e
14	13	1	12	11	1	1267225.718	-0.563	-0.568	3543284.6398	e
14	13	1	12	11	1	1267225.718	-0.563	-0.568	3543284.6398	e
14	14	0	12	12	0	1294734.674	-0.996	-0.991	3699777.8012	e
13	7	6	13	6	7	78149.210	0.005	0.004	3520311.3815	b
13	9	4	13	8	5	84847.605	0.017	-0.005	3661037.6880	b
13	8	6	13	7	7	106072.960	0.003	-0.011	3528064.4777	b
13	9	5	13	8	6	107000.600	0.012	-0.005	3634137.4340	b
13	6	7	13	5	8	111702.180	0.004	-0.001	3408609.2069	b
13	10	3	13	9	4	115727.940	0.016	-0.002	3745885.2754	b
13	7	7	13	6	8	118645.000	0.014	0.003	3409419.4929	b
14	14	1	13	13	0	671557.726	0.002	0.008	4322955.7400	c
14	14	0	13	13	1	671557.726	-0.005	0.001	4322955.7343	c
14	13	2	13	12	1	657810.677	0.336	0.337	4152700.4313	c
14	13	1	13	12	2	657810.677	-0.324	-0.324	4152699.9142	c
14	7	8	13	6	7	491274.497	0.006	-0.001	3520311.3815	c
14	11	4	13	11	3	492711.635	-0.008	-0.005	3998497.5134	c
14	11	3	13	11	2	492834.738	-0.003	0.000	3998517.2490	c
14	8	7	13	8	6	495286.920	-0.005	-0.001	3634137.4340	c
14	10	5	13	10	4	496349.106	-0.004	0.001	3861204.6352	c
14	10	4	13	10	3	497927.147	-0.011	-0.006	3861613.1986	c
14	9	6	13	9	5	498795.477	-0.012	-0.007	3741138.0207	c
14	9	5	13	9	4	509143.169	-0.007	0.001	3745885.2754	c
14	7	7	13	7	6	513104.276	0.000	-0.002	3598460.5861	c
14	8	6	13	8	5	521394.331	-0.005	-0.001	3661037.6880	c
14	8	7	13	7	6	530963.786	0.013	-0.004	3598460.5861	c
14	9	6	13	8	5	578895.850	0.028	0.008	3661037.6880	c
14	10	5	13	9	4	611668.485	0.014	0.000	3745885.2754	c
14	10	4	13	9	5	618402.355	0.018	0.008	3741138.0207	c
14	9	5	13	8	6	620891.016	-0.002	-0.009	3634137.4340	c
14	11	4	13	10	3	629595.970	0.011	0.001	3861613.1986	c
14	11	3	13	10	4	630147.366	0.009	0.000	3861204.6352	c
14	12	3	13	11	2	643957.436	0.008	0.003	3998517.2490	c
14	12	2	13	11	3	643983.237	0.006	0.001	3998497.5134	c

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J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
14	8	6	13	7	7	654367.554	0.006	0.005	3528064.4777	c
14	7	7	13	6	8	702145.377	0.007	-0.001	3409419.4929	c
14	9	6	13	6	7	719622.169	0.039	0.005	3520311.3815	c
14	8	7	13	5	8	720815.175	0.021	-0.002	3408609.2069	c
14	6	8	13	5	9	736990.033	0.013	-0.005	3271999.3201	c
14	9	5	13	7	6	656567.889	0.022	-0.005	3598460.5861	c
14	6	8	13	5	8	600380.132	0.000	-0.007	3408609.2069	c
14	7	8	13	6	8	602166.381	0.000	-0.009	3409419.4929	c
14	5	9	13	4	9	604308.673	0.010	-0.001	3271949.5585	c
14	6	9	13	5	9	604469.604	-0.001	-0.011	3271999.3201	c
14	4	10	13	3	10	606391.309	0.009	-0.003	3115299.0938	c
14	1	13	13	0	13	609705.665	0.015	-0.002	2535394.6470	c
14	2	13	13	1	13	609705.665	0.015	-0.002	2535394.6470	c
14	10	4	13	9	4	613655.100	0.018	0.004	3745885.2754	c
14	10	5	13	9	5	616415.714	-0.011	-0.023	3741138.0207	c
14	11	3	13	10	3	629738.778	-0.015	-0.025	3861613.1986	c
14	11	4	13	10	4	630004.527	0.004	-0.004	3861204.6352	c
14	8	6	13	6	7	662120.657	0.013	0.003	3520311.3815	c
14	10	5	13	8	6	723416.325	0.012	-0.017	3634137.4340	c
15	0	15	13	0	13	789752.266	-3.000	-2.999	2535394.6470	e
15	0	15	13	0	13	789755.264	-0.006	-0.001	2535394.6470	e
15	1	14	13	1	12	823637.807	-4.760	-4.753	2746594.5648	e
15	1	14	13	1	12	823646.801	4.230	4.241	2746594.5648	e
15	2	13	13	2	11	857571.316	-3.130	-3.120	2939998.4073	e
15	2	13	13	2	11	857574.314	-0.128	-0.122	2939998.4073	e
15	3	12	13	3	10	891618.745	-10.600	-10.569	3115299.0938	e
15	3	12	13	3	10	891633.735	4.420	4.421	3115299.0938	e
15	4	11	13	4	9	925989.950	-6.640	-6.629	3271949.5585	e
15	12	3	13	10	3	1308051.455	-6.270	-6.278	3861613.1986	e
15	13	2	13	11	2	1336342.869	7.360	7.359	3998517.2490	e
15	13	2	13	11	2	1336345.867	10.400	10.356	3998517.2490	e
15	14	1	13	12	1	1363998.723	3.870	3.875	4152700.4313	e
15	14	1	13	12	1	1364001.721	6.860	6.873	4152700.4313	e
15	15	0	13	13	0	1391474.702	-0.722	-0.703	4322955.7400	e
15	15	0	13	13	0	1391477.700	2.280	2.295	4322955.7400	e
14	8	6	14	7	7	70867.180	0.016	0.011	4111564.8565	b
14	9	5	14	8	6	72596.450	0.023	0.003	4182432.0195	b
14	7	7	14	6	8	102575.520	-0.005	-0.006	4008989.3326	b
14	10	4	14	9	5	104511.930	0.023	0.002	4255028.4462	b
14	9	6	14	8	7	110509.170	0.018	0.002	4129424.3539	b
14	10	5	14	9	6	117620.250	0.014	-0.003	4239933.5047	b
14	8	7	14	7	8	117838.500	0.013	0.001	4011585.8681	b
15	14	2	14	13	1	706184.413	0.079	0.087	4810510.9087	c
15	14	1	14	13	2	706184.413	-0.103	-0.095	4810510.7654	c
15	15	1	14	14	0	719917.688	-0.011	0.002	4994513.4590	c

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J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
15	15	0	14	14	1	719917.688	-0.012	0.000	4994513.4575	c
15	10	5	14	9	6	659455.438	-0.002	-0.009	4239933.5047	c
15	13	3	14	12	2	692370.189	-0.004	-0.003	4642480.7382	c
15	13	2	14	12	3	692378.081	0.002	0.003	4642474.6713	c
15	5	10	14	6	9	493543.956	-0.001	0.003	3876468.9186	c
15	6	10	14	6	9	493594.604	-0.004	-0.001	3876468.9186	c
15	5	10	14	5	9	493754.653	-0.007	-0.004	3876258.2158	c
15	6	10	14	5	9	493805.307	-0.004	-0.001	3876258.2158	c
15	8	7	14	9	6	499824.065	-0.025	0.002	4239933.5047	c
15	6	9	14	7	8	510150.286	0.000	0.004	4011585.8681	c
15	7	9	14	7	8	510908.026	-0.003	0.000	4011585.8681	c
15	6	9	14	6	8	512746.824	0.002	0.004	4008989.3326	c
15	7	9	14	6	8	513504.565	0.001	0.001	4008989.3326	c
15	7	8	14	8	7	518882.391	-0.014	-0.001	4129424.3539	c
15	14	2	14	14	1	522181.798	0.015	0.019	4994513.4575	c
15	14	1	14	14	0	522181.798	-0.023	-0.019	4994513.4590	c
15	8	8	14	8	7	525980.519	-0.009	-0.005	4129424.3539	c
15	12	4	14	12	3	527148.283	0.002	0.005	4642474.6713	c
15	12	3	14	12	2	527190.183	0.010	0.014	4642480.7382	c
15	11	5	14	11	4	530782.909	-0.011	-0.005	4491209.1516	c
15	11	4	14	11	3	531413.156	-0.008	-0.003	4491351.9856	c
15	9	7	14	9	6	534249.701	-0.004	0.002	4239933.5047	c
15	10	6	14	10	5	534420.497	-0.006	0.000	4357553.7401	c
15	7	8	14	7	7	536741.904	0.002	0.000	4111564.8565	c
15	10	5	14	10	4	539848.591	0.000	0.008	4359540.3517	c
15	8	8	14	7	7	543840.033	0.007	-0.003	4111564.8565	c
15	9	6	14	9	5	554859.937	-0.010	0.000	4255028.4462	c
15	9	7	14	8	6	591751.201	0.011	-0.008	4182432.0195	c
15	10	6	14	9	5	636945.810	0.012	-0.003	4255028.4462	c
15	11	5	14	10	4	662451.726	0.005	-0.004	4359540.3517	c
15	11	4	14	10	5	665211.414	0.003	-0.004	4357553.7401	c
15	12	4	14	11	3	678270.973	0.005	0.000	4491351.9856	c
15	12	3	14	11	4	678461.769	0.008	0.004	4491209.1516	c
15	9	6	14	8	7	680464.036	-0.005	-0.005	4129424.3539	c
15	8	7	14	7	8	728171.723	-0.006	-0.007	4011585.8681	c
15	8	7	14	8	6	557325.583	0.007	0.010	4182432.0195	c
15	9	6	14	8	6	627456.381	0.007	-0.003	4182432.0195	c
15	8	8	14	7	8	643819.026	0.011	0.003	4011585.8681	c
15	10	5	14	9	5	644360.489	-0.009	-0.022	4255028.4462	c
15	6	9	14	5	9	645477.969	0.029	0.022	3876258.2158	c
15	7	9	14	6	9	646024.997	0.018	0.009	3876468.9186	c
15	5	10	14	4	10	648322.500	0.010	0.001	3721690.3875	c
15	10	6	14	9	6	652040.759	0.020	0.010	4239933.5047	c
15	2	13	14	1	13	652472.575	0.018	0.004	3145100.2908	c
15	3	13	14	2	13	652472.575	0.017	0.003	3145100.2908	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
15	11	4	14	10	4	663224.823	0.024	0.015	4359540.3517	c
15	11	5	14	10	5	664438.352	0.020	0.011	4357553.7401	c
15	12	3	14	11	3	678318.940	0.013	0.010	4491351.9856	c
15	10	5	14	8	6	716956.955	0.030	-0.002	4182432.0195	c
16	0	16	14	0	14	843022.388	0.120	0.126	2916954.8372	e
16	0	16	14	0	14	843022.388	0.120	0.126	2916954.8372	e
16	1	15	14	1	13	876898.935	-3.230	-3.222	3145100.2908	e
16	1	15	14	1	13	876901.933	-0.232	-0.224	3145100.2908	e
16	2	14	14	2	12	910814.456	-2.900	-2.889	3355474.5928	e
16	2	14	14	2	12	910820.452	3.100	3.107	3355474.5928	e
16	3	13	14	3	11	944828.909	0.371	0.379	3547815.1826	e
16	4	12	14	4	10	979059.211	-3.620	-3.610	3721690.3875	e
16	4	12	14	4	10	979062.209	-0.621	-0.612	3721690.3875	e
16	14	2	14	12	2	1433121.870	-1.310	-1.295	4642480.7382	e
16	15	1	14	13	1	1460714.768	-6.310	-6.292	4810510.9087	e
16	15	1	14	13	1	1460717.766	-3.320	-3.294	4810510.9087	e
16	16	0	14	14	0	1488169.762	-4.410	-4.375	4994513.4590	e
16	16	0	14	14	0	1488175.757	1.590	1.621	4994513.4590	e
15	9	6	15	8	7	70130.820	0.021	0.009	4739757.5898	b
15	10	5	15	9	6	89500.575	0.024	0.001	4809888.3879	b
15	8	7	15	7	8	91450.840	0.003	0.002	4648306.7534	b
15	10	6	15	9	7	117791.050	0.015	-0.001	4774183.2041	b
15	9	7	15	8	8	118778.340	0.012	-0.002	4655404.8768	b
16	11	6	15	10	5	691826.523	0.003	-0.007	4899388.9379	c
16	11	5	15	10	6	702517.684	0.001	-0.005	4891974.2376	c
16	12	5	15	11	4	711956.591	-0.002	-0.005	5022765.1444	c
16	12	4	15	11	5	713014.574	0.014	0.011	5021992.0660	c
16	13	4	15	12	3	726778.268	-0.008	-0.005	5169670.9062	c
16	4	12	15	5	11	502804.820	0.000	0.004	4197948.3924	c
16	5	12	15	4	11	502807.515	-0.012	-0.007	4197946.1344	c
16	9	7	15	10	6	514742.161	-0.040	-0.005	4891974.2376	c
16	5	11	15	6	10	520070.705	-0.006	-0.001	4370063.5221	c
16	6	11	15	6	10	520082.153	-0.006	-0.001	4370063.5221	c
16	5	11	15	5	10	520121.357	-0.005	0.000	4370012.8709	c
16	6	11	15	5	10	520132.804	-0.006	-0.001	4370012.8709	c
16	6	10	15	7	9	537389.314	-0.007	-0.002	4522493.8916	c
16	7	10	15	7	9	537590.113	-0.002	0.003	4522493.8916	c
16	6	10	15	6	9	538147.057	-0.007	-0.002	4521736.1494	c
16	7	10	15	6	9	538347.855	-0.002	0.001	4521736.1494	c
16	8	8	15	9	7	550605.803	-0.023	0.000	4774183.2041	c
16	7	9	15	8	8	552105.553	-0.008	0.001	4655404.8768	c
16	14	3	15	14	2	558908.378	0.242	0.247	5516695.2355	c
16	14	2	15	14	1	558908.378	-0.253	-0.248	5516695.2747	c
16	8	9	15	7	8	561561.727	0.000	-0.003	4648306.7534	c
16	13	4	15	13	3	561598.254	-0.001	0.003	5334850.9247	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
16	12	5	15	12	4	565098.782	-0.006	-0.001	5169622.9475	c
16	12	4	15	12	3	565335.717	-0.002	0.004	5169670.9062	c
16	9	8	15	9	7	567118.352	-0.008	-0.001	4774183.2041	c
16	11	6	15	11	5	569223.385	-0.006	0.002	5021992.0660	c
16	10	7	15	10	6	571536.143	-0.015	-0.006	4891974.2376	c
16	11	5	15	11	4	571726.763	-0.012	-0.003	5022765.1444	c
16	8	8	15	8	7	585031.435	-0.005	-0.004	4739757.5898	c
16	10	6	15	10	5	585243.770	-0.010	0.002	4899388.9379	c
16	9	7	15	9	6	596828.046	-0.006	0.003	4809888.3879	c
16	9	8	15	8	7	601543.993	0.018	0.004	4739757.5898	c
16	10	7	15	9	6	653622.022	0.014	-0.003	4809888.3879	c
16	10	6	15	9	7	710449.510	-0.005	-0.006	4774183.2041	c
16	13	3	15	12	4	726841.812	-0.002	0.000	5169622.9475	c
16	15	2	15	15	1	556800.821	0.000	0.006	5714431.1505	c
16	15	1	15	15	0	556800.821	-0.010	-0.004	5714431.1508	c
16	9	7	15	8	7	666958.834	-0.016	-0.020	4739757.5898	c
16	8	8	15	7	8	676482.284	0.006	0.007	4648306.7534	c
16	9	8	15	8	8	685896.710	0.021	0.015	4655404.8768	c
16	10	7	15	9	7	689327.213	0.021	0.013	4774183.2041	c
16	6	10	15	5	10	689870.340	-0.004	-0.010	4370012.8709	c
16	7	10	15	6	10	690020.499	0.013	0.007	4370063.5221	c
16	4	12	15	3	12	693825.038	0.228	0.219	4006928.4049	c
16	5	12	15	4	12	693825.038	-0.153	-0.162	4006928.4720	c
16	11	5	15	10	5	695102.965	-0.017	-0.026	4899388.9379	c
16	12	4	15	11	4	712241.486	0.004	0.001	5022765.1444	c
16	13	4	15	12	4	726826.218	-0.016	-0.014	5169622.9475	c
16	16	0	15	15	1	768254.347	-2.120	-2.104	5714431.1505	d
16	16	1	15	15	0	768254.347	-2.120	-2.103	5714431.1508	d
16	15	1	15	14	2	754534.332	-2.420	-2.401	5516695.2355	d
16	15	2	15	14	1	754534.332	-2.370	-2.352	5516695.2747	d
17	0	17	15	0	15	896280.518	-3.020	-3.018	3325149.9096	e
17	0	17	15	0	15	896286.514	2.970	2.978	3325149.9096	e
17	1	16	15	1	14	930157.066	0.802	0.810	3570237.1231	e
17	2	15	15	2	13	964060.595	3.500	3.508	3797572.8411	e
17	2	15	15	2	13	964060.595	3.500	3.508	3797572.8411	e
17	3	14	15	3	12	998027.080	-7.500	-7.492	4006928.4049	e
17	3	14	15	3	12	998039.072	4.490	4.499	4006928.4049	e
17	4	13	15	4	11	1032182.435	0.095	0.106	4197946.1344	e
17	14	3	15	12	3	1502014.177	12.600	12.598	5169670.9062	e
17	15	2	15	13	2	1529852.905	-1.970	-1.949	5334852.7435	e
17	15	2	15	13	2	1529852.905	-1.970	-1.949	5334852.7435	e
17	16	1	15	14	1	1557400.834	-2.290	-2.254	5516695.2747	e
17	16	1	15	14	1	1557403.832	0.707	0.744	5516695.2747	e
17	17	0	15	15	0	1584828.846	-0.261	-0.213	5714431.1508	e
17	17	0	15	15	0	1584828.846	-0.261	-0.213	5714431.1508	e

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
16	10	6	16	9	7	77916.300	0.021	0.002	5406716.4334	b
16	9	7	16	8	8	81927.410	0.000	-0.004	5324789.0243	b
16	11	5	16	10	6	109859.220	0.017	-0.004	5484632.7118	b
16	8	8	16	7	9	117278.590	-0.003	-0.004	5207510.4320	b
17	2	15	16	3	14	495337.988	-0.008	-0.003	4266291.9375	c
17	3	15	16	2	14	495337.988	-0.008	-0.003	4266291.9373	c
17	3	14	16	4	13	512319.256	-0.004	0.002	4492643.7236	c
17	4	14	16	3	13	512319.256	-0.018	-0.012	4492643.7116	c
17	4	13	16	5	12	529375.078	0.265	0.271	4700753.6569	c
17	5	13	16	4	12	529375.078	-0.270	-0.264	4700753.2075	c
17	11	7	16	10	6	713999.128	0.017	0.005	5484632.7118	c
17	10	7	16	11	6	524686.296	-0.042	-0.006	5591215.4508	c
17	5	12	16	6	11	546577.687	-0.006	0.001	4890145.6760	c
17	6	12	16	5	11	546591.595	-0.006	0.000	4890134.2281	c
17	6	11	16	7	10	563994.892	-0.004	0.002	5060084.0009	c
17	7	11	16	7	10	564044.341	-0.008	-0.001	5060084.0009	c
17	6	11	16	6	10	564195.683	-0.006	-0.001	5059883.2077	c
17	7	11	16	6	10	564245.136	-0.006	0.000	5059883.2077	c
17	9	8	16	10	7	574022.915	-0.036	-0.005	5463510.3899	c
17	7	10	16	8	9	580902.806	-0.008	0.001	5209868.4745	c
17	8	10	16	8	9	581595.751	-0.011	-0.003	5209868.4745	c
17	7	10	16	7	9	583260.862	0.006	0.010	5207510.4320	c
17	8	10	16	7	9	583953.801	-0.003	0.000	5207510.4320	c
17	8	9	16	9	8	590902.687	-0.014	0.002	5341301.5590	c
17	15	3	16	15	2	593475.555	0.062	0.067	6271231.9660	c
17	15	2	16	15	1	593475.555	-0.082	-0.076	6271231.9764	c
17	14	4	16	14	3	596064.198	0.000	0.005	6075603.3658	c
17	14	3	16	14	2	596068.590	0.002	0.007	6075603.8997	c
17	9	9	16	9	8	597293.156	-0.010	-0.002	5341301.5590	c
17	13	5	16	13	4	599396.689	-0.009	-0.003	5896449.1746	c
17	13	4	16	13	3	599481.685	-0.001	0.005	5896464.7548	c
17	12	6	16	12	5	603587.622	-0.003	0.005	5734721.7304	c
17	12	5	16	12	4	604642.714	-0.008	0.000	5735006.6192	c
17	10	8	16	10	7	606594.957	-0.016	-0.006	5463510.3899	c
17	9	9	16	8	8	613805.709	0.008	0.002	5324789.0243	c
17	11	6	16	11	5	615098.643	-0.017	-0.005	5594491.9134	c
17	9	8	16	9	7	630816.902	-0.006	0.000	5406716.4334	c
17	10	7	16	10	6	631269.060	-0.018	-0.004	5484632.7118	c
17	10	8	16	9	7	663388.953	0.023	0.007	5406716.4334	c
17	12	6	16	11	5	743817.441	-0.002	-0.006	5594491.9134	c
17	11	6	16	10	7	746080.190	0.005	0.004	5463510.3899	c
16	12	4	16	7	9	527496.248	0.056	-0.001	5207510.4320	c
16	7	10	16	4	13	567440.358	0.075	0.036	4492643.7236	c
17	16	2	16	16	1	591410.767	-0.007	0.001	6482687.6140	c
17	16	1	16	16	0	591410.767	-0.010	-0.002	6482687.6140	c

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J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
17	11	6	16	10	6	724957.882	0.019	0.011	5484632.7118	c
17	17	0	16	16	1	816568.948	-3.690	-3.660	6482687.6140	d
17	17	1	16	16	0	816568.948	-3.690	-3.660	6482687.6140	d
17	16	1	16	15	2	802869.319	2.890	2.915	6271231.9660	d
17	16	2	16	15	1	802869.319	2.910	2.928	6271231.9764	d
17	13	5	16	12	4	760835.376	-3.880	-3.876	5735006.6192	d
17	13	4	16	12	5	761221.509	-3.200	-3.201	5734721.7304	d
17	9	9	16	6	10	878709.092	-2.430	-2.442	5059883.2077	d
18	0	18	16	0	16	949538.648	-0.073	-0.066	3759977.0969	e
18	0	18	16	0	16	949541.646	2.920	2.932	3759977.0969	e
18	1	17	16	1	15	983403.204	-1.150	-1.139	4022002.4472	e
18	1	17	16	1	15	983403.204	-1.150	-1.139	4022002.4472	e
18	2	16	16	2	14	1017294.742	2.350	2.359	4266291.9373	e
18	3	15	16	3	13	1051243.239	0.671	0.685	4492643.7116	e
18	3	15	16	3	13	1051243.239	0.671	0.685	4492643.7116	e
18	4	14	16	4	12	1085329.642	2.280	2.294	4700753.2075	e
18	4	14	16	4	12	1085332.640	5.280	5.292	4700753.2075	e
18	5	13	16	5	11	1119688.856	-1.360	-1.345	4890134.2281	e
18	15	3	16	13	3	1598793.179	6.410	6.440	5896464.7548	e
18	16	2	16	14	2	1626529.977	-3.950	-3.911	6075603.8997	e
18	16	2	16	14	2	1626535.973	2.050	2.085	6075603.8997	e
18	17	1	16	15	1	1654053.922	15.200	15.282	6271231.9764	e
18	18	0	16	16	0	1681424.974	-12.400	-12.384	6482687.6140	e
18	18	0	16	16	0	1681442.961	5.540	5.604	6482687.6140	e
17	10	7	17	9	8	78368.460	0.011	0.000	6037533.3355	b
17	11	6	17	10	7	93688.810	0.026	0.003	6115901.7837	b
17	9	8	17	8	9	105329.080	-0.003	-0.002	5932204.2537	b
18	2	16	17	3	15	521954.390	-0.007	-0.001	4761629.9286	c
18	3	16	17	2	15	521954.390	-0.007	-0.001	4761629.9286	c
18	4	14	17	5	13	555952.058	0.045	0.052	5230128.5507	c
18	5	14	17	4	13	555952.058	-0.058	-0.050	5230128.4647	c
18	10	9	17	11	6	499421.770	-0.021	0.003	6209590.5672	c
18	11	8	17	12	5	503311.602	-0.026	-0.001	6339649.3350	c
18	1	17	17	2	16	505013.410	-0.007	-0.002	4500393.3781	c
18	2	17	17	1	16	505013.410	-0.007	-0.002	4500393.3781	c
18	11	7	17	12	6	533065.870	-0.046	-0.013	6338309.3490	c
18	3	15	17	4	14	538923.291	-0.003	0.004	5004962.9805	c
18	4	15	17	3	14	538923.291	-0.005	0.002	5004962.9784	c
18	5	13	17	6	12	573098.608	-0.006	0.002	5436725.8239	c
18	6	13	17	5	12	573101.577	-0.005	0.003	5436723.3632	c
18	10	8	17	11	7	589203.017	-0.028	0.010	6198631.8155	c
18	6	12	17	7	11	590455.866	-0.004	0.004	5624128.3445	c
18	7	12	17	7	11	590467.344	-0.013	-0.004	5624128.3445	c
18	6	12	17	6	11	590505.317	-0.006	0.003	5624078.8916	c
18	7	12	17	6	11	590516.797	-0.013	-0.005	5624078.8916	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
18	7	11	17	8	10	607943.907	-0.009	0.000	5791464.2304	c
18	8	11	17	8	10	608130.357	0.007	0.015	5791464.2304	c
18	7	11	17	7	10	608636.857	-0.007	0.001	5790771.2827	c
18	8	11	17	7	10	608823.292	-0.005	0.001	5790771.2827	c
18	8	10	17	9	9	623271.933	-0.020	-0.007	5938594.7193	c
18	9	9	17	10	8	623896.852	-0.026	0.000	6070105.3571	c
18	9	10	17	9	9	625380.190	-0.016	-0.006	5938594.7193	c
18	8	10	17	8	9	629662.411	-0.007	-0.002	5932204.2537	c
18	9	10	17	8	9	631770.669	-0.003	-0.001	5932204.2537	c
18	13	6	17	13	5	637773.370	-0.006	0.002	6495845.8665	c
18	13	5	17	13	4	638190.087	-0.003	0.005	6495946.4352	c
18	10	9	17	10	8	638906.998	-0.005	0.006	6070105.3571	c
18	12	7	17	12	6	642308.828	-0.021	-0.010	6338309.3490	c
18	11	8	17	11	7	644329.138	-0.011	0.001	6198631.8155	c
18	12	6	17	12	5	646061.463	-0.006	0.006	6339649.3350	c
18	9	9	17	9	8	656468.904	0.004	0.009	6037533.3355	c
18	10	9	17	9	8	671479.026	0.001	-0.009	6037533.3355	c
18	10	8	17	10	7	671933.068	-0.010	0.002	6115901.7837	c
18	11	8	17	10	7	727059.194	0.012	-0.001	6115901.7837	c
17	15	3	17	12	6	526398.144	0.035	0.043	6338309.3490	c
17	7	10	17	4	13	560642.858	0.034	0.001	5230128.4647	c
17	7	11	17	4	14	619165.416	0.046	0.009	5004962.9805	c
18	17	2	17	17	1	626010.400	-0.017	-0.006	7299260.2422	c
18	17	1	17	17	0	626010.400	-0.017	-0.007	7299260.2422	c
18	14	5	17	14	4	633713.841	-0.004	0.003	6671667.5579	c
18	14	4	17	14	3	633743.197	0.002	0.008	6671672.4817	c
18	11	7	17	11	6	661784.689	-0.010	0.007	6209590.5672	c
18	17	1	17	16	2	851166.531	-5.750	-5.718	7074098.3819	d
18	17	2	17	16	1	851166.531	-5.750	-5.715	7074098.3849	d
18	15	4	17	14	3	823574.805	-2.700	-2.688	6671672.4817	d
18	14	5	17	13	4	809430.883	-4.090	-4.077	6495946.4352	d
18	14	4	17	13	5	809567.288	-2.520	-2.515	6495845.8665	d
18	13	6	17	12	5	793966.073	-3.840	-3.833	6339649.3350	d
18	18	0	17	17	1	864859.865	-4.920	-4.884	7299260.2422	d
18	18	1	17	17	0	864859.865	-4.920	-4.884	7299260.2422	d
18	16	2	17	15	3	837423.432	-6.930	-6.910	6864707.4531	d
18	16	3	17	15	2	837423.432	-6.740	-6.712	6864707.6072	d
18	13	5	17	12	6	795824.489	-2.690	-2.686	6338309.3490	d
18	12	6	17	11	7	787078.035	-0.955	-0.955	6198631.8155	d
18	11	8	17	8	9	910753.640	-3.070	-3.098	5932204.2537	d
19	0	19	17	0	17	1002784.787	-2.650	-2.640	4221433.4437	e
19	0	19	17	0	17	1002787.784	0.351	0.358	4221433.4437	e
19	1	18	17	1	16	1036646.345	0.379	0.389	4500393.3781	e
19	2	17	17	2	15	1070516.897	-5.380	-5.367	4761629.9286	e
19	2	17	17	2	15	1070522.892	0.615	0.628	4761629.9286	e

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
19	3	16	17	3	14	1104450.405	0.931	0.946	5004962.9784	e
19	4	15	17	4	13	1138479.847	-5.590	-5.570	5230128.4647	e
19	5	14	17	5	12	1172734.133	-2.420	-2.407	5436723.3632	e
19	5	14	17	5	12	1172740.129	3.570	3.589	5436723.3632	e
19	15	4	17	13	4	1667355.714	-17.200	-17.215	6495946.4352	e
19	16	3	17	14	3	1695494.234	0.029	0.071	6671672.4817	e
19	17	2	17	15	2	1723156.084	-4.410	-4.354	6864707.6072	e
19	17	2	17	15	2	1723174.071	13.600	13.633	6864707.6072	e
19	18	1	17	16	1	1750623.069	-2.210	-2.142	7074098.3849	e
19	18	1	17	16	1	1750626.067	0.788	0.856	7074098.3849	e
19	19	0	17	17	0	1778000.116	3.830	3.905	7299260.2422	e
19	19	0	17	17	0	1778000.116	3.830	3.905	7299260.2422	e
18	11	7	18	10	8	83540.420	0.014	-0.004	6787834.8551	b
18	10	8	18	9	9	93832.630	0.003	0.000	6694002.2291	b
18	12	6	18	11	7	114335.560	0.021	0.000	6871375.2601	b
19	0	19	18	1	18	514705.061	-0.002	0.001	4709515.8088	c
19	1	19	18	0	18	514705.061	-0.002	0.001	4709515.8088	c
19	1	18	18	2	17	531632.537	-0.012	-0.007	5005406.7900	c
19	2	18	18	1	17	531632.537	-0.012	-0.007	5005406.7900	c
19	2	17	18	3	16	548567.878	-0.001	0.005	5283584.3209	c
19	3	17	18	2	16	548567.878	-0.001	0.005	5283584.3209	c
19	3	16	18	4	15	565526.171	-0.007	0.001	5543886.2693	c
19	4	16	18	3	15	565526.171	-0.007	0.001	5543886.2690	c
19	13	7	18	14	4	504834.420	-0.015	-0.006	7305415.6706	c
19	10	10	18	11	7	506189.214	-0.014	0.006	6871375.2601	c
19	13	6	18	14	5	507048.183	-0.002	0.008	7305381.3965	c
19	12	8	18	13	5	526999.767	-0.018	0.004	7134136.5194	c
19	11	9	18	12	6	536156.213	-0.024	0.004	6985710.7978	c
19	12	7	18	13	6	543030.121	-0.029	-0.002	7133619.2359	c
19	4	15	18	5	14	582533.316	-0.002	0.007	5786080.5746	c
19	5	15	18	4	14	582533.316	-0.021	-0.012	5786080.5587	c
19	11	8	18	12	7	598385.723	-0.043	-0.003	6980618.1919	c
19	5	14	18	6	13	599635.270	0.294	0.304	6009824.9394	c
19	6	14	18	5	13	599635.270	-0.314	-0.304	6009824.4321	c
19	6	13	18	7	12	616911.466	-0.009	0.001	6214595.6955	c
19	7	13	18	6	12	616925.495	-0.008	0.001	6214584.2090	c
19	7	12	18	8	11	634445.661	-0.003	0.007	6399594.5743	c
19	8	12	18	8	11	634492.494	-0.010	0.000	6399594.5743	c
19	7	12	18	7	11	634632.086	-0.012	-0.002	6399408.1408	c
19	8	12	18	7	11	634678.927	-0.011	0.000	6399408.1408	c
19	10	9	18	11	8	648615.243	-0.038	-0.003	6842960.9585	c
19	8	11	18	9	10	651643.738	-0.017	-0.005	6563974.9191	c
19	9	11	18	9	10	652266.711	-0.007	0.004	6563974.9191	c
19	8	11	18	8	10	653751.991	-0.018	-0.008	6561866.6661	c
19	9	11	18	8	10	654374.965	-0.006	0.001	6561866.6661	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
19	9	10	18	10	9	662875.678	-0.025	-0.005	6709012.3539	c
19	15	5	18	15	4	668058.060	0.003	0.010	7495249.9831	c
19	15	4	18	15	3	668067.866	-0.012	-0.005	7495251.5031	c
19	10	10	18	10	9	668552.123	-0.012	0.000	6709012.3539	c
19	14	5	18	14	4	672076.954	-0.005	0.003	7305415.6706	c
19	13	7	18	13	6	676630.866	-0.005	0.006	7133619.2359	c
19	9	10	18	9	9	677885.825	-0.003	0.003	6694002.2291	c
19	13	6	18	13	5	678293.057	-0.007	0.005	7134136.5194	c
19	11	9	18	11	8	678906.068	-0.010	0.004	6842960.9585	c
19	12	8	18	12	7	680518.104	-0.010	0.004	6980618.1919	c
19	10	10	18	9	9	683562.263	0.003	0.001	6694002.2291	c
19	12	7	18	12	6	690938.567	-0.022	-0.005	6985710.7978	c
19	11	9	18	10	8	734032.191	0.009	-0.002	6787834.8551	c
18	15	3	18	12	6	509540.721	0.011	0.013	6985710.7978	c
18	15	4	18	12	7	514631.797	0.001	0.004	6980618.1919	c
18	8	10	18	5	13	552042.269	0.030	0.003	6009824.4321	c
18	9	10	18	6	13	554150.018	0.033	0.003	6009824.9394	c
19	17	3	18	17	2	662597.418	-0.008	0.001	7925270.6528	c
19	17	2	18	17	1	662597.418	-0.020	-0.011	7925270.6534	c
19	16	4	18	16	3	665028.658	0.209	0.216	7702137.7672	c
19	16	3	18	16	2	665028.658	-0.207	-0.200	7702137.8109	c
19	14	6	18	14	5	671920.386	0.003	0.011	7305381.3965	c
19	11	8	18	11	7	707628.684	-0.015	0.003	6871375.2601	c
19	17	2	18	16	3	885726.641	-3.680	-3.653	7702137.7672	d
19	17	3	18	16	2	885726.641	-3.630	-3.597	7702137.8109	d
19	14	5	18	13	6	843869.276	-4.120	-4.110	7133619.2359	d
19	14	6	18	13	5	843162.365	-2.900	-2.887	7134136.5194	d
19	15	5	18	14	4	857889.984	-2.390	-2.371	7305415.6706	d
19	16	3	18	15	4	871912.790	-3.910	-3.881	7495249.9831	d
19	16	4	18	15	3	871912.790	-1.930	-1.901	7495251.5031	d
19	18	1	18	17	2	899449.654	-3.350	-3.311	7925270.6528	d
19	18	2	18	17	1	899449.654	-3.350	-3.310	7925270.6534	d
19	19	0	18	18	1	913127.998	-3.510	-3.463	8164125.0186	d
19	19	1	18	18	0	913127.998	-3.510	-3.463	8164125.0186	d
19	11	8	18	10	9	869989.020	-2.590	-2.576	6709012.3539	d
19	12	7	18	11	8	833686.515	-1.920	-1.911	6842960.9585	d
19	13	6	18	12	7	831809.513	-1.880	-1.877	6980618.1919	d
19	10	10	18	7	11	978153.048	-3.300	-3.312	6399408.1408	d
19	7	12	18	6	13	1024213.207	-2.100	-2.106	6009824.9394	d
20	0	20	18	0	18	1056030.925	1.610	1.621	4709515.8088	e
20	1	19	18	1	17	1089877.494	-3.180	-3.166	5005406.7900	e
20	1	19	18	1	17	1089880.491	-0.179	-0.168	5005406.7900	e
20	2	18	18	2	16	1123739.052	-6.920	-6.904	5283584.3209	e
20	2	18	18	2	16	1123751.043	5.070	5.088	5283584.3209	e
20	3	17	18	3	15	1157651.574	-1.660	-1.640	5543886.2690	e

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J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
20	5	15	18	5	13	1225815.386	-2.630	-2.611	6009824.4321	e
20	16	4	18	14	4	1764191.676	11.400	11.415	7305415.6706	e
20	17	3	18	15	3	1792126.337	-7.840	-7.787	7495251.5031	e
20	17	3	18	15	3	1792135.331	1.150	1.207	7495251.5031	e
20	18	2	18	16	2	1819734.224	0.806	0.878	7702137.8109	e
20	18	2	18	16	2	1819740.220	6.800	6.874	7702137.8109	e
20	19	1	18	17	1	1847159.238	-1.030	-0.944	7925270.6534	e
20	19	1	18	17	1	1847168.232	7.970	8.050	7925270.6534	e
20	20	0	18	18	0	1874512.302	9.420	9.510	8164125.0186	e
19	11	8	19	10	9	87427.730	0.010	0.000	7491576.2334	b
19	12	7	19	11	8	97645.450	0.021	-0.001	7579003.9524	b
19	10	9	19	9	10	119688.180	-0.004	-0.003	7371888.0503	b
20	0	20	19	1	19	541324.246	-0.002	0.002	5224220.8673	c
20	1	20	19	0	19	541324.246	-0.002	0.002	5224220.8673	c
20	2	18	19	3	17	575178.087	-0.003	0.004	5832152.1948	c
20	3	18	19	2	17	575178.087	-0.003	0.004	5832152.1948	c
20	3	17	19	4	16	592127.050	-0.003	0.006	6109412.4417	c
20	4	17	19	3	16	592127.050	-0.003	0.006	6109412.4417	c
20	4	16	19	5	15	609116.357	-0.007	0.003	6368613.8894	c
20	5	16	19	4	15	609116.357	-0.010	-0.001	6368613.8864	c
20	5	15	19	6	14	626182.485	0.052	0.062	6609460.0103	c
20	6	15	19	5	14	626182.485	-0.069	-0.059	6609459.9093	c
20	10	11	19	11	8	494815.777	-0.013	0.002	7579003.9524	c
20	15	6	19	16	3	502228.990	0.006	-0.004	8367166.6698	c
20	15	5	19	16	4	502297.315	0.017	0.007	8367166.2100	c
20	14	7	19	15	4	524677.381	-0.015	-0.013	8163319.3743	c
20	14	6	19	15	5	525566.153	-0.003	-0.001	8163308.0340	c
20	13	8	19	14	5	548309.355	-0.016	0.001	7977492.6229	c
20	11	10	19	12	7	555839.913	-0.023	0.004	7676649.3806	c
20	13	7	19	14	6	556060.805	-0.014	0.004	7977301.7729	c
20	1	19	19	2	18	558248.114	-0.007	-0.001	5537039.3339	c
20	2	19	19	1	18	558248.114	-0.007	-0.001	5537039.3339	c
20	12	9	19	13	6	565829.245	-0.033	-0.006	7812429.5765	c
20	12	8	19	13	7	605027.006	-0.030	0.006	7810250.1007	c
20	6	14	19	7	13	643389.115	-0.019	-0.008	6831509.7062	c
20	7	14	19	6	13	643392.206	-0.010	0.001	6831507.1643	c
20	7	13	19	8	12	660837.525	-0.005	0.007	7034087.0722	c
20	8	13	19	7	12	660895.487	-0.014	-0.002	7034040.2321	c
20	11	9	19	12	8	664461.288	-0.048	-0.006	7661136.2997	c
20	8	12	19	9	11	678488.813	-0.010	0.003	7216241.6308	c
20	9	12	19	9	11	678658.521	-0.011	0.002	7216241.6308	c
20	8	12	19	8	11	679111.779	-0.006	0.005	7215618.6680	c
20	9	12	19	8	11	679281.483	-0.011	0.000	7215618.6680	c
20	9	11	19	10	10	694393.658	-0.010	0.007	7377564.4826	c
20	10	10	19	11	9	697170.621	-0.030	-0.001	7521867.0298	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(\text{SP})$ / MHz	$\Delta_{O-C}(\text{LP})$ / MHz	E''/h (MHz)	Source
20	10	11	19	9	10	701931.687	-0.007	-0.001	7371888.0503	c
20	11	10	19	10	9	740913.093	0.008	0.003	7491576.2334	c
19	15	5	19	12	8	502171.764	0.025	0.021	7661136.2997	c
19	9	10	19	6	13	540380.884	-0.007	-0.028	6831507.1643	c
20	10	10	19	12	7	542388.254	-0.045	-0.005	7676649.3806	c
20	8	13	19	8	12	660848.636	-0.025	-0.012	7034087.0722	c
20	7	13	19	7	12	660884.369	-0.001	0.011	7034040.2321	c
20	19	2	19	19	1	695174.381	-0.014	0.003	9077256.5135	c
20	19	1	19	19	0	695174.381	-0.014	0.003	9077256.5135	c
20	10	11	19	10	10	696255.250	-0.011	0.003	7377564.4826	c
20	18	3	19	18	2	697147.563	-0.004	0.006	8824723.6467	c
20	18	2	19	18	1	697147.563	-0.008	0.003	8824723.6470	c
20	17	4	19	17	3	699517.512	0.048	0.055	8587868.0722	c
20	17	3	19	17	2	699517.512	-0.077	-0.069	8587868.0845	c
20	9	11	19	9	10	700070.089	-0.011	-0.002	7371888.0503	c
20	16	5	19	16	4	702426.087	-0.007	0.000	8367166.2100	c
20	15	6	19	15	5	706087.598	-0.024	-0.017	8163308.0340	c
20	15	5	19	15	4	706144.115	-0.020	-0.013	8163319.3743	c
20	11	10	19	11	9	710622.272	-0.016	0.000	7521867.0298	c
20	14	7	19	14	6	710694.988	-0.011	-0.001	7977301.7729	c
20	14	6	19	14	5	711381.552	-0.017	-0.006	7977492.6229	c
20	13	8	19	13	7	715551.879	-0.016	-0.001	7810250.1007	c
20	12	9	19	12	8	717122.537	-0.020	-0.003	7661136.2997	c
20	13	7	19	13	6	720933.006	-0.011	0.004	7812429.5765	c
20	14	6	19	13	7	878621.252	-2.840	-2.832	7810250.1007	d
20	14	7	19	13	6	875564.266	-2.930	-2.922	7812429.5765	d
20	15	6	19	14	5	891900.573	-2.460	-2.445	7977492.6229	d
20	15	5	19	14	6	892157.195	-4.540	-4.527	7977301.7729	d
20	17	3	19	16	4	920213.600	-5.870	-5.833	8367166.2100	d
20	17	4	19	16	3	920213.600	-5.270	-5.236	8367166.6698	d
20	19	1	19	18	2	947704.296	-2.970	-2.922	8824723.6467	d
20	19	2	19	18	1	947704.296	-2.970	-2.922	8824723.6470	d
20	20	0	19	19	1	961367.951	-3.430	-3.379	9077256.5135	d
20	20	1	19	19	0	961367.951	-3.430	-3.379	9077256.5135	d
20	18	2	19	17	3	933999.270	-3.880	-3.838	8587868.0722	d
20	18	3	19	17	2	933999.270	-3.860	-3.822	8587868.0845	d
20	13	7	19	12	8	872223.075	-3.220	-3.216	7661136.2997	d
20	13	8	19	12	7	849150.125	-2.490	-2.492	7676649.3806	d
20	12	9	19	11	8	799252.319	-2.590	-2.595	7579003.9524	d
20	12	8	19	11	9	893407.631	-2.480	-2.468	7521867.0298	d
20	9	11	19	8	12	1037867.568	-3.510	-3.515	7034087.0722	d
20	10	11	19	7	12	1039776.348	-3.170	-3.172	7034040.2321	d
21	0	21	19	0	19	1109259.076	-4.910	-4.905	5224220.8673	e
21	1	20	19	1	18	1143108.642	0.593	0.604	5537039.3339	e
21	1	20	19	1	18	1143111.640	3.590	3.602	5537039.3339	e

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
21	2	19	19	2	17	1176964.205	1.390	1.404	5832152.1948	e
21	2	19	19	2	17	1176967.203	4.390	4.402	5832152.1948	e
21	3	18	19	3	16	1210849.746	-2.570	-2.555	6109412.4417	e
21	3	18	19	3	16	1210855.742	3.420	3.441	6109412.4417	e
21	4	17	19	4	15	1244804.240	-11.600	-11.555	6368613.8864	e
21	5	16	19	5	14	1278926.618	7.250	7.273	6609459.9093	e
21	6	15	19	6	13	1313291.827	11.800	11.867	6831507.1643	e
21	18	3	19	16	3	1888707.475	-2.910	-2.841	8367166.6698	e
21	19	2	19	17	2	1916249.408	-1.500	-1.408	8587868.0845	e
21	19	2	19	17	2	1916252.406	1.500	1.590	8587868.0845	e
21	20	1	19	18	1	1943638.447	-2.520	-2.424	8824723.6470	e
21	21	0	19	19	0	1970949.540	-4.830	-4.733	9077256.5135	e
21	21	0	19	19	0	1970958.534	4.160	4.261	9077256.5135	e
20	12	8	20	11	9	89679.520	0.017	0.000	8325597.6287	b
20	11	9	20	10	10	106559.955	-0.001	-0.003	8219037.6739	b
20	13	7	20	12	8	118085.480	0.023	0.002	8415277.1306	b
21	6	15	20	7	14	669888.085	0.317	0.329	7474899.3737	c
21	7	15	20	6	14	669888.085	-0.333	-0.321	7474898.8338	c
21	0	21	20	1	20	567939.738	-0.002	0.001	5765545.1096	c
21	1	21	20	0	20	567939.738	-0.002	0.001	5765545.1096	c
21	1	20	20	2	19	584859.927	-0.001	0.004	6095287.4490	c
21	2	20	20	1	19	584859.927	-0.001	0.004	6095287.4490	c
21	2	19	20	3	18	601784.718	-0.007	0.000	6407330.2788	c
21	3	19	20	2	18	601784.718	-0.007	0.000	6407330.2788	c
21	4	17	20	5	16	635699.439	-0.009	0.002	6977730.2477	c
21	5	17	20	4	16	635699.439	-0.009	0.001	6977730.2471	c
21	5	16	20	6	15	652736.810	-0.003	0.009	7235642.4572	c
21	6	16	20	5	15	652736.810	-0.027	-0.014	7235642.4377	c
21	16	5	20	17	4	522522.009	0.017	-0.002	9287385.5295	c
21	15	7	20	16	4	544485.791	0.006	-0.001	9069595.9552	c
21	14	8	20	15	5	568401.479	-0.011	-0.003	8869463.5028	c
21	14	7	20	15	6	571845.539	-0.012	-0.004	8869395.6493	c
21	13	9	20	14	6	590600.874	-0.022	0.001	8688874.1847	c
21	12	10	20	13	7	596041.619	-0.029	0.002	8533362.5866	c
21	13	8	20	14	7	612678.400	-0.031	-0.003	8687996.7650	c
21	12	9	20	13	8	673265.957	-0.040	0.003	8525801.9881	c
21	7	14	20	8	13	687238.550	-0.011	0.003	7694935.7261	c
21	8	14	20	7	13	687252.206	-0.010	0.003	7694924.5955	c
21	8	13	20	9	12	704886.120	-0.020	-0.006	7894900.1557	c
21	9	13	20	8	12	705099.195	-0.009	0.004	7894730.4467	c
21	9	12	20	10	11	722356.620	-0.014	0.001	8073819.7371	c
21	11	10	20	12	9	723404.667	-0.043	-0.003	8378258.8490	c
21	10	12	20	9	11	724770.752	-0.009	0.003	8071958.1438	c
20	10	10	20	7	13	524113.077	-0.007	-0.020	7694924.5955	c
20	16	4	20	13	7	536233.367	-0.007	0.009	8533362.5866	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
20	16	5	20	13	8	543790.298	-0.016	0.001	8525801.9881	c
21	11	11	20	12	8	556951.737	-0.017	0.005	8415277.1306	c
20	9	11	20	6	14	597059.340	0.024	0.002	7474898.8338	c
21	9	13	20	9	12	704929.478	-0.017	-0.004	7894900.1557	c
21	8	13	20	8	12	705055.828	-0.021	-0.007	7894730.4467	c
21	10	12	20	10	11	722909.162	-0.005	0.010	8073819.7371	c
21	9	12	20	9	11	724218.219	-0.009	0.004	8071958.1438	c
21	14	8	20	13	7	904497.265	-5.140	-5.138	8533362.5866	d
21	14	7	20	13	8	915436.403	-2.810	-2.804	8525801.9881	d
21	15	7	20	14	6	925205.150	-2.410	-2.394	8688874.1847	d
21	15	6	20	14	7	926419.910	-1.900	-1.886	8687996.7650	d
21	16	6	20	15	5	940416.934	-3.710	-3.681	8869463.5028	d
21	16	5	20	15	6	940508.671	-3.210	-3.182	8869395.6493	d
21	17	4	20	16	5	954601.029	-5.110	-5.073	9069592.2968	d
21	17	5	20	16	4	954601.029	-0.292	-0.260	9069595.9552	d
21	18	3	20	17	4	968488.928	-2.590	-2.552	9287385.5295	d
21	18	4	20	17	3	968488.928	-2.420	-2.375	9287385.6662	d
21	19	2	20	18	3	982247.917	0.145	0.193	9521871.2074	d
21	19	3	20	18	2	982247.917	0.150	0.197	9521871.2110	d
21	20	1	20	19	2	995932.257	-1.450	-1.397	9772430.9014	d
21	20	2	20	19	1	995932.257	-1.450	-1.397	9772430.9014	d
21	21	0	20	20	1	1009581.222	-1.770	-1.720	10038627.8829	d
21	21	1	20	20	0	1009581.222	-1.770	-1.720	10038627.8829	d
21	10	12	20	7	13	1101802.870	-1.440	-1.445	7694924.5955	d
21	8	14	20	5	15	1146528.352	-6.030	-6.032	7235642.4377	d
21	7	14	20	6	15	1146528.352	-3.480	-3.488	7235642.4572	d
21	13	8	20	12	9	922412.880	-3.470	-3.460	8378258.8490	d
21	13	9	20	12	8	864195.824	-2.130	-2.133	8415277.1306	d
21	11	10	20	10	11	1027840.999	-2.830	-2.811	8073819.7371	d
21	11	11	20	8	12	1077495.374	-3.070	-3.072	7894730.4467	d
21	8	13	20	7	14	1124883.615	-3.310	-3.315	7474899.3737	d
22	0	22	20	0	20	1162490.225	-0.874	-0.868	5765545.1096	e
22	0	22	20	0	20	1162496.221	5.120	5.128	5765545.1096	e
22	1	21	20	1	19	1196330.797	3.090	3.105	6095287.4490	e
22	2	20	20	2	18	1230168.372	-3.870	-3.854	6407330.2788	e
22	2	20	20	2	18	1230171.370	-0.871	-0.856	6407330.2788	e
22	3	19	20	3	17	1264044.920	-0.641	-0.623	6701539.4888	e
22	3	19	20	3	17	1264056.912	11.400	11.369	6701539.4888	e
22	4	18	20	4	16	1297981.426	0.653	0.674	6977730.2471	e
22	4	18	20	4	16	1297981.426	0.653	0.674	6977730.2471	e
22	5	17	20	5	15	1332028.856	-2.960	-2.932	7235642.4377	e
22	5	17	20	5	15	1332034.851	3.040	3.063	7235642.4377	e
22	6	16	20	6	14	1366283.142	-6.810	-6.788	7474898.8338	e
22	7	15	20	7	13	1400924.160	2.290	2.314	7694924.5955	e
22	18	4	20	16	4	1957488.859	-1.370	-1.293	9069595.9552	e

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
22	19	3	20	17	3	1985225.657	2.010	2.098	9287385.6662	e
22	20	2	20	18	2	2012710.629	-0.190	-0.088	9521871.2110	e
22	22	0	20	20	0	2067347.805	-0.131	-0.020	10038627.8829	e
21	13	8	21	12	9	101607.230	0.018	-0.003	9199067.9788	b
22	8	14	21	9	13	731207.219	-0.018	-0.002	8599829.6441	c
22	9	14	21	9	13	731217.726	-0.015	0.000	8599829.6441	c
22	8	14	21	8	13	731250.579	-0.013	0.002	8599786.2890	c
22	9	14	21	8	13	731261.083	-0.013	0.002	8599786.2890	c
22	0	22	21	1	21	594551.357	-0.002	0.001	6333484.8442	c
22	1	22	21	0	21	594551.357	-0.002	0.001	6333484.8442	c
22	1	21	21	2	20	611467.775	0.001	0.005	6680147.3716	c
22	2	21	21	1	20	611467.775	0.001	0.005	6680147.3716	c
22	2	20	21	3	19	628387.509	-0.006	0.001	7009114.9982	c
22	3	20	21	2	19	628387.509	-0.006	0.001	7009114.9982	c
22	3	19	21	4	18	645320.288	-0.008	0.002	7320264.7481	c
22	4	19	21	3	18	645320.288	-0.008	0.002	7320264.7481	c
22	4	18	21	5	17	662281.320	-0.005	0.007	7613429.6894	c
22	5	18	21	4	17	662281.320	-0.005	0.007	7613429.6891	c
22	5	17	21	6	16	679294.966	-0.009	0.003	7888379.2677	c
22	6	17	21	5	16	679294.966	-0.014	-0.001	7888379.2641	c
22	6	16	21	7	15	696401.591	0.053	0.067	8144787.2457	c
22	7	16	21	6	15	696401.591	-0.080	-0.066	8144787.1348	c
22	19	4	21	20	1	504244.728	0.037	0.006	10768364.5971	c
22	19	3	21	20	2	504244.728	0.025	-0.006	10768364.5971	c
22	18	5	21	19	2	522967.054	0.216	0.182	10504118.9698	c
22	18	4	21	19	3	522967.054	-0.143	-0.176	10504118.9689	c
22	11	12	21	12	9	540238.070	-0.025	-0.008	9199067.9788	c
22	17	6	21	18	3	542852.159	0.025	-0.004	10255877.0406	c
22	17	5	21	18	4	542860.051	0.030	0.002	10255877.0007	c
22	16	7	21	17	4	564376.922	0.016	-0.001	10024198.4219	c
22	16	6	21	17	5	564502.476	0.018	0.001	10024197.2674	c
22	15	8	21	16	5	588002.222	-0.006	-0.008	9809907.5164	c
22	15	7	21	16	6	589438.484	-0.010	-0.012	9809884.1326	c
22	12	11	21	13	8	610970.538	-0.030	-0.001	9300675.1894	c
22	14	9	21	15	6	612350.441	-0.021	-0.006	9614418.5668	c
22	13	10	21	14	7	628106.273	-0.024	0.005	9441241.1945	c
22	13	9	21	14	8	678434.281	-0.031	0.008	9437864.9873	c
22	7	15	21	8	14	713669.638	-0.019	-0.005	8382176.8048	c
22	8	15	21	7	14	713672.724	-0.008	0.006	8382174.2803	c
21	11	10	21	8	13	501877.278	0.010	0.002	8599786.2890	c
21	16	5	21	13	8	509232.341	0.009	0.011	9300675.1894	c
21	10	11	21	7	14	585067.829	0.013	-0.004	8382174.2803	c
21	17	5	21	14	8	586332.260	-0.026	0.015	9437864.9873	c
21	11	11	21	8	14	590052.095	0.015	-0.010	8382176.8048	c
21	15	6	21	10	11	647176.515	0.032	-0.009	8967242.0904	c

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J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
21	10	12	21	7	15	651941.684	0.026	0.002	8144787.2457	c
22	10	12	21	11	11	765443.191	-6.870	-6.852	8972228.8795	d
22	15	8	21	14	7	956667.200	-1.350	-1.339	9441241.1945	d
22	15	7	21	14	8	961456.090	-1.550	-1.539	9437864.9873	d
22	16	7	21	15	6	974153.512	-3.250	-3.230	9614418.5668	d
22	16	6	21	15	7	974615.493	-2.500	-2.478	9614081.7350	d
22	17	5	21	16	6	988850.253	-2.640	-2.608	9809884.1326	d
22	17	6	21	16	5	988818.475	-3.190	-3.156	9809907.5164	d
22	18	4	21	17	5	1002884.751	-4.150	-4.112	10024197.2674	d
22	18	5	21	17	4	1002884.751	-2.640	-2.599	10024198.4219	d
22	19	3	21	18	4	1016730.080	-2.220	-2.176	10255877.0007	d
22	19	4	21	18	3	1016730.080	-2.170	-2.125	10255877.0406	d
22	20	2	21	19	3	1030459.989	-3.060	-3.008	10504118.9689	d
22	20	3	21	19	2	1030459.989	-3.060	-3.007	10504118.9698	d
22	21	1	21	20	2	1044128.440	-2.520	-2.460	10768364.5971	d
22	21	2	21	20	1	1044128.440	-2.520	-2.460	10768364.5971	d
22	22	0	21	21	1	1057762.115	-2.820	-2.768	11048210.8688	d
22	22	1	21	21	0	1057762.115	-2.820	-2.768	11048210.8688	d
22	13	10	21	10	11	1102101.164	-4.240	-4.254	8967242.0904	d
22	11	12	21	8	13	1139517.399	-2.390	-2.391	8599786.2890	d
22	10	13	21	7	14	1163716.670	-2.880	-2.881	8382174.2803	d
22	9	13	21	8	14	1163560.778	-4.150	-4.148	8382176.8048	d
22	8	15	21	5	16	1207466.027	-1.730	-1.729	7888379.2641	d
22	7	15	21	6	16	1207466.027	-1.170	-1.175	7888379.2677	d
22	14	9	21	13	8	926091.337	-2.510	-2.502	9300675.1894	d
22	12	11	21	11	10	809976.206	-6.000	-6.003	9101663.5519	d
22	14	8	21	13	9	958107.705	-1.640	-1.629	9279475.0750	d
22	13	9	21	12	10	986892.906	-2.170	-2.152	9129404.2286	d
22	12	10	21	11	11	1047551.473	-0.429	-0.409	8972228.8795	d
22	12	11	21	9	12	1115466.825	-2.570	-2.575	8796176.3644	d
22	11	12	21	8	13	1139517.399	-2.390	-2.391	8599786.2890	d
23	0	23	21	0	21	1215706.384	-3.900	-3.890	6333484.8442	e
23	0	23	21	0	21	1215709.382	-0.897	-0.893	6333484.8442	e
23	1	22	21	1	20	1249537.963	-1.280	-1.268	6680147.3716	e
23	1	22	21	1	20	1249537.963	-1.280	-1.268	6680147.3716	e
23	2	21	21	2	19	1283372.540	-1.190	-1.174	7009114.9982	e
23	3	20	21	3	18	1317231.100	-0.912	-0.894	7320264.7481	e
23	3	20	21	3	18	1317240.094	8.080	8.100	7320264.7481	e
23	4	19	21	4	17	1351134.629	-7.750	-7.731	7613429.6891	e
23	4	19	21	4	17	1351140.625	-1.760	-1.735	7613429.6891	e
23	5	18	21	5	16	1385149.081	-0.545	-0.520	7888379.2641	e
23	5	18	21	5	16	1385161.073	11.400	11.472	7888379.2641	e
23	7	16	21	7	14	1453792.560	-7.350	-7.318	8382174.2803	e
23	18	5	21	16	5	2025994.433	12.700	12.767	9809907.5164	e
23	19	4	21	17	4	2054019.032	-3.880	-3.788	10024198.4219	e

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
23	20	3	21	18	3	2081683.880	10.500	10.586	10255877.0406	e
23	21	2	21	19	2	2109111.892	1.070	1.181	10504118.9698	e
23	22	1	21	20	1	2136425.983	-2.610	-2.492	10768364.5971	e
23	23	0	21	21	0	2163680.115	-0.623	-0.507	11048210.8688	e
23	5	18	22	6	17	705854.634	-0.012	0.001	8567674.2372	c
23	6	18	22	5	17	705854.634	-0.013	0.000	8567674.2363	c
23	1	22	22	2	21	638071.460	-0.006	-0.001	7291615.1400	c
23	2	22	22	1	21	638071.460	-0.006	-0.001	7291615.1400	c
23	2	21	22	3	20	654986.207	-0.005	0.001	7637502.5075	c
23	3	21	22	2	20	654986.207	-0.005	0.001	7637502.5075	c
23	3	20	22	4	19	671911.712	-0.004	0.005	7965585.0373	c
23	4	20	22	3	19	671911.712	-0.004	0.005	7965585.0373	c
23	4	19	22	5	18	688861.041	-0.016	-0.005	8275711.0074	c
23	5	19	22	4	18	688861.041	-0.016	-0.005	8275711.0074	c
23	6	17	22	7	16	722925.232	0.001	0.015	8841188.7987	c
23	7	17	22	6	16	722925.232	-0.025	-0.011	8841188.7768	c
23	7	16	22	8	15	740127.496	0.321	0.336	9095847.0053	c
23	8	16	22	7	15	740127.496	-0.345	-0.330	9095846.4552	c
23	19	5	22	20	2	543639.281	0.085	0.045	11534582.0104	c
23	19	4	22	20	3	543639.281	-0.024	-0.064	11534582.0101	c
23	17	7	22	18	4	584383.474	0.026	-0.002	11027086.1605	c
23	17	6	22	18	5	584428.296	0.019	-0.009	11027085.8028	c
23	12	12	22	13	9	606189.289	-0.033	-0.009	10116299.2923	c
23	16	8	22	17	5	607503.223	0.016	0.004	10798737.0159	c
23	16	7	22	17	6	608073.532	0.024	0.011	10798729.1698	c
23	15	9	22	16	6	632468.828	-0.008	-0.002	10588699.7193	c
23	15	8	22	16	7	637623.130	-0.016	-0.009	10588575.3225	c
23	14	10	22	15	7	654280.786	-0.030	-0.006	10399322.6209	c
23	13	11	22	14	8	655045.935	-0.028	0.005	10237584.4090	c
23	14	9	22	15	8	683817.091	-0.037	-0.008	10397909.7386	c
23	21	3	22	22	0	507254.001	0.020	0.005	12105975.7984	c
23	21	2	22	22	1	507254.001	0.020	0.004	12105975.7984	c
23	11	13	22	12	10	513039.082	-0.024	-0.010	10019780.7708	c
22	16	7	22	13	10	519227.841	-0.001	-0.007	10069347.4851	c
22	13	10	22	10	13	523453.684	0.014	-0.017	9545893.8199	c
23	20	4	22	21	1	525054.916	0.041	0.007	11812495.5444	c
23	20	3	22	21	2	525054.916	0.038	0.004	11812495.5444	c
22	17	5	22	14	8	561152.558	-0.055	-0.027	10237584.4090	c
22	11	11	22	8	14	568698.213	0.023	0.012	9331036.8736	c
22	17	6	22	14	9	571960.155	0.003	0.033	10226769.0231	c
22	12	11	22	9	14	580598.403	0.023	-0.001	9331047.3777	c
22	18	5	22	15	8	629175.986	-0.084	-0.017	10397909.7386	c
23	12	11	22	14	8	629985.601	-0.056	-0.004	10237584.4090	c
22	10	12	22	7	15	641832.500	0.014	-0.005	9095846.4552	c
23	12	12	22	11	11	822745.578	-7.980	-7.974	9899735.0582	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
23	15	9	22	14	8	983580.196	-3.950	-3.943	10237584.4090	d
23	16	8	22	15	7	1006915.465	-2.140	-2.120	10399322.6209	d
23	16	7	22	15	8	1008890.499	-2.440	-2.424	10397909.7386	d
23	17	7	22	16	6	1022767.906	-1.990	-1.958	10588699.7193	d
23	17	6	22	16	7	1022936.689	-2.070	-2.043	10588575.3225	d
23	19	4	22	18	5	1051131.599	-3.920	-3.871	11027085.8028	d
23	19	5	22	18	4	1051131.599	-3.450	-3.404	11027086.1605	d
23	20	3	22	19	4	1064938.254	-2.890	-2.835	11272609.2833	d
23	20	4	22	19	3	1064938.254	-2.880	-2.820	11272609.2950	d
23	22	1	22	21	2	1092294.943	-2.690	-2.632	11812495.5444	d
23	22	2	22	21	1	1092294.943	-2.690	-2.632	11812495.5444	d
23	23	0	22	22	1	1105913.928	-1.870	-1.811	12105975.7984	d
23	23	1	22	22	0	1105913.928	-1.870	-1.811	12105975.7984	d
23	11	12	22	10	13	1172251.470	-2.640	-2.634	9545893.8199	d
23	12	12	22	9	13	1176742.366	-4.530	-4.532	9545741.7202	d
23	10	13	22	9	14	1201286.399	-1.390	-1.385	9331047.3777	d
23	8	16	22	5	17	1268295.776	-4.290	-4.290	8567674.2363	d
23	7	16	22	6	17	1268295.776	-4.170	-4.173	8567674.2372	d
23	14	10	22	13	9	937302.087	-2.060	-2.062	10116299.2923	d
23	13	11	22	12	10	872844.546	-5.060	-5.061	10019780.7708	d
23	14	9	22	13	10	1012378.588	-0.797	-0.783	10069347.4851	d
23	7	17	22	4	18	1288401.378	-1.650	-1.656	8275711.0074	d
23	6	17	22	5	18	1288401.378	-1.650	-1.651	8275711.0074	d
24	0	24	22	0	22	1268922.543	1.380	1.381	6928036.1971	e
24	0	24	22	0	22	1268922.543	1.380	1.381	6928036.1971	e
24	1	23	22	1	21	1302742.130	-0.146	-0.138	7291615.1400	e
24	1	23	22	1	21	1302748.126	5.850	5.858	7291615.1400	e
24	2	22	22	2	20	1336561.718	-5.080	-5.066	7637502.5075	e
24	2	22	22	2	20	1336570.711	3.910	3.928	7637502.5075	e
24	3	21	22	3	19	1370402.290	-8.590	-8.572	7965585.0373	e
24	3	21	22	3	19	1370402.290	-8.590	-8.572	7965585.0373	e
24	5	19	22	5	17	1438266.309	-2.500	-2.471	8567674.2363	e
24	5	19	22	5	17	1438275.303	6.500	6.523	8567674.2363	e
24	6	18	22	6	16	1472370.699	-9.500	-9.472	8841188.7768	e
24	8	16	22	8	14	1541499.842	1.980	2.008	9331036.8736	e
24	19	5	22	17	5	2122581.567	5.650	5.733	10798737.0159	e
24	20	4	22	18	4	2150486.249	5.310	5.412	11027086.1605	e
24	21	3	22	19	3	2178055.164	-3.170	-3.058	11272609.2950	e
24	22	2	22	20	2	2205444.203	-4.250	-4.124	11534582.0104	e
24	23	1	22	21	1	2232734.310	4.320	4.444	11812495.5444	e
24	24	0	22	22	0	2259949.470	-0.486	-0.369	12105975.7984	e
23	14	9	23	13	10	105806.970	0.011	-0.010	10975919.9024	b
24	3	21	23	4	20	698499.160	-0.004	0.005	8637496.7470	c
24	4	21	23	3	20	698499.160	-0.004	0.005	8637496.7470	c
24	0	24	23	1	23	647762.247	0.002	0.003	7549195.1117	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(\text{SP})$ / MHz	$\Delta_{O-C}(\text{LP})$ / MHz	E''/h (MHz)	Source
24	1	24	23	0	23	647762.247	0.002	0.003	7549195.1117	c
24	1	23	23	2	22	664670.804	-0.007	-0.003	7929686.5993	c
24	2	23	23	1	22	664670.804	-0.007	-0.003	7929686.5993	c
24	2	22	23	3	21	681580.574	-0.010	-0.004	8292488.7133	c
24	3	22	23	2	21	681580.574	-0.010	-0.004	8292488.7133	c
24	4	20	23	5	19	715437.905	-0.010	0.001	8964572.0575	c
24	5	20	23	4	19	715437.905	-0.010	0.001	8964572.0575	c
24	5	19	23	6	18	732414.144	-0.014	-0.001	9273528.8762	c
24	6	19	23	5	18	732414.144	-0.014	-0.001	9273528.8759	c
24	12	13	23	13	10	584406.125	-0.018	0.000	10975919.9024	c
24	18	7	23	19	4	604502.591	0.035	-0.003	12078221.3101	c
24	18	6	23	19	5	604518.162	0.037	-0.001	12078221.2013	c
24	17	8	23	18	5	627080.562	0.027	0.003	11835889.2343	c
24	17	7	23	18	6	627298.188	0.027	0.002	11835886.6621	c
24	16	9	23	17	6	651865.854	0.018	0.012	11611514.0744	c
24	16	8	23	17	7	654093.379	0.016	0.009	11611469.6032	c
24	13	12	23	14	9	664651.541	-0.038	-0.008	11081726.8603	c
24	15	10	23	16	7	676686.280	-0.016	-0.001	11406802.6720	c
24	14	11	23	15	8	689946.198	-0.037	-0.006	11226198.4617	c
23	15	9	23	12	12	498679.973	0.027	-0.006	10722488.6086	c
24	11	13	23	14	10	505312.412	-0.051	-0.004	11053603.4309	c
24	12	12	23	15	9	514771.234	-0.064	-0.008	11221168.5496	c
24	21	4	23	22	1	545874.475	0.030	-0.004	12904793.1707	c
24	21	3	23	22	2	545874.475	0.029	-0.005	12904793.1707	c
23	12	11	23	9	14	546368.907	-0.004	-0.009	10321201.1543	c
24	20	5	23	21	2	564337.340	0.062	0.017	12613229.7743	c
24	20	4	23	21	3	564337.340	0.029	-0.016	12613229.7740	c
23	13	11	23	10	14	571389.826	0.020	-0.005	10321240.5647	c
24	19	6	23	20	3	583762.134	0.456	0.411	12337550.4173	c
24	19	5	23	20	4	583762.134	-0.373	-0.418	12337550.4140	c
23	18	6	23	15	9	614718.065	-0.054	0.003	11221168.5496	c
23	12	12	23	9	15	633887.331	0.006	-0.014	10088601.2903	c
23	19	4	23	16	7	671418.553	-0.092	0.003	11406802.6720	c
24	12	13	23	11	12	842174.847	-3.280	-3.266	10718147.9220	d
24	9	16	23	8	15	783933.509	-2.910	-2.892	10088598.8568	d
24	8	16	23	9	15	783933.509	0.067	0.083	10088601.2903	d
24	8	17	23	7	16	766598.292	-5.710	-5.695	9835974.1736	d
24	7	17	23	8	16	766598.292	-5.570	-5.556	9835974.2893	d
24	16	8	23	15	9	1044391.958	-2.460	-2.445	11221168.5496	d
24	17	7	23	16	8	1056941.282	-3.330	-3.301	11406240.2170	d
24	17	8	23	16	7	1056166.918	-0.183	-0.155	11406802.6720	d
24	18	7	23	17	6	1071207.520	-2.280	-2.239	11611514.0744	d
24	18	6	23	17	7	1071266.580	-3.150	-3.110	11611469.6032	d
24	19	5	23	18	6	1085422.194	-4.070	-4.024	11835886.6621	d
24	19	6	23	18	5	1085422.194	-0.672	-0.625	11835889.2343	d

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J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
24	20	4	23	19	5	1099343.670	-2.220	-2.164	12078221.2013	d
24	20	5	23	19	4	1099343.670	-2.080	-2.023	12078221.3101	d
24	21	3	23	20	4	1113113.451	-3.760	-3.696	12337550.4140	d
24	21	4	23	20	3	1113113.451	-3.750	-3.692	12337550.4173	d
24	23	1	23	22	2	1140429.668	-2.690	-2.622	12904793.1707	d
24	23	2	23	22	1	1140429.668	-2.690	-2.622	12904793.1707	d
24	24	0	23	23	1	1154031.865	-2.290	-2.234	13211891.5859	d
24	24	1	23	23	0	1154031.865	-2.290	-2.234	13211891.5859	d
24	12	12	23	11	13	1203117.533	-2.450	-2.434	10532819.8723	d
24	13	12	23	10	13	1214041.981	-1.310	-1.307	10532335.1547	d
24	12	13	23	9	14	1239123.543	-1.350	-1.349	10321201.1543	d
24	10	14	23	9	15	1263724.536	-0.621	-0.616	10088601.2903	d
24	11	14	23	8	15	1263860.642	-1.560	-1.559	10088598.8568	d
24	9	16	23	6	17	1308419.140	-2.120	-2.114	9564114.0225	d
24	8	16	23	7	17	1308419.140	-1.570	-1.567	9564114.0267	d
24	13	12	23	12	11	878806.524	-1.860	-1.856	10867570.0598	d
24	14	11	23	13	10	940221.769	-3.030	-3.031	10975919.9024	d
24	15	9	23	14	10	1044878.821	-2.710	-2.695	11053603.4309	d
24	14	10	23	13	11	1081713.758	-2.930	-2.909	10892630.3652	d
24	15	10	23	12	11	1215911.489	-7.420	-7.446	10867570.0598	d
24	6	19	23	3	20	1368445.444	-0.849	-0.849	8637496.7470	d
24	5	19	23	4	20	1368445.444	-0.849	-0.849	8637496.7470	d
25	0	25	23	0	23	1322123.713	0.318	0.319	7549195.1117	e
25	1	24	23	1	22	1355931.308	-5.120	-5.118	7929686.5993	e
25	1	24	23	1	22	1355943.300	6.870	6.874	7929686.5993	e
25	2	23	23	2	21	1389741.902	-9.090	-9.082	8292488.7133	e
25	2	23	23	2	21	1389750.895	-0.100	-0.088	8292488.7133	e
25	3	22	23	3	20	1423576.479	-5.000	-4.986	8637496.7470	e
25	3	22	23	3	20	1423603.460	22.000	21.995	8637496.7470	e
25	4	21	23	4	19	1457447.030	-2.200	-2.174	8964572.0575	e
25	4	21	23	4	19	1457450.028	0.803	0.824	8964572.0575	e
25	5	20	23	5	18	1491389.533	3.120	3.140	9273528.8759	e
25	6	19	23	6	17	1525442.958	0.188	0.215	9564114.0225	e
25	7	18	23	7	16	1559691.248	-6.290	-6.258	9835974.1736	e
25	20	5	23	18	5	2219078.764	5.710	5.814	11835889.2343	e
25	21	4	23	19	4	2246848.539	-17.100	-16.942	12078221.3101	e
25	22	3	23	20	3	2274378.481	1.750	1.876	12337550.4173	e
25	23	2	23	21	2	2301725.549	4.410	4.542	12613229.7743	e
25	25	0	23	23	0	2356158.865	6.100	6.215	13211891.5859	e
25	0	25	24	1	24	674361.149	-0.001	0.000	8196957.3505	c
25	1	25	24	0	24	674361.149	-0.001	0.000	8196957.3505	c
25	1	24	24	2	23	691265.622	0.000	0.003	8594357.4035	c
25	2	24	24	1	23	691265.622	0.000	0.003	8594357.4035	c
25	2	23	24	3	22	708170.405	-0.006	-0.001	8974069.2907	c
25	3	23	24	2	22	708170.405	-0.006	-0.001	8974069.2907	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(\text{SP})$ / MHz	$\Delta_{O-C}(\text{LP})$ / MHz	E''/h (MHz)	Source
25	3	22	24	4	21	725082.316	-0.002	0.006	9335995.9040	c
25	4	22	24	3	21	725082.316	-0.002	0.006	9335995.9040	c
25	4	21	24	5	20	742011.302	-0.009	0.001	9680009.9653	c
25	5	21	24	4	20	742011.302	-0.009	0.001	9680009.9653	c
25	20	6	24	21	3	604294.583	0.187	0.133	13450667.6117	c
25	20	5	24	21	4	604294.583	-0.075	-0.128	13450667.6105	c
25	17	9	24	18	6	671061.169	0.021	0.003	12682739.3200	c
25	17	8	24	18	7	671975.530	0.016	-0.004	12682723.8600	c
24	16	9	24	13	12	517001.501	0.025	0.000	11746378.4328	c
24	13	11	24	10	14	517807.710	-0.004	-0.006	11352326.4353	c
24	15	10	24	12	13	523162.965	0.039	0.007	11560326.0396	c
25	13	12	24	16	9	525694.606	-0.080	-0.024	12263379.9039	c
25	12	13	24	15	10	540993.763	-0.046	0.005	12083488.9610	c
24	17	8	24	14	11	546825.087	0.009	0.010	11916144.6898	c
25	12	14	24	13	11	554264.916	-0.016	-0.002	11870134.1445	c
24	14	11	24	11	14	563683.674	0.029	0.002	11352461.0506	c
25	22	4	24	23	1	566701.658	0.041	0.008	14045225.5142	c
25	22	3	24	23	2	566701.658	0.041	0.008	14045225.5142	c
25	21	5	24	22	2	585056.481	0.041	-0.008	13740030.4406	c
25	21	4	24	22	3	585056.481	0.031	-0.017	13740030.4406	c
24	13	12	24	10	15	623571.065	0.006	-0.014	11122807.3795	c
25	19	7	24	20	4	624719.898	0.058	0.009	13177567.0792	c
25	19	6	24	20	5	624725.167	0.049	0.000	13177567.0466	c
25	18	8	24	19	5	646793.333	0.026	-0.010	12921312.9154	c
25	18	7	24	19	6	646873.667	0.040	0.004	12921312.0895	c
25	13	13	24	14	10	653884.536	-0.016	0.006	11974347.0424	c
24	19	6	24	16	9	657932.099	-0.093	-0.008	12263379.9039	c
24	11	13	24	8	16	686381.185	0.014	0.000	10872534.7242	c
24	12	13	24	9	16	687790.816	0.036	0.019	10872535.2666	c
25	16	10	24	17	7	696959.005	-0.003	0.000	12463184.8168	c
25	16	9	24	17	8	704429.100	-0.010	-0.007	12462969.7628	c
25	14	12	24	15	9	712954.537	-0.026	0.007	12098484.9503	c
25	15	11	24	16	8	717885.880	-0.026	-0.001	12265562.9602	c
25	12	13	24	13	12	878101.112	-3.230	-3.202	11746378.4328	d
25	9	17	24	8	16	810346.450	-1.240	-1.224	10872534.7242	d
25	8	17	24	9	16	810346.450	-0.581	-0.565	10872535.2666	d
25	8	18	24	7	17	793086.481	-7.080	-7.066	10602578.1447	d
25	7	18	24	8	17	793086.481	-7.050	-7.038	10602578.1684	d
25	7	19	24	6	18	775985.103	-2.720	-2.708	10313568.9612	d
25	6	19	24	7	18	775985.103	-2.720	-2.707	10313568.9621	d
25	6	20	24	5	19	758968.566	-3.690	-3.680	10005943.0270	d
25	5	20	24	6	19	758968.566	-3.690	-3.680	10005943.0270	d
25	10	15	24	11	14	845697.412	-3.800	-3.780	11352461.0506	d
25	11	15	24	10	14	845868.594	-2.540	-2.521	11352326.4353	d
25	11	14	24	12	13	863648.103	-3.570	-3.550	11560326.0396	d

Table S4_2: Assigned transitions v , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
25	12	14	24	11	13	865481.336	-1.850	-1.838	11558915.8890	d
25	16	10	24	15	9	1061653.125	-5.750	-5.739	12098484.9503	d
25	16	9	24	15	10	1083907.341	-2.570	-2.558	12083488.9610	d
25	17	8	24	16	9	1091317.619	-1.860	-1.831	12263379.9039	d
25	18	7	24	17	8	1105213.313	-2.640	-2.610	12462969.7628	d
25	18	8	24	17	7	1104918.317	-3.090	-3.059	12463184.8168	d
25	20	5	24	19	6	1133647.157	-3.030	-2.974	12921312.0895	d
25	20	6	24	19	5	1133647.157	-1.940	-1.887	12921312.9154	d
25	21	4	24	20	5	1147517.968	-1.880	-1.820	13177567.0466	d
25	21	5	24	20	4	1147517.968	-1.840	-1.778	13177567.0792	d
25	22	3	24	21	4	1161256.871	-2.660	-2.590	13450667.6105	d
25	22	4	24	21	3	1161256.871	-2.650	-2.589	13450667.6117	d
25	23	2	24	22	3	1174918.127	-2.330	-2.266	13740030.4406	d
25	23	3	24	22	2	1174918.127	-2.330	-2.266	13740030.4406	d
25	24	1	24	23	2	1188531.416	-2.300	-2.235	14045225.5142	d
25	24	2	24	23	1	1188531.416	-2.300	-2.235	14045225.5142	d
25	25	0	24	24	1	1202116.825	-1.780	-1.727	14365925.7327	d
25	25	1	24	24	0	1202116.825	-1.780	-1.727	14365925.7327	d
25	11	14	24	10	15	1301166.553	-3.780	-3.776	11122807.3795	d
25	12	14	24	9	15	1301599.154	-2.260	-2.251	11122797.6710	d
25	10	15	24	9	16	1325624.546	-2.450	-2.446	10872535.2666	d
25	11	15	24	8	16	1325658.722	-4.130	-4.119	10872534.7242	d
25	10	16	24	7	17	1348071.229	-3.380	-3.374	10602578.1447	d
25	9	16	24	8	17	1348071.229	-1.070	-1.059	10602578.1684	d
25	7	19	24	4	20	1409544.033	-2.790	-2.789	9680009.9653	d
25	6	19	24	5	20	1409544.033	-2.790	-2.789	9680009.9653	d
25	13	13	24	12	12	892289.704	-2.050	-2.041	11735939.8429	d
25	13	12	24	14	11	872926.689	-3.210	-3.172	11916144.6898	d
26	0	26	24	0	24	1375315.889	-0.715	-0.716	8196957.3505	e
26	0	26	24	0	24	1375318.887	2.280	2.282	8196957.3505	e
26	1	25	24	1	23	1409117.488	-3.850	-3.841	8594357.4035	e
26	2	24	24	2	22	1442910.094	-15.800	-15.790	8974069.2907	e
26	2	24	24	2	22	1442928.082	2.190	2.198	8974069.2907	e
26	3	23	24	3	21	1476744.671	1.460	1.476	9335995.9040	e
26	3	23	24	3	21	1476750.667	7.460	7.472	9335995.9040	e
26	4	22	24	4	20	1510594.237	2.170	2.188	9680009.9653	e
26	4	22	24	4	20	1510597.235	5.170	5.186	9680009.9653	e
26	5	21	24	5	19	1544494.769	-5.470	-5.443	10005943.0270	e
26	5	21	24	5	19	1544497.766	-2.470	-2.445	10005943.0270	e
26	6	20	24	6	18	1578512.219	2.620	2.644	10313568.9612	e
26	7	19	24	7	17	1612685.561	0.443	0.472	10602578.1447	e
26	8	18	24	8	16	1647119.723	-11.700	-11.645	10872534.7242	e
26	21	5	24	19	5	2315474.031	-7.180	-7.065	12921312.9154	e
26	22	4	24	20	4	2343168.858	-7.950	-7.821	13177567.0792	e
26	24	2	24	22	2	2397925.950	-0.311	-0.175	13740030.4406	e

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J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
26	26	0	24	24	0	2452287.317	0.969	1.078	14365925.7327	e
26	0	26	25	1	25	700955.459	0.005	0.004	8871318.4938	c
26	1	26	25	0	25	700955.459	0.005	0.004	8871318.4938	c
26	1	25	25	2	24	717855.712	0.000	0.001	9285623.0187	c
26	2	25	25	1	24	717855.712	0.000	0.001	9285623.0187	c
26	18	9	25	19	6	690307.029	0.030	-0.002	13802292.1588	c
26	18	8	25	19	7	690667.167	0.032	-0.001	13802286.9136	c
26	11	15	25	14	12	502921.532	-0.065	-0.031	12811439.5063	c
26	14	12	25	17	9	522589.610	-0.044	0.005	13353800.4612	c
26	12	15	25	13	12	525404.415	-0.014	0.001	12789074.5851	c
25	16	10	25	13	13	531912.266	0.031	0.003	12628231.5883	c
25	17	9	25	14	12	542360.976	0.016	0.004	12811439.5063	c
25	18	7	25	15	10	548375.451	-0.013	0.005	13019810.2509	c
26	12	14	25	15	11	552098.860	-0.063	-0.018	12983448.8584	c
25	15	11	25	12	14	559049.820	0.027	-0.001	12424399.0707	c
26	13	13	25	16	10	567357.391	-0.056	-0.002	13160143.8179	c
26	24	2	25	25	1	569912.365	0.011	0.021	15568044.3293	c
26	24	3	25	25	0	569912.365	0.011	0.021	15568044.3293	c
26	23	4	25	24	1	587534.959	0.033	0.005	15233759.2182	c
26	23	3	25	24	2	587534.959	0.033	0.005	15233759.2182	c
25	13	12	25	10	15	590912.343	0.004	0.003	12198162.2521	c
25	14	12	25	11	15	613241.961	0.008	-0.013	12198197.5590	c
26	21	6	25	22	3	624867.016	0.116	0.055	14611927.1257	c
26	21	5	25	22	4	624867.016	0.034	-0.026	14611927.1254	c
26	13	14	25	14	11	627417.053	-0.022	-0.007	12909343.9980	c
25	19	7	25	16	10	642143.028	-0.074	-0.004	13160143.8179	c
26	19	8	25	20	5	666647.127	0.041	-0.008	14054962.2624	c
26	19	7	25	20	6	666675.947	0.056	0.008	14054962.0016	c
25	12	13	25	9	16	673832.339	0.017	0.008	11950650.4494	c
25	13	13	25	10	16	677578.880	0.025	0.009	11950652.7399	c
26	17	10	25	18	7	716213.737	0.017	0.007	13568185.7099	c
26	14	13	25	15	10	716759.212	-0.021	0.008	13019810.2509	c
26	17	9	25	18	8	719553.866	0.012	0.001	13568106.2163	c
26	7	20	25	6	19	802518.861	-2.920	-2.903	11089556.7780	d
26	6	20	25	7	19	802518.861	-2.920	-2.903	11089556.7783	d
26	6	21	25	5	20	785523.310	-4.670	-4.655	10764915.2780	d
26	5	21	25	6	20	785523.310	-4.670	-4.655	10764915.2780	d
26	5	22	25	4	21	768576.325	-4.430	-4.424	10422021.2686	d
26	4	22	25	5	21	768576.325	-4.430	-4.424	10422021.2686	d
26	9	18	25	8	17	836783.374	-0.476	-0.460	11682882.2895	d
26	8	18	25	9	17	836783.374	-0.334	-0.319	11682882.4064	d
26	10	17	25	9	16	854171.954	-4.710	-4.698	11950650.4494	d
26	9	17	25	10	16	854171.954	-1.900	-1.887	11950652.7399	d
26	11	15	25	12	14	889958.515	-3.520	-3.503	12424399.0707	d
26	12	15	25	11	14	890498.742	-2.570	-2.554	12423977.7043	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
26	12	14	25	13	13	907312.019	-4.180	-4.155	12628231.5883	d
26	13	13	25	14	12	916059.672	-2.090	-2.055	12811439.5063	d
26	17	10	25	16	9	1116997.866	-2.700	-2.681	13167398.8658	d
26	17	9	25	16	10	1127513.697	-2.560	-2.539	13160143.8179	d
26	16	10	25	15	11	1132692.617	0.146	0.163	12983448.8584	d
26	18	9	25	17	8	1137896.719	-3.080	-3.045	13354699.3673	d
26	18	8	25	17	9	1139151.652	-1.940	-1.909	13353800.4612	d
26	19	8	25	18	7	1153422.087	-1.560	-1.515	13568185.7099	d
26	19	7	25	18	8	1153528.813	-2.870	-2.827	13568106.2163	d
26	20	6	25	19	7	1167816.336	-4.710	-4.664	13802286.9136	d
26	20	7	25	19	6	1167816.336	2.270	2.323	13802292.1588	d
26	21	5	25	20	6	1181830.748	-1.360	-1.304	14054962.0016	d
26	21	6	25	20	5	1181830.748	-1.020	-0.962	14054962.2624	d
26	22	4	25	21	5	1195654.792	-2.210	-2.141	14325086.8747	d
26	22	5	25	21	4	1195654.792	-2.190	-2.129	14325086.8843	d
26	23	3	25	22	4	1209364.914	-2.110	-2.042	14611927.1254	d
26	23	4	25	22	3	1209364.914	-2.110	-2.041	14611927.1257	d
26	24	2	25	23	3	1223004.286	-1.510	-1.445	14914950.8899	d
26	24	3	25	23	2	1223004.286	-1.510	-1.445	14914950.8899	d
26	25	1	25	24	2	1236598.688	-1.630	-1.571	15233759.2182	d
26	25	2	25	24	1	1236598.688	-1.630	-1.571	15233759.2182	d
26	14	12	25	13	13	1248156.298	-2.240	-2.208	12628231.5883	d
26	26	1	25	25	0	1250165.210	-2.530	-2.477	15568044.3293	d
26	26	0	25	25	1	1250165.210	-2.530	-2.477	15568044.3293	d
26	14	13	25	11	14	1312590.156	-1.630	-1.624	12423977.7043	d
26	13	14	25	10	15	1338595.979	-2.850	-2.839	12198162.2521	d
26	12	15	25	9	16	1363825.038	-3.530	-3.526	11950650.4494	d
26	10	17	25	7	18	1409153.404	-2.030	-2.018	11395671.6940	d
26	9	17	25	8	18	1409153.404	-1.500	-1.493	11395671.6985	d
26	9	18	25	6	19	1430108.018	-1.350	-1.342	11089556.7780	d
26	8	18	25	7	19	1430108.018	-1.320	-1.317	11089556.7783	d
26	8	19	25	5	20	1450346.727	-1.260	-1.250	10764915.2780	d
26	7	19	25	6	20	1450346.727	-1.260	-1.249	10764915.2780	d
26	17	9	25	14	12	1476220.641	0.069	0.071	12811439.5063	d
26	6	21	25	3	22	1489365.054	0.007	0.014	10061078.2147	d
26	5	21	25	4	22	1489365.054	0.007	0.014	10061078.2147	d
26	13	14	25	12	13	912275.987	-2.320	-2.310	12624482.7651	d
26	8	19	25	7	18	819587.561	-4.000	-3.986	11395671.6940	d
26	7	19	25	8	18	819587.561	-4.000	-3.981	11395671.6985	d
26	15	12	25	14	11	1009196.588	-5.520	-5.519	12909343.9980	d
26	15	11	25	14	12	1177832.712	-2.090	-2.062	12811439.5063	d
27	0	27	25	0	25	1428499.071	-1.360	-1.363	8871318.4938	e
27	1	26	25	1	24	1462297.672	1.060	1.067	9285623.0187	e
27	1	26	25	1	24	1462297.672	1.060	1.067	9285623.0187	e
27	2	25	25	2	23	1496093.276	2.200	2.209	9682239.6951	e

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
27	3	24	25	3	22	1529894.876	-0.638	-0.626	10061078.2147	e
27	4	23	25	4	21	1563723.457	-3.140	-3.127	10422021.2686	e
27	6	21	25	6	19	1631581.480	4.490	4.513	11089556.7780	e
27	7	20	25	7	18	1665685.870	-0.221	-0.194	11395671.6940	e
27	8	19	25	8	17	1700018.102	-2.150	-2.118	11682882.2895	e
27	22	5	25	20	5	2411806.341	2.130	2.251	14054962.2624	e
27	23	4	25	21	4	2439417.227	3.530	3.660	14325086.8843	e
27	24	3	25	22	3	2466809.263	3.690	3.830	14611927.1257	e
27	0	27	26	1	26	727544.980	0.004	0.001	9572273.9409	c
27	1	27	26	0	26	727544.980	0.004	0.001	9572273.9409	c
27	1	26	26	2	25	744440.896	0.001	0.000	10003478.7237	c
27	2	26	26	1	25	744440.896	0.001	0.000	10003478.7237	c
27	12	16	26	13	13	503069.395	-0.022	-0.006	13727501.2590	c
26	17	10	26	14	13	547829.966	0.014	-0.007	13736569.4766	c
26	16	11	26	13	14	559141.697	0.037	0.009	13536761.0663	c
26	14	12	26	11	15	562029.009	-0.008	-0.005	13314361.0986	c
26	18	9	26	15	12	574053.060	-0.005	0.002	13918546.0918	c
27	14	13	26	17	10	581564.552	-0.056	-0.004	14284399.4231	c
27	13	14	26	16	11	590215.137	-0.064	-0.017	14095902.7209	c
27	25	2	26	26	1	590799.931	-0.034	-0.009	16818212.0569	c
27	25	3	26	26	0	590799.931	-0.034	-0.009	16818212.0569	c
27	13	15	26	14	12	594951.354	-0.008	0.002	13876390.1101	c
26	15	12	26	12	15	604067.101	0.012	-0.010	13314479.0085	c
26	19	7	26	16	10	605496.537	-0.037	0.012	14116141.3182	c
26	19	8	26	16	11	625706.574	-0.053	-0.002	14095902.7209	c
27	23	5	26	24	2	626543.929	0.041	-0.010	16137956.6776	c
27	23	4	26	24	3	626543.929	0.040	-0.011	16137956.6776	c
27	22	6	26	23	3	645472.368	0.073	0.008	15821294.1383	c
27	22	5	26	23	4	645472.368	0.048	-0.017	15821294.1380	c
26	13	13	26	10	16	657423.905	-0.004	-0.007	13070077.3568	c
27	21	7	26	22	4	665387.176	0.343	0.276	15520743.8613	c
27	21	6	26	22	5	665387.176	-0.227	-0.295	15520743.8583	c
27	20	8	26	21	5	686627.674	0.062	0.002	15236794.1009	c
27	14	14	26	15	11	700059.526	-0.026	-0.008	13989274.2935	c
27	19	9	26	20	6	709700.263	0.027	-0.018	14970107.9528	c
27	19	8	26	20	7	709837.325	0.058	0.013	14970106.2107	c
27	8	20	26	7	19	846090.740	-3.790	-3.777	12215263.2467	d
27	7	20	26	8	19	846090.740	-3.790	-3.776	12215263.2476	d
27	6	22	26	5	21	812076.554	-3.990	-3.976	11550443.2469	d
27	5	22	26	6	21	812076.554	-3.990	-3.976	11550443.2469	d
27	5	23	26	4	22	795141.261	-4.580	-4.574	11190602.0193	d
27	4	23	26	5	22	795141.261	-4.580	-4.574	11190602.0193	d
27	3	24	26	4	23	778230.251	-4.370	-4.366	10812739.0991	d
27	4	24	26	3	23	778230.251	-4.370	-4.366	10812739.0991	d
27	2	25	26	3	24	761332.133	-3.460	-3.457	10416995.1701	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
27	3	25	26	2	24	761332.133	-3.460	-3.457	10416995.1701	d
27	7	21	26	6	20	829052.319	-2.900	-2.884	11892078.5468	d
27	6	21	26	7	20	829052.319	-2.900	-2.884	11892078.5468	d
27	9	19	26	8	18	863233.790	-2.640	-2.625	12519666.1065	d
27	8	19	26	9	18	863233.790	-2.610	-2.596	12519666.1311	d
27	10	18	26	9	17	880539.027	-2.770	-2.754	12804826.5886	d
27	9	18	26	10	17	880539.027	-2.130	-2.119	12804827.1091	d
27	11	16	26	12	15	916059.672	-0.746	-0.730	13314479.0085	d
27	13	15	26	12	14	935788.733	-4.970	-4.952	13535547.7757	d
27	14	14	26	13	13	961827.833	-4.760	-4.747	13727501.2590	d
27	17	11	26	16	10	1138601.532	-2.710	-2.690	14116141.3182	d
27	18	10	26	17	9	1169096.751	-1.430	-1.406	14287660.0636	d
27	17	10	26	16	11	1169018.205	-3.750	-3.735	14095902.7209	d
27	18	9	26	17	10	1173743.539	-1.390	-1.359	14284399.4231	d
27	19	9	26	18	8	1186851.378	-2.770	-2.736	14492954.0421	d
27	19	8	26	18	9	1187342.138	-2.190	-2.156	14492599.1514	d
27	16	11	26	15	12	1196332.024	1.110	1.129	13918546.0918	d
27	20	7	26	19	8	1201820.330	-2.040	-1.992	14721609.3419	d
27	20	8	26	19	7	1201781.956	-1.880	-1.828	14721637.8864	d
27	21	6	26	20	7	1216023.911	-1.150	-1.089	14970106.2107	d
27	21	7	26	20	6	1216023.911	1.160	1.220	14970107.9528	d
27	22	5	26	21	6	1229970.870	-1.570	-1.509	15236794.0203	d
27	22	6	26	21	5	1229970.870	-1.470	-1.404	15236794.1009	d
27	23	4	26	22	5	1243755.041	-1.670	-1.605	15520743.8583	d
27	23	5	26	22	4	1243755.041	-1.670	-1.601	15520743.8613	d
27	24	3	26	23	4	1257436.983	-1.570	-1.496	15821294.1380	d
27	24	4	26	23	3	1257436.983	-1.570	-1.496	15821294.1383	d
27	15	12	26	14	13	1262516.671	-1.970	-1.939	13736569.4766	d
27	26	1	26	25	2	1284628.786	-1.990	-1.930	16470359.5288	d
27	26	2	26	25	1	1284628.786	-1.990	-1.930	16470359.5288	d
27	27	1	26	26	0	1298178.219	-1.930	-1.879	16818212.0569	d
27	27	0	26	26	1	1298178.219	-1.930	-1.879	16818212.0569	d
27	13	14	26	12	15	1371634.640	-4.280	-4.266	13314479.0085	d
27	13	15	26	10	16	1401262.259	-1.860	-1.854	13070077.3568	d
27	12	15	26	11	16	1400889.017	-2.800	-2.792	13070086.1806	d
27	11	17	26	8	18	1448525.786	-2.880	-2.869	12519666.1065	d
27	10	17	26	9	18	1448525.786	-0.737	-0.729	12519666.1311	d
27	12	16	26	9	17	1425741.836	-2.260	-2.251	12804826.5886	d
27	11	16	26	10	17	1425711.557	-0.766	-0.757	12804827.1091	d
27	10	18	26	7	19	1470103.070	-2.070	-2.066	12215263.2467	d
27	9	18	26	8	19	1470103.070	-1.960	-1.951	12215263.2476	d
27	9	19	26	6	20	1490822.347	-1.650	-1.640	11892078.5468	d
27	8	19	26	7	20	1490822.347	-1.640	-1.635	11892078.5468	d
27	8	20	26	5	21	1510914.158	-0.379	-0.370	11550443.2469	d
27	7	20	26	6	21	1510914.158	-0.378	-0.370	11550443.2469	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
27	7	21	26	4	22	1530530.797	-0.952	-0.943	11190602.0193	d
27	6	21	26	5	22	1530530.797	-0.952	-0.943	11190602.0193	d
27	12	15	26	13	14	934214.222	-2.710	-2.689	13536761.0663	d
27	13	14	26	14	13	949546.223	-2.230	-2.199	13736569.4766	d
27	16	12	26	15	11	1079636.793	-3.190	-3.192	13989274.2935	d
27	15	13	26	12	14	1350158.985	-2.050	-2.045	13535547.7757	d
28	0	28	26	0	26	1481673.259	-1.250	-1.259	9572273.9409	e
28	0	28	26	0	26	1481673.259	-1.250	-1.259	9572273.9409	e
28	1	27	26	1	25	1515468.863	6.980	6.978	10003478.7237	e
28	2	26	26	2	24	1549249.477	3.340	3.346	10416995.1701	e
28	3	25	26	3	23	1583030.091	-7.790	-7.784	10812739.0991	e
28	3	25	26	3	23	1583033.089	-4.800	-4.786	10812739.0991	e
28	4	24	26	4	22	1616849.678	-2.370	-2.351	11190602.0193	e
28	4	24	26	4	22	1616855.674	3.630	3.644	11190602.0193	e
28	5	23	26	5	21	1650711.236	1.380	1.397	11550443.2469	e
28	7	21	26	7	19	1718686.178	-8.280	-8.251	12215263.2467	e
28	8	20	26	8	18	1752937.467	1.230	1.260	12519666.1065	e
28	26	2	26	24	2	2590134.887	11.800	11.914	16137956.6776	e
27	15	12	27	12	15	528110.122	0.000	0.003	14470977.9871	c
28	12	16	27	15	13	546004.855	-0.028	0.000	14885708.7953	c
27	17	11	27	14	14	565411.736	0.025	0.001	14689333.8388	c
28	13	16	27	14	13	565852.003	-0.029	-0.021	14865964.0255	c
27	18	10	27	15	13	571049.453	0.006	-0.001	14885708.7953	c
28	15	13	27	18	10	581514.034	-0.050	-0.005	15456758.2369	c
27	16	12	27	13	15	597572.840	0.032	0.009	14471341.4663	c
28	13	15	27	16	12	598530.370	-0.039	-0.001	15068914.2679	c
27	19	9	27	16	12	610893.885	-0.035	-0.003	15068914.2679	c
28	14	14	27	17	11	619524.172	-0.046	0.002	15254745.5441	c
27	20	8	27	17	11	668676.084	-0.085	-0.003	15254745.5441	c
28	14	15	27	15	12	669393.969	-0.012	-0.004	14999088.1043	c
28	22	7	27	23	4	685810.775	0.169	0.095	16764500.5608	c
28	22	6	27	23	5	685810.775	-0.013	-0.088	16764500.5599	c
28	25	3	27	26	2	629215.266	0.000	-0.011	17754990.2920	c
28	25	4	27	26	1	629215.266	0.000	-0.011	17754990.2920	c
28	4	24	27	5	23	821699.601	-6.600	-6.594	11985747.8543	d
28	5	24	27	4	23	821699.601	-6.600	-6.594	11985747.8543	d
28	3	25	27	4	24	804799.384	-3.880	-3.875	11590973.7138	d
28	4	25	27	3	24	804799.384	-3.880	-3.875	11590973.7138	d
28	2	26	27	3	25	787906.962	-3.580	-3.579	11178330.7552	d
28	3	26	27	2	25	787906.962	-3.580	-3.579	11178330.7552	d
28	1	28	27	0	27	754124.215	-5.320	-5.324	10299818.9099	d
28	0	28	27	1	27	754124.215	-5.320	-5.324	10299818.9099	d
28	6	23	27	5	22	838626.200	-3.120	-3.109	12362523.7790	d
28	5	23	27	6	22	838626.200	-3.120	-3.109	12362523.7790	d
28	7	22	27	6	21	855584.577	-2.330	-2.324	12721133.7536	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
28	6	22	27	7	21	855584.577	-2.330	-2.324	12721133.7536	d
28	8	21	27	7	20	872597.517	-2.410	-2.395	13061357.7685	d
28	7	21	27	8	20	872597.517	-2.410	-2.395	13061357.7688	d
28	9	20	27	8	19	889697.995	-1.810	-1.802	13382902.5227	d
28	8	20	27	9	19	889697.995	-1.810	-1.796	13382902.5278	d
28	10	19	27	9	18	906932.781	-2.650	-2.633	13685368.2618	d
28	9	19	27	10	18	906932.781	-2.510	-2.494	13685368.3763	d
28	11	18	27	10	17	924381.319	-5.730	-5.714	13968192.6400	d
28	10	18	27	11	17	924381.319	-3.120	-3.110	13968194.7556	d
28	12	16	27	13	15	960366.343	-5.870	-5.858	14471341.4663	d
28	13	16	27	12	15	960834.919	-3.160	-3.141	14470977.9871	d
28	14	14	27	15	13	988558.854	-2.120	-2.084	14885708.7953	d
28	17	12	27	16	11	1149046.312	-1.990	-1.982	15114876.9969	d
28	18	11	27	17	10	1196006.749	-2.300	-2.281	15264924.6682	d
28	18	10	27	17	11	1210918.141	-2.890	-2.865	15254745.5441	d
28	19	10	27	18	9	1219310.839	-2.840	-2.803	15458144.3358	d
28	19	9	27	18	10	1221260.391	-3.280	-3.244	15456758.2369	d
28	20	9	27	19	8	1235446.285	-2.550	-2.504	15679943.4711	d
28	20	8	27	19	9	1235632.456	-1.720	-1.673	15679808.1817	d
28	23	5	27	22	6	1278072.318	1.000	1.071	16466766.4265	d
28	23	6	27	22	5	1278072.318	1.040	1.104	16466766.4514	d
28	15	13	27	14	14	1348938.829	0.339	0.370	14689333.8388	d
28	14	14	27	13	15	1402926.108	-2.200	-2.175	14471341.4663	d
28	15	14	27	12	15	1411107.753	-2.060	-2.051	14470977.9871	d
28	14	15	27	11	16	1437940.703	-1.970	-1.961	14230539.4179	d
28	12	16	27	11	17	1463517.223	-1.710	-1.699	13968194.7556	d
28	13	16	27	10	17	1463621.551	-1.880	-1.866	13968192.6400	d
28	12	17	27	9	18	1487371.732	-7.000	-6.995	13685368.2618	d
28	11	17	27	10	18	1487371.732	1.020	1.030	13685368.3763	d
28	11	18	27	8	19	1509676.014	-1.160	-1.148	13382902.5227	d
28	10	18	27	9	19	1509676.014	-0.662	-0.654	13382902.5278	d
28	10	19	27	7	20	1530944.211	-1.720	-1.707	13061357.7685	d
28	9	19	27	8	20	1530944.211	-1.690	-1.682	13061357.7688	d
28	8	21	27	5	22	1571431.523	-2.400	-2.387	12362523.7790	d
28	7	21	27	6	22	1571431.523	-2.400	-2.387	12362523.7790	d
28	13	15	27	14	14	978108.678	-2.160	-2.144	14689333.8388	d
28	14	15	27	13	14	982361.538	-2.630	-2.623	14686117.9159	d
28	25	3	27	24	4	1305471.277	-1.610	-1.543	17078732.6748	d
28	25	4	27	24	3	1305471.277	-1.610	-1.543	17078732.6748	d
28	26	2	27	25	3	1319065.380	-2.380	-2.310	17409012.0160	d
28	26	3	27	25	2	1319065.380	-2.380	-2.310	17409012.0160	d
28	27	1	27	26	2	1332622.608	-1.070	-1.012	17754990.2920	d
28	27	2	27	26	1	1332622.608	-1.070	-1.012	17754990.2920	d
28	28	1	27	27	0	1346152.555	-1.860	-1.823	18116392.1891	d
28	28	0	27	27	1	1346152.555	-1.860	-1.823	18116392.1891	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
28	13	15	27	12	16	1436871.043	-2.970	-2.958	14230570.6712	d
29	0	29	27	0	27	1534838.453	-0.032	-0.042	10299818.9099	e
29	1	28	27	1	26	1568619.068	2.280	2.270	10747919.6116	e
29	2	27	27	2	25	1602384.692	-5.990	-5.985	11178330.7552	e
29	3	26	27	3	24	1636171.302	1.460	1.464	11590973.7138	e
29	4	25	27	4	23	1669963.908	-3.810	-3.795	11985747.8543	e
29	6	23	27	6	21	1737696.018	-6.780	-6.766	12721133.7536	e
29	7	22	27	7	20	1771692.483	-13.300	-13.240	13061357.7685	e
29	26	3	27	24	3	2658943.252	1.570	1.707	17078732.6748	e
29	27	2	27	25	2	2686119.438	10.000	10.162	17409012.0160	e
28	19	9	28	16	12	517134.166	0.004	0.001	16160887.7352	c
29	12	17	28	15	14	536106.462	-0.023	-0.003	15882087.7848	c
28	18	11	28	15	14	578845.956	0.027	0.012	15882087.7848	c
28	17	12	28	14	15	595443.231	0.018	-0.003	15668482.0787	c
29	13	16	28	16	13	596773.127	-0.016	0.012	16076427.7523	c
28	19	10	28	16	13	601030.235	-0.018	-0.004	16076427.7523	c
28	15	13	28	12	16	606558.650	0.003	0.013	15431713.6733	c
28	20	8	28	17	11	624848.335	-0.057	-0.001	16290593.9567	c
29	15	14	28	18	11	637101.029	-0.042	0.003	16460933.7085	c
29	14	15	28	17	12	638992.163	-0.045	-0.005	16263925.2857	c
28	16	13	28	13	16	644611.723	0.017	0.001	15431816.0522	c
29	24	6	28	25	3	686760.771	0.067	-0.001	18384205.5514	c
29	24	5	28	25	4	686760.771	0.065	-0.004	18384205.5514	c
29	23	7	28	24	4	706281.301	0.126	0.046	18056318.7417	c
29	23	6	28	24	5	706281.301	0.069	-0.011	18056318.7414	c
29	26	3	28	27	2	650060.386	0.002	0.003	19087613.9544	c
29	26	4	28	27	1	650060.386	0.002	0.003	19087613.9544	c
29	5	25	28	4	24	848258.242	-3.270	-3.265	12807454.0477	d
29	4	25	28	5	24	848258.242	-3.270	-3.265	12807454.0477	d
29	4	26	28	3	25	831362.821	-3.760	-3.759	12395776.9686	d
29	3	26	28	4	25	831362.821	-3.760	-3.759	12395776.9686	d
29	2	27	28	3	26	814475.795	-4.340	-4.341	11966241.2896	d
29	3	27	28	2	26	814475.795	-4.340	-4.341	11966241.2896	d
29	2	28	28	1	27	797593.865	-1.940	-1.944	11518940.5917	d
29	1	28	28	2	27	797593.865	-1.940	-1.944	11518940.5917	d
29	1	29	28	0	28	780703.242	-5.710	-5.714	11053948.4377	d
29	0	29	28	1	28	780703.242	-5.710	-5.714	11053948.4377	d
29	6	24	28	5	23	865168.052	-5.730	-5.722	13201153.0887	d
29	5	24	28	6	23	865168.052	-5.730	-5.722	13201153.0887	d
29	7	23	28	6	22	882112.339	-3.550	-3.544	13576720.6564	d
29	6	23	28	7	22	882112.339	-3.550	-3.544	13576720.6564	d
29	8	22	28	7	21	899102.194	-3.630	-3.616	13933957.6837	d
29	7	22	28	8	21	899102.194	-3.630	-3.616	13933957.6840	d
29	9	21	28	8	20	916169.696	-0.299	-0.288	14272602.3227	d
29	8	21	28	9	20	916169.696	-0.297	-0.287	14272602.3236	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
29	10	20	28	9	19	933344.223	-4.180	-4.166	14592303.6555	d
29	9	20	28	10	19	933344.223	-4.150	-4.136	14592303.6801	d
29	11	19	28	10	18	950700.125	-3.940	-3.925	14892579.1892	d
29	10	19	28	11	18	950700.125	-3.340	-3.327	14892579.6781	d
29	12	17	28	13	16	986374.864	-3.360	-3.344	15431816.0522	d
29	13	17	28	12	16	986506.173	-1.820	-1.803	15431713.6733	d
29	13	16	28	14	15	1004716.485	-2.340	-2.320	15668482.0787	d
29	14	16	28	13	15	1006064.053	-3.640	-3.632	15667444.6715	d
29	14	15	28	15	14	1020820.752	-8.960	-8.938	15882087.7848	d
29	15	15	28	14	14	1031388.147	-2.220	-2.218	15874269.7557	d
29	15	14	28	16	13	1021604.710	-2.320	-2.282	16076427.7523	d
29	17	13	28	16	12	1148989.351	-3.440	-3.445	16160887.7352	d
29	18	12	28	17	11	1214305.499	-3.100	-3.088	16290593.9567	d
29	19	11	28	18	10	1249415.428	-2.480	-2.455	16465666.5599	d
29	19	10	28	18	11	1256222.822	-2.200	-2.177	16460933.7085	d
29	20	10	28	19	9	1268541.606	-1.920	-1.885	16678021.8923	d
29	20	9	28	19	10	1269326.164	-2.480	-2.446	16677457.9989	d
29	21	9	28	20	8	1283845.427	-1.710	-1.660	16915442.3423	d
29	21	8	28	20	9	1283912.581	-2.650	-2.596	16915392.2914	d
29	17	12	28	16	13	1290394.400	-2.600	-2.577	16076427.7523	d
29	22	7	28	21	8	1298245.972	-4.900	-4.844	17173482.4337	d
29	22	8	28	21	7	1298245.972	-0.332	-0.274	17173485.8552	d
29	16	13	28	15	14	1362779.661	-2.130	-2.098	15882087.7848	d
29	29	0	28	28	1	1394088.817	-0.335	-0.305	19462546.5926	d
29	29	1	28	28	0	1394088.817	-0.335	-0.305	19462546.5926	d
29	15	14	28	14	15	1429551.603	-1.110	-1.079	15668482.0787	d
29	15	15	28	12	16	1473947.612	1.150	1.164	15431713.6733	d
29	14	16	28	11	17	1500770.070	-3.230	-3.221	15172739.0722	d
29	12	18	28	9	19	1548777.683	-2.660	-2.650	14592303.6555	d
29	11	18	28	10	19	1548777.683	-0.710	-0.702	14592303.6801	d
29	9	21	28	6	22	1612049.844	-1.820	-1.814	13576720.6564	d
29	8	21	28	7	22	1612049.844	-1.820	-1.814	13576720.6564	d
29	6	23	28	5	24	1651380.855	-1.650	-1.639	12807454.0477	d
29	7	23	28	4	24	1651380.855	-1.650	-1.639	12807454.0477	d
29	16	14	28	15	13	1077024.999	-3.010	-3.015	16038272.3150	d
29	24	5	28	23	6	1326125.200	-3.340	-3.274	17744837.7206	d
29	24	6	28	23	5	1326125.200	-3.330	-3.264	17744837.7281	d
29	25	4	28	24	5	1339838.620	-1.880	-1.809	18056318.7414	d
29	25	5	28	24	4	1339838.620	-1.880	-1.809	18056318.7417	d
29	26	3	28	25	4	1353466.299	-2.490	-2.427	18384205.5514	d
29	26	4	28	25	3	1353466.299	-2.490	-2.427	18384205.5514	d
29	27	2	28	26	3	1367040.316	-1.330	-1.270	18728079.7587	d
29	27	3	28	26	2	1367040.316	-1.330	-1.270	18728079.7587	d
29	28	1	28	27	2	1380575.659	-1.960	-1.912	19087613.9544	d
29	28	2	28	27	1	1380575.659	-1.960	-1.912	19087613.9544	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
29	10	20	28	7	21	1591691.518	-2.860	-2.852	13933957.6837	d
29	9	20	28	8	21	1591691.518	-2.860	-2.847	13933957.6840	d
30	0	30	28	0	28	1587988.658	-3.330	-3.346	11053948.4377	e
30	1	29	28	1	27	1621763.277	2.310	2.298	11518940.5917	e
30	2	28	28	2	26	1655528.901	4.590	4.584	11966241.2896	e
30	3	27	28	3	25	1689288.530	-2.410	-2.406	12395776.9686	e
30	6	24	28	6	22	1790756.285	-0.971	-0.957	13576720.6564	e
30	7	23	28	7	21	1824722.771	6.230	6.243	13933957.6837	e
30	28	2	28	26	2	2782029.041	11.700	11.861	18728079.7587	e
30	12	18	29	15	15	524977.920	-0.015	-0.002	16905660.1171	c
30	13	18	29	14	15	527727.571	-0.003	0.003	16902917.4871	c
30	17	13	29	20	10	542385.526	0.022	0.024	17946565.4097	c
29	16	13	29	13	16	571668.682	0.002	0.015	16673200.8896	c
30	13	17	29	16	14	588942.862	-0.010	0.007	17115300.3134	c
29	18	12	29	15	15	599242.441	0.007	-0.009	16905660.1171	c
29	19	11	29	16	14	599784.144	-0.007	-0.006	17115300.3134	c
29	20	10	29	17	13	636684.860	-0.040	0.000	17309880.5163	c
30	16	14	29	19	11	640419.367	-0.038	-0.001	17715084.4589	c
30	14	16	29	17	13	644586.973	-0.031	-0.004	17309880.5163	c
30	15	15	29	18	12	671191.808	-0.045	-0.007	17504902.5454	c
29	15	14	29	12	17	679840.512	-0.004	0.007	16418194.2641	c
29	16	14	29	13	17	697078.686	0.018	0.011	16418221.6523	c
30	25	6	29	26	3	707435.662	0.067	0.001	19737674.3318	c
30	25	5	29	26	4	707435.662	0.066	0.001	19737674.3318	c
30	15	16	29	16	13	710480.123	-0.012	-0.016	17244869.5642	c
30	27	3	29	28	2	670907.720	-0.019	-0.003	20468191.5604	c
30	27	4	29	28	1	670907.720	-0.019	-0.003	20468191.5604	c
30	2	28	29	3	27	841039.832	-4.350	-4.349	12780721.4166	d
30	3	28	29	2	27	841039.832	-4.350	-4.349	12780721.4166	d
30	2	29	29	1	28	824162.699	-2.470	-2.471	12316536.3891	d
30	1	29	29	2	28	824162.699	-2.470	-2.471	12316536.3891	d
30	1	30	29	0	29	807278.970	-4.070	-4.078	11834657.3799	d
30	0	30	29	1	29	807278.970	-4.070	-4.078	11834657.3799	d
30	4	26	29	5	25	874808.488	-2.990	-2.990	13655715.5511	d
30	5	26	29	4	25	874808.488	-2.990	-2.990	13655715.5511	d
30	5	25	29	6	24	891711.403	-2.070	-2.069	14066326.8608	d
30	6	25	29	5	24	891711.403	-2.070	-2.069	14066326.8608	d
30	7	24	29	6	23	908638.002	-3.360	-3.357	14458836.5389	d
30	6	24	29	7	23	908638.002	-3.360	-3.357	14458836.5389	d
30	8	23	29	7	22	925608.071	-2.650	-2.647	14833063.4946	d
30	7	23	29	8	22	925608.071	-2.650	-2.647	14833063.4946	d
30	9	22	29	8	21	942643.795	-0.233	-0.225	15188772.3080	d
30	8	22	29	9	21	942643.795	-0.233	-0.225	15188772.3083	d
30	10	21	29	9	20	959767.657	-6.850	-6.837	15525652.0415	d
30	9	21	29	10	20	959767.657	-6.840	-6.830	15525652.0466	d

Table S4_2: Assigned transitions v , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
30	11	20	29	10	19	977051.609	-1.340	-1.330	15843283.1323	d
30	10	20	29	11	19	977051.609	-1.210	-1.197	15843283.2417	d
30	12	19	29	11	18	994558.007	-3.290	-3.283	16141082.0580	d
30	11	19	29	12	18	994558.007	-0.918	-0.908	16141083.9815	d
30	15	16	29	14	15	1052426.703	-5.510	-5.505	16902917.4871	d
30	14	17	29	13	16	1031128.526	-2.000	-1.995	16673200.8896	d
30	13	17	29	14	16	1030728.903	-1.930	-1.917	16673512.3584	d
30	12	18	29	13	17	1012411.265	-5.140	-5.129	16418221.6523	d
30	13	18	29	12	17	1012447.540	-3.260	-3.253	16418194.2641	d
30	17	14	29	16	13	1144775.464	-3.250	-3.259	17244869.5642	d
30	19	12	29	18	11	1274080.278	-1.220	-1.203	17518841.9285	d
30	19	11	29	18	12	1294721.608	-1.330	-1.311	17504902.5454	d
30	20	11	29	19	10	1300359.511	0.562	0.597	17717158.7226	d
30	20	10	29	19	11	1303299.878	-1.480	-1.443	17715084.4589	d
30	18	12	29	17	13	1311958.793	-1.600	-1.576	17309880.5163	d
30	21	10	29	20	9	1317268.422	-1.060	-1.012	17946786.6349	d
30	21	9	29	20	10	1317574.810	-0.040	0.005	17946565.4097	d
30	17	13	29	16	14	1373649.547	-1.060	-1.027	17115300.3134	d
30	30	1	29	29	0	1441981.910	-1.040	-1.020	20856635.7313	d
30	30	0	29	29	1	1441981.910	-1.040	-1.020	20856635.7313	d
30	29	1	29	28	2	1428489.137	-2.070	-2.032	20468191.5604	d
30	29	2	29	28	1	1428489.137	-2.070	-2.032	20468191.5604	d
30	16	14	29	15	15	1449840.977	-2.780	-2.745	16905660.1171	d
30	17	14	29	14	15	1486728.677	-2.120	-2.115	16902917.4871	d
30	18	13	29	15	14	1489411.822	-1.320	-1.332	17098034.7732	d
30	16	15	29	13	16	1509586.676	-2.540	-2.528	16673200.8896	d
30	14	16	29	13	17	1536243.948	-1.930	-1.916	16418221.6523	d
30	15	16	29	12	17	1537152.919	-2.520	-2.514	16418194.2641	d
30	14	17	29	11	18	1563248.980	-0.388	-0.379	16141082.0580	d
30	12	19	29	9	20	1609988.769	-2.550	-2.547	15525652.0415	d
30	11	19	29	10	20	1609988.769	-2.100	-2.091	15525652.0466	d
30	10	21	29	7	22	1652362.077	-0.979	-0.972	14833063.4946	d
30	9	21	29	8	22	1652362.077	-0.978	-0.971	14833063.4946	d
30	9	22	29	6	23	1672581.300	1.500	1.505	14458836.5389	d
30	8	22	29	7	23	1672581.300	1.500	1.505	14458836.5389	d
30	14	16	29	15	15	1048807.305	-0.102	-0.087	16905660.1171	d
30	15	15	29	16	14	1060790.621	-3.470	-3.441	17115300.3134	d
30	22	9	29	21	8	1332121.654	-1.530	-1.473	18199307.5049	d
30	22	8	29	21	9	1332145.938	-1.640	-1.581	18199289.4664	d
30	23	7	29	22	8	1346378.899	-3.420	-3.361	18471732.1468	d
30	23	8	29	22	7	1346378.899	-1.900	-1.834	18471733.2950	d
30	25	5	29	24	6	1374141.507	-2.180	-2.108	19070966.2490	d
30	25	6	29	24	5	1374141.507	-2.180	-2.105	19070966.2511	d
30	26	4	29	25	5	1387821.950	-0.639	-0.570	19396159.2280	d
30	26	5	29	25	4	1387821.950	-0.639	-0.569	19396159.2280	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
30	13	17	29	12	18	1563158.442	-0.772	-0.763	16141083.9815	d
31	0	31	29	0	29	1641141.861	7.200	7.179	11834657.3799	e
31	1	30	29	1	28	1674886.500	-7.550	-7.561	12316536.3891	e
31	2	29	29	2	27	1708646.129	-0.530	-0.539	12780721.4166	e
31	3	28	29	3	26	1742405.758	5.030	5.027	13227143.5416	e
31	4	27	29	4	25	1776168.384	1.070	1.072	13655715.5511	e
31	5	26	29	5	24	1809963.988	2.500	2.510	14066326.8608	e
31	6	25	29	6	23	1843801.563	-2.480	-2.468	14458836.5389	e
31	8	23	29	8	21	1911758.517	-5.170	-5.155	15188772.3080	e
31	29	2	29	27	2	2877848.707	4.670	4.776	20095121.3919	e
30	1	29	30	0	30	498761.125	-0.013	-0.002	12641940.4121	c
30	2	29	30	1	30	498761.125	-0.013	-0.002	12641940.4121	c
31	12	19	30	15	16	513817.977	-0.005	0.001	17955349.6924	c
30	17	13	30	14	16	534483.388	-0.012	0.003	17954467.5141	c
31	13	18	30	16	15	578189.636	-0.008	-0.002	18182790.0884	c
31	14	18	30	15	15	584909.139	0.001	-0.002	18176094.3911	c
30	19	12	30	16	15	610133.343	0.008	0.003	18182790.0884	c
30	18	13	30	15	16	632098.220	0.004	-0.005	17955349.6924	c
31	14	17	30	17	14	640853.650	-0.018	-0.004	18389648.2667	c
31	15	17	30	16	14	675263.430	-0.007	-0.019	18355503.8574	c
31	15	16	30	18	13	687289.522	-0.035	-0.010	18587447.9018	c
31	16	15	30	19	12	692168.524	-0.024	0.008	18792923.4178	c
30	21	9	30	18	12	642299.296	-0.062	-0.001	18621840.8954	c
31	26	6	30	27	3	728126.762	0.061	-0.001	21139099.2934	c
31	26	5	30	27	4	728126.762	0.060	-0.001	21139099.2934	c
31	1	31	30	0	30	833849.003	-2.620	-2.632	12641940.4121	d
31	0	31	30	1	30	833849.003	-2.620	-2.632	12641940.4121	d
31	2	30	30	1	29	850725.236	-3.650	-3.655	13140701.5452	d
31	1	30	30	2	29	850725.236	-3.650	-3.655	13140701.5452	d
31	3	29	30	2	28	867599.671	-2.810	-2.815	13621765.5863	d
31	2	29	30	3	28	867599.671	-2.810	-2.815	13621765.5863	d
31	3	28	30	4	27	884472.308	-4.060	-4.066	14085067.8890	d
31	4	28	30	3	27	884472.308	-4.060	-4.066	14085067.8890	d
31	4	27	30	5	26	901352.738	-3.100	-3.097	14530527.0222	d
31	5	27	30	4	26	901352.738	-3.100	-3.097	14530527.0222	d
31	5	26	30	6	25	918244.561	-3.450	-3.445	14958040.3282	d
31	6	26	30	5	25	918244.561	-3.450	-3.445	14958040.3282	d
31	7	25	30	6	24	935157.969	-4.710	-4.703	15367477.8946	d
31	6	25	30	7	24	935157.969	-4.710	-4.703	15367477.8946	d
31	8	24	30	7	23	952109.451	-4.010	-4.002	15758674.2107	d
31	7	24	30	8	23	952109.451	-4.010	-4.002	15758674.2107	d
31	9	23	30	8	22	969117.893	-1.760	-1.760	16131416.3268	d
31	8	23	30	9	22	969117.893	-1.760	-1.760	16131416.3268	d
31	10	22	30	9	21	986206.380	-2.880	-2.870	16485426.5332	d
31	9	22	30	10	21	986206.380	-2.870	-2.868	16485426.5344	d

Table S4_2: Assigned transitions v , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
31	11	21	30	10	20	1003421.680	-2.280	-2.275	16820336.0466	d
31	10	21	30	11	20	1003421.680	-2.250	-2.246	16820336.0705	d
31	12	20	30	11	19	1020820.752	-7.740	-7.737	17135642.8965	d
31	11	20	30	12	19	1020820.752	-7.190	-7.183	17135643.3480	d
31	13	19	30	12	18	1038523.814	-7.540	-7.539	17430638.0465	d
31	15	17	30	14	16	1076298.001	-1.780	-1.777	17954467.5141	d
31	16	16	30	15	15	1100969.746	-0.250	-0.249	18176094.3911	d
31	17	15	30	16	14	1144556.915	-1.770	-1.777	18355503.8574	d
31	18	14	30	17	13	1217255.460	-2.130	-2.135	18488950.9083	d
31	19	13	30	18	12	1288675.988	-2.610	-2.601	18621840.8954	d
31	20	12	30	19	11	1329100.043	-1.520	-1.489	18799625.4746	d
31	20	11	30	19	12	1338827.719	-1.460	-1.435	18792923.4178	d
31	21	11	30	20	10	1349958.424	-1.720	-1.676	19018385.8009	d
31	21	10	30	20	11	1351177.681	-0.513	-0.473	19017517.6583	d
31	22	9	30	21	10	1365840.545	-0.650	-0.599	19264056.1008	d
31	22	10	30	21	9	1365730.821	4.930	4.978	19264140.2468	d
31	29	2	30	28	3	1462866.672	-1.710	-1.664	21510097.0275	d
31	29	3	30	28	2	1462866.672	-1.710	-1.664	21510097.0275	d
31	17	14	30	16	15	1463589.173	-2.860	-2.819	18182790.0884	d
31	30	2	30	29	1	1476361.544	-1.500	-1.469	21896682.7559	d
31	30	1	30	29	2	1476361.544	-1.500	-1.469	21896682.7559	d
31	31	1	30	30	0	1489832.731	-1.680	-1.668	22298618.6669	d
31	31	0	30	30	1	1489832.731	-1.680	-1.668	22298618.6669	d
31	16	15	30	15	16	1529742.042	-0.240	-0.213	17955349.6924	d
31	15	16	30	14	17	1570404.433	-1.620	-1.609	17704331.4104	d
31	14	17	30	13	18	1599853.376	-3.510	-3.502	17430645.0565	d
31	15	17	30	12	18	1600125.887	-3.370	-3.361	17430638.0465	d
31	13	19	30	10	20	1648831.418	-1.950	-1.943	16820336.0466	d
31	12	19	30	11	20	1648831.418	-0.197	-0.193	16820336.0705	d
31	12	20	30	9	21	1671043.063	-1.800	-1.799	16485426.5332	d
31	11	20	30	10	21	1671043.063	-1.700	-1.695	16485426.5344	d
31	9	23	30	6	24	1733056.394	-1.700	-1.695	15367477.8946	d
31	8	23	30	7	24	1733056.394	-1.700	-1.695	15367477.8946	d
31	8	24	30	5	25	1752746.783	-0.565	-0.552	14958040.3282	d
31	7	24	30	6	25	1752746.783	-0.565	-0.552	14958040.3282	d
31	6	25	30	5	26	1772113.395	-0.161	-0.144	14530527.0222	d
31	7	25	30	4	26	1772113.395	-0.161	-0.144	14530527.0222	d
31	14	17	30	15	16	1075148.896	-3.350	-3.342	17955349.6924	d
31	19	12	30	18	13	1341747.700	-1.560	-1.541	18587447.9018	d
31	24	7	30	23	8	1394458.762	-1.090	-1.023	19818114.0778	d
31	24	8	30	23	7	1394458.762	-0.588	-0.522	19818114.4562	d
31	26	5	30	25	6	1422114.644	-1.440	-1.369	20445109.9197	d
31	26	6	30	25	5	1422114.644	-1.440	-1.368	20445109.9206	d
31	27	4	30	26	5	1435760.311	-3.030	-2.966	20783981.8032	d
31	27	5	30	26	4	1435760.311	-3.030	-2.966	20783981.8032	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
31	28	3	30	27	4	1449337.925	-2.200	-2.142	21139099.2934	d
31	28	4	30	27	3	1449337.925	-2.200	-2.142	21139099.2934	d
32	0	32	30	0	30	1694262.087	-4.060	-4.082	12641940.4121	e
32	1	31	30	1	29	1728012.722	-2.940	-2.958	13140701.5452	e
32	2	30	30	2	28	1761763.357	6.020	6.008	13621765.5863	e
32	3	29	30	3	27	1795499.002	0.211	0.202	14085067.8890	e
32	4	28	30	4	26	1829243.641	-6.510	-6.518	14530527.0222	e
32	5	27	30	5	25	1863033.249	8.220	8.220	14958040.3282	e
32	6	26	30	6	24	1896837.846	-4.100	-4.092	15367477.8946	e
32	7	25	30	7	23	1930729.384	2.870	2.876	15758674.2107	e
32	30	2	30	28	2	2973572.439	-14.400	-14.325	21510097.0275	e
31	2	29	31	1	30	497937.631	-0.013	0.003	13991430.4195	c
31	3	29	31	2	30	497937.631	-0.013	0.003	13991430.4195	c
31	1	30	31	0	31	515638.376	-0.020	-0.007	13475792.0286	c
31	2	30	31	1	31	515638.376	-0.020	-0.007	13475792.0286	c
31	18	13	31	15	16	500761.339	-0.014	-0.002	19274737.4521	c
32	12	20	31	15	17	503093.309	-0.009	-0.009	19030767.2876	c
32	13	20	31	14	17	503359.092	0.005	0.003	19030501.9284	c
32	13	19	31	16	16	566556.742	0.014	0.011	19277064.3761	c
32	14	19	31	15	16	568889.808	0.004	-0.002	19274737.4521	c
31	17	14	31	14	17	615880.157	-0.024	0.004	19030501.9284	c
31	20	12	31	17	15	628664.486	-0.013	0.000	19500062.5287	c
31	19	13	31	16	16	633455.110	-0.002	-0.004	19277064.3761	c
32	15	18	31	16	15	646783.025	0.024	0.008	19485091.9594	c
31	21	11	31	18	14	662137.406	-0.046	0.003	19706208.4823	c
32	15	17	31	18	14	690259.297	-0.010	-0.001	19706208.4823	c
32	17	15	31	20	12	699086.871	-0.038	-0.016	20128727.0217	c
32	16	16	31	19	13	722300.989	-0.020	0.000	19910519.4816	c
32	1	32	31	0	31	860411.540	-2.980	-2.995	13475792.0286	d
32	0	32	31	1	31	860411.540	-2.980	-2.995	13475792.0286	d
32	2	31	31	1	30	877283.577	-3.200	-3.212	13991430.4195	d
32	1	31	31	2	30	877283.577	-3.200	-3.212	13991430.4195	d
32	2	30	31	3	29	894150.817	-4.040	-4.045	14489368.0584	d
32	3	30	31	2	29	894150.817	-4.040	-4.045	14489368.0584	d
32	3	29	31	4	28	911019.556	-2.860	-2.870	14969544.2516	d
32	4	29	31	3	28	911019.556	-2.860	-2.870	14969544.2516	d
32	4	28	31	5	27	927891.293	-3.030	-3.031	15431882.8474	d
32	5	28	31	4	27	927891.293	-3.030	-3.031	15431882.8474	d
32	6	27	31	5	26	944774.422	-2.600	-2.601	15876288.3267	d
32	5	27	31	6	26	944774.422	-2.600	-2.601	15876288.3267	d
32	7	26	31	6	25	961676.737	-2.530	-2.530	16302640.5608	d
32	6	26	31	7	25	961676.737	-2.530	-2.530	16302640.5608	d
32	8	25	31	7	24	978609.932	-3.120	-3.123	16710787.6586	d
32	7	25	31	8	24	978609.932	-3.120	-3.123	16710787.6586	d
32	9	24	31	8	23	995591.692	-3.440	-3.436	17100535.9753	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
32	8	24	31	9	23	995591.692	-3.440	-3.436	17100535.9753	d
32	10	23	31	9	22	1012647.802	-1.510	-1.508	17471635.7785	d
32	9	23	31	10	22	1012647.802	-1.510	-1.508	17471635.7788	d
32	11	22	31	10	21	1029807.939	-2.420	-2.422	17823759.9927	d
32	10	22	31	11	21	1029807.939	-2.420	-2.416	17823759.9978	d
32	12	21	31	11	20	1047127.567	-3.110	-3.103	18156471.2791	d
32	11	21	31	12	20	1047127.567	-2.980	-2.978	18156471.3816	d
32	13	20	31	12	19	1064689.126	-4.230	-4.224	18469167.6691	d
32	12	20	31	13	19	1064689.126	-2.090	-2.087	18469169.3953	d
32	13	19	31	14	18	1082610.138	-7.450	-7.446	18761003.5234	d
32	14	19	31	13	18	1082642.216	-5.320	-5.316	18760979.7271	d
32	15	18	31	14	17	1101371.169	-1.870	-1.865	19030501.9284	d
32	14	18	31	15	17	1101030.005	-2.130	-2.124	19030767.2876	d
32	15	17	31	16	16	1119399.206	-4.210	-4.205	19277064.3761	d
32	17	16	31	16	15	1153422.087	-7.690	-7.702	19485091.9594	d
32	18	15	31	17	14	1211666.123	-2.280	-2.291	19646382.1036	d
32	20	13	31	19	12	1351086.844	-1.900	-1.883	19929197.1522	d
32	20	12	31	19	13	1379051.513	-0.411	-0.385	19910519.4816	d
32	21	12	31	20	11	1380973.784	-1.760	-1.727	20131752.5878	d
32	22	11	31	21	10	1398866.615	-0.740	-0.693	20368695.8390	d
32	22	10	31	21	11	1399354.377	0.509	0.556	20368345.9281	d
32	26	6	31	25	7	1456334.788	0.800	0.869	21531315.4254	d
32	26	7	31	25	6	1456334.788	0.807	0.876	21531315.4311	d
32	28	4	31	27	5	1483661.497	-0.090	-0.028	22219745.1323	d
32	28	5	31	27	4	1483661.497	-0.090	-0.028	22219745.1323	d
32	29	3	31	28	4	1497212.130	-0.788	-0.735	22588439.4051	d
32	29	4	31	28	3	1497212.130	-0.788	-0.735	22588439.4051	d
32	30	2	31	29	3	1510718.393	-0.074	-0.034	22972965.3974	d
32	30	3	31	29	2	1510718.393	-0.074	-0.034	22972965.3974	d
32	31	1	31	30	2	1524189.881	-1.850	-1.823	23373045.7853	d
32	31	2	31	30	1	1524189.881	-1.850	-1.823	23373045.7853	d
32	32	0	31	31	1	1537640.382	-1.750	-1.751	23788453.0614	d
32	32	1	31	31	0	1537640.382	-1.750	-1.751	23788453.0614	d
32	12	21	31	9	22	1731965.748	-0.431	-0.432	17471635.7785	d
32	11	21	31	10	22	1731965.748	-0.408	-0.409	17471635.7788	d
32	11	22	31	8	23	1753033.684	-0.704	-0.703	17100535.9753	d
32	10	22	31	9	23	1753033.684	-0.703	-0.702	17100535.9753	d
32	16	17	31	15	16	1122474.181	-2.710	-2.707	19274737.4521	d
32	17	15	31	18	14	1121600.884	-4.570	-4.531	19706208.4823	d
32	16	16	31	17	15	1132757.072	-0.894	-0.876	19500062.5287	d
32	21	11	31	20	12	1385298.594	-3.670	-3.635	20128727.0217	d
32	23	9	31	22	10	1414063.409	-0.757	-0.700	20629866.1270	d
32	24	8	31	23	9	1428426.181	-2.460	-2.395	20911747.7367	d
32	24	9	31	23	8	1428426.181	0.475	0.538	20911749.9282	d
32	25	7	31	24	8	1442484.962	0.150	0.218	21212573.7921	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
32	25	8	31	24	7	1442484.962	0.312	0.380	21212573.9151	d
32	27	5	31	26	6	1470043.411	-1.510	-1.439	21867225.9878	d
32	27	6	31	26	5	1470043.411	-1.510	-1.439	21867225.9878	d
33	0	33	31	0	31	1747391.306	5.230	5.204	13475792.0286	e
33	1	32	31	1	30	1781123.954	-1.490	-1.518	13991430.4195	e
33	4	29	31	4	27	1882306.906	-14.100	-14.124	15431882.8474	e
33	6	27	31	6	25	1949877.128	7.200	7.198	16302640.5608	e
33	7	26	31	7	24	1983723.697	1.910	1.909	16710787.6586	e
32	4	29	32	2	30	497043.745	-0.019	-0.001	15383522.9030	c
32	4	29	32	3	30	497043.745	-0.019	-0.001	15383522.9030	c
32	2	30	32	1	31	514805.705	-0.014	0.003	14868717.1893	c
32	3	30	32	2	31	514805.705	-0.014	0.003	14868717.1893	c
32	1	31	32	0	32	532510.645	-0.007	0.007	14336206.5430	c
32	2	31	32	1	32	532510.645	-0.007	0.007	14336206.5430	c
32	21	11	32	18	14	540840.886	-0.015	-0.007	20973188.3773	c
32	18	14	32	15	17	576720.570	-0.030	0.003	20396467.7825	c
33	15	19	32	16	16	625939.796	0.008	-0.011	20632820.4836	c
32	21	12	32	18	15	654677.630	-0.007	0.031	20858050.4903	c
32	19	14	32	16	17	669125.562	-0.005	0.003	20397214.3293	c
33	18	15	32	21	12	690575.556	0.009	0.012	21512728.1206	c
32	18	15	32	15	18	726175.542	-0.001	0.009	20131874.9541	c
32	22	10	32	19	13	657867.147	-0.067	0.000	21109832.5754	c
33	15	18	32	18	15	684676.570	0.001	-0.005	20858050.4903	c
33	2	32	32	1	31	903835.922	-2.750	-2.760	14868717.1893	d
33	1	32	32	2	31	903835.922	-2.750	-2.760	14868717.1893	d
33	2	31	32	3	30	920698.065	-3.040	-3.056	15383522.9030	d
33	3	31	32	2	30	920698.065	-3.040	-3.056	15383522.9030	d
33	3	30	32	4	29	937559.309	-2.990	-2.999	15880566.6625	d
33	4	30	32	3	29	937559.309	-2.990	-2.999	15880566.6625	d
33	5	29	32	4	28	954423.851	-2.850	-2.855	16359777.1590	d
33	4	29	32	5	28	954423.851	-2.850	-2.855	16359777.1590	d
33	5	28	32	6	27	971297.387	-2.810	-2.816	16821065.3388	d
33	6	28	32	5	27	971297.387	-2.810	-2.816	16821065.3388	d
33	8	26	32	7	25	1005105.016	-3.720	-3.717	17689400.7060	d
33	7	26	32	8	25	1005105.016	-3.720	-3.717	17689400.7060	d
33	9	25	32	8	24	1022066.391	-2.660	-2.659	18096131.0956	d
33	8	25	32	9	24	1022066.391	-2.660	-2.659	18096131.0956	d
33	10	24	32	9	23	1039090.722	-1.390	-1.387	18484285.0815	d
33	9	24	32	10	23	1039090.722	-1.390	-1.387	18484285.0815	d
33	12	22	32	11	21	1073454.467	-3.130	-3.135	19203601.9182	d
33	11	22	32	12	21	1073454.467	-3.110	-3.107	19203601.9410	d
33	13	21	32	12	20	1090906.903	-2.320	-2.325	19533860.6001	d
33	12	21	32	13	20	1090906.903	-1.820	-1.820	19533861.0108	d
33	14	20	32	13	19	1108664.827	-5.870	-5.873	19843621.0989	d
33	13	20	32	14	19	1108664.827	1.810	1.811	19843627.2503	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
33	15	18	32	16	17	1145509.656	-3.080	-3.079	20397214.3293	d
33	16	18	32	15	17	1146483.383	-0.819	-0.822	20396467.7825	d
33	18	16	32	17	15	1212014.183	-3.350	-3.361	20827813.9243	d
33	21	13	32	20	12	1408038.774	-1.920	-1.890	21289571.3922	d
33	21	12	32	20	13	1421640.072	-1.760	-1.723	21280285.8853	d
33	20	13	32	19	14	1429669.721	-2.300	-2.267	21066339.8896	d
33	22	11	32	21	12	1432907.183	-0.443	-0.399	21512728.1206	d
33	23	11	32	22	10	1447405.760	-1.760	-1.703	21767699.7828	d
33	23	10	32	22	11	1447597.927	1.940	1.990	21767563.1800	d
33	25	8	32	24	9	1476476.964	-0.164	-0.097	22340175.6204	d
33	25	9	32	24	8	1476476.964	0.825	0.892	22340176.3627	d
33	27	6	32	26	7	1504254.861	-1.110	-1.041	22987649.3978	d
33	27	7	32	26	6	1504254.861	-1.110	-1.038	22987649.3993	d
33	28	5	32	27	6	1517927.809	-1.450	-1.381	23337270.8908	d
33	28	6	32	27	5	1517927.809	-1.450	-1.381	23337270.8908	d
33	29	4	32	28	5	1531517.115	1.020	1.074	23703406.7042	d
33	29	5	32	28	4	1531517.115	1.020	1.074	23703406.7042	d
33	30	3	32	29	4	1545039.567	-2.440	-2.397	24085652.3084	d
33	30	4	32	29	3	1545039.567	-2.440	-2.397	24085652.3084	d
33	31	3	32	30	2	1558522.747	-1.770	-1.733	24483683.8496	d
33	31	2	32	30	3	1558522.747	-1.770	-1.733	24483683.8496	d
33	32	1	32	31	2	1571974.148	-1.710	-1.696	24897237.4966	d
33	32	2	32	31	1	1571974.148	-1.710	-1.696	24897237.4966	d
33	33	1	32	32	0	1585403.964	-0.764	-0.771	25326095.1799	d
33	33	0	32	32	1	1585403.964	-0.764	-0.771	25326095.1799	d
33	17	17	32	14	18	1671588.686	-2.010	-2.001	20131799.4085	d
33	14	20	32	11	21	1748687.888	-2.000	-1.999	19203601.9182	d
33	13	20	32	12	21	1748687.888	-0.441	-0.444	19203601.9410	d
33	13	21	32	10	22	1771195.729	-3.760	-3.764	18853570.3450	d
33	12	21	32	11	22	1771195.729	-3.660	-3.668	18853570.3459	d
33	12	22	32	9	23	1792773.613	-0.831	-0.836	18484285.0815	d
33	11	22	32	10	23	1792773.613	-0.826	-0.831	18484285.0815	d
33	11	23	32	8	24	1813644.285	-2.210	-2.212	18096131.0956	d
33	10	23	32	9	24	1813644.285	-2.210	-2.212	18096131.0956	d
33	10	24	32	7	25	1833975.630	-0.861	-0.860	17689400.7060	d
33	9	24	32	8	25	1833975.630	-0.861	-0.860	17689400.7060	d
33	0	33	32	1	32	886971.380	-0.174	-0.188	14336206.5430	d
33	1	33	32	0	32	886971.380	-0.174	-0.188	14336206.5430	d
33	7	27	32	6	26	988188.011	-2.650	-2.652	17264319.8186	d
33	6	27	32	7	26	988188.011	-2.650	-2.652	17264319.8186	d
33	22	12	32	21	11	1431069.453	1.040	1.079	21514029.2730	d
33	26	7	32	25	8	1490456.600	-1.550	-1.479	22655058.5503	d
33	26	8	32	25	7	1490456.600	-1.500	-1.428	22655058.5896	d
34	0	34	32	0	32	1800505.536	11.400	11.415	14336206.5430	e
34	1	33	32	1	31	1834217.198	-5.840	-5.873	14868717.1893	e

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
34	5	29	32	5	27	1969114.810	-2.630	-2.645	16821065.3388	e
34	7	27	32	7	25	2036685.032	-23.500	-23.519	17689400.7060	e
33	4	29	33	3	30	496074.884	-0.018	0.000	16818128.9520	c
33	5	29	33	4	30	496074.884	-0.018	0.000	16818128.9520	c
33	3	30	33	2	31	513904.931	-0.022	-0.003	16304224.0037	c
33	4	30	33	3	31	513904.931	-0.022	-0.003	16304224.0037	c
33	2	31	33	1	32	531668.132	-0.027	-0.008	15772555.8495	c
33	3	31	33	2	32	531668.132	-0.027	-0.008	15772555.8495	c
33	1	32	33	0	33	549377.759	-0.008	0.006	15223178.0881	c
33	2	32	33	1	33	549377.759	-0.008	0.006	15223178.0881	c
33	21	12	33	18	15	498624.030	-0.013	-0.010	22203303.6613	c
33	19	14	33	16	17	539269.904	-0.040	-0.003	21801424.9402	c
34	13	21	33	16	18	544115.234	0.028	0.012	21542951.9737	c
34	14	21	33	15	18	544340.514	0.018	0.001	21542727.0526	c
33	22	11	33	19	14	604940.817	-0.043	-0.003	22340694.8784	c
34	14	20	33	17	17	608136.243	0.052	0.031	21803390.0896	c
33	18	15	33	15	18	660576.581	-0.034	0.013	21542727.0526	c
33	20	14	33	17	17	668088.164	-0.025	-0.003	21803390.0896	c
34	19	15	33	22	12	668192.700	0.042	0.018	22945097.6765	c
34	16	19	33	17	16	687339.881	0.043	0.007	22026947.2017	c
33	22	12	33	19	15	687356.792	-0.061	0.007	22257740.8306	c
34	0	34	33	1	33	913519.828	-2.710	-2.726	15223178.0881	d
34	1	34	33	0	33	913519.828	-2.710	-2.726	15223178.0881	d
34	2	33	33	1	32	930381.072	-3.300	-3.317	15772555.8495	d
34	1	33	33	2	32	930381.072	-3.300	-3.317	15772555.8495	d
34	3	31	33	4	30	964093.067	-2.740	-2.753	16818128.9520	d
34	4	31	33	3	30	964093.067	-2.740	-2.753	16818128.9520	d
34	5	30	33	4	29	980949.514	-3.230	-3.235	17314203.8491	d
34	4	30	33	5	29	980949.514	-3.230	-3.235	17314203.8491	d
34	6	29	33	5	28	997815.255	-1.990	-1.997	17792365.5281	d
34	5	29	33	6	28	997815.255	-1.990	-1.997	17792365.5281	d
34	7	28	33	6	27	1014693.588	-2.850	-2.851	18252510.4693	d
34	6	28	33	7	27	1014693.588	-2.850	-2.851	18252510.4693	d
34	7	27	33	8	26	1031597.102	-2.710	-2.716	18694509.4273	d
34	8	27	33	7	26	1031597.102	-2.710	-2.716	18694509.4273	d
34	9	26	33	8	25	1048537.492	-2.790	-2.796	19118200.1349	d
34	8	26	33	9	25	1048537.492	-2.790	-2.796	19118200.1349	d
34	10	25	33	9	24	1065533.343	-2.290	-2.292	19523377.1792	d
34	9	25	33	10	24	1065533.343	-2.290	-2.292	19523377.1792	d
34	11	24	33	10	23	1082610.138	-0.737	-0.742	19909777.5717	d
34	10	24	33	11	23	1082610.138	-0.736	-0.741	19909777.5720	d
34	12	23	33	11	22	1099800.255	-1.830	-1.834	20277059.5030	d
34	11	23	33	12	22	1099800.255	-1.820	-1.828	20277059.5078	d
34	14	21	33	13	20	1134774.378	-2.920	-2.931	20952290.2531	d
34	13	21	33	14	20	1134774.378	-1.020	-1.030	20952291.7850	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
34	14	20	33	15	19	1152763.742	-2.280	-2.287	21258760.2649	d
34	15	20	33	14	19	1152789.824	-2.070	-2.080	21258739.7423	d
34	16	19	33	15	18	1171558.949	-1.040	-1.050	21542727.0526	d
34	17	17	33	18	16	1204456.707	0.476	0.482	22039831.4406	d
34	22	13	33	21	12	1461092.799	1.200	1.242	22701927.6991	d
34	21	13	33	20	14	1464050.254	-1.460	-1.422	22471478.2718	d
34	22	12	33	21	13	1467311.999	-0.591	-0.551	22697612.0715	d
34	23	12	33	22	11	1480219.876	-1.120	-1.073	22945635.7323	d
34	23	11	33	22	12	1480976.853	2.510	2.564	22945097.6765	d
34	24	11	33	23	10	1495739.548	2.980	3.042	23215159.1567	d
34	24	10	33	23	11	1495805.502	-2.160	-2.096	23215107.2855	d
34	26	8	33	25	9	1524466.889	0.234	0.304	23816652.4868	d
34	26	9	33	25	8	1524466.889	0.562	0.632	23816652.7341	d
34	27	7	33	26	8	1538379.072	-1.280	-1.214	24145516.6723	d
34	27	8	33	26	7	1538379.072	-1.270	-1.198	24145516.6849	d
34	28	6	33	27	7	1552131.765	1.040	1.109	24491905.3525	d
34	28	7	33	27	6	1552131.765	1.040	1.109	24491905.3531	d
34	29	5	33	28	6	1565768.438	0.377	0.438	24855200.1302	d
34	29	6	33	28	5	1565768.438	0.377	0.438	24855200.1302	d
34	30	4	33	29	5	1579323.567	-2.050	-2.003	25234922.7872	d
34	30	5	33	29	4	1579323.567	-2.050	-2.003	25234922.7872	d
34	31	3	33	30	4	1592824.435	-1.620	-1.577	25630694.3040	d
34	31	4	33	30	3	1592824.435	-1.620	-1.577	25630694.3040	d
34	32	3	33	31	2	1606285.129	-0.005	0.021	26042208.3472	d
34	32	2	33	31	3	1606285.129	-0.005	0.021	26042208.3472	d
34	33	1	33	32	2	1619712.247	-1.800	-1.789	26469213.3398	d
34	33	2	33	32	1	1619712.247	-1.800	-1.789	26469213.3398	d
34	34	1	33	33	0	1633119.279	-1.520	-1.531	26911499.8929	d
34	34	0	33	33	1	1633119.279	-1.520	-1.531	26911499.8929	d
34	16	18	33	15	19	1734525.978	-1.050	-1.039	21258760.2649	d
34	15	20	33	12	21	1786757.671	-4.250	-4.258	20624769.7208	d
34	14	20	33	13	21	1786757.671	1.190	1.190	20624769.8156	d
34	14	21	33	11	22	1810006.600	-1.460	-1.467	20277059.5030	d
34	13	21	33	12	22	1810006.600	-1.080	-1.093	20277059.5078	d
34	2	32	33	3	31	947241.716	0.653	0.639	16304224.0037	d
34	3	32	33	2	31	947241.716	0.653	0.639	16304224.0037	d
34	13	22	33	12	21	1117160.654	-2.280	-2.284	20624769.7208	d
34	12	22	33	13	21	1117160.654	-2.160	-2.167	20624769.8156	d
34	16	18	33	17	17	1189894.874	-2.320	-2.326	21803390.0896	d
34	25	9	33	24	10	1510309.776	-1.990	-1.923	23506137.5756	d
34	25	10	33	24	9	1510309.776	3.380	3.448	23506141.5625	d
35	0	35	33	0	33	1853592.784	2.950	2.920	15223178.0881	e
35	1	34	33	1	32	1887310.442	2.360	2.326	15772555.8495	e
35	4	31	33	4	29	1988424.442	-0.520	-0.541	17314203.8491	e
35	5	30	33	5	28	2022154.092	8.960	8.944	17792365.5281	e

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(\text{SP})$ / MHz	$\Delta_{O-C}(\text{LP})$ / MHz	E''/h (MHz)	Source
35	6	29	33	6	27	2055889.737	-2.910	-2.919	18252510.4693	e
34	5	29	34	4	30	495026.173	-0.015	0.002	18295156.5797	c
34	6	29	34	5	30	495026.173	-0.015	0.002	18295156.5797	c
34	4	30	34	3	31	512931.808	-0.026	-0.005	17782224.7508	c
34	5	30	34	4	31	512931.808	-0.026	-0.005	17782224.7508	c
34	3	31	34	2	32	530759.679	-0.020	0.003	17251465.0571	c
34	4	31	34	3	32	530759.679	-0.020	0.003	17251465.0571	c
34	2	32	34	1	33	548524.837	-0.012	0.010	16702940.2139	c
34	3	32	34	2	33	548524.837	-0.012	0.010	16702940.2139	c
34	1	33	34	0	34	566239.596	-0.006	0.007	16136700.6170	c
34	2	33	34	1	34	566239.596	-0.006	0.007	16136700.6170	c
34	20	14	34	17	17	510180.523	-0.052	-0.013	23244287.6602	c
35	14	22	34	15	19	533785.008	0.050	0.029	22714222.7169	c
34	22	12	34	19	15	551634.312	-0.013	0.014	23613290.3283	c
35	14	21	34	17	18	596365.735	0.021	-0.007	22993916.3031	c
35	15	21	34	16	18	596996.119	0.031	0.000	22993287.2750	c
35	15	20	34	18	17	662191.809	0.040	0.005	23249117.2417	c
34	23	11	34	20	14	671603.701	-0.079	0.000	23754468.2301	c
34	22	13	34	19	16	681556.245	-0.069	-0.005	23481462.9735	c
35	0	35	34	1	34	940064.078	-3.220	-3.233	16136700.6170	d
35	1	35	34	0	34	940064.078	-3.220	-3.233	16136700.6170	d
35	1	34	34	2	33	956921.724	-1.990	-2.004	16702940.2139	d
35	2	34	34	1	33	956921.724	-1.990	-2.004	16702940.2139	d
35	3	33	34	2	32	973771.576	-2.950	-2.968	17251465.0571	d
35	2	33	34	3	32	973771.576	-2.950	-2.968	17251465.0571	d
35	3	32	34	4	31	990621.129	-1.620	-1.638	17782224.7508	d
35	4	32	34	3	31	990621.129	-1.620	-1.638	17782224.7508	d
35	5	31	34	4	30	1007470.081	-2.140	-2.153	18295156.5797	d
35	4	31	34	5	30	1007470.081	-2.140	-2.153	18295156.5797	d
35	5	30	34	6	29	1024326.529	-1.360	-1.367	18790182.7632	d
35	6	30	34	5	29	1024326.529	-1.360	-1.367	18790182.7632	d
35	6	29	34	7	28	1041194.068	-2.140	-2.149	19267206.8928	d
35	7	29	34	6	28	1041194.068	-2.140	-2.149	19267206.8928	d
35	8	28	34	7	27	1058084.092	-1.640	-1.649	19726109.2309	d
35	7	28	34	8	27	1058084.092	-1.640	-1.649	19726109.2309	d
35	9	27	34	8	26	1075005.895	-2.010	-2.013	20166740.4083	d
35	8	27	34	9	26	1075005.895	-2.010	-2.013	20166740.4083	d
35	11	25	34	10	24	1109016.783	-1.630	-1.636	20992388.4354	d
35	10	25	34	11	24	1109016.783	-1.630	-1.636	20992388.4357	d
35	12	24	34	11	23	1126155.336	-3.470	-3.482	21376861.5740	d
35	11	24	34	12	23	1126155.336	-3.470	-3.481	21376861.5752	d
35	14	22	34	13	21	1160937.891	-2.620	-2.628	22087067.1744	d
35	13	22	34	14	21	1160937.891	-2.160	-2.173	22087067.5434	d
35	15	20	34	16	19	1197020.648	-1.340	-1.349	22714287.0329	d
35	17	19	34	16	18	1216613.304	-1.710	-1.721	22993287.2750	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
35	22	13	34	21	14	1504763.010	-0.465	-0.423	23922916.1824	d
35	23	13	34	22	12	1511828.826	3.640	3.691	24164924.6476	d
35	24	12	34	23	11	1528875.941	-1.970	-1.907	24426072.0032	d
35	24	11	34	23	12	1529177.233	0.319	0.381	24425856.7187	d
35	26	9	34	25	10	1558330.879	-1.900	-1.828	25016447.9431	d
35	26	10	34	25	9	1558330.879	-0.045	0.029	25016449.3275	d
35	27	8	34	26	9	1572397.156	-1.650	-1.571	25341119.0463	d
35	27	9	34	26	8	1572397.156	-1.540	-1.464	25341119.1273	d
35	28	7	34	27	8	1586249.979	-1.560	-1.491	25683897.0100	d
35	28	8	34	27	7	1586249.979	-1.560	-1.486	25683897.0139	d
35	29	6	34	28	7	1599955.905	-1.630	-1.566	26044036.0610	d
35	29	7	34	28	6	1599955.905	-1.630	-1.565	26044036.0610	d
35	30	5	34	29	6	1613558.401	-1.830	-1.776	26420968.1754	d
35	30	6	34	29	5	1613558.401	-1.830	-1.776	26420968.1754	d
35	31	4	34	30	5	1627085.950	-2.930	-2.879	26814248.3932	d
35	31	5	34	30	4	1627085.950	-2.930	-2.879	26814248.3932	d
35	32	3	34	31	4	1640562.534	-1.150	-1.115	27223520.3411	d
35	32	4	34	31	3	1640562.534	-1.150	-1.115	27223520.3411	d
35	33	3	34	32	2	1653998.346	-0.598	-0.575	27648493.4658	d
35	33	2	34	32	3	1653998.346	-0.598	-0.575	27648493.4658	d
35	34	1	34	33	2	1667404.179	-0.716	-0.708	28088927.3698	d
35	34	2	34	33	1	1667404.179	-0.716	-0.708	28088927.3698	d
35	35	1	34	34	0	1680787.227	-1.740	-1.742	28544620.6776	d
35	35	0	34	34	1	1680787.227	-1.740	-1.742	28544620.6776	d
35	16	19	34	15	20	1798179.775	-1.120	-1.111	22411531.6271	d
35	17	19	34	14	20	1798374.341	-1.680	-1.673	22411526.2749	d
35	13	23	34	12	22	1143441.986	-1.850	-1.863	21741932.6190	d
35	12	23	34	13	22	1143441.986	-1.830	-1.837	21741932.6402	d
35	15	21	34	14	20	1178751.577	-5.520	-5.530	22411526.2749	d
35	14	21	34	15	20	1178751.577	1.180	1.168	22411531.6271	d
35	16	19	34	17	18	1215793.970	-2.240	-2.250	22993916.3031	d
36	0	36	34	0	34	1906671.039	-1.900	-1.932	16136700.6170	e
36	1	35	34	1	33	1940379.703	-0.504	-0.542	16702940.2139	e
36	4	32	34	4	30	2041454.730	-2.420	-2.448	18295156.5797	e
36	5	31	34	5	29	2075181.382	21.600	21.608	18790182.7632	e
35	6	29	35	5	30	493892.439	-0.018	-0.005	19814510.6390	c
35	7	29	35	6	30	493892.439	-0.018	-0.005	19814510.6390	c
35	5	30	35	4	31	511881.831	-0.022	-0.004	19302628.7913	c
35	6	30	35	5	31	511881.831	-0.022	-0.004	19302628.7913	c
35	4	31	35	3	32	529781.277	-0.026	-0.003	18772847.4936	c
35	5	31	35	4	32	529781.277	-0.026	-0.003	18772847.4936	c
35	3	32	35	2	33	547607.892	-0.032	-0.007	18225239.5747	c
35	4	32	35	3	33	547607.892	-0.032	-0.007	18225239.5747	c
35	2	33	35	1	34	565375.652	-0.014	0.008	17659863.9143	c
35	3	33	35	2	34	565375.652	-0.014	0.008	17659863.9143	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
35	1	34	35	0	35	583096.001	-0.018	-0.004	17076767.9016	c
35	2	34	35	1	35	583096.001	-0.018	-0.004	17076767.9016	c
35	22	13	35	19	16	512374.843	-0.035	-0.001	24915304.7700	c
35	20	15	35	17	18	579344.661	-0.060	0.011	24482817.7309	c
36	15	21	35	18	18	649712.168	0.075	0.030	24484470.4846	c
35	22	14	35	19	17	687213.310	-0.100	-0.030	24734431.4750	c
35	23	13	35	20	16	712446.197	-0.083	0.016	24964303.5452	c
36	14	22	35	17	19	585186.836	0.034	-0.001	24209902.2750	c
36	1	36	35	0	35	966603.532	-2.110	-2.128	17076767.9016	d
36	0	36	35	1	35	966603.532	-2.110	-2.128	17076767.9016	d
36	1	35	35	2	34	983454.283	-2.210	-2.234	17659863.9143	d
36	2	35	35	1	34	983454.283	-2.210	-2.234	17659863.9143	d
36	3	34	35	2	33	1000300.837	-0.482	-0.501	18225239.5747	d
36	2	34	35	3	33	1000300.837	-0.482	-0.501	18225239.5747	d
36	3	33	35	4	32	1017140.796	-2.140	-2.158	18772847.4936	d
36	4	33	35	3	32	1017140.796	-2.140	-2.158	18772847.4936	d
36	4	32	35	5	31	1033981.954	-2.980	-2.990	19302628.7913	d
36	5	32	35	4	31	1033981.954	-2.980	-2.990	19302628.7913	d
36	5	31	35	6	30	1050828.208	-3.660	-3.669	19814510.6390	d
36	6	31	35	5	30	1050828.208	-3.660	-3.669	19814510.6390	d
36	6	30	35	7	29	1067687.953	-1.690	-1.705	20308403.0914	d
36	7	30	35	6	29	1067687.953	-1.690	-1.705	20308403.0914	d
36	8	29	35	7	28	1084564.787	-1.200	-1.215	20784194.9535	d
36	7	29	35	8	28	1084564.787	-1.200	-1.215	20784194.9535	d
36	9	28	35	8	27	1101468.901	-2.220	-2.225	21241748.2985	d
36	8	28	35	9	27	1101468.901	-2.220	-2.225	21241748.2985	d
36	10	27	35	9	26	1118415.586	-3.150	-3.164	21680891.0638	d
36	9	27	35	10	26	1118415.586	-3.150	-3.164	21680891.0638	d
36	11	26	35	10	25	1135424.928	-2.660	-2.673	22101406.8349	d
36	10	26	35	11	25	1135424.928	-2.660	-2.673	22101406.8349	d
36	12	25	35	11	24	1152517.312	-6.420	-6.436	22503020.3708	d
36	11	25	35	12	24	1152517.312	-6.420	-6.436	22503020.3711	d
36	13	24	35	12	23	1169744.903	0.550	0.535	22885376.4404	d
36	12	24	35	13	23	1169744.903	0.556	0.540	22885376.4449	d
36	14	23	35	13	22	1187144.875	0.738	0.721	23248007.5834	d
36	13	23	35	14	22	1187144.875	0.844	0.827	23248007.6697	d
36	15	22	35	14	21	1204805.366	-2.030	-2.053	23590282.0108	d
36	14	22	35	15	21	1204805.366	-0.360	-0.378	23590283.3575	d
36	16	20	35	17	19	1241437.943	-3.670	-3.689	24209902.2750	d
36	17	20	35	16	19	1241683.773	-2.090	-2.114	24209712.5001	d
36	18	19	35	17	18	1262464.807	-3.350	-3.370	24482817.7309	d
36	19	18	35	18	17	1290982.293	-2.900	-2.923	24723415.5882	d
36	24	13	35	23	12	1561306.023	1.290	1.352	25677557.3124	d
36	24	12	35	23	13	1562444.935	1.960	2.022	25676749.8178	d
36	27	10	35	26	9	1606285.129	-2.190	-2.112	26574780.7084	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(\text{SP})$ / MHz	$\Delta_{O-C}(\text{LP})$ / MHz	E''/h (MHz)	Source
36	28	8	35	27	9	1620277.956	3.330	3.405	26913517.8064	d
36	28	9	35	27	8	1620277.956	3.360	3.440	26913517.8325	d
36	29	7	35	28	8	1634071.121	-0.383	-0.309	27270148.5350	d
36	29	8	35	28	7	1634071.121	-0.381	-0.308	27270148.5362	d
36	30	6	35	29	7	1647734.476	-1.090	-1.021	27643993.5819	d
36	30	7	35	29	6	1647734.476	-1.090	-1.021	27643993.5819	d
36	31	5	35	30	6	1661304.895	0.274	0.330	28034528.3950	d
36	31	6	35	30	5	1661304.895	0.274	0.330	28034528.3950	d
36	32	4	35	31	5	1674804.563	0.003	0.048	28441337.2538	d
36	32	5	35	31	4	1674804.563	0.003	0.048	28441337.2538	d
36	33	4	35	32	3	1688251.767	-1.780	-1.741	28864084.0102	d
36	33	3	35	32	4	1688251.767	-1.780	-1.741	28864084.0102	d
36	34	3	35	33	2	1701663.296	-1.260	-1.235	29302492.3938	d
36	34	2	35	33	3	1701663.296	-1.260	-1.235	29302492.3938	d
36	35	1	35	34	2	1715046.045	-0.971	-0.957	29756332.2491	d
36	35	2	35	34	1	1715046.045	-0.971	-0.957	29756332.2491	d
36	36	1	35	35	0	1728406.908	-0.917	-0.914	30225409.6236	d
36	36	0	35	35	1	1728406.908	-0.917	-0.914	30225409.6236	d
36	18	19	35	15	20	1833975.630	-1.260	-1.250	23911309.0045	d
37	0	37	35	0	35	1959740.300	-2.740	-2.779	17076767.9016	e
37	1	36	35	1	34	1993436.972	-2.080	-2.121	17659863.9143	e
37	4	33	35	4	31	2094470.029	-5.560	-5.588	19302628.7913	e
37	5	32	35	5	30	2128184.688	23.900	23.860	19814510.6390	e
36	7	29	36	6	30	492668.202	-0.010	-0.001	21376092.7274	c
36	8	29	36	7	30	492668.202	-0.010	-0.001	21376092.7274	c
36	6	30	36	5	31	510750.218	-0.021	-0.006	20865342.4937	c
36	7	30	36	6	31	510750.218	-0.021	-0.006	20865342.4937	c
36	5	31	36	4	32	528728.764	-0.024	-0.003	20336613.7107	c
36	6	31	36	5	32	528728.764	-0.024	-0.003	20336613.7107	c
36	4	32	36	3	33	546623.275	-0.020	0.005	19789990.4211	c
36	5	32	36	4	33	546623.275	-0.020	0.005	19789990.4211	c
36	3	33	36	2	34	564449.518	-0.025	0.002	19225540.8841	c
36	4	33	36	3	34	564449.518	-0.025	0.002	19225540.8841	c
36	2	34	36	1	35	582220.471	-0.017	0.006	18643320.4024	c
36	3	34	36	2	35	582220.471	-0.017	0.006	18643320.4024	c
36	1	35	36	0	36	599946.864	-0.010	0.002	18043373.5337	c
36	2	35	36	1	36	599946.864	-0.010	0.002	18043373.5337	c
36	21	15	36	18	18	545265.891	-0.095	-0.011	26010328.3324	c
36	23	13	36	20	16	562117.542	-0.062	0.000	26408917.9654	c
36	20	16	36	17	19	664159.925	-0.099	-0.003	25744757.9482	c
36	24	12	36	21	15	683598.375	-0.099	0.006	26555594.3128	c
37	1	37	36	0	36	993134.291	-3.110	-3.128	18043373.5337	d
37	0	37	36	1	36	993134.291	-3.110	-3.128	18043373.5337	d
37	2	36	36	1	35	1009980.546	-2.010	-2.030	18643320.4024	d
37	1	36	36	2	35	1009980.546	-2.010	-2.030	18643320.4024	d

Table S4_2: Assigned transitions v , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
37	2	35	36	3	34	1026818.706	-2.550	-2.569	19225540.8841	d
37	3	35	36	2	34	1026818.706	-2.550	-2.569	19225540.8841	d
37	3	34	36	4	33	1043654.168	-2.000	-2.023	19789990.4211	d
37	4	34	36	3	33	1043654.168	-2.000	-2.023	19789990.4211	d
37	4	33	36	5	32	1060488.430	-2.230	-2.242	20336613.7107	d
37	5	33	36	4	32	1060488.430	-2.230	-2.242	20336613.7107	d
37	6	32	36	5	31	1077328.689	-0.248	-0.262	20865342.4937	d
37	5	32	36	6	31	1077328.689	-0.248	-0.262	20865342.4937	d
37	7	31	36	6	30	1094174.344	-2.090	-2.102	21376092.7274	d
37	6	31	36	7	30	1094174.344	-2.090	-2.102	21376092.7274	d
37	8	30	36	7	29	1111036.187	-3.960	-3.975	21868760.9344	d
37	7	30	36	8	29	1111036.187	-3.960	-3.975	21868760.9344	d
37	8	29	36	9	28	1127926.511	-2.750	-2.765	22343219.4040	d
37	9	29	36	8	28	1127926.511	-2.750	-2.765	22343219.4040	d
37	10	28	36	9	27	1144852.811	-3.140	-3.149	22799309.7923	d
37	9	28	36	10	27	1144852.811	-3.140	-3.149	22799309.7923	d
37	11	27	36	10	26	1161834.272	-2.330	-2.344	23236834.4123	d
37	10	27	36	11	26	1161834.272	-2.330	-2.344	23236834.4123	d
37	12	26	36	11	25	1178890.980	-2.740	-2.755	23655544.0933	d
37	11	26	36	12	25	1178890.980	-2.740	-2.755	23655544.0936	d
37	13	25	36	12	24	1196056.814	-2.000	-2.017	24055120.7804	d
37	12	25	36	13	24	1196056.814	-2.000	-2.016	24055120.7813	d
37	14	24	36	13	23	1213374.642	-2.600	-2.620	24435151.6888	d
37	13	24	36	14	23	1213374.642	-2.570	-2.596	24435151.7086	d
37	16	22	36	15	21	1248778.968	-5.910	-5.937	25134182.5715	d
37	15	22	36	16	21	1248778.968	-0.116	-0.141	25134187.1943	d
37	17	21	36	16	20	1267181.147	-2.760	-2.782	25451343.8770	d
37	16	21	36	17	20	1267114.593	0.148	0.124	25451398.3553	d
37	17	20	36	18	19	1285995.241	-3.590	-3.612	25745285.8771	d
37	18	20	36	17	19	1286684.464	-1.760	-1.780	25744757.9482	d
37	19	19	36	18	18	1309798.186	-2.190	-2.216	26010328.3324	d
37	22	15	36	21	16	1609329.225	-2.070	-2.007	26489608.8161	d
37	28	9	36	27	10	1654178.521	-0.975	-0.887	28181068.0134	d
37	28	10	36	27	9	1654178.521	-0.764	-0.676	28181068.1723	d
37	29	8	36	28	9	1668093.702	-1.020	-0.935	28533792.4109	d
37	29	9	36	28	8	1668093.702	-1.010	-0.924	28533792.4193	d
37	30	7	36	29	8	1681838.001	-1.800	-1.725	28904220.0222	d
37	30	8	36	29	7	1681838.001	-1.800	-1.724	28904220.0225	d
37	31	6	36	30	7	1695463.582	-0.266	-0.200	29291729.1278	d
37	31	7	36	30	6	1695463.582	-0.266	-0.200	29291729.1278	d
37	32	5	36	31	6	1708998.925	-1.090	-1.035	29695832.9994	d
37	32	6	36	31	5	1708998.925	-1.090	-1.035	29695832.9994	d
37	33	4	36	32	5	1722470.712	-0.642	-0.596	30116141.7974	d
37	33	5	36	32	4	1722470.712	-0.642	-0.596	30116141.7974	d
37	34	3	36	33	4	1735893.033	-1.220	-1.185	30552337.5357	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
37	34	4	36	33	3	1735893.033	-1.220	-1.185	30552337.5357	d
37	35	3	36	34	2	1749279.679	-0.900	-0.869	31004156.9317	d
37	35	2	36	34	3	1749279.679	-0.900	-0.869	31004156.9317	d
37	36	1	36	35	2	1762637.245	-1.770	-1.746	31471379.2480	d
37	36	2	36	35	1	1762637.245	-1.770	-1.746	31471379.2480	d
37	37	1	36	36	0	1775974.426	-1.580	-1.555	31953817.4319	d
37	37	0	36	36	1	1775974.426	-1.580	-1.555	31953817.4319	d
37	15	23	36	14	22	1230914.917	-1.790	-1.815	24795089.0712	d
37	14	23	36	15	22	1230914.917	-1.390	-1.409	24795089.3992	d
37	18	19	36	19	18	1304341.958	-1.190	-1.207	26014400.7695	d
38	0	38	36	0	36	2012797.569	-2.220	-2.259	18043373.5337	e
37	8	29	37	7	30	491347.578	-0.009	-0.006	22979801.0738	c
37	9	29	37	8	30	491347.578	-0.009	-0.006	22979801.0738	c
37	7	30	37	6	31	509531.919	-0.010	-0.001	22470269.1495	c
37	8	30	37	7	31	509531.919	-0.010	-0.001	22470269.1495	c
37	6	31	37	5	32	527597.722	-0.013	0.003	21942671.4196	c
37	7	31	37	6	32	527597.722	-0.013	0.003	21942671.4196	c
37	5	32	37	4	33	545567.042	-0.027	-0.004	21397104.3555	c
37	6	32	37	5	33	545567.042	-0.027	-0.004	21397104.3555	c
37	4	33	37	3	34	563457.745	-0.033	-0.006	20833646.5835	c
37	5	33	37	4	34	563457.745	-0.033	-0.006	20833646.5835	c
37	3	34	37	2	35	581284.432	-0.029	0.000	20252362.1287	c
37	4	34	37	3	35	581284.432	-0.029	0.000	20252362.1287	c
37	2	35	37	1	36	599059.164	-0.023	0.001	19653302.9477	c
37	3	35	37	2	36	599059.164	-0.023	0.001	19653302.9477	c
37	1	36	37	0	37	616792.024	-0.005	0.005	19036510.9249	c
37	2	36	37	1	37	616792.024	-0.005	0.005	19036510.9249	c
37	22	15	37	19	18	524627.500	-0.090	0.010	27574312.5115	c
37	23	14	37	20	17	526942.302	-0.102	-0.015	27782056.7118	c
37	21	16	37	18	19	620864.433	-0.120	-0.003	27318743.9040	c
37	37	0	37	36	1	495775.360	0.183	0.010	33234018.2486	c
37	37	1	37	36	2	495775.360	0.183	0.010	33234018.2486	c
38	15	23	37	18	20	626299.922	0.064	0.005	27031444.1557	c
38	16	23	37	17	20	626459.668	0.060	0.001	27031284.6943	c
38	17	22	37	18	19	692669.891	0.090	0.014	27318743.9040	c
38	0	38	37	1	37	1019659.655	-2.740	-2.754	19036510.9249	d
38	1	38	37	0	37	1019659.655	-2.740	-2.754	19036510.9249	d
38	1	37	37	2	36	1036499.314	-2.390	-2.410	19653302.9477	d
38	2	37	37	1	36	1036499.314	-2.390	-2.410	19653302.9477	d
38	2	36	37	3	35	1053331.478	-2.670	-2.694	20252362.1287	d
38	3	36	37	2	35	1053331.478	-2.670	-2.694	20252362.1287	d
38	4	35	37	3	34	1070158.845	-3.420	-3.443	20833646.5835	d
38	3	35	37	4	34	1070158.845	-3.420	-3.443	20833646.5835	d
38	4	34	37	5	33	1086986.812	-2.380	-2.400	21397104.3555	d
38	5	34	37	4	33	1086986.812	-2.380	-2.400	21397104.3555	d

Table S4_2: Assigned transitions v , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
38	5	33	37	6	32	1103818.377	-0.490	-0.506	21942671.4196	d
38	6	33	37	5	32	1103818.377	-0.490	-0.506	21942671.4196	d
38	7	32	37	6	31	1120654.139	-2.140	-2.152	22470269.1495	d
38	6	32	37	7	31	1120654.139	-2.140	-2.152	22470269.1495	d
38	8	31	37	7	30	1137506.089	-1.730	-1.739	22979801.0738	d
38	7	31	37	8	30	1137506.089	-1.730	-1.739	22979801.0738	d
38	8	30	37	9	29	1154380.224	-1.540	-1.554	23471148.6560	d
38	9	30	37	8	29	1154380.224	-1.540	-1.554	23471148.6560	d
38	11	28	37	10	27	1188241.816	-2.160	-2.175	24398671.0013	d
38	10	28	37	11	27	1188241.816	-2.160	-2.175	24398671.0013	d
38	12	27	37	11	26	1205264.949	-1.320	-1.341	24834437.7997	d
38	11	27	37	12	26	1205264.949	-1.320	-1.341	24834437.7997	d
38	13	26	37	12	25	1222376.819	-6.050	-6.074	25251179.5806	d
38	12	26	37	13	25	1222376.819	-6.050	-6.074	25251179.5806	d
38	14	25	37	13	24	1239629.293	-2.590	-2.617	25648528.9132	d
38	13	25	37	14	24	1239629.293	-2.590	-2.612	25648528.9177	d
38	15	24	37	14	23	1257066.139	-2.650	-2.678	26026005.6903	d
38	14	24	37	15	23	1257066.139	-2.560	-2.583	26026005.7679	d
38	16	23	37	15	22	1274772.799	-5.240	-5.272	26382966.2664	d
38	15	23	37	16	22	1274772.799	-3.780	-3.810	26382967.4398	d
38	19	19	37	20	18	1347089.707	-0.681	-0.701	27583676.1850	d
38	29	9	37	28	10	1702010.456	1.360	1.461	29835247.4408	d
38	29	10	37	28	9	1702010.456	1.430	1.531	29835247.4933	d
38	30	8	37	29	9	1715859.083	-0.182	-0.091	30201887.1126	d
38	30	9	37	29	8	1715859.083	-0.179	-0.088	30201887.1153	d
38	31	7	37	30	8	1729556.913	1.100	1.183	30586059.8076	d
38	31	8	37	30	7	1729556.913	1.100	1.183	30586059.8076	d
38	32	6	37	31	7	1743139.324	-2.040	-1.967	30987192.9596	d
38	32	7	37	31	6	1743139.324	-2.040	-1.967	30987192.9596	d
38	33	5	37	32	6	1756644.088	-1.100	-1.038	31404832.9988	d
38	33	6	37	32	5	1756644.088	-1.100	-1.038	31404832.9988	d
38	34	4	37	33	5	1770086.796	-1.130	-1.081	31838613.1349	d
38	34	5	37	33	4	1770086.796	-1.130	-1.081	31838613.1349	d
38	35	4	37	34	3	1783483.335	-1.120	-1.071	32288231.7742	d
38	35	3	37	34	4	1783483.335	-1.120	-1.071	32288231.7742	d
38	36	3	37	35	2	1796843.599	-2.030	-1.986	32753437.4937	d
38	36	2	37	35	3	1796843.599	-2.030	-1.986	32753437.4937	d
38	37	1	37	36	2	1810178.381	-1.130	-1.084	33234018.2486	d
38	37	2	37	36	1	1810178.381	-1.130	-1.084	33234018.2486	d
38	38	1	37	37	0	1823491.578	-0.546	-0.485	33729793.4207	d
38	38	0	37	37	1	1823491.578	-0.546	-0.485	33729793.4207	d
38	9	29	37	10	28	1171288.536	-0.459	-0.474	23944165.7273	d
38	10	29	37	9	28	1171288.536	-0.459	-0.474	23944165.7273	d
39	0	39	37	0	37	2065839.849	-2.980	-3.010	19036510.9249	e
39	1	38	37	1	36	2099518.534	3.070	3.030	19653302.9477	e

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(\text{SP})$ / MHz	$\Delta_{O-C}(\text{LP})$ / MHz	E''/h (MHz)	Source
38	8	30	38	7	31	508221.526	-0.010	-0.008	24117308.8771	c
38	9	30	38	8	31	508221.526	-0.010	-0.008	24117308.8771	c
38	7	31	38	6	32	526383.458	-0.009	0.001	23590925.4155	c
38	8	31	38	7	32	526383.458	-0.009	0.001	23590925.4155	c
38	6	32	38	5	33	544435.128	-0.017	0.001	23046490.2760	c
38	7	32	38	6	33	544435.128	-0.017	0.001	23046490.2760	c
38	5	33	38	4	34	562396.717	-0.026	-0.001	22484093.5390	c
38	6	33	38	5	34	562396.717	-0.026	-0.001	22484093.5390	c
38	3	35	38	2	36	598112.538	-0.039	-0.009	21305696.2692	c
38	4	35	38	3	36	598112.538	-0.039	-0.009	21305696.2692	c
38	2	36	38	1	37	615891.626	-0.009	0.014	20689804.6404	c
38	3	36	38	2	37	615891.626	-0.009	0.014	20689804.6404	c
38	1	37	38	0	38	633631.320	-0.020	-0.014	20056173.3064	c
38	2	37	38	1	38	633631.320	-0.020	-0.014	20056173.3064	c
38	38	0	38	37	1	509087.963	0.178	0.014	35044197.7463	c
38	38	1	38	37	2	509087.963	0.178	0.014	35044197.7463	c
38	23	15	38	20	18	522854.377	-0.114	0.014	29172672.5031	c
38	4	34	38	3	35	580284.675	-0.029	0.000	21903808.8406	c
38	5	34	38	4	35	580284.675	-0.029	0.000	21903808.8406	c
38	22	16	38	19	19	582238.237	-0.149	-0.007	28930766.5601	c
38	37	1	38	36	2	493914.744	0.100	0.001	34550283.1072	c
38	37	2	38	36	3	493914.744	0.100	0.001	34550283.1072	c
39	19	20	38	22	17	875393.752	0.158	0.030	29433628.0149	c
39	32	7	38	33	6	931356.157	-0.030	-0.016	33161478.1679	c
39	32	8	38	33	5	931356.157	-0.030	-0.016	33161478.1679	c
39	31	9	38	32	6	950980.173	-0.013	-0.017	32730334.3042	c
39	31	8	38	32	7	950980.173	-0.014	-0.017	32730334.3042	c
39	30	10	38	31	7	971418.739	-0.002	-0.020	32315615.6018	c
39	30	9	38	31	8	971418.739	-0.008	-0.026	32315615.6018	c
39	29	11	38	30	8	992870.018	0.078	0.049	31917746.3608	c
39	29	10	38	30	9	992870.018	-0.024	-0.052	31917746.3599	c
39	27	12	38	28	11	1040067.274	0.041	-0.002	31174823.5922	c
39	1	39	38	0	38	1046178.123	-2.310	-2.326	20056173.3064	d
39	0	39	38	1	38	1046178.123	-2.310	-2.326	20056173.3064	d
39	1	38	38	2	37	1063011.486	-2.270	-2.294	20689804.6404	d
39	2	38	38	1	37	1063011.486	-2.270	-2.294	20689804.6404	d
39	3	37	38	2	36	1079837.355	-2.470	-2.492	21305696.2692	d
39	2	37	38	3	36	1079837.355	-2.470	-2.492	21305696.2692	d
39	3	36	38	4	35	1096659.026	-2.010	-2.030	21903808.8406	d
39	4	36	38	3	35	1096659.026	-2.010	-2.030	21903808.8406	d
39	6	34	38	5	33	1130298.772	-2.660	-2.675	23046490.2760	d
39	5	34	38	6	33	1130298.772	-2.660	-2.675	23046490.2760	d
39	7	33	38	6	32	1147121.642	-7.260	-7.279	23590925.4155	d
39	6	33	38	7	32	1147121.642	-7.260	-7.279	23590925.4155	d
39	7	32	38	8	31	1163966.398	-2.230	-2.243	24117308.8771	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
39	8	32	38	7	31	1163966.398	-2.230	-2.243	24117308.8771	d
39	8	31	38	9	30	1180825.543	-2.570	-2.582	24625530.4085	d
39	9	31	38	8	30	1180825.543	-2.570	-2.582	24625530.4085	d
39	9	30	38	10	29	1197712.569	-4.550	-4.564	25115454.7105	d
39	10	30	38	9	29	1197712.569	-4.550	-4.564	25115454.7105	d
39	11	29	38	10	28	1214646.064	-2.430	-2.445	25586914.9638	d
39	10	29	38	11	28	1214646.064	-2.430	-2.445	25586914.9638	d
39	12	28	38	11	27	1231635.019	-4.370	-4.390	26039704.0585	d
39	11	28	38	12	27	1231635.019	-4.370	-4.390	26039704.0585	d
39	13	27	38	12	26	1248711.515	-1.610	-1.638	26473562.4398	d
39	12	27	38	13	26	1248711.515	-1.610	-1.638	26473562.4398	d
39	15	25	38	14	24	1283251.538	-0.900	-0.929	27283074.4502	d
39	14	25	38	15	24	1283251.538	-0.878	-0.908	27283074.4682	d
39	16	24	38	15	23	1300829.586	-2.730	-2.762	27657744.0075	d
39	15	24	38	16	23	1300829.586	-2.370	-2.404	27657744.2962	d
39	17	23	38	16	22	1318744.002	-4.530	-4.565	28011409.7315	d
39	16	23	38	17	22	1318744.002	0.451	0.417	28011413.6980	d
39	32	7	38	31	8	1777217.666	-1.100	-1.006	32315615.6018	d
39	32	8	38	31	7	1777217.666	-1.100	-1.006	32315615.6018	d
39	33	6	38	32	7	1790770.098	3.090	3.172	32730334.3042	d
39	33	7	38	32	6	1790770.098	3.090	3.172	32730334.3042	d
39	34	5	38	33	6	1804237.688	-1.180	-1.112	33161478.1679	d
39	34	6	38	33	5	1804237.688	-1.180	-1.112	33161478.1679	d
39	35	5	38	34	4	1817651.915	-1.030	-0.963	33608701.0463	d
39	35	4	38	34	5	1817651.915	-1.030	-0.963	33608701.0463	d
39	36	3	38	35	4	1831021.772	-0.988	-0.922	34071716.2096	d
39	36	4	38	35	3	1831021.772	-0.988	-0.922	34071716.2096	d
39	9	30	39	8	31	506813.315	0.001	-0.003	25806358.5078	c
39	10	30	39	9	31	506813.315	0.001	-0.003	25806358.5078	c
39	8	31	39	7	32	525081.016	-0.004	-0.001	25281277.4930	c
39	9	31	39	8	32	525081.016	-0.004	-0.001	25281277.4930	c
39	7	32	39	6	33	543223.178	-0.010	0.000	24738054.3101	c
39	8	32	39	7	33	543223.178	-0.010	0.000	24738054.3101	c
39	6	33	39	5	34	561262.597	-0.023	-0.003	24176791.6961	c
39	7	33	39	6	34	561262.597	-0.023	-0.003	24176791.6961	c
39	4	35	39	3	36	597103.988	-0.027	0.005	23000469.8648	c
39	5	35	39	4	36	597103.988	-0.027	0.005	23000469.8648	c
39	3	36	39	2	37	614933.761	-0.026	0.004	22385536.0837	c
39	4	36	39	3	37	614933.761	-0.026	0.004	22385536.0837	c
39	2	37	39	1	38	632717.683	-0.018	0.004	21752818.3889	c
39	3	37	39	2	38	632717.683	-0.018	0.004	21752818.3889	c
39	1	38	39	0	39	650464.676	0.010	0.012	21102353.7294	c
39	2	38	39	1	39	650464.676	0.010	0.012	21102353.7294	c
39	38	1	39	37	2	507223.518	0.076	-0.007	36394641.4157	c
39	38	2	39	37	3	507223.518	0.076	-0.007	36394641.4157	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(\text{SP})$ / MHz	$\Delta_{O-C}(\text{LP})$ / MHz	E''/h (MHz)	Source
39	39	0	39	38	1	522375.621	0.161	0.021	36901864.8533	c
39	39	1	39	38	2	522375.621	0.161	0.021	36901864.8533	c
39	24	15	39	21	18	542633.504	-0.143	0.028	30803238.4786	c
39	5	34	39	4	35	579217.800	-0.028	-0.001	23597573.8738	c
39	6	34	39	5	35	579217.800	-0.028	-0.001	23597573.8738	c
39	25	14	39	22	17	633392.412	-0.171	0.011	30972701.3591	c
39	22	17	39	19	20	663679.577	-0.188	-0.013	30309021.6002	c
40	20	21	39	21	18	908060.522	0.154	0.007	30803238.4786	c
40	21	19	39	24	16	928137.509	0.189	0.009	31334673.8644	c
40	31	10	39	32	7	991686.373	-0.024	-0.003	34092834.3455	c
40	31	9	39	32	8	991686.373	-0.026	-0.005	34092834.3455	c
40	30	11	39	31	8	1012878.157	0.009	0.017	33681314.4815	c
40	30	10	39	31	9	1012878.157	-0.025	-0.017	33681314.4812	c
40	21	20	39	22	17	1035577.043	0.154	0.005	30972701.3591	c
40	28	13	39	29	10	1059157.895	0.052	0.037	32910616.3920	c
40	28	12	39	29	11	1059165.132	0.016	0.001	32910616.2912	c
40	0	40	39	1	39	1072689.396	-1.950	-1.963	21102353.7294	d
40	1	40	39	0	39	1072689.396	-1.950	-1.963	21102353.7294	d
40	2	39	39	1	38	1089516.164	-2.380	-2.399	21752818.3889	d
40	1	39	39	2	38	1089516.164	-2.380	-2.399	21752818.3889	d
40	3	38	39	2	37	1106335.737	-2.360	-2.378	22385536.0837	d
40	2	38	39	3	37	1106335.737	-2.360	-2.378	22385536.0837	d
40	3	37	39	4	36	1123149.314	-2.970	-2.993	23000469.8648	d
40	4	37	39	3	36	1123149.314	-2.970	-2.993	23000469.8648	d
40	4	36	39	5	35	1139961.991	-1.920	-1.939	23597573.8738	d
40	5	36	39	4	35	1139961.991	-1.920	-1.939	23597573.8738	d
40	5	35	39	6	34	1156774.070	-2.340	-2.355	24176791.6961	d
40	6	35	39	5	34	1156774.070	-2.340	-2.355	24176791.6961	d
40	8	32	39	9	31	1207266.365	-1.490	-1.501	25806358.5078	d
40	9	32	39	8	31	1207266.365	-1.490	-1.501	25806358.5078	d
40	9	31	39	10	30	1224136.603	-3.050	-3.064	26313171.8163	d
40	10	31	39	9	30	1224136.603	-3.050	-3.064	26313171.8163	d
40	11	30	39	10	29	1241047.313	-1.820	-1.836	26801563.4434	d
40	10	30	39	11	29	1241047.313	-1.820	-1.836	26801563.4434	d
40	12	29	39	11	28	1258010.486	-0.949	-0.969	27271343.4349	d
40	11	29	39	12	28	1258010.486	-0.949	-0.969	27271343.4349	d
40	13	28	39	12	27	1275045.310	-1.570	-1.594	27722275.5576	d
40	12	28	39	13	27	1275045.310	-1.570	-1.594	27722275.5576	d
40	14	27	39	13	26	1292182.963	-0.288	-0.315	28154062.8677	d
40	13	27	39	14	26	1292182.963	-0.288	-0.315	28154062.8677	d
40	15	26	39	14	25	1309458.221	-1.210	-1.239	28566326.8711	d
40	14	26	39	15	25	1309458.221	-1.200	-1.234	28566326.8753	d
40	16	25	39	15	24	1326928.644	-2.830	-2.865	28958576.2414	d
40	15	25	39	16	24	1326928.644	-2.750	-2.780	28958576.3104	d
40	17	24	39	16	23	1344682.072	-1.680	-1.712	29330157.2365	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
40	16	24	39	17	23	1344682.072	-0.408	-0.444	29330158.2519	d
40	20	21	39	19	20	1402275.858	-1.390	-1.426	30309021.6002	d
40	8	33	39	7	32	1190423.108	0.848	0.836	25281277.4930	d
40	7	33	39	8	32	1190423.108	0.848	0.836	25281277.4930	d
40	19	22	39	18	21	1381732.559	-0.131	-0.167	30007260.1713	d
41	1	40	39	1	38	2205534.140	-0.281	-0.314	21752818.3889	e
40	10	30	40	9	31	505301.120	0.009	-0.003	27537311.4575	c
40	11	30	40	10	31	505301.120	0.009	-0.003	27537311.4575	c
40	9	31	40	8	32	523685.102	-0.012	-0.018	27013626.3486	c
40	10	31	40	9	32	523685.102	-0.012	-0.018	27013626.3486	c
40	8	32	40	7	33	541926.607	-0.006	-0.003	26471699.7408	c
40	9	32	40	8	33	541926.607	-0.006	-0.003	26471699.7408	c
40	7	33	40	6	34	560051.371	-0.014	-0.003	25911648.3612	c
40	8	33	40	7	34	560051.371	-0.014	-0.003	25911648.3612	c
40	6	34	40	5	35	578080.251	-0.022	0.000	25333568.0943	c
40	7	34	40	6	35	578080.251	-0.022	0.000	25333568.0943	c
40	5	35	40	4	36	596030.293	-0.032	-0.002	24737537.7749	c
40	6	35	40	5	36	596030.293	-0.032	-0.002	24737537.7749	c
40	4	36	40	3	37	613915.606	-0.034	0.001	24123622.1414	c
40	5	36	40	4	37	613915.606	-0.034	0.001	24123622.1414	c
40	3	37	40	2	38	631747.937	-0.043	-0.011	23491874.1678	c
40	4	37	40	3	38	631747.937	-0.043	-0.011	23491874.1678	c
40	2	38	40	1	39	649537.228	-0.024	-0.004	22842336.9223	c
40	3	38	40	2	39	649537.228	-0.024	-0.004	22842336.9223	c
40	38	2	40	37	3	505211.968	0.018	-0.007	37781246.7346	c
40	38	3	40	37	4	505211.968	0.018	-0.007	37781246.7346	c
40	39	1	40	38	2	520506.680	0.055	0.002	38286458.6796	c
40	39	2	40	38	3	520506.680	0.055	0.002	38286458.6796	c
40	24	16	40	21	19	546729.832	-0.200	0.024	32262811.1755	c
40	25	15	40	22	18	583437.675	-0.232	0.000	32465290.1076	c
40	23	17	40	20	20	621026.495	-0.212	0.005	32005417.2388	c
40	1	39	40	0	40	667291.866	0.002	-0.003	22175045.0650	c
40	2	39	40	1	40	667291.866	0.002	-0.003	22175045.0650	c
40	40	0	40	39	1	535637.774	0.118	0.018	38806965.2998	c
40	40	1	40	39	2	535637.774	0.118	0.018	38806965.2998	c
41	19	22	40	22	19	857588.857	0.171	0.001	32279856.8482	c
41	20	21	40	23	18	921155.485	0.195	-0.002	32532303.5849	c
41	21	20	40	24	17	957591.155	0.189	-0.031	32781047.1226	c
41	32	10	40	33	7	1011993.571	-0.072	-0.005	35917662.0969	c
41	32	9	40	33	8	1011993.571	-0.073	-0.006	35917662.0969	c
41	31	11	40	32	8	1032950.776	-0.018	0.038	35492535.4384	c
41	31	10	40	32	9	1032950.776	-0.029	0.027	35492535.4384	c
41	30	12	40	31	9	1054997.601	0.052	0.094	35084520.7346	c
41	30	11	40	31	10	1054997.601	-0.135	-0.093	35084520.7328	c
41	0	41	40	1	40	1099192.575	-2.380	-2.383	22175045.0650	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(\text{SP})$ / MHz	$\Delta_{O-C}(\text{LP})$ / MHz	E''/h (MHz)	Source
41	1	41	40	0	40	1099192.575	-2.380	-2.383	22175045.0650	d
41	1	40	40	2	39	1116012.447	-3.430	-3.445	22842336.9223	d
41	2	40	40	1	39	1116012.447	-3.430	-3.445	22842336.9223	d
41	2	39	40	3	38	1132826.624	-2.160	-2.173	23491874.1678	d
41	3	39	40	2	38	1132826.624	-2.160	-2.173	23491874.1678	d
41	4	38	40	3	37	1149633.905	-1.930	-1.951	24123622.1414	d
41	3	38	40	4	37	1149633.905	-1.930	-1.951	24123622.1414	d
41	8	33	40	9	32	1233698.793	-1.790	-1.801	27013626.3486	d
41	9	33	40	8	32	1233698.793	-1.790	-1.801	27013626.3486	d
41	9	32	40	10	31	1250554.940	-1.080	-1.094	27537311.4575	d
41	10	32	40	9	31	1250554.940	-1.080	-1.094	27537311.4575	d
41	11	31	40	10	30	1267443.166	-1.860	-1.876	28042612.5634	d
41	10	31	40	11	30	1267443.166	-1.860	-1.876	28042612.5634	d
41	12	30	40	11	29	1284379.958	-1.100	-1.113	28529354.8577	d
41	11	30	40	12	29	1284379.958	-1.100	-1.113	28529354.8577	d
41	13	29	40	12	28	1301380.006	-1.930	-1.949	28997322.4257	d
41	12	29	40	13	28	1301380.006	-1.930	-1.949	28997322.4257	d
41	14	28	40	13	27	1318471.191	-0.526	-0.552	29446246.1056	d
41	13	28	40	14	27	1318471.191	-0.526	-0.552	29446246.1056	d
41	15	27	40	14	26	1335680.494	-3.020	-3.052	29875786.2868	d
41	14	27	40	15	26	1335680.494	-3.020	-3.051	29875786.2877	d
41	17	25	40	16	24	1370679.800	-2.110	-2.150	30674840.7188	d
41	16	25	40	17	24	1370679.800	-1.800	-1.837	30674840.9709	d
41	19	22	40	20	21	1426146.257	-0.445	-0.481	31711298.8375	d
41	20	21	40	21	20	1445179.199	-1.440	-1.476	32008278.2380	d
41	5	36	40	6	35	1183239.175	-4.410	-4.427	25333568.0943	d
41	6	36	40	5	35	1183239.175	-4.410	-4.427	25333568.0943	d
41	6	35	40	7	34	1200049.454	-2.050	-2.056	25911648.3612	d
41	7	35	40	6	34	1200049.454	-2.050	-2.056	25911648.3612	d
41	16	26	40	15	25	1353061.579	-2.540	-2.570	30285507.6872	d
41	15	26	40	16	25	1353061.579	-2.520	-2.550	30285507.7034	d
42	1	41	40	1	39	2258519.460	-2.000	-2.020	22842336.9223	e
41	10	31	41	9	32	522190.127	0.011	-0.004	28787867.4691	c
41	11	31	41	10	32	522190.127	0.011	-0.004	28787867.4691	c
41	9	32	41	8	33	540540.561	0.008	0.000	28247326.9208	c
41	10	32	41	9	33	540540.561	0.008	0.000	28247326.9208	c
41	8	33	41	7	34	558758.789	-0.001	0.001	27688568.1359	c
41	9	33	41	8	34	558758.789	-0.001	0.001	27688568.1359	c
41	5	36	41	4	37	612834.195	-0.021	0.011	25903977.4628	c
41	6	36	41	5	37	612834.195	-0.021	0.011	25903977.4628	c
41	4	37	41	3	38	630719.458	-0.042	-0.006	25273257.9692	c
41	5	37	41	4	38	630719.458	-0.042	-0.006	25273257.9692	c
41	3	38	41	2	39	648555.001	-0.039	-0.007	24624702.9358	c
41	4	38	41	3	39	648555.001	-0.039	-0.007	24624702.9358	c
41	2	39	41	1	40	666350.140	-0.014	0.004	23958352.7884	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
41	3	39	41	2	40	666350.140	-0.014	0.004	23958352.7884	c
41	38	3	41	37	4	503043.024	-0.021	-0.008	39204141.8784	c
41	38	4	41	37	5	503043.024	-0.021	-0.008	39204141.8784	c
41	39	2	41	38	3	518494.840	-0.024	-0.014	39707184.9185	c
41	39	3	41	38	4	518494.840	-0.024	-0.014	39707184.9185	c
41	40	1	41	39	2	533763.675	0.009	0.004	40225679.7772	c
41	40	2	41	39	3	533763.675	0.009	0.004	40225679.7772	c
41	7	34	41	6	35	576868.274	-0.018	-0.006	27111699.8493	c
41	8	34	41	7	35	576868.274	-0.018	-0.006	27111699.8493	c
41	1	40	41	0	41	684112.810	0.019	0.007	23274240.0044	c
41	2	40	41	1	41	684112.810	0.019	0.007	23274240.0044	c
41	41	0	41	40	1	548873.873	0.041	0.004	40759443.4378	c
41	41	1	41	40	2	548873.873	0.041	0.004	40759443.4378	c
41	26	15	41	23	18	641485.341	-0.311	-0.001	34161075.6869	c
42	32	11	41	33	8	1053079.152	-0.113	0.003	37351352.6376	c
42	32	10	41	33	9	1053079.152	-0.117	-0.001	37351352.6376	c
42	1	42	41	0	41	1125688.558	-2.510	-2.508	23274240.0044	d
42	0	42	41	1	41	1125688.558	-2.510	-2.508	23274240.0044	d
42	1	41	41	2	40	1142503.335	-2.240	-2.253	23958352.7884	d
42	2	41	41	1	40	1142503.335	-2.240	-2.253	23958352.7884	d
42	3	40	41	2	39	1159309.117	-2.580	-2.592	24624702.9358	d
42	2	40	41	3	39	1159309.117	-2.580	-2.592	24624702.9358	d
42	3	39	41	4	38	1176109.203	-2.300	-2.315	25273257.9692	d
42	4	39	41	3	38	1176109.203	-2.300	-2.315	25273257.9692	d
42	4	38	41	5	37	1192905.393	-2.120	-2.131	25903977.4628	d
42	5	38	41	4	37	1192905.393	-2.120	-2.131	25903977.4628	d
42	5	37	41	6	36	1209701.582	-1.180	-1.189	26516811.6723	d
42	6	37	41	5	36	1209701.582	-1.180	-1.189	26516811.6723	d
42	6	36	41	7	35	1226504.066	3.080	3.078	27111699.8493	d
42	7	36	41	6	35	1226504.066	3.080	3.078	27111699.8493	d
42	8	35	41	7	34	1243304.452	-2.330	-2.336	27688568.1359	d
42	7	35	41	8	34	1243304.452	-2.330	-2.336	27688568.1359	d
42	7	35	41	8	34	1243304.452	-2.330	-2.336	27688568.1359	d
42	8	35	41	7	34	1243304.452	-2.330	-2.336	27688568.1359	d
42	9	34	41	8	33	1260123.725	-2.210	-2.214	28247326.9208	d
42	8	34	41	9	33	1260123.725	-2.210	-2.214	28247326.9208	d
42	10	33	41	9	32	1276961.586	-4.130	-4.137	28787867.4691	d
42	9	33	41	10	32	1276961.586	-4.130	-4.137	28787867.4691	d
42	11	32	41	10	31	1293832.723	-2.710	-2.719	29310057.5798	d
42	10	32	41	11	31	1293832.723	-2.710	-2.719	29310057.5798	d
42	12	31	41	11	30	1310744.632	-2.480	-2.487	29813735.8998	d
42	11	31	41	12	30	1310744.632	-2.480	-2.487	29813735.8998	d
42	14	29	41	13	28	1344762.416	-2.170	-2.188	30764717.8102	d
42	13	29	41	14	28	1344762.416	-2.170	-2.188	30764717.8102	d
42	15	28	41	14	27	1361919.256	-0.581	-0.607	31211469.7903	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
42	14	28	41	15	27	1361919.256	-0.581	-0.606	31211469.7903	d
42	17	26	41	16	25	1396724.595	-2.260	-2.296	32045522.5586	d
42	16	26	41	17	25	1396724.595	-2.190	-2.221	32045522.6194	d
42	18	25	41	17	24	1414516.996	-2.150	-2.188	32431659.8529	d
42	17	25	41	18	24	1414516.996	-1.060	-1.097	32431660.7259	d
42	20	22	41	21	21	1470825.271	-0.456	-0.488	33454421.2718	d
42	12	30	42	11	31	501937.864	0.023	-0.002	31124482.9949	c
42	13	30	42	12	31	501937.864	0.023	-0.002	31124482.9949	c
42	11	31	42	10	32	520590.018	0.020	-0.004	30603893.0018	c
42	12	31	42	11	32	520590.018	0.020	-0.004	30603893.0018	c
42	10	32	42	9	33	539059.854	0.022	0.004	30064833.1750	c
42	11	32	42	10	33	539059.854	0.022	0.004	30064833.1750	c
42	8	34	42	7	35	575577.934	-0.007	-0.005	28931874.9081	c
42	9	34	42	8	35	575577.934	-0.007	-0.005	28931874.9081	c
42	7	35	42	6	36	593674.079	-0.015	-0.001	28338200.8198	c
42	8	35	42	7	36	593674.079	-0.015	-0.001	28338200.8198	c
42	6	36	42	5	37	611686.375	-0.027	-0.001	27726514.4242	c
42	7	36	42	6	37	611686.375	-0.027	-0.001	27726514.4242	c
42	5	37	42	4	38	629629.433	-0.032	0.002	27096884.9649	c
42	6	37	42	5	38	629629.433	-0.032	0.002	27096884.9649	c
42	4	38	42	3	39	647515.476	-0.032	0.005	26449369.4630	c
42	5	38	42	4	39	647515.476	-0.032	0.005	26449369.4630	c
42	3	39	42	2	40	665354.817	-0.033	0.000	25784014.6200	c
42	4	39	42	3	40	665354.817	-0.033	0.000	25784014.6200	c
42	2	40	42	1	41	683156.251	-0.021	-0.006	25100858.3554	c
42	3	40	42	2	41	683156.251	-0.021	-0.006	25100858.3554	c
42	38	4	42	37	5	500705.483	-0.033	-0.001	40663461.4698	c
42	38	5	42	37	6	500705.483	-0.033	-0.001	40663461.4698	c
42	39	3	42	38	4	516330.440	-0.072	-0.025	41164166.9807	c
42	39	4	42	38	5	516330.440	-0.072	-0.025	41164166.9807	c
42	40	2	42	39	3	531750.664	-0.063	-0.002	41680497.4871	c
42	40	3	42	39	4	531750.664	-0.063	-0.002	41680497.4871	c
42	41	1	42	40	2	546993.968	-0.072	-0.006	42212248.2093	c
42	41	2	42	40	3	546993.968	-0.072	-0.006	42212248.2093	c
42	9	33	42	8	34	557380.343	0.006	-0.002	29507452.8437	c
42	10	33	42	9	34	557380.343	0.006	-0.002	29507452.8437	c
42	26	16	42	23	19	594935.578	-0.411	-0.019	35725275.4872	c
42	1	41	42	0	42	700927.317	0.014	-0.008	24399931.0590	c
42	2	41	42	1	42	700927.317	0.014	-0.008	24399931.0590	c
42	24	18	42	21	21	661522.106	-0.325	-0.017	35234085.5439	c
43	1	43	42	0	42	1152177.647	-1.870	-1.856	24399931.0590	d
43	0	43	42	1	42	1152177.647	-1.870	-1.856	24399931.0590	d
43	2	42	42	1	41	1168984.928	-2.540	-2.541	25100858.3554	d
43	1	42	42	2	41	1168984.928	-2.540	-2.541	25100858.3554	d
43	3	41	42	2	40	1185785.914	-0.750	-0.756	25784014.6200	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
43	2	41	42	3	40	1185785.914	-0.750	-0.756	25784014.6200	d
43	3	40	42	4	39	1202576.407	-2.690	-2.700	26449369.4630	d
43	4	40	42	3	39	1202576.407	-2.690	-2.700	26449369.4630	d
43	5	39	42	4	38	1219364.802	-2.360	-2.366	27096884.9649	d
43	4	39	42	5	38	1219364.802	-2.360	-2.366	27096884.9649	d
43	6	37	42	7	36	1252940.091	-2.190	-2.188	28338200.8198	d
43	7	37	42	6	36	1252940.091	-2.190	-2.188	28338200.8198	d
43	7	36	42	8	35	1269735.081	-2.040	-2.036	28931874.9081	d
43	8	36	42	7	35	1269735.081	-2.040	-2.036	28931874.9081	d
43	9	35	42	8	34	1286542.962	-0.603	-0.598	29507452.8437	d
43	8	35	42	9	34	1286542.962	-0.603	-0.598	29507452.8437	d
43	10	34	42	9	33	1303366.432	-1.850	-1.843	30064833.1750	d
43	9	34	42	10	33	1303366.432	-1.850	-1.843	30064833.1750	d
43	11	33	42	10	32	1320217.783	-1.920	-1.915	30603893.0018	d
43	10	33	42	11	32	1320217.783	-1.920	-1.915	30603893.0018	d
43	13	31	42	12	30	1354044.899	-4.180	-4.186	31626420.8309	d
43	12	31	42	13	30	1354044.899	-4.180	-4.186	31626420.8309	d
43	14	30	42	13	29	1371058.738	-0.748	-0.760	32109482.3807	d
43	13	30	42	14	29	1371058.738	-0.748	-0.760	32109482.3807	d
43	16	28	42	15	27	1405398.199	0.235	0.212	33017793.5454	d
43	15	28	42	16	27	1405398.199	0.236	0.213	33017793.5463	d
43	18	26	42	17	25	1440459.262	-0.921	-0.952	33846178.7681	d
43	17	26	42	18	25	1440459.262	-0.649	-0.680	33846178.9867	d
43	19	25	42	18	24	1458461.218	-0.751	-0.784	34228808.4121	d
43	18	25	42	19	24	1458461.218	2.870	2.834	34228811.2841	d
43	13	30	43	12	31	500071.991	0.028	-0.002	32980469.8952	c
43	14	30	43	13	31	500071.991	0.028	-0.002	32980469.8952	c
43	12	31	43	11	32	518878.311	0.021	-0.009	32461591.6107	c
43	13	31	43	12	32	518878.311	0.021	-0.009	32461591.6107	c
43	11	32	43	10	33	537478.946	0.019	-0.009	31924112.6887	c
43	12	32	43	11	33	537478.946	0.019	-0.009	31924112.6887	c
43	10	33	43	9	34	555911.274	0.021	0.002	31368201.4414	c
43	11	33	43	10	34	555911.274	0.021	0.002	31368201.4414	c
43	9	34	43	8	35	574205.064	0.013	0.003	30793996.3964	c
43	10	34	43	9	35	574205.064	0.013	0.003	30793996.3964	c
43	8	35	43	7	36	592384.384	-0.001	0.002	30201612.0168	c
43	9	35	43	8	36	592384.384	-0.001	0.002	30201612.0168	c
43	7	36	43	6	37	610468.918	-0.015	0.001	29591143.0894	c
43	8	36	43	7	37	610468.918	-0.015	0.001	29591143.0894	c
43	6	37	43	5	38	628474.933	-0.024	0.005	28962668.1390	c
43	7	37	43	6	38	628474.933	-0.024	0.005	28962668.1390	c
43	3	40	43	2	41	682147.253	-0.034	-0.002	26969801.2724	c
43	4	40	43	3	41	682147.253	-0.034	-0.002	26969801.2724	c
43	39	4	43	38	5	514002.970	-0.068	-0.004	42657534.2962	c
43	39	5	43	38	6	514002.970	-0.068	-0.004	42657534.2962	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
43	40	3	43	39	4	529589.615	-0.110	-0.010	43171537.3294	c
43	40	4	43	39	5	529589.615	-0.110	-0.010	43171537.3294	c
43	41	2	43	40	3	544978.898	-0.156	-0.021	43701127.0498	c
43	41	3	43	40	4	544978.898	-0.156	-0.021	43701127.0498	c
43	42	1	43	41	2	560197.065	-0.165	-0.002	44246106.0988	c
43	42	2	43	41	3	560197.065	-0.165	-0.002	44246106.0988	c
43	5	38	43	4	39	646415.993	-0.034	0.003	28316252.1179	c
43	6	38	43	5	39	646415.993	-0.034	0.003	28316252.1179	c
43	4	39	43	3	40	664303.534	-0.038	0.003	27651948.5529	c
43	5	39	43	4	40	664303.534	-0.038	0.003	27651948.5529	c
43	2	41	43	1	42	699955.464	-0.004	0.006	26269845.8112	c
43	3	41	43	2	42	699955.464	-0.004	0.006	26269845.8112	c
43	1	42	43	0	43	717735.290	0.032	-0.001	25552110.5599	c
43	2	42	43	1	43	717735.290	0.032	-0.001	25552110.5599	c
43	27	16	43	24	19	649381.048	-0.515	-0.005	37504337.3459	c
44	0	44	43	1	43	1178658.341	-1.770	-1.747	25552110.5599	d
44	1	44	43	0	43	1178658.341	-1.770	-1.747	25552110.5599	d
44	1	43	43	2	42	1195459.627	-1.740	-1.728	26269845.8112	d
44	2	43	43	1	42	1195459.627	-1.740	-1.728	26269845.8112	d
44	3	42	43	2	41	1212251.319	-2.180	-2.179	26969801.2724	d
44	2	42	43	3	41	1212251.319	-2.180	-2.179	26969801.2724	d
44	3	41	43	4	40	1229036.715	-1.730	-1.725	27651948.5529	d
44	4	41	43	3	40	1229036.715	-1.730	-1.725	27651948.5529	d
44	4	40	43	5	39	1245816.416	-2.050	-2.041	28316252.1179	d
44	5	40	43	4	39	1245816.416	-2.050	-2.041	28316252.1179	d
44	5	39	43	6	38	1262594.617	-1.660	-1.652	28962668.1390	d
44	6	39	43	5	38	1262594.617	-1.660	-1.652	28962668.1390	d
44	7	38	43	6	37	1279372.819	-2.360	-2.345	29591143.0894	d
44	6	38	43	7	37	1279372.819	-2.360	-2.345	29591143.0894	d
44	8	37	43	7	36	1296158.515	-0.646	-0.630	30201612.0168	d
44	7	37	43	8	36	1296158.515	-0.646	-0.630	30201612.0168	d
44	9	36	43	8	35	1312951.107	-2.050	-2.034	30793996.3964	d
44	8	36	43	9	35	1312951.107	-2.050	-2.034	30793996.3964	d
44	10	35	43	9	34	1329761.686	-1.610	-1.590	31368201.4414	d
44	9	35	43	10	34	1329761.686	-1.610	-1.590	31368201.4414	d
44	12	33	43	11	32	1363462.889	-1.900	-1.884	32461591.6107	d
44	11	33	43	12	32	1363462.889	-1.900	-1.884	32461591.6107	d
44	14	31	43	13	30	1397352.961	-1.520	-1.520	33480541.8532	d
44	13	31	43	14	30	1397352.961	-1.520	-1.520	33480541.8532	d
44	15	30	43	14	29	1414412.368	-2.160	-2.161	33961554.1390	d
44	14	30	43	15	29	1414412.368	-2.160	-2.161	33961554.1390	d
44	16	29	43	15	28	1431587.195	-0.411	-0.423	34423191.4954	d
44	15	29	43	16	28	1431587.195	-0.411	-0.423	34423191.4957	d
44	18	27	43	17	26	1466445.898	-3.780	-3.801	35286638.8839	d
44	17	27	43	18	26	1466445.898	-3.710	-3.736	35286638.9373	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
44	19	26	43	18	25	1484276.072	-2.900	-2.924	35687269.6215	d
44	18	26	43	19	25	1484276.072	-1.970	-1.990	35687270.3674	d
44	10	34	43	11	33	1346595.949	-1.300	-1.286	31924112.6887	d
44	11	34	43	10	33	1346595.949	-1.300	-1.286	31924112.6887	d
44	13	32	43	12	31	1380376.297	-2.130	-2.121	32980469.8952	d
44	12	32	43	13	31	1380376.297	-2.130	-2.121	32980469.8952	d
44	14	30	44	13	31	498072.368	0.035	0.003	34877896.3203	c
44	15	30	44	14	31	498072.368	0.035	0.003	34877896.3203	c
44	13	31	44	12	32	517048.058	0.039	0.003	34360848.3062	c
44	14	31	44	13	32	517048.058	0.039	0.003	34360848.3062	c
44	12	32	44	11	33	535791.970	0.040	0.004	33825056.3817	c
44	13	32	44	12	33	535791.970	0.040	0.004	33825056.3817	c
44	11	33	44	10	34	554346.499	0.037	0.006	33270709.9255	c
44	12	33	44	11	34	554346.499	0.037	0.006	33270709.9255	c
44	10	34	44	9	35	572745.233	0.023	0.001	32697964.7217	c
44	11	34	44	10	35	572745.233	0.023	0.001	32697964.7217	c
44	9	35	44	8	36	591015.195	0.010	0.000	32106949.5424	c
44	10	35	44	9	36	591015.195	0.010	0.000	32106949.5424	c
44	8	36	44	7	37	609178.380	-0.003	0.002	31497771.1653	c
44	9	36	44	8	37	609178.380	-0.003	0.002	31497771.1653	c
44	7	37	44	6	38	627252.901	-0.016	0.003	30870518.2546	c
44	8	37	44	7	38	627252.901	-0.016	0.003	30870518.2546	c
44	4	40	44	3	41	681083.554	-0.037	0.007	28880986.9857	c
44	5	40	44	4	41	681083.554	-0.037	0.007	28880986.9857	c
44	39	5	44	38	6	511500.881	-0.032	0.030	44187422.9292	c
44	39	6	44	38	7	511500.881	-0.032	0.030	44187422.9292	c
44	40	4	44	39	5	527270.617	-0.135	-0.022	44698923.8369	c
44	40	5	44	39	6	527270.617	-0.135	-0.022	44698923.8369	c
44	41	3	44	40	4	542820.078	-0.185	-0.011	45226194.5835	c
44	41	4	44	40	5	542820.078	-0.185	-0.011	45226194.5835	c
44	6	38	44	5	39	645253.818	-0.036	-0.004	30225264.4063	c
44	7	38	44	6	39	645253.818	-0.036	-0.004	30225264.4063	c
44	5	39	44	4	40	663193.803	-0.040	0.001	29562070.5695	c
44	6	39	44	5	40	663193.803	-0.040	0.001	29562070.5695	c
44	3	41	44	2	42	698932.193	-0.036	-0.004	28182054.7638	c
44	4	41	44	3	42	698932.193	-0.036	-0.004	28182054.7638	c
44	2	42	44	1	43	716747.597	-0.009	-0.004	27465307.1646	c
44	3	42	44	2	43	716747.597	-0.009	-0.004	27465307.1646	c
44	38	6	44	37	7	495474.020	-0.020	0.004	43691948.8938	c
44	38	7	44	37	8	495474.020	-0.020	0.004	43691948.8938	c
44	26	18	44	23	21	600804.004	-0.517	0.004	38904526.6239	c
45	1	45	44	0	44	1205130.641	-2.040	-2.000	26730770.6592	d
45	0	45	44	1	44	1205130.641	-2.040	-2.000	26730770.6592	d
45	2	43	44	3	42	1238709.829	-2.200	-2.185	28182054.7638	d
45	3	43	44	2	42	1238709.829	-2.200	-2.185	28182054.7638	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
45	3	42	44	4	41	1255488.630	-0.722	-0.704	28880986.9857	d
45	4	42	44	3	41	1255488.630	-0.722	-0.704	28880986.9857	d
45	5	41	44	4	40	1272260.535	-0.687	-0.666	29562070.5695	d
45	4	41	44	5	40	1272260.535	-0.687	-0.666	29562070.5695	d
45	6	40	44	5	39	1289028.844	-1.380	-1.355	30225264.4063	d
45	5	40	44	6	39	1289028.844	-1.380	-1.355	30225264.4063	d
45	7	39	44	6	38	1305798.052	-1.400	-1.373	30870518.2546	d
45	6	39	44	7	38	1305798.052	-1.400	-1.373	30870518.2546	d
45	8	38	44	7	37	1322570.257	-2.400	-2.370	31497771.1653	d
45	7	38	44	8	37	1322570.257	-2.400	-2.370	31497771.1653	d
45	8	37	44	9	36	1339353.255	-1.160	-1.131	32106949.5424	d
45	9	37	44	8	36	1339353.255	-1.160	-1.131	32106949.5424	d
45	10	36	44	9	35	1356149.444	-0.937	-0.903	32697964.7217	d
45	9	36	44	10	35	1356149.444	-0.937	-0.903	32697964.7217	d
45	10	35	44	11	34	1372965.420	-2.160	-2.123	33270709.9255	d
45	11	35	44	10	34	1372965.420	-2.160	-2.123	33270709.9255	d
45	12	34	44	11	33	1389814.372	-0.479	-0.451	33825056.3817	d
45	11	34	44	12	33	1389814.372	-0.479	-0.451	33825056.3817	d
45	13	33	44	12	32	1406701.399	-2.070	-2.048	34360848.3062	d
45	12	33	44	13	32	1406701.399	-2.070	-2.048	34360848.3062	d
45	14	32	44	13	31	1423642.987	-4.960	-4.944	34877896.3203	d
45	13	32	44	14	31	1423642.987	-4.960	-4.944	34877896.3203	d
45	15	31	44	14	30	1440665.819	-1.440	-1.434	35375968.6482	d
45	14	31	44	15	30	1440665.819	-1.440	-1.434	35375968.6482	d
45	16	30	44	15	29	1457784.286	-2.370	-2.363	35854779.0873	d
45	15	30	44	16	29	1457784.286	-2.370	-2.362	35854779.0873	d
45	17	29	44	16	28	1475037.659	-2.690	-2.696	36313970.1331	d
45	16	29	44	17	28	1475037.659	-2.690	-2.695	36313970.1337	d
45	20	26	44	19	25	1528197.810	-3.470	-3.483	37568571.8763	d
45	19	26	44	20	25	1528197.810	-0.413	-0.423	37568574.3019	d
45	2	44	44	1	43	1221925.631	-1.460	-1.435	27465307.1646	d
45	1	44	44	2	43	1221925.631	-1.460	-1.435	27465307.1646	d
45	14	31	45	13	32	515091.690	0.042	0.003	36301544.2547	c
45	15	31	45	14	32	515091.690	0.042	0.003	36301544.2547	c
45	13	32	45	12	33	533992.543	0.046	0.004	35767551.7631	c
45	14	32	45	13	33	533992.543	0.046	0.004	35767551.7631	c
45	12	33	45	11	34	552680.591	0.042	0.001	35214871.2193	c
45	13	33	45	12	34	552680.591	0.042	0.001	35214871.2193	c
45	11	34	45	10	35	571193.770	0.033	-0.002	34643677.4876	c
45	12	34	45	11	35	571193.770	0.033	-0.002	34643677.4876	c
45	10	35	45	9	36	589562.421	0.017	-0.007	34054115.0895	c
45	11	35	45	10	36	589562.421	0.017	-0.007	34054115.0895	c
45	9	36	45	8	37	607811.157	0.011	0.001	33446303.9491	c
45	10	36	45	9	37	607811.157	0.011	0.001	33446303.9491	c
45	8	37	45	7	38	625960.132	-0.011	-0.005	32820343.8119	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
45	9	37	45	8	38	625960.132	-0.011	-0.005	32820343.8119	c
45	5	40	45	4	41	679962.794	-0.051	-0.006	30834331.7787	c
45	6	40	45	5	41	679962.794	-0.051	-0.006	30834331.7787	c
45	39	6	45	38	7	508811.400	-0.042	0.004	45753976.2936	c
45	39	7	45	38	8	508811.400	-0.042	0.004	45753976.2936	c
45	40	5	45	39	6	524782.884	-0.104	0.002	46262787.7303	c
45	40	6	45	39	7	524782.884	-0.104	0.002	46262787.7303	c
45	41	4	45	40	5	540508.153	-0.177	0.008	46787570.7130	c
45	41	5	45	40	6	540508.153	-0.177	0.008	46787570.7130	c
45	27	18	45	24	21	599212.886	-0.646	0.051	40790352.8784	c
45	7	38	45	6	39	644026.098	-0.025	-0.002	32176317.6955	c
45	8	38	45	7	39	644026.098	-0.025	-0.002	32176317.6955	c
45	6	39	45	5	40	662023.051	-0.033	0.003	31514294.6175	c
45	7	39	45	6	40	662023.051	-0.033	0.003	31514294.6175	c
45	4	41	45	3	42	697855.424	-0.037	0.009	30136476.3250	c
45	5	41	45	4	42	697855.424	-0.037	0.009	30136476.3250	c
45	3	42	45	2	43	715709.521	-0.027	0.004	29420766.7839	c
45	4	42	45	3	43	715709.521	-0.027	0.004	29420766.7839	c
45	38	7	45	37	8	492551.384	0.001	0.004	45261424.9157	c
45	38	8	45	37	9	492551.384	0.001	0.004	45261424.9157	c
46	1	46	45	0	45	1231594.547	-2.500	-2.436	27935903.3288	d
46	0	46	45	1	45	1231594.547	-2.500	-2.436	27935903.3288	d
46	2	45	45	1	44	1248382.342	-2.120	-2.079	28687234.2433	d
46	1	45	45	2	44	1248382.342	-2.120	-2.079	28687234.2433	d
46	2	44	45	3	43	1265160.544	-1.530	-1.491	29420766.7839	d
46	3	44	45	2	43	1265160.544	-1.530	-1.491	29420766.7839	d
46	3	43	45	4	42	1281930.051	-1.590	-1.553	30136476.3250	d
46	4	43	45	3	42	1281930.051	-1.590	-1.553	30136476.3250	d
46	5	42	45	4	41	1298694.462	-0.790	-0.752	30834331.7787	d
46	4	42	45	5	41	1298694.462	-0.790	-0.752	30834331.7787	d
46	6	41	45	5	40	1315456.775	1.410	1.455	31514294.6175	d
46	5	41	45	6	40	1315456.775	1.410	1.455	31514294.6175	d
46	7	39	45	8	38	1348976.303	-1.080	-1.023	32820343.8119	d
46	8	39	45	7	38	1348976.303	-1.080	-1.023	32820343.8119	d
46	10	37	45	9	36	1382527.909	-1.290	-1.229	34054115.0895	d
46	9	37	45	10	36	1382527.909	-1.290	-1.229	34054115.0895	d
46	12	35	45	11	34	1416156.562	-1.630	-1.579	35214871.2193	d
46	11	35	45	12	34	1416156.562	-1.630	-1.579	35214871.2193	d
46	14	33	45	13	32	1449938.709	0.184	0.225	36301544.2547	d
46	13	33	45	14	32	1449938.709	0.184	0.225	36301544.2547	d
46	15	32	45	14	31	1466918.371	-2.300	-2.270	36816635.8975	d
46	14	32	45	15	31	1466918.371	-2.300	-2.270	36816635.8975	d
46	17	30	45	16	29	1501176.889	-4.660	-4.642	37789010.4713	d
46	16	30	45	17	29	1501176.889	-4.660	-4.642	37789010.4713	d
46	19	28	45	18	27	1536092.852	-1.900	-1.888	38681710.2183	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
46	18	28	45	19	27	1536092.852	-1.840	-1.830	38681710.2648	d
46	6	40	45	7	39	1332212.492	-2.410	-2.359	32176317.6955	d
46	7	40	45	6	39	1332212.492	-2.410	-2.359	32176317.6955	d
46	14	32	46	13	33	532073.828	0.030	-0.016	37751482.7653	c
46	15	32	46	14	33	532073.828	0.030	-0.016	37751482.7653	c
46	12	34	46	11	35	569545.706	0.050	0.004	36631029.3982	c
46	13	34	46	12	35	569545.706	0.050	0.004	36631029.3982	c
46	10	36	46	9	37	606363.439	0.014	-0.011	35436644.2704	c
46	11	36	46	10	37	606363.439	0.014	-0.011	35436644.2704	c
46	9	37	46	8	38	624593.285	0.013	0.004	34812051.0042	c
46	10	37	46	9	38	624593.285	0.013	0.004	34812051.0042	c
46	39	7	46	38	8	505920.567	-0.006	0.010	47357345.9989	c
46	39	8	46	38	9	505920.567	-0.006	0.010	47357345.9989	c
46	15	31	46	14	32	513001.024	0.033	-0.004	38283556.5576	c
46	16	31	46	15	32	513001.024	0.033	-0.004	38283556.5576	c
46	40	6	46	39	7	522114.479	-0.082	-0.001	47863266.5672	c
46	40	7	46	39	8	522114.479	-0.082	-0.001	47863266.5672	c
46	41	5	46	40	6	538032.912	-0.171	-0.001	48385381.1230	c
46	41	6	46	40	7	538032.912	-0.171	-0.001	48385381.1230	c
46	13	33	46	12	34	550907.775	0.053	0.005	37200575.0488	c
46	14	33	46	13	34	550907.775	0.053	0.005	37200575.0488	c
46	43	3	46	42	4	569193.140	-0.442	-0.032	49477129.6203	c
46	43	4	46	42	5	569193.140	-0.442	-0.032	49477129.6203	c
46	7	39	46	6	40	660788.586	-0.016	0.011	33508532.5825	c
46	8	39	46	7	40	660788.586	-0.016	0.011	33508532.5825	c
46	6	40	46	5	41	678782.577	-0.044	-0.001	32829749.9684	c
46	7	40	46	6	41	678782.577	-0.044	-0.001	32829749.9684	c
46	5	41	46	4	42	696722.904	-0.053	-0.002	32133027.0185	c
46	6	41	46	5	42	696722.904	-0.053	-0.002	32133027.0185	c
47	0	47	46	1	46	1258050.359	-2.660	-2.573	29167500.3610	d
47	1	47	46	0	46	1258050.359	-2.660	-2.573	29167500.3610	d
47	2	46	46	1	45	1274828.260	-5.050	-4.981	29935618.6962	d
47	1	46	46	2	45	1274828.260	-5.050	-4.981	29935618.6962	d
47	2	45	46	3	44	1291601.965	-1.470	-1.415	30685928.8426	d
47	3	45	46	2	44	1291601.965	-1.470	-1.415	30685928.8426	d
47	3	44	46	4	43	1308364.278	-0.850	-0.792	31418407.9527	d
47	4	44	46	3	43	1308364.278	-0.850	-0.792	31418407.9527	d
47	5	43	46	4	42	1325119.695	-0.675	-0.613	32133027.0185	d
47	4	43	46	5	42	1325119.695	-0.675	-0.613	32133027.0185	d
47	7	41	46	6	40	1358619.737	-1.570	-1.499	33508532.5825	d
47	6	41	46	7	40	1358619.737	-1.570	-1.499	33508532.5825	d
47	7	40	46	8	39	1375370.357	-2.730	-2.655	34169321.1778	d
47	8	40	46	7	39	1375370.357	-2.730	-2.655	34169321.1778	d
47	8	39	46	9	38	1392129.072	-1.770	-1.685	34812051.0042	d
47	9	39	46	8	38	1392129.072	-1.770	-1.685	34812051.0042	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
47	10	38	46	9	37	1408897.381	-2.030	-1.943	35436644.2704	d
47	9	38	46	10	37	1408897.381	-2.030	-1.943	35436644.2704	d
47	10	37	46	11	36	1425681.878	-2.870	-2.789	36043007.6893	d
47	11	37	46	10	36	1425681.878	-2.870	-2.789	36043007.6893	d
47	13	35	46	12	34	1459336.912	-0.203	-0.125	37200575.0488	d
47	12	35	46	13	34	1459336.912	-0.203	-0.125	37200575.0488	d
47	13	34	47	12	35	567795.708	0.053	-0.002	38659912.1492	c
47	14	34	47	13	35	567795.708	0.053	-0.002	38659912.1492	c
47	16	31	47	15	32	510767.158	0.034	0.004	40306757.9984	c
47	17	31	47	16	32	510767.158	0.034	0.004	40306757.9984	c
47	15	32	47	14	33	530028.470	0.023	-0.021	39776729.5569	c
47	16	32	47	15	33	530028.470	0.023	-0.021	39776729.5569	c
47	14	33	47	13	34	549021.818	0.055	0.002	39227707.7988	c
47	15	33	47	14	34	549021.818	0.055	0.002	39227707.7988	c
47	43	4	47	42	5	566891.221	-0.453	-0.043	51106392.2302	c
47	43	5	47	42	6	566891.221	-0.453	-0.043	51106392.2302	c
47	12	35	47	11	36	586388.582	0.055	0.004	38073523.6278	c
47	13	35	47	12	36	586388.582	0.055	0.004	38073523.6278	c
47	10	37	47	9	38	623148.784	0.017	-0.009	36845543.6662	c
47	11	37	47	10	38	623148.784	0.017	-0.009	36845543.6662	c
47	8	39	47	7	40	659487.577	-0.005	0.007	35544694.2554	c
47	9	39	47	8	40	659487.577	-0.005	0.007	35544694.2554	c
47	7	40	47	6	41	677540.356	-0.027	0.005	34867153.8790	c
47	8	40	47	7	41	677540.356	-0.027	0.005	34867153.8790	c
47	6	41	47	5	42	695532.373	-0.051	-0.003	34171621.4619	c
47	7	41	47	6	42	695532.373	-0.051	-0.003	34171621.4619	c
47	40	7	47	39	8	519252.334	-0.039	0.004	49500505.5022	c
47	40	8	47	39	9	519252.334	-0.039	0.004	49500505.5022	c
47	41	6	47	40	7	535383.265	-0.133	0.003	50019757.8702	c
47	41	7	47	40	8	535383.265	-0.133	0.003	50019757.8702	c
47	42	5	47	41	6	551250.645	-0.328	-0.068	50555141.2624	c
47	42	6	47	41	7	551250.645	-0.328	-0.068	50555141.2624	c
48	0	48	47	1	47	1284499.575	-0.855	-0.734	30425553.3692	d
48	1	48	47	0	47	1284499.575	-0.855	-0.734	30425553.3692	d
48	2	47	47	1	46	1301271.780	-1.660	-1.565	31210451.9928	d
48	1	47	47	2	46	1301271.780	-1.660	-1.565	31210451.9928	d
48	2	46	47	3	45	1318034.393	-1.560	-1.476	31977532.2694	d
48	3	46	47	2	45	1318034.393	-1.560	-1.476	31977532.2694	d
48	4	45	47	3	44	1334788.311	-1.320	-1.236	32726773.0678	d
48	3	45	47	4	44	1334788.311	-1.320	-1.236	32726773.0678	d
48	5	44	47	4	43	1351535.334	-1.060	-0.965	33458147.3758	d
48	4	44	47	5	43	1351535.334	-1.060	-0.965	33458147.3758	d
48	5	43	47	6	42	1368276.661	-1.800	-1.702	34171621.4619	d
48	6	43	47	5	42	1368276.661	-1.800	-1.702	34171621.4619	d
48	9	40	47	8	39	1418503.940	-1.540	-1.423	36204181.8309	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
48	8	40	47	9	39	1418503.940	-1.540	-1.423	36204181.8309	d
48	9	39	47	10	38	1435258.457	-2.260	-2.143	36845543.6662	d
48	10	39	47	9	38	1435258.457	-2.260	-2.143	36845543.6662	d
48	10	38	47	11	37	1452028.864	-1.940	-1.816	37468692.4271	d
48	11	38	47	10	37	1452028.864	-1.940	-1.816	37468692.4271	d
48	15	34	47	14	33	1519422.276	-0.535	-0.433	39776729.5569	d
48	14	34	47	15	33	1519422.276	-0.535	-0.433	39776729.5569	d
48	16	33	47	15	32	1536409.433	-0.910	-0.816	40306757.9984	d
48	15	33	47	16	32	1536409.433	-0.910	-0.816	40306757.9984	d
48	7	42	47	6	41	1385016.789	-1.690	-1.587	34867153.8790	d
48	6	42	47	7	41	1385016.789	-1.690	-1.587	34867153.8790	d
48	39	9	48	38	10	499470.191	0.050	-0.008	50675188.0476	c
48	39	10	48	38	11	499470.191	0.050	-0.008	50675188.0476	c
48	17	31	48	16	32	508380.293	0.024	0.006	42371016.7496	c
48	18	31	48	17	32	508380.293	0.024	0.006	42371016.7496	c
48	15	33	48	14	34	547016.033	0.054	0.001	41296152.3530	c
48	16	33	48	15	34	547016.033	0.054	0.001	41296152.3530	c
48	42	6	48	41	7	548617.663	-0.228	-0.014	52223387.0988	c
48	42	7	48	41	8	548617.663	-0.228	-0.014	52223387.0988	c
48	43	5	48	42	6	564436.030	-0.370	0.010	52772004.9847	c
48	43	6	48	42	7	564436.030	-0.370	0.010	52772004.9847	c
48	14	34	48	13	35	565938.117	0.061	0.001	40730214.3027	c
48	15	34	48	14	35	565938.117	0.061	0.001	40730214.3027	c
48	12	36	48	11	37	603210.309	0.062	0.007	39542346.1094	c
48	13	36	48	12	37	603210.309	0.062	0.007	39542346.1094	c
48	12	36	48	11	37	603210.309	0.062	0.007	39542346.1094	c
48	13	36	48	12	37	603210.309	0.062	0.007	39542346.1094	c
48	11	37	48	10	38	621622.939	0.038	-0.005	38920723.2148	c
48	12	37	48	11	38	621622.939	0.038	-0.005	38920723.2148	c
48	8	40	48	7	41	676233.477	-0.012	0.006	36946453.8154	c
48	9	40	48	8	41	676233.477	-0.012	0.006	36946453.8154	c
48	6	42	48	5	43	712272.397	-0.047	0.009	35539899.9100	c
48	7	42	48	6	43	712272.397	-0.047	0.009	35539899.9100	c
48	41	7	48	40	8	532546.959	-0.076	0.009	51690840.0686	c
48	41	8	48	40	9	532546.959	-0.076	0.009	51690840.0686	c
49	0	49	48	1	48	1310936.200	-2.890	-2.734	31710053.7866	d
49	1	49	48	0	48	1310936.200	-2.890	-2.734	31710053.7866	d
49	3	47	48	2	46	1344461.124	1.680	1.802	33295568.2140	d
49	2	47	48	3	46	1344461.124	1.680	1.802	33295568.2140	d
49	4	46	48	3	45	1361204.550	-0.427	-0.305	34061562.6887	d
49	3	46	48	4	45	1361204.550	-0.427	-0.305	34061562.6887	d
49	7	43	48	6	42	1411403.948	-2.270	-2.121	36252172.3467	d
49	6	43	48	7	42	1411403.948	-2.270	-2.121	36252172.3467	d
49	8	41	48	9	40	1444867.715	-3.030	-2.871	37622687.2978	d
49	9	41	48	8	40	1444867.715	-3.030	-2.871	37622687.2978	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
49	10	39	48	11	38	1478365.958	-2.050	-1.885	38920723.2148	d
49	11	39	48	10	38	1478365.958	-2.050	-1.885	38920723.2148	d
49	12	37	48	13	36	1511942.747	-1.230	-1.072	40145556.3506	d
49	13	37	48	12	36	1511942.747	-1.230	-1.072	40145556.3506	d
49	5	45	48	4	44	1377941.380	-1.750	-1.620	34809683.7521	d
49	4	45	48	5	44	1377941.380	-1.750	-1.620	34809683.7521	d
49	6	44	48	5	43	1394674.313	-1.720	-1.589	35539899.9100	d
49	5	44	48	6	43	1394674.313	-1.720	-1.589	35539899.9100	d
49	8	42	48	7	41	1428134.782	-1.830	-1.675	36946453.8154	d
49	7	42	48	8	41	1428134.782	-1.830	-1.675	36946453.8154	d
49	11	38	48	12	37	1495139.962	-2.530	-2.363	39542346.1094	d
49	12	38	48	11	37	1495139.962	-2.530	-2.363	39542346.1094	d
49	18	31	49	17	32	505829.659	-0.003	0.001	44476196.0348	c
49	19	31	49	18	32	505829.659	-0.003	0.000	44476196.0348	c
49	40	9	49	39	10	512886.962	0.076	0.021	52885887.8145	c
49	40	10	49	39	11	512886.962	0.076	0.021	52885887.8145	c
49	17	32	49	16	33	525525.032	0.025	0.000	43950671.0328	c
49	18	32	49	17	33	525525.032	0.025	0.000	43950671.0328	c
49	16	33	49	15	34	544883.181	0.049	0.002	43405787.9056	c
49	17	33	49	16	34	544883.181	0.049	0.002	43405787.9056	c
49	15	34	49	14	35	563966.822	0.059	-0.002	42841821.1481	c
49	16	34	49	15	35	563966.822	0.059	-0.002	42841821.1481	c
49	14	35	49	13	36	582824.873	0.073	0.005	42258996.3537	c
49	15	35	49	14	36	582824.873	0.073	0.005	42258996.3537	c
49	13	36	49	12	37	601496.106	0.064	-0.003	41657500.3174	c
49	14	36	49	13	37	601496.106	0.064	-0.003	41657500.3174	c
49	12	37	49	11	38	620011.799	0.061	0.003	41037488.5860	c
49	13	37	49	12	38	620011.799	0.061	0.003	41037488.5860	c
49	11	38	49	10	39	638397.425	0.043	-0.001	40399091.2103	c
49	12	38	49	11	39	638397.425	0.043	-0.001	40399091.2103	c
49	10	39	49	9	40	656674.051	0.035	0.012	39742417.2012	c
49	11	39	49	10	40	656674.051	0.035	0.012	39742417.2012	c
49	9	40	49	8	41	674859.169	-0.009	-0.008	39067558.0298	c
49	10	40	49	9	41	674859.169	-0.009	-0.008	39067558.0298	c
49	8	41	49	7	42	692967.593	-0.032	-0.006	38374590.4118	c
49	9	41	49	8	42	692967.593	-0.032	-0.006	38374590.4118	c
49	7	42	49	6	43	711011.836	-0.036	0.012	37663578.5462	c
49	8	42	49	7	43	711011.836	-0.036	0.012	37663578.5462	c
49	41	8	49	40	9	529510.418	-0.049	-0.025	53398774.6952	c
49	41	9	49	40	10	529510.418	-0.049	-0.025	53398774.6952	c
49	42	7	49	41	8	545804.545	-0.177	-0.028	53928285.1568	c
49	42	8	49	41	9	545804.545	-0.177	-0.028	53928285.1568	c
50	2	49	49	1	48	1354126.143	-0.718	-0.540	33839430.0960	d
50	1	49	49	2	48	1354126.143	-0.718	-0.540	33839430.0960	d
50	3	48	49	2	47	1370872.866	-0.857	-0.691	34640027.6458	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
50	2	48	49	3	47	1370872.866	-0.857	-0.691	34640027.6458	d
50	5	46	49	4	45	1404342.329	1.930	2.101	36187626.8656	d
50	4	46	49	5	45	1404342.329	1.930	2.101	36187626.8656	d
50	5	45	49	6	44	1421062.071	-1.980	-1.796	36934575.9338	d
50	6	45	49	5	44	1421062.071	-1.980	-1.796	36934575.9338	d
50	6	44	49	7	43	1437782.713	-1.600	-1.405	37663578.5462	d
50	7	44	49	6	43	1437782.713	-1.600	-1.405	37663578.5462	d
50	7	43	49	8	42	1454500.356	-3.630	-3.430	38374590.4118	d
50	8	43	49	7	42	1454500.356	-3.630	-3.430	38374590.4118	d
50	8	42	49	9	41	1471223.695	-2.710	-2.494	39067558.0298	d
50	9	42	49	8	41	1471223.695	-2.710	-2.494	39067558.0298	d
50	19	31	50	18	32	503103.351	-0.037	-0.002	46622153.7362	c
50	20	31	50	19	32	503103.351	-0.037	-0.003	46622153.7362	c
50	18	32	50	17	33	523048.606	-0.012	-0.015	46099105.1233	c
50	19	32	50	18	33	523048.606	-0.012	-0.015	46099105.1233	c
50	17	33	50	16	34	542615.411	0.036	0.003	45556489.7537	c
50	18	33	50	17	34	542615.411	0.036	0.003	45556489.7537	c
50	16	34	50	15	35	561875.286	0.070	0.015	44994614.5432	c
50	17	34	50	16	35	561875.286	0.070	0.015	44994614.5432	c
50	15	35	50	14	36	580883.551	0.066	-0.003	44413731.0642	c
50	16	35	50	15	36	580883.551	0.066	-0.003	44413731.0642	c
50	14	36	50	13	37	599683.877	0.074	-0.001	43814047.2667	c
50	15	36	50	14	37	599683.877	0.074	-0.001	43814047.2667	c
50	12	38	50	11	39	636793.851	0.065	0.004	42558942.3801	c
50	13	38	50	12	39	636793.851	0.065	0.004	42558942.3801	c
50	9	41	50	8	42	691588.273	-0.005	0.002	40538784.4161	c
50	10	41	50	9	42	691588.273	-0.005	0.002	40538784.4161	c
50	8	42	50	7	43	709690.011	-0.026	0.009	39829094.3865	c
50	9	42	50	8	43	709690.011	-0.026	0.009	39829094.3865	c
50	7	43	50	6	44	727731.480	-0.072	-0.013	39101362.8420	c
50	8	43	50	7	44	727731.480	-0.072	-0.013	39101362.8420	c
50	39	11	50	38	12	491999.401	0.107	-0.013	54142369.1332	c
50	39	12	50	38	13	491999.401	0.107	-0.013	54142369.1332	c
50	40	10	50	39	11	509349.233	0.112	0.009	54634368.4223	c
50	40	11	50	39	12	509349.233	0.112	0.009	54634368.4223	c
50	41	9	50	40	10	526258.692	0.047	0.005	55143717.5379	c
50	41	10	50	40	11	526258.692	0.047	0.005	55143717.5379	c
50	2	48	50	1	49	817344.465	0.046	-0.005	35193556.9445	c
50	3	48	50	2	49	817344.465	0.046	-0.005	35193556.9445	c
50	1	49	50	0	50	835195.432	0.167	-0.008	34358361.6876	c
50	2	49	50	1	50	835195.432	0.167	-0.008	34358361.6876	c
51	0	51	50	1	50	1363788.164	-1.300	-1.041	34358361.6876	d
51	1	51	50	0	50	1363788.164	-1.300	-1.041	34358361.6876	d
51	2	49	50	3	48	1397277.113	-1.500	-1.281	36010901.3557	d
51	3	49	50	2	48	1397277.113	-1.500	-1.281	36010901.3557	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(\text{SP})$ / MHz	$\Delta_{O-C}(\text{LP})$ / MHz	E''/h (MHz)	Source
51	5	47	50	4	46	1430726.490	-1.530	-1.309	37591967.2504	d
51	4	47	50	5	46	1430726.490	-1.530	-1.309	37591967.2504	d
51	6	46	50	5	45	1447439.037	-3.270	-3.031	38355639.9672	d
51	5	46	50	6	45	1447439.037	-3.270	-3.031	38355639.9672	d
51	8	44	50	7	43	1480859.634	-1.870	-1.606	39829094.3865	d
51	7	44	50	8	43	1480859.634	-1.870	-1.606	39829094.3865	d
51	10	42	50	9	41	1514287.726	-0.709	-0.427	41230372.6872	d
51	9	42	50	10	41	1514287.726	-0.709	-0.427	41230372.6872	d
51	11	41	50	10	40	1531013.164	-1.430	-1.147	41903787.2412	d
51	10	41	50	11	40	1531013.164	-1.430	-1.147	41903787.2412	d
51	2	50	50	1	49	1380538.485	-1.300	-1.072	35193556.9445	d
51	1	50	50	2	49	1380538.485	-1.300	-1.072	35193556.9445	d
51	20	31	51	19	32	500188.104	-0.076	-0.001	48808741.9359	c
51	21	31	51	20	32	500188.104	-0.078	-0.003	48808741.9359	c
51	19	32	51	18	33	520408.712	-0.027	0.002	48288333.2024	c
51	20	32	51	19	33	520408.712	-0.027	0.002	48288333.2024	c
51	18	33	51	17	34	540204.178	0.023	0.013	47748129.0522	c
51	19	33	51	18	34	540204.178	0.023	0.013	47748129.0522	c
51	17	34	51	16	35	559656.373	0.047	0.005	47188472.7316	c
51	18	34	51	17	35	559656.373	0.047	0.005	47188472.7316	c
51	16	35	51	15	36	578828.098	0.061	-0.003	46609644.7001	c
51	17	35	51	16	36	578828.098	0.061	-0.003	46609644.7001	c
51	15	36	51	14	37	597768.510	0.086	0.009	46011876.2821	c
51	16	36	51	15	37	597768.510	0.086	0.009	46011876.2821	c
51	14	37	51	13	38	616516.696	0.088	0.007	45395359.6801	c
51	15	37	51	14	38	616516.696	0.088	0.007	45395359.6801	c
51	13	38	51	12	39	635104.277	0.077	0.002	44760255.4868	c
51	14	38	51	13	39	635104.277	0.077	0.002	44760255.4868	c
51	12	39	51	11	40	653557.137	0.072	0.010	44106698.4283	c
51	13	39	51	12	40	653557.137	0.072	0.010	44106698.4283	c
51	3	48	51	2	49	816206.075	-0.029	-0.005	37408179.9538	c
51	4	48	51	3	49	816206.075	-0.029	-0.005	37408179.9538	c
51	2	49	51	1	50	834083.304	0.062	-0.004	36574096.7194	c
51	3	49	51	2	50	834083.304	0.062	-0.004	36574096.7194	c
51	1	50	51	0	51	851945.795	0.209	0.003	35722151.1420	c
51	2	50	51	1	51	851945.795	0.209	0.003	35722151.1420	c
52	1	52	51	0	51	1390201.105	0.285	0.614	35722151.1420	d
52	0	52	51	1	51	1390201.105	0.285	0.614	35722151.1420	d
52	2	51	51	1	50	1406942.732	-0.557	-0.263	36574096.7194	d
52	1	51	51	2	50	1406942.732	-0.557	-0.263	36574096.7194	d
52	3	50	51	2	49	1423672.667	-1.260	-0.986	37408179.9538	d
52	2	50	51	3	49	1423672.667	-1.260	-0.986	37408179.9538	d
52	3	49	51	4	48	1440396.905	2.690	2.964	38224386.0495	d
52	4	49	51	3	48	1440396.905	2.690	2.964	38224386.0495	d
52	5	48	51	4	47	1457104.356	-1.460	-1.173	39022695.2585	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν /MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
52	4	48	51	5	47	1457104.356	-1.460	-1.173	39022695.2585	d
52	6	47	51	5	46	1473810.607	-0.011	0.288	39803082.2556	d
52	5	47	51	6	46	1473810.607	-0.011	0.288	39803082.2556	d
52	7	45	51	8	44	1507207.220	-1.720	-1.393	41309955.8737	d
52	8	45	51	7	44	1507207.220	-1.720	-1.393	41309955.8737	d
52	11	42	51	10	41	1557320.578	-2.800	-2.431	43434801.8251	d
52	10	42	51	11	41	1557320.578	-2.800	-2.431	43434801.8251	d
52	11	41	51	12	40	1574046.016	-2.880	-2.509	44106698.4283	d
52	12	41	51	11	40	1574046.016	-2.880	-2.509	44106698.4283	d
52	21	31	52	20	32	497069.044	-0.132	-0.004	51035806.3780	c
52	22	31	52	21	32	497069.044	-0.139	-0.011	51035806.3783	c
52	19	33	52	18	34	537640.113	-0.005	0.018	49980572.5388	c
52	20	33	52	19	34	537640.113	-0.005	0.018	49980572.5388	c
52	17	35	52	16	36	576652.077	0.050	-0.001	48846618.1155	c
52	18	35	52	17	36	576652.077	0.050	-0.001	48846618.1155	c
52	15	37	52	14	38	614623.611	0.084	0.000	47636250.1577	c
52	16	37	52	15	38	614623.611	0.084	0.000	47636250.1577	c
52	14	38	52	13	39	633324.620	0.084	-0.002	47002925.6284	c
52	15	38	52	14	39	633324.620	0.084	-0.002	47002925.6284	c
52	13	39	52	12	40	651876.267	0.081	0.002	46351049.4486	c
52	14	39	52	13	40	651876.267	0.081	0.002	46351049.4486	c
52	12	40	52	11	41	670302.198	0.051	-0.010	45680747.3081	c
52	13	40	52	12	41	670302.198	0.051	-0.010	45680747.3081	c
52	11	41	52	10	42	688622.166	0.037	0.000	44992125.1854	c
52	12	41	52	11	42	688622.166	0.037	0.000	44992125.1854	c
52	9	43	52	8	44	725007.882	-0.038	-0.010	43560264.5751	c
52	10	43	52	9	44	725007.882	-0.038	-0.010	43560264.5751	c
52	10	42	52	9	43	706852.706	0.002	-0.004	44285272.4881	c
52	11	42	52	10	43	706852.706	0.002	-0.004	44285272.4881	c
52	4	48	52	3	49	815020.724	-0.089	-0.007	39664780.2544	c
52	5	48	52	4	49	815020.724	-0.089	-0.007	39664780.2544	c
52	3	49	52	2	50	832926.365	-0.026	-0.003	38831853.8715	c
52	4	49	52	3	50	832926.365	-0.026	-0.003	38831853.8715	c
52	1	51	52	0	52	868688.286	0.231	-0.010	37112351.9480	c
52	2	51	52	1	52	868688.286	0.231	-0.010	37112351.9480	c
53	0	53	52	1	52	1416601.755	-0.955	-0.548	37112351.9480	d
53	1	53	52	0	52	1416601.755	-0.955	-0.548	37112351.9480	d
53	2	52	52	1	51	1433336.186	-0.997	-0.629	37981039.9943	d
53	1	52	52	2	51	1433336.186	-0.997	-0.629	37981039.9943	d
53	2	51	52	3	50	1450058.926	-0.578	-0.227	38831853.8715	d
53	3	51	52	2	50	1450058.926	-0.578	-0.227	38831853.8715	d
53	4	50	52	3	49	1466771.173	0.069	0.420	39664780.2544	d
53	3	50	52	4	49	1466771.173	0.069	0.420	39664780.2544	d
53	6	48	52	5	47	1500166.587	-2.220	-1.845	41276892.8596	d
53	5	48	52	6	47	1500166.587	-2.220	-1.845	41276892.8596	d

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
53	21	32	53	20	33	514590.529	-0.127	0.002	52788595.1839	c
53	22	32	53	21	33	514590.529	-0.128	0.001	52788595.1839	c
53	20	33	53	19	34	534912.903	-0.074	-0.005	52253682.2125	c
53	21	33	53	20	34	534912.903	-0.074	-0.005	52253682.2125	c
53	18	35	53	17	36	574348.559	0.047	0.021	51124528.6231	c
53	19	35	53	18	36	574348.559	0.047	0.021	51124528.6231	c
53	17	36	53	16	37	593606.068	0.064	0.006	50530922.6249	c
53	18	36	53	17	37	593606.068	0.064	0.006	50530922.6249	c
53	16	37	53	15	38	612626.949	0.089	0.009	49918295.7707	c
53	17	37	53	16	38	612626.949	0.089	0.009	49918295.7707	c
53	11	42	53	10	43	705332.036	0.034	0.004	46575747.2676	c
53	12	42	53	11	43	705332.036	0.034	0.004	46575747.2676	c
53	22	31	53	21	32	493729.416	-0.189	0.006	53303185.8346	c
53	23	31	53	22	32	493729.416	-0.212	-0.017	53303185.8364	c
53	15	38	53	14	39	631450.542	0.081	-0.010	49286845.3163	c
53	16	38	53	15	39	631450.542	0.081	-0.010	49286845.3163	c
53	12	41	53	11	42	687029.582	0.060	0.002	47281079.2631	c
53	13	41	53	12	42	687029.582	0.060	0.002	47281079.2631	c
53	10	43	53	9	44	723550.652	-0.010	-0.004	45852196.6131	c
53	11	43	53	10	44	723550.652	-0.010	-0.004	45852196.6131	c
53	5	48	53	4	49	813786.901	-0.121	0.002	41963274.6396	c
53	6	48	53	5	49	813786.901	-0.121	0.002	41963274.6396	c
53	3	50	53	2	51	849637.969	-0.022	0.000	40281913.3613	c
53	4	50	53	3	51	849637.969	-0.022	0.000	40281913.3613	c
53	2	51	53	1	52	867536.301	0.095	-0.002	39414377.1631	c
53	3	51	53	2	52	867536.301	0.095	-0.002	39414377.1631	c
53	1	52	53	0	53	885422.828	0.300	0.020	38528954.6435	c
53	2	52	53	1	53	885422.828	0.300	0.020	38528954.6435	c
54	2	53	53	1	52	1459720.647	-0.645	-0.191	39414377.1631	d
54	1	53	53	2	52	1459720.647	-0.645	-0.191	39414377.1631	d
54	5	49	53	6	48	1526515.973	-0.716	-0.249	42777061.6535	d
54	6	49	53	5	48	1526515.973	-0.716	-0.249	42777061.6535	d
54	22	32	54	21	33	511384.822	-0.206	-0.007	55099326.3276	c
54	23	32	54	22	33	511384.822	-0.212	-0.013	55099326.3282	c
54	21	33	54	20	34	532011.268	-0.100	0.028	54567314.9647	c
54	22	33	54	21	34	532011.268	-0.101	0.028	54567314.9647	c
54	20	34	54	19	35	552155.164	-0.056	0.008	54015159.7497	c
54	21	34	54	20	35	552155.164	-0.056	0.008	54015159.7497	c
54	18	36	54	17	37	591346.836	0.030	-0.004	52851902.9925	c
54	19	36	54	18	37	591346.836	0.030	-0.004	52851902.9925	c
54	17	37	54	16	38	610521.297	0.043	-0.025	52241381.7442	c
54	18	37	54	17	38	610521.297	0.043	-0.025	52241381.7442	c
54	16	38	54	15	39	629477.458	0.091	0.003	51611904.3831	c
54	17	38	54	16	39	629477.458	0.091	0.003	51611904.3831	c
54	14	40	54	13	41	666870.228	0.089	-0.004	50296783.5982	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{\text{obs.}} - \nu_{\text{cal.}}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(\text{SP})$ / MHz	$\Delta_{O-C}(\text{LP})$ / MHz	E''/h (MHz)	Source
54	15	40	54	14	41	666870.228	0.089	-0.004	50296783.5982	c
54	13	41	54	12	42	685359.860	0.077	-0.001	49611423.8215	c
54	14	41	54	13	42	685359.860	0.077	-0.001	49611423.8215	c
54	11	43	54	10	44	722026.490	0.012	-0.007	48185657.7503	c
54	12	43	54	11	44	722026.490	0.012	-0.007	48185657.7503	c
54	6	48	54	5	49	812503.011	-0.148	-0.001	44303578.3276	c
54	7	48	54	6	49	812503.011	-0.148	-0.001	44303578.3276	c
54	3	51	54	2	52	866340.722	-0.044	-0.021	41758348.4959	c
54	4	51	54	3	52	866340.722	-0.044	-0.021	41758348.4959	c
54	2	52	54	1	53	884250.181	0.118	0.003	40874098.4413	c
54	3	52	54	2	53	884250.181	0.118	0.003	40874098.4413	c
54	1	53	54	0	54	902149.181	0.319	-0.003	39971949.5879	c
54	2	53	54	1	54	902149.181	0.319	-0.003	39971949.5879	c
55	1	55	54	0	54	1469375.473	-1.910	-1.313	39971949.5879	d
55	0	55	54	1	54	1469375.473	-1.910	-1.313	39971949.5879	d
55	3	52	54	4	51	1519491.828	-2.670	-2.137	42624689.2534	d
55	4	52	54	3	51	1519491.828	-2.670	-2.137	42624689.2534	d
55	5	51	54	4	50	1536176.794	-1.600	-1.049	43473105.8059	d
55	4	51	54	5	50	1536176.794	-1.600	-1.049	43473105.8059	d
55	22	33	55	21	34	528922.456	-0.212	-0.008	56921322.1496	c
55	23	33	55	22	34	528922.456	-0.213	-0.009	56921322.1496	c
55	21	34	55	20	35	549342.604	-0.145	-0.017	56371979.4054	c
55	22	34	55	21	35	549342.604	-0.146	-0.018	56371979.4054	c
55	18	37	55	17	38	608301.020	0.051	0.009	54605390.2186	c
55	19	37	55	18	38	608301.020	0.051	0.009	54605390.2186	c
55	16	39	55	15	40	646297.856	0.106	0.012	53331692.1374	c
55	17	39	55	16	40	646297.856	0.106	0.012	53331692.1374	c
55	19	36	55	18	37	588960.047	0.001	0.004	55213691.1812	c
55	20	36	55	19	37	588960.047	0.001	0.004	55213691.1812	c
55	17	38	55	16	39	627400.406	0.062	-0.012	53977989.8808	c
55	18	38	55	17	39	627400.406	0.062	-0.012	53977989.8808	c
55	12	43	55	11	44	720432.807	0.049	0.004	50560551.8114	c
55	13	43	55	12	44	720432.807	0.049	0.004	50560551.8114	c
55	6	49	55	5	50	829172.411	-0.163	0.011	45856432.3885	c
55	7	49	55	6	50	829172.411	-0.163	0.011	45856432.3885	c
55	4	51	55	3	52	865100.334	-0.119	-0.001	44144183.7391	c
55	5	51	55	4	52	865100.334	-0.119	-0.001	44144183.7391	c
55	3	52	55	2	53	883034.553	-0.024	-0.001	43261149.1702	c
55	4	52	55	3	53	883034.553	-0.024	-0.001	43261149.1702	c
55	2	53	55	1	54	900955.446	0.132	-0.002	42360193.8653	c
55	3	53	55	2	54	900955.446	0.132	-0.002	42360193.8653	c
56	2	55	55	1	54	1512457.791	-1.650	-0.981	42360193.8653	d
56	1	55	55	2	54	1512457.791	-1.650	-0.981	42360193.8653	d
56	23	33	56	22	34	525632.472	-0.294	0.004	59315549.0828	c
56	24	33	56	23	34	525632.472	-0.299	-0.001	59315549.0831	c

Table S4_2: Assigned transitions ν , ground state of monodeutero-oxirane, calculated energies E'' with parameters of WANG(SP) from Table 4, $\Delta_{O-C} = \nu_{obs.} - \nu_{cal.}$ values using LP and SP parameters, all given in MHz. Source **a** represents transitions from Hirose [43]; **b** from Albert et al. [14]; **c** from Müller et al [17]; **d** from reanalysis of the ground state in this work; **e** from ground state combination differences of rovibrational spectra in this work.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν / MHz	$\Delta_{O-C}(SP)$ / MHz	$\Delta_{O-C}(LP)$ / MHz	E''/h (MHz)	Source
56	21	35	56	20	36	566594.110	-0.132	-0.005	58202598.2715	c
56	22	35	56	21	36	566594.110	-0.132	-0.005	58202598.2715	c
56	15	41	56	14	42	681775.717	0.097	-0.005	54395875.3427	c
56	16	41	56	15	42	681775.717	0.097	-0.005	54395875.3427	c
56	14	42	56	13	43	700328.023	0.090	-0.001	53695547.4169	c
56	15	42	56	14	43	700328.023	0.090	-0.001	53695547.4169	c
56	13	43	56	12	44	718766.838	0.064	-0.003	52976780.6502	c
56	14	43	56	13	44	718766.838	0.064	-0.003	52976780.6502	c
56	5	51	56	4	52	863813.764	-0.187	0.002	46571799.2171	c
56	6	51	56	5	52	863813.764	-0.187	0.002	46571799.2171	c
56	4	52	56	3	53	881774.720	-0.128	0.005	45690024.3776	c
56	5	52	56	4	53	881774.720	-0.128	0.005	45690024.3776	c
56	3	53	56	2	54	899719.270	-0.017	0.008	44790305.0999	c
56	4	53	56	3	54	899719.270	-0.017	0.008	44790305.0999	c
57	1	57	56	0	56	1522106.321	-5.750	-4.892	42937076.7654	d
57	0	57	56	1	56	1522106.321	-5.750	-4.892	42937076.7654	d
57	2	55	56	3	54	1555500.536	-0.201	0.582	44790305.0999	d
57	3	55	56	2	54	1555500.536	-0.201	0.582	44790305.0999	d
57	16	41	57	15	42	679854.158	0.065	-0.037	56849772.1319	c
57	17	41	57	16	42	679854.158	0.065	-0.037	56849772.1319	c
57	18	39	57	17	40	642089.070	0.053	-0.003	58190684.7566	c
57	19	39	57	18	40	642089.070	0.053	-0.003	58190684.7566	c
57	17	40	57	16	41	661058.626	0.082	-0.006	57529626.2186	c
57	18	40	57	17	41	661058.626	0.082	-0.006	57529626.2186	c
57	7	50	57	6	51	844464.800	-0.229	-0.001	49903589.6793	c
57	8	50	57	7	51	844464.800	-0.229	-0.001	49903589.6793	c
57	6	51	57	5	52	862479.664	-0.241	-0.001	49041109.7828	c
57	7	51	57	6	52	862479.664	-0.241	-0.001	49041109.7828	c
57	5	52	57	4	53	880469.378	-0.242	-0.023	48160640.1710	c
57	6	52	57	5	53	880469.378	-0.242	-0.023	48160640.1710	c
57	4	53	57	3	54	898439.472	-0.141	0.011	47262200.5667	c
57	5	53	57	4	54	898439.472	-0.141	0.011	47262200.5667	c
57	3	54	57	2	55	916394.731	-0.023	0.003	46345805.8216	c
57	4	54	57	3	55	916394.731	-0.023	0.003	46345805.8216	c
58	9	49	58	8	50	824961.756	-0.171	0.013	53256172.9216	c
58	10	49	58	9	50	824961.756	-0.171	0.013	53256172.9216	c
58	8	50	58	7	51	843046.974	-0.237	-0.002	52413125.7188	c
58	9	50	58	8	51	843046.974	-0.237	-0.002	52413125.7188	c
58	6	52	58	5	53	879117.320	-0.282	0.000	50672911.2162	c
58	7	52	58	6	53	879117.320	-0.282	0.000	50672911.2162	c

Table C1(Corrected version of Table 1 in Albert et al. [14]): Spectroscopic parameters for the ground state of monodeutero-oxirane in the MW and GHz ranges in MHz (values in parenthesis provide statistical 1σ uncertainties in units of the last specified digits.).

	MW previous ^[43]	GHz
<i>A</i> /MHz	24252.47(17)	24252.6477 (44)
<i>B</i> /MHz	19905.34(17)	19905.5213 (44)
<i>C</i> /MHz	13327.40(17)	13327.5813 (44)
Δ_J /kHz		16.98 (18)
Δ_K /kHz		25.398 (18)
Δ_{JK} /kHz		17.369 (23)
δ_j /kHz		4.7521 (33)
δ_k /kHz		13.145 (13)
d_{rms} / kHz	-	27.59
N	20	112

[43] C. Hirose, *Bull. Chem. Soc. Jpn.*, 1974, **47**, 1311-1318.

Table C2 (Corrected version of Table 2 in Albert et al. [14]): Spectroscopic parameters for the ground state of C₂H₃DO in cm⁻¹.

	Only MW and GHz corresponding to Table CS1	MW,GHz and THz combined corresponding to Table CS2	CCSD(T)/cc-pVTZ ^b
A /cm ⁻¹	0.808981249	0.808981249	0.8089040
B /cm ⁻¹	0.663976720	0.663976720	0.6640071
C /cm ⁻¹	0.444560260	0.444560260	0.4445481
Δ_J / 10 ⁻⁶ cm ⁻¹	0.5715 (84) ^a	0.56955 (23) ^a	0.52333
Δ_K / 10 ⁻⁶ cm ⁻¹	0.8468 (15)	0.84983 (79)	0.58233
Δ_{JK} / 10 ⁻⁶ cm ⁻¹	0.5799 (17)	0.57554 (72)	0.74725
δ_J / 10 ⁻⁶ cm ⁻¹	0.15858 (21)	0.158118 (69)	0.1376
δ_K / 10 ⁻⁶ cm ⁻¹	0.4382 (11)	0.44194 (35)	0.54084
ϕ_J / 10 ⁻¹² cm ⁻¹	-	0.49 (7)	0.20
ϕ_{JK} / 10 ⁻¹² cm ⁻¹	-	6.2 (7)	5.681
ϕ_{KJ} / 10 ⁻¹² cm ⁻¹	-	-31 (2)	-28.98
ϕ_K / 10 ⁻¹² cm ⁻¹	-	29 (2)	25.27
η_J / 10 ⁻¹² cm ⁻¹	-	0.073 ^c	0.073
η_{JK} / 10 ⁻¹² cm ⁻¹	-	2.71 ^c	2.71
η_K / 10 ⁻¹² cm ⁻¹	-	2.06 ^c	2.06
d_{rms} /cm ⁻¹	0.0000035	0.000079	
n	132	530	

^a Values in parenthesis indicate uncertainties as 1 σ in units of the last digits given. Rotational constants without parenthesis were held fixed to the respective values of the ground state obtained by fitting only transitions in the GHz region of this study.

^b Scaled values from Ref. [28].

^c Fixed at the ab initio estimate from Ref. [28].

[14] S. Albert, Z. Chen, K. Keppler, P. Lerch, M. Quack, V. Schurig and O. Trapp, *Phys. Chem. Chem. Phys.* 2019, **21**, 3669.

[28] C. Puzzarini, M. Biczysko, J. Bloino and V. Barone, *Astrophys. J.*, 2014, **785**, 107.

Table CS1(Corrected version of Table S1 in Albert et al. [14]): Observed pure rotational transitions (ν , $\tilde{\nu}$, in MHz and cm^{-1}) of the ground state of oxirane- D_1 in **only MW and GHz regions**. J , K_a and K_c are quantum numbers, $\nu_{\text{obs.}}$ and $\tilde{\nu}_{\text{obs.}}$ = observed transition frequencies in MHz and cm^{-1} , and $\tilde{\nu}_{\text{calc.}}$ = wavenumbers using the reported spectroscopic parameters (lower states ", upper states '). Spectroscopic parameters used in fitting are presented in Table C2(2019).

J'	K_a'	K_c'	J''	K_a''	K_c''	$\nu_{\text{obs.}}/\text{MHz}$	$\tilde{\nu}_{\text{obs.}}/\text{cm}^{-1}$	$(\tilde{\nu}_{\text{obs.}} - \tilde{\nu}_{\text{calc.}})/10^{-6} \text{ cm}^{-1}$
1	1	0	1	0	1	10925.000	0.3644188	1.33
2	2	0	2	1	1	16822.390	0.5611345	-0.68
3	2	1	3	1	2	21212.880	0.7075855	-0.57
2	1	1	2	0	2	21284.050	0.7099595	-1.68
4	3	1	4	2	2	25443.480	0.8487031	-0.70
3	3	0	3	2	1	27356.030	0.9124989	0.80
5	3	2	5	2	3	31522.220	1.0514681	-0.22
2	2	1	2	1	2	32774.050	1.0932246	-6.89
6	4	2	6	3	3	33776.670	1.1266684	1.03
4	2	2	4	1	3	33890.100	1.1304521	1.49
5	4	1	5	3	2	35048.150	1.1690804	1.05
1	1	1	0	0	0	37580.170	1.2535395	0.77
3	1	2	3	0	3	38190.670	1.2739036	1.50
3	3	1	3	2	2	40137.710	1.3388499	1.05
4	4	0	4	3	1	41664.470	1.3897771	0.17
7	5	2	7	4	3	42052.250	1.4027121	-2.69
7	4	3	7	3	4	42232.500	1.4087246	2.58
8	5	3	8	4	4	42246.240	1.4091829	-1.49
2	0	2	1	1	1	58336.180	1.9458855	-29.70
4	2	3	4	1	4	59363.970	1.9801689	-24.00
6	4	3	6	3	4	62656.825	2.0900067	-0.31
6	5	2	6	4	3	62699.865	2.0914424	-0.62
2	1	2	1	0	1	64234.970	2.1426480	0.25
11	6	5	11	5	6	65496.695	2.1847346	-0.65
7	6	1	7	5	2	65932.715	2.1992786	-0.25
7	3	4	7	2	5	67338.650	2.2461756	-0.07
12	8	4	12	7	5	67347.590	2.2464738	-0.29
7	5	3	7	4	4	67514.320	2.2520353	-0.42
15	9	6	15	8	7	70130.820	2.3393124	-0.17
14	8	6	14	7	7	70867.180	2.3638747	-0.74
6	2	4	6	1	5	72394.960	2.4148359	0.34
6	6	0	6	5	1	72516.095	2.4188766	0.18
14	9	5	14	8	6	72596.450	2.4215569	-0.13
9	7	2	9	6	3	73267.970	2.4439564	-0.30
7	6	2	7	5	3	73448.350	2.4499732	-0.71

6	3	4	6	2	5	75075.845	2.5042606	0.43
7	4	4	7	3	5	75163.800	2.5071945	-0.09
5	2	4	5	1	5	75641.550	2.5231305	0.57
8	5	4	8	4	5	76727.350	2.5593489	-0.60
16	10	6	16	9	7	77916.300	2.5990080	0.13
13	7	6	13	6	7	78149.210	2.6067771	-1.09
17	10	7	17	9	8	78368.460	2.6140904	0.01
11	8	3	11	7	4	79506.710	2.6520584	-0.24
9	6	4	9	5	5	80528.270	2.6861340	-0.82
16	9	7	16	8	8	81927.410	2.7328042	-1.08
9	4	5	9	3	6	82055.520	2.7370775	-0.17
8	7	1	8	6	2	82247.660	2.7434866	-0.17
18	11	7	18	10	8	83540.420	2.7866085	0.72
13	9	4	13	8	5	84847.605	2.8302115	-0.32
9	7	3	9	6	4	84934.140	2.8330980	-0.68
8	7	2	8	6	3	85758.420	2.8605930	-0.27
2	2	1	1	1	0	86084.260	2.8714618	0.03
10	7	4	10	6	5	86993.135	2.9017786	-1.11
7	7	0	7	6	1	87035.740	2.9031998	0.16
19	11	8	19	10	9	87427.730	2.9162752	1.63
3	0	3	2	1	2	87497.970	2.9186181	0.23
8	3	5	8	2	6	87611.670	2.9224107	0.19
7	7	1	7	6	2	87677.750	2.9246149	0.10
12	6	6	12	5	7	88102.860	2.9387951	-0.92
3	1	3	2	0	2	89421.945	2.9827950	0.61
15	10	5	15	9	6	89500.575	2.9854178	-0.13
20	12	8	20	11	9	89679.520	2.9913868	2.43
9	5	5	9	4	6	89833.785	2.9965325	-0.44
8	4	5	8	3	6	90399.850	3.0154144	0.22
10	6	5	10	5	6	90544.615	3.0202433	-0.57
7	2	5	7	1	6	90710.475	3.0257758	0.64
10	8	2	10	7	3	90781.870	3.0281572	-0.58
15	8	7	15	7	8	91450.840	3.0504717	-1.23
7	3	5	7	2	6	91454.150	3.0505821	0.54
6	1	5	6	0	6	92326.200	3.0796705	1.05
6	2	5	6	1	6	92462.185	3.0842065	0.82
3	1	2	2	2	1	92914.360	3.0992894	0.92
11	7	5	11	6	6	93346.380	3.1137001	-0.99
17	11	6	17	10	7	93688.810	3.1251223	0.06
18	10	8	18	9	9	93832.630	3.1299196	0.04
11	8	4	11	7	5	96079.325	3.2048613	-0.89
2	2	0	1	1	1	96443.580	3.2170116	0.00
10	8	3	10	7	4	96740.480	3.2269151	-0.21
11	5	6	11	4	7	96853.615	3.2306888	-0.13
9	8	1	9	7	2	97557.390	3.2541643	0.30
19	12	7	19	11	8	97645.450	3.2571016	0.24
12	9	3	12	8	4	98181.120	3.2749696	-0.08

12	8	5	12	7	6	98794.820	3.2954405	-1.01
9	8	2	9	7	3	98984.540	3.3017689	0.47
8	8	0	8	7	1	101145.270	3.3738430	1.14
8	8	1	8	7	2	101362.465	3.3810879	1.11
21	13	8	21	12	9	101607.230	3.3892524	1.09
14	7	7	14	6	8	102575.520	3.4215511	-1.16
10	4	6	10	3	7	102729.985	3.4267034	0.38
12	7	6	12	6	7	104224.340	3.4765498	-0.46
11	6	6	11	5	7	104301.940	3.4791382	0.00
14	10	4	14	9	5	104511.930	3.4861427	-0.38
17	9	8	17	8	9	105329.080	3.5133999	-0.98
10	5	6	10	4	7	105466.650	3.5179888	0.45
23	14	9	23	13	10	105806.970	3.5293406	2.89
13	8	6	13	7	7	106072.960	3.5382131	-1.23
9	3	6	9	2	7	106180.250	3.5417919	0.91
20	11	9	20	10	10	106559.955	3.5544575	2.36
9	4	6	9	3	7	106975.370	3.5683143	0.67
13	9	5	13	8	6	107000.600	3.5691558	-1.38
11	9	2	11	8	3	107119.820	3.5731326	0.27
12	9	4	12	8	5	107327.490	3.5800597	-0.91
8	2	6	8	1	7	108180.625	3.6085172	1.77
8	3	6	8	2	7	108356.975	3.6143996	1.43
7	1	6	7	0	7	109393.200	3.6489644	1.98
7	2	6	7	1	7	109420.270	3.6498673	1.80
11	9	3	11	8	4	109749.690	3.6608556	0.05
16	11	5	16	10	6	109859.220	3.6645091	-0.96
14	9	6	14	8	7	110509.170	3.6861891	-1.08
13	6	7	13	5	8	111702.180	3.7259837	-0.23
10	9	1	10	8	2	112120.740	3.7399453	1.28
10	9	2	10	8	3	112648.970	3.7575652	1.09
3	2	2	2	1	1	112738.000	3.7605349	0.82
18	12	6	18	11	7	114335.560	3.8138238	-1.33
4	0	4	3	1	3	114895.670	3.8325070	1.10
9	9	0	9	8	1	115068.600	3.8382753	2.53
9	9	1	9	8	2	115137.940	3.8405883	2.25
4	1	4	3	0	3	115342.600	3.8474150	1.49
13	10	3	13	9	4	115727.940	3.8602686	-0.26
16	8	8	16	7	9	117278.590	3.9119927	-0.93
14	10	5	14	9	6	117620.250	3.9233892	-1.49
12	5	7	12	4	8	117766.965	3.9282831	0.50
15	10	6	15	9	7	117791.050	3.9290865	-1.47
14	8	7	14	7	8	117838.500	3.9306693	-0.26
20	13	7	20	12	8	118085.480	3.9389076	-2.09
13	7	7	13	6	8	118645.000	3.9575712	0.20
15	9	7	15	8	8	118778.340	3.9620190	-0.66
19	10	9	19	9	10	119688.180	3.9923679	0.43

[14] S. Albert, Z. Chen, K. Keppler, P. Lerch, M. Quack, V. Schurig and O. Trapp, *Phys. Chem. Chem. Phys.* 2019, **21**, 3669.

Table CS2 (Corrected version of Table S2 in Albert et al. [14]): 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 C2 (2019).

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	0.3644188	1.30
2	2	0	2	1	1	0.5611345	-0.66
3	2	1	3	1	2	0.7075855	-0.52
2	1	1	2	0	2	0.7099595	-1.69
4	3	1	4	2	2	0.8487031	-0.61
3	3	0	3	2	1	0.9124989	0.78
5	3	2	5	2	3	1.0514681	-0.08
2	2	1	2	1	2	1.0932246	-6.88
6	4	2	6	3	3	1.1266684	1.26
4	2	2	4	1	3	1.1304521	1.51
5	4	1	5	3	2	1.1690804	1.08
1	1	1	0	0	0	1.2535395	0.79
3	1	2	3	0	3	1.2739036	1.46
3	3	1	3	2	2	1.3388499	1.02
4	4	0	4	3	1	1.3897771	0.03
7	5	2	7	4	3	1.4027121	-2.59
7	4	3	7	3	4	1.4087246	2.93
8	5	3	8	4	4	1.4091829	-1.05
2	0	2	1	1	1	1.9458855	-29.80
4	2	3	4	1	4	1.9801689	-24.30
6	4	3	6	3	4	2.0900067	-0.21
6	5	2	6	4	3	2.0914424	-0.58
2	1	2	1	0	1	2.1426480	0.12
11	6	5	11	5	6	2.1847346	0.41
7	6	1	7	5	2	2.1992786	-0.49
7	3	4	7	2	5	2.2461756	-0.14
12	8	4	12	7	5	2.2464738	0.16
7	5	3	7	4	4	2.2520353	-0.16
15	9	6	15	8	7	2.3393124	0.55
14	8	6	14	7	7	2.3638747	0.52
6	2	4	6	1	5	2.4148359	-0.10
6	6	0	6	5	1	2.4188766	-0.41
14	9	5	14	8	6	2.4215569	0.48
9	7	2	9	6	3	2.4439564	-0.41
7	6	2	7	5	3	2.4499732	-0.69
10	5	5	10	4	6	2.4663851	0.05
6	6	1	6	5	2	2.4770893	-0.52
8	6	3	8	5	4	2.5019495	-0.05
5	1	4	5	0	5	2.5026510	-0.37
6	3	4	6	2	5	2.5042606	-0.01

7	4	4	7	3	5	2.5071945	-0.20
5	2	4	5	1	5	2.5231305	-0.23
8	5	4	8	4	5	2.5593489	-0.35
16	10	6	16	9	7	2.5990080	0.53
13	7	6	13	6	7	2.6067771	0.25
17	10	7	17	9	8	2.6140904	0.15
11	8	3	11	7	4	2.6520584	-0.08
9	6	4	9	5	5	2.6861340	-0.33
16	9	7	16	8	8	2.7328042	-0.03
9	4	5	9	3	6	2.7370775	-0.10
8	7	1	8	6	2	2.7434866	-0.59
18	11	7	18	10	8	2.7866085	0.14
13	9	4	13	8	5	2.8302115	0.17
9	7	3	9	6	4	2.8330980	-0.36
8	7	2	8	6	3	2.8605930	-0.51
2	2	1	1	1	0	2.8714618	-0.06
10	7	4	10	6	5	2.9017786	-0.31
7	7	0	7	6	1	2.9031998	-0.81
19	11	8	19	10	9	2.9162752	-0.07
3	0	3	2	1	2	2.9186181	0.00
8	3	5	8	2	6	2.9224107	-0.34
7	7	1	7	6	2	2.9246149	-0.76
12	6	6	12	5	7	2.9387951	0.01
3	1	3	2	0	2	2.9827950	0.37
15	10	5	15	9	6	2.9854178	0.73
20	12	8	20	11	9	2.9913868	-0.28
9	5	5	9	4	6	2.9965325	-0.47
8	4	5	8	3	6	3.0154144	-0.36
10	6	5	10	5	6	3.0202433	-0.17
7	2	5	7	1	6	3.0257758	-0.53
10	8	2	10	7	3	3.0281572	-0.68
15	8	7	15	7	8	3.0504717	0.19
7	3	5	7	2	6	3.0505821	-0.60
6	1	5	6	0	6	3.0796705	-0.53
6	2	5	6	1	6	3.0842065	-0.78
3	1	2	2	2	1	3.0992894	0.66
11	7	5	11	6	6	3.1137001	-0.15
17	11	6	17	10	7	3.1251223	0.89
18	10	8	18	9	9	3.1299196	0.05
11	8	4	11	7	5	3.2048613	0.06
2	2	0	1	1	1	3.2170116	-0.14
10	8	3	10	7	4	3.2269151	0.06
11	5	6	11	4	7	3.2306888	0.11
9	8	1	9	7	2	3.2541643	-0.47
19	12	7	19	11	8	3.2571016	0.39
12	9	3	12	8	4	3.2749696	0.37
12	8	5	12	7	6	3.2954405	0.19
9	8	2	9	7	3	3.3017689	-0.16

8	8	0	8	7	1	3.3738430	-0.46
8	8	1	8	7	2	3.3810879	-0.52
21	13	8	21	12	9	3.3892524	-0.72
14	7	7	14	6	8	3.4215511	-0.08
10	4	6	10	3	7	3.4267034	-0.20
12	7	6	12	6	7	3.4765498	0.11
11	6	6	11	5	7	3.4791382	0.03
14	10	4	14	9	5	3.4861427	0.77
17	9	8	17	8	9	3.5133999	0.07
10	5	6	10	4	7	3.5179888	-0.27
23	14	9	23	13	10	3.5293406	-2.79
13	8	6	13	7	7	3.5382131	-0.14
9	3	6	9	2	7	3.5417919	-0.48
20	11	9	20	10	10	3.5544575	0.03
9	4	6	9	3	7	3.5683143	-0.78
13	9	5	13	8	6	3.5691558	0.23
11	9	2	11	8	3	3.5731326	0.09
12	9	4	12	8	5	3.5800597	0.19
8	2	6	8	1	7	3.6085172	-0.31
8	3	6	8	2	7	3.6143996	-0.65
7	1	6	7	0	7	3.6489644	-0.82
7	2	6	7	1	7	3.6498673	-0.94
11	9	3	11	8	4	3.6608556	0.19
16	11	5	16	10	6	3.6645091	0.97
14	9	6	14	8	7	3.6861891	0.50
13	6	7	13	5	8	3.7259837	0.03
10	9	1	10	8	2	3.7399453	0.03
10	9	2	10	8	3	3.7575652	-0.12
3	2	2	2	1	1	3.7605349	0.46
18	12	6	18	11	7	3.8138238	1.19
4	0	4	3	1	3	3.8325070	0.58
9	9	0	9	8	1	3.8382753	-0.22
9	9	1	9	8	2	3.8405883	-0.55
4	1	4	3	0	3	3.8474150	0.96
13	10	3	13	9	4	3.8602686	0.49
16	8	8	16	7	9	3.9119927	0.06
14	10	5	14	9	6	3.9233892	0.58
12	5	7	12	4	8	3.9282831	-0.17
15	10	6	15	9	7	3.9290865	0.64
14	8	7	14	7	8	3.9306693	0.26
20	13	7	20	12	8	3.9389076	0.72
13	7	7	13	6	8	3.9575712	0.16
15	9	7	15	8	8	3.9620190	0.32
19	10	9	19	9	10	3.9923679	0.21
16	15	1	15	14	2	25.16907	453.00
23	8	15	22	9	14	25.26925	98.30
24	7	17	23	8	16	25.57088	-216.00
28	1	27	27	2	26	25.71829	-117.00

24	8	16	23	9	15	26.14916	16.20
26	5	21	25	6	20	26.20216	-164.00
25	7	18	24	8	17	26.45447	-216.00
27	4	23	26	5	22	26.52302	-118.00
29	1	28	28	2	27	26.60477	-76.80
26	6	20	25	7	19	26.76907	-107.00
17	16	1	16	15	2	26.78081	94.70
30	0	30	29	1	29	26.92788	-88.80
25	8	17	24	9	16	27.03017	-33.80
27	5	22	26	6	21	27.08788	-130.00
29	2	27	28	3	26	27.16790	-141.00
26	7	19	25	8	18	27.33846	-104.00
28	4	24	27	5	23	27.40891	-179.00
30	1	29	29	2	28	27.49102	-73.10
25	9	16	24	10	15	27.61405	238.00
27	6	21	26	7	20	27.65415	-75.70
31	0	31	30	1	30	27.81414	-51.20
26	8	18	25	9	17	27.91200	-31.50
28	5	23	27	6	22	27.97348	-104.00
30	2	28	29	3	27	28.05400	-119.00
27	7	20	26	8	19	28.22246	-134.00
29	4	25	28	5	24	28.29476	-111.00
31	1	30	30	2	29	28.37709	-62.20
18	17	1	17	16	2	28.39178	-243.00
26	9	17	25	10	16	28.49202	-78.00
28	6	22	27	7	21	28.53914	-80.60
30	3	27	29	4	26	28.61724	59.80
32	0	32	31	1	31	28.70016	-68.00
27	8	19	26	9	18	28.79429	-98.10
18	18	0	17	17	1	28.84857	-177.00
29	5	24	28	6	23	28.85881	-189.00
31	2	29	30	3	28	28.93996	-36.40
28	7	21	27	8	20	29.10664	-76.90
30	4	26	29	5	25	29.18037	-102.00
32	1	31	31	2	30	29.26296	-64.10
27	9	18	26	10	17	29.37154	-74.20
29	6	23	28	7	22	29.42402	-104.00
31	3	28	30	4	27	29.50274	-108.00
33	0	33	32	1	32	29.58613	67.90
28	8	20	27	9	19	29.67700	-103.00
30	5	25	29	6	24	29.74419	-67.80
32	2	30	31	3	29	29.82559	-91.00
27	10	17	26	11	16	29.95764	109.00
29	7	22	28	8	21	29.99077	-81.70
19	18	1	18	17	2	30.00236	-124.00
31	4	27	30	5	26	30.06582	-68.50
33	1	32	32	2	31	30.14861	-83.70
28	9	19	27	10	18	30.25194	-74.80

30	6	24	29	7	23	30.30886	-55.40
32	3	29	31	4	28	30.38824	-81.20
19	19	0	18	18	1	30.45915	396.00
34	0	34	33	1	33	30.47168	-23.60
31	5	26	30	6	25	30.62927	-77.80
33	2	31	32	3	30	30.71113	-34.50
28	10	18	27	11	17	30.83398	-79.30
30	7	23	29	8	22	30.87487	-79.30
32	4	28	31	5	27	30.95106	-47.50
34	1	33	33	2	32	31.03413	-23.10
29	9	20	28	10	19	31.13296	-92.40
31	6	25	30	7	24	31.19346	-98.20
33	3	30	32	4	29	31.27356	-29.90
35	0	35	34	1	34	31.35712	-17.70
32	5	27	31	6	26	31.51419	-64.70
34	2	32	33	3	31	31.59654	104.00
20	19	1	19	18	2	31.61191	-159.00
29	10	19	28	11	18	31.71189	-65.20
31	7	24	30	8	23	31.75889	-88.20
33	4	29	32	5	28	31.83607	-54.80
35	1	34	34	2	33	31.91938	-25.30
30	9	21	29	10	20	32.01427	-258.00
20	20	0	19	19	1	32.06770	-157.00
32	6	26	31	7	25	32.07800	-52.50
34	3	31	33	4	30	32.15862	-31.20
36	0	36	35	1	35	32.24233	-27.20
29	11	18	28	12	17	32.30018	94.00
31	8	23	30	9	22	32.32624	-6.64
33	5	28	32	6	27	32.39889	-75.80
35	2	33	34	3	32	32.48146	-30.10
30	10	20	29	11	19	32.59086	-8.43
32	7	25	31	8	24	32.64284	-57.40
34	4	30	33	5	29	32.72085	-81.80
36	1	35	35	2	34	32.80444	-1.28
31	9	22	30	10	21	32.89623	-54.90
33	6	27	32	7	26	32.96238	8.65
22	17	5	21	16	6	32.98443	-105.00
35	3	32	34	4	31	33.04348	-6.65
37	0	37	36	1	36	33.12734	-12.40
30	11	19	29	12	18	33.17480	-8.48
32	8	24	31	9	23	33.20927	-87.80
21	20	1	20	19	2	33.22122	497.00
34	5	29	33	6	28	33.28345	-18.50
36	2	34	35	3	33	33.36636	36.10
31	10	21	30	11	20	33.47045	-54.50
33	7	26	32	8	25	33.52663	-61.70
35	4	31	34	5	30	33.60553	9.97
37	1	36	36	2	35	33.68926	11.90

32	9	23	31	10	22	33.77823	3.45
34	6	28	33	7	27	33.84644	-62.70
36	3	33	35	4	32	33.92808	-16.90
38	0	38	37	1	37	34.01210	-23.20
31	11	20	30	12	19	34.05087	-173.00
35	5	30	34	6	29	34.16774	-19.60
37	2	35	36	3	34	34.25091	-15.40
32	10	22	31	11	21	34.35062	-37.90
34	7	27	33	8	26	34.41031	-18.70
36	4	32	35	5	31	34.48983	-47.60
38	1	37	37	2	36	34.57381	-13.00
23	18	5	22	17	6	34.59551	-375.00
33	9	24	32	10	23	34.66024	-17.40
35	6	29	34	7	28	34.73040	-23.00
37	3	34	36	4	33	34.81249	9.44
22	21	1	21	20	2	34.82829	-118.00
39	0	39	38	1	38	34.89669	25.10
32	11	21	31	12	20	34.92833	-57.90
34	8	26	33	9	25	34.97538	-27.70
36	5	31	35	6	30	35.05179	-44.60
23	19	4	22	18	5	35.06189	-163.00
38	2	36	37	3	35	35.13526	-37.50
35	7	28	34	8	27	35.29384	42.50
37	4	33	36	5	32	35.37398	-28.40
39	1	38	38	2	37	35.45818	16.20
34	9	25	33	10	24	35.54230	-1.32
36	6	30	35	7	29	35.61415	8.92
38	3	35	37	4	34	35.69661	-10.50
40	0	40	39	1	39	35.78097	-0.42
33	11	22	32	12	21	35.80653	-30.50
35	8	27	34	9	26	35.85825	-5.69
37	5	32	36	6	31	35.93574	71.50
34	10	24	33	11	23	36.11192	50.90
36	7	29	35	8	28	36.17710	19.50
24	19	5	23	18	6	36.20568	-180.00
38	4	34	37	5	33	36.25789	-5.98
40	1	39	39	2	38	36.34225	-17.70
35	9	26	34	10	25	36.42435	17.10
23	22	1	22	21	2	36.43495	-117.00
37	6	31	36	7	30	36.49763	-10.50
39	3	36	38	4	35	36.58054	24.50
41	0	41	40	1	40	36.66505	22.00
24	20	4	23	19	5	36.67008	-84.90
34	11	23	33	12	22	36.68530	-3.96
36	8	28	35	9	27	36.74097	-1.89
38	5	33	37	6	32	36.81929	14.50
40	2	38	39	3	37	36.90332	18.50
35	10	25	34	11	24	36.99276	36.80

37	7	30	36	8	29	37.06007	-77.30
39	4	35	38	5	34	37.14166	112.00
41	1	40	40	2	39	37.22611	-9.87
36	9	27	35	10	26	37.30623	-48.80
38	6	32	37	7	31	37.38093	18.40
40	3	37	39	4	36	37.46415	-15.40
42	0	42	41	1	41	37.54886	16.40
35	11	24	34	12	23	37.56446	-3.09
37	8	29	36	9	28	37.62351	2.86
39	5	34	38	6	33	37.70262	-7.16
41	2	39	40	3	38	37.78695	11.40
25	20	5	24	19	6	37.81434	-89.50
36	10	26	35	11	25	37.87361	-20.20
38	7	31	37	8	30	37.94304	27.30
40	4	36	39	5	35	38.02493	-8.68
24	23	1	23	22	2	38.04058	-78.00
42	1	41	41	2	40	38.10972	8.68
37	9	28	36	10	27	38.18811	-13.20
39	6	33	38	7	32	38.26380	-136.00
25	21	4	24	20	5	38.27699	-77.40
41	3	38	40	4	37	38.34759	35.90
43	0	43	42	1	42	38.43241	4.49
36	11	25	35	12	24	38.44379	-98.60
24	24	0	23	23	1	38.49428	-82.40
38	8	30	37	9	29	38.50588	13.70
40	5	35	39	6	34	38.58578	46.70
42	2	40	41	3	39	38.67034	32.60
37	10	27	36	11	26	38.75454	12.40
39	7	32	38	8	31	38.82573	85.10
41	4	37	40	5	36	38.90807	-1.97
43	1	42	42	2	41	38.99307	14.80
38	9	29	37	10	28	39.06978	-43.00
42	3	39	41	4	38	39.23069	1.33
44	0	44	43	1	43	39.31573	33.20
37	11	26	36	12	25	39.32347	-20.70
39	8	31	38	9	30	39.38803	17.60
26	21	5	25	20	6	39.42152	-77.70
41	5	36	40	6	35	39.46855	-34.00
43	2	41	42	3	40	39.55345	35.00
38	10	28	37	11	27	39.63538	0.52
25	24	1	24	23	2	39.64504	-96.40
40	7	33	39	8	32	39.70816	129.00
42	4	38	41	5	37	39.79100	61.90
44	1	43	43	2	42	39.87613	5.30
26	22	4	25	21	5	39.88269	-59.80
39	9	30	38	10	29	39.95123	-130.00
41	6	35	40	7	34	40.02927	38.40
25	25	0	24	24	1	40.09821	-68.60

43	3	40	42	4	39	40.11358	30.00
45	0	45	44	1	44	40.19874	6.34
38	11	27	37	12	26	40.20324	61.30
40	8	32	39	9	31	40.26994	7.40
42	5	37	41	6	36	40.35119	32.60
44	2	42	43	3	41	40.43627	14.30
39	10	29	38	11	28	40.51618	55.70
43	4	39	42	5	38	40.67354	12.20
45	1	44	44	2	43	40.75886	-66.90
40	9	31	39	10	30	40.83273	19.60
42	6	36	41	7	35	40.91171	227.00
44	3	41	43	4	40	40.99627	139.00
27	22	5	26	21	6	41.02732	-63.30
46	0	46	45	1	45	41.08148	-6.23
39	11	28	38	12	27	41.08285	-26.60
41	8	33	40	9	32	41.15166	34.60
26	25	1	25	24	2	41.24838	-80.20
45	2	43	44	3	42	41.31883	14.60
40	10	30	39	11	29	41.39681	60.90
42	7	35	41	8	34	41.47211	49.60
27	23	4	26	22	5	41.48710	-73.30
44	4	40	43	5	39	41.55586	15.00
46	1	45	45	2	44	41.64146	9.01
26	26	0	25	25	1	41.70097	-46.50
41	9	32	40	10	31	41.71395	84.10
43	6	37	42	7	36	41.79351	43.50
45	3	42	44	4	41	41.87866	221.00
40	11	29	39	12	28	41.96263	87.00
47	0	47	46	1	46	41.96396	-11.70
42	8	34	41	9	33	42.03312	45.30
44	5	39	43	6	38	42.11554	54.50
46	2	44	45	3	43	42.20112	24.70
41	10	31	40	11	30	42.27728	66.00
43	7	36	42	8	35	42.35372	48.70
45	4	41	44	5	40	42.43796	81.50
47	1	46	46	2	45	42.52359	-109.00
42	9	33	41	10	32	42.59478	-6.18
28	23	5	27	22	6	42.63175	-32.80
44	6	38	43	7	37	42.67513	-33.40
46	3	43	45	4	42	42.76050	42.30
29	21	9	28	20	8	42.82440	-46.60
41	11	30	40	12	29	42.84227	138.00
48	0	48	47	1	47	42.84622	52.80
27	26	1	26	25	2	42.85052	-59.00
43	8	35	42	9	34	42.91430	30.90
45	5	40	44	6	39	42.99728	50.70
47	2	45	46	3	44	43.08311	22.50
28	24	4	27	23	5	43.09027	-55.40

42	10	32	41	11	31	43.15753	33.80
44	7	37	43	8	36	43.23512	103.00
27	27	0	26	26	1	43.30249	-41.30
46	4	42	45	5	41	43.31964	13.90
48	1	47	47	2	46	43.40566	7.50
43	9	34	42	10	33	43.47552	50.80
45	6	39	44	7	38	43.55665	71.10
47	3	44	46	4	43	43.64220	7.49
42	11	31	41	12	30	43.72166	57.90
49	0	49	48	1	48	43.72807	-7.01
46	5	41	45	6	40	43.87873	49.40
48	2	46	47	3	45	43.96480	12.70
43	10	33	42	11	32	44.03765	77.80
45	7	38	44	8	37	44.11607	1.36
47	4	43	46	5	42	44.20112	41.00
29	24	5	28	23	6	44.23470	-89.30
49	1	48	48	2	47	44.28744	129.00
44	9	35	43	10	34	44.35598	64.80
46	6	40	45	7	39	44.43772	10.90
28	27	1	27	26	2	44.45141	-30.10
48	3	45	47	4	44	44.52364	18.70
43	11	32	42	12	31	44.60099	69.40
50	0	50	49	1	49	44.60965	-29.30
45	8	37	44	9	36	44.67591	65.60
47	5	42	46	6	41	44.75964	-188.00
49	2	47	48	3	46	44.84620	11.20
28	28	0	27	27	1	44.90275	-24.10
44	10	34	43	11	33	44.91751	90.10
46	7	39	45	8	38	44.99692	80.80
48	4	44	47	5	43	45.08226	36.10
50	1	49	49	2	48	45.16867	-0.77
45	9	36	44	10	35	45.23619	103.00
47	6	41	46	7	40	45.31862	89.80
49	3	46	48	4	45	45.40482	72.60
44	11	33	43	12	32	45.48013	73.10
51	0	51	50	1	50	45.49100	8.71
48	5	43	47	6	42	45.64073	57.00
50	2	48	49	3	47	45.72728	3.85
45	10	35	44	11	34	45.79711	74.50
30	25	5	29	24	6	45.83637	-31.00
47	7	40	46	8	39	45.87736	62.50
49	4	45	48	5	44	45.96310	37.90
31	23	9	30	22	8	46.04222	108.00
51	1	50	50	2	49	46.04979	70.90
29	28	1	28	27	2	46.05093	-72.80
46	9	37	45	10	36	46.11607	90.70
48	6	42	47	7	41	46.19911	59.30
50	3	47	49	4	46	46.28553	-36.80

45	11	34	44	12	33	46.35907	79.20
52	0	52	51	1	51	46.37197	-32.20
47	8	39	46	9	38	46.43630	30.50
29	29	0	28	28	1	46.50167	-31.10
49	5	44	48	6	43	46.52123	26.30
51	2	49	50	3	48	46.60806	-3.62
48	7	41	47	8	40	46.75747	12.50
50	4	46	49	5	45	46.84372	126.00
52	1	51	51	2	50	46.93042	-40.50
47	9	38	46	10	37	46.99569	90.70
49	6	43	48	7	42	47.07928	32.00
51	3	48	50	4	47	47.16640	335.00
46	11	35	45	12	34	47.23784	131.00
53	0	53	52	1	52	47.25256	-127.00
50	5	45	49	6	44	47.40143	13.80
31	26	5	30	25	6	47.43653	-42.10
52	2	50	51	3	49	47.48853	-0.41
49	7	42	48	8	41	47.63735	41.00
32	24	9	31	23	8	47.64707	26.00
30	29	1	29	28	2	47.64917	-57.60
51	4	47	50	5	46	47.72379	-3.30
53	1	52	52	2	51	47.81086	-27.30
48	9	39	47	10	38	47.87500	89.50
31	27	4	30	26	5	47.89174	-56.10
50	6	44	49	7	43	47.95919	59.20
52	3	49	51	4	48	48.04630	53.60
30	30	0	29	29	1	48.09922	-37.80
47	11	36	46	12	35	48.11603	-149.00
51	5	46	50	6	45	48.28128	-27.40
53	2	51	52	3	50	48.36868	6.25
50	7	43	49	8	42	48.51681	-17.10
52	4	48	51	5	47	48.60368	10.50
54	1	53	53	2	52	48.69098	1.38
49	9	40	48	10	39	48.75400	76.30
51	6	45	50	7	44	48.83854	-156.00
53	3	50	52	4	49	48.92614	39.90
48	11	37	47	12	36	48.99417	-216.00
55	0	55	54	1	54	49.01300	-104.00
32	27	5	31	26	6	49.03527	-36.30
52	5	47	51	6	46	49.16080	-71.40
31	30	1	30	29	2	49.24605	5.11
51	7	44	50	8	43	49.39607	46.90
53	4	49	52	5	48	49.48325	29.60
32	28	4	31	27	5	49.48949	-17.80
50	9	41	49	10	40	49.63279	165.00
31	31	0	30	30	1	49.69539	-11.60
52	6	46	51	7	45	49.71804	121.00
54	3	51	53	4	50	49.80559	-27.80

49	11	38	48	12	37	49.87242	94.80
56	0	56	55	1	55	49.89241	-409.00
53	5	48	52	6	47	50.04009	-9.17
52	7	45	51	8	44	50.27491	20.60
54	4	50	53	5	49	50.36239	-44.00
56	1	55	55	2	54	50.45003	-155.00
53	6	47	52	7	46	50.59654	-267.00
33	28	5	32	27	6	50.63252	-29.70
55	3	52	54	4	51	50.68470	-104.00
50	11	39	49	12	38	50.75017	191.00
57	0	57	56	1	56	50.77191	-297.00
32	31	1	31	30	2	50.84142	-16.10
34	26	9	33	25	8	50.85059	-15.80
33	29	4	32	28	5	51.08573	-26.10
32	32	0	31	31	1	51.29009	1.11
57	1	56	56	2	55	51.32923	-51.10
56	3	53	55	4	52	51.56359	-46.80
58	0	58	57	1	57	51.65130	57.60
34	29	5	33	28	6	52.22830	23.10
33	32	1	32	31	2	52.43534	5.22
35	27	9	34	26	8	52.44942	-28.10
34	30	4	33	29	5	52.68045	-47.30
33	33	0	32	32	1	52.88329	18.60
35	30	5	34	29	6	53.82243	-18.20
34	33	1	33	32	2	54.02771	5.45
36	28	9	35	27	8	54.04640	-17.60
35	31	4	34	30	5	54.27368	-23.90
34	34	0	33	33	1	54.47491	8.23
35	34	1	34	33	2	55.61853	38.90
37	29	9	36	28	8	55.64152	-1.32
36	32	4	35	31	5	55.86537	48.50
35	35	0	34	34	1	56.06495	8.15
37	32	5	36	31	6	57.00597	9.81
36	35	1	35	34	2	57.20767	7.87
38	30	9	37	29	8	57.23477	-5.72
37	33	4	36	32	5	57.45533	9.75
36	36	0	35	35	1	57.65333	0.48
38	33	5	37	32	6	58.59524	3.08
37	36	1	36	35	2	58.79514	-19.60
38	34	4	37	33	5	59.04364	3.95
37	37	0	36	36	1	59.24004	6.18
39	34	5	38	33	6	60.18279	-1.56
38	37	1	37	36	2	60.38094	10.70
40	32	9	39	31	8	60.41570	1.00
39	35	4	38	34	5	60.63024	10.60
38	38	0	37	37	1	60.82502	25.10
40	35	5	39	34	6	61.76859	12.50
39	38	1	38	37	2	61.96497	15.60

40	36	4	39	35	5	62.21509	25.60
39	39	0	38	38	1	62.40822	41.10
41	36	5	40	35	6	63.35259	11.30
40	39	1	39	38	2	63.54719	31.10
41	37	4	40	36	5	63.79823	142.00
42	37	5	41	36	6	64.93474	12.60
41	40	1	40	39	2	65.12749	-23.30
43	38	5	42	37	6	66.51496	-19.70
44	39	5	43	38	6	68.09330	-2.52
45	40	5	44	39	6	69.66964	-12.40

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Table CS3 (Corrected version of Table S3 in Albert et al. [14]): 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 C2 using transitions listed in Table CS2 (2019).

J'	K_a'	K_c'	J''	K_a''	K_c''	<i>Predicted Frequency / MHz</i>
11	1	11	10	0	10	301640.634835
11	0	11	10	1	10	301640.633454
9	4	6	8	3	5	301895.269413
9	4	5	8	5	4	303420.007836
10	3	8	9	2	7	309031.992292
10	2	8	9	3	7	308985.617240
8	5	4	7	4	3	313911.738482
7	5	2	6	4	3	316586.849796
7	6	2	6	5	1	317358.512835
11	2	10	10	1	9	318600.141169
11	1	10	10	2	9	318599.966075
7	6	1	6	5	2	319819.696639
10	3	7	9	4	6	325821.601577
10	4	7	9	3	6	326860.450333
12	1	12	11	0	11	328282.593441
12	0	12	11	1	11	328282.593241
9	5	5	8	4	4	331568.679313
7	7	0	6	6	1	332594.177353
7	7	1	6	6	0	332520.180681
11	3	9	10	2	8	335620.736563
11	2	9	10	3	8	335611.599264
10	4	6	9	5	5	338717.792589
12	2	11	11	1	10	345236.717114
12	1	11	11	2	10	345236.688534
8	6	3	7	5	2	346865.972692
10	5	6	9	4	5	350271.580599
11	4	8	10	3	7	352939.677816
11	3	8	10	4	7	352688.627089
13	1	13	12	0	12	354922.365742
13	0	13	12	1	12	354922.365713
8	6	2	7	5	3	358772.682526
12	3	10	11	2	9	362233.634992
12	2	10	11	3	9	362231.924490
8	7	2	7	6	1	366691.680247
8	7	1	7	6	2	367571.989583
11	4	7	10	5	6	368707.924279
9	6	4	8	5	3	369850.686077
7	3	4	6	2	5	370034.785304
13	2	12	12	1	11	371871.957363
13	1	12	12	2	11	371871.952810
11	5	7	10	4	6	372490.025935
12	4	9	11	3	8	379381.736232

12	3	9	11	4	8	379326.069511
8	8	0	7	7	1	381039.503890
8	8	1	7	7	0	381018.399868
14	1	14	13	0	13	381559.747191
14	0	14	13	1	13	381559.747187
10	6	5	9	5	4	387286.873877
13	3	11	12	2	10	388853.695660
13	2	11	12	3	10	388853.388167
12	4	8	11	5	7	396308.827580
12	5	8	11	4	7	397362.564661
14	2	13	13	1	12	398505.286264
14	1	13	13	2	12	398505.285553
9	7	3	8	6	2	398755.416581

[14] S. Albert, Z. Chen, K. Keppler, P. Lerch, M. Quack, V. Schurig and O. Trapp, *Phys. Chem. Chem. Phys.* 2019, **21**, 3669.

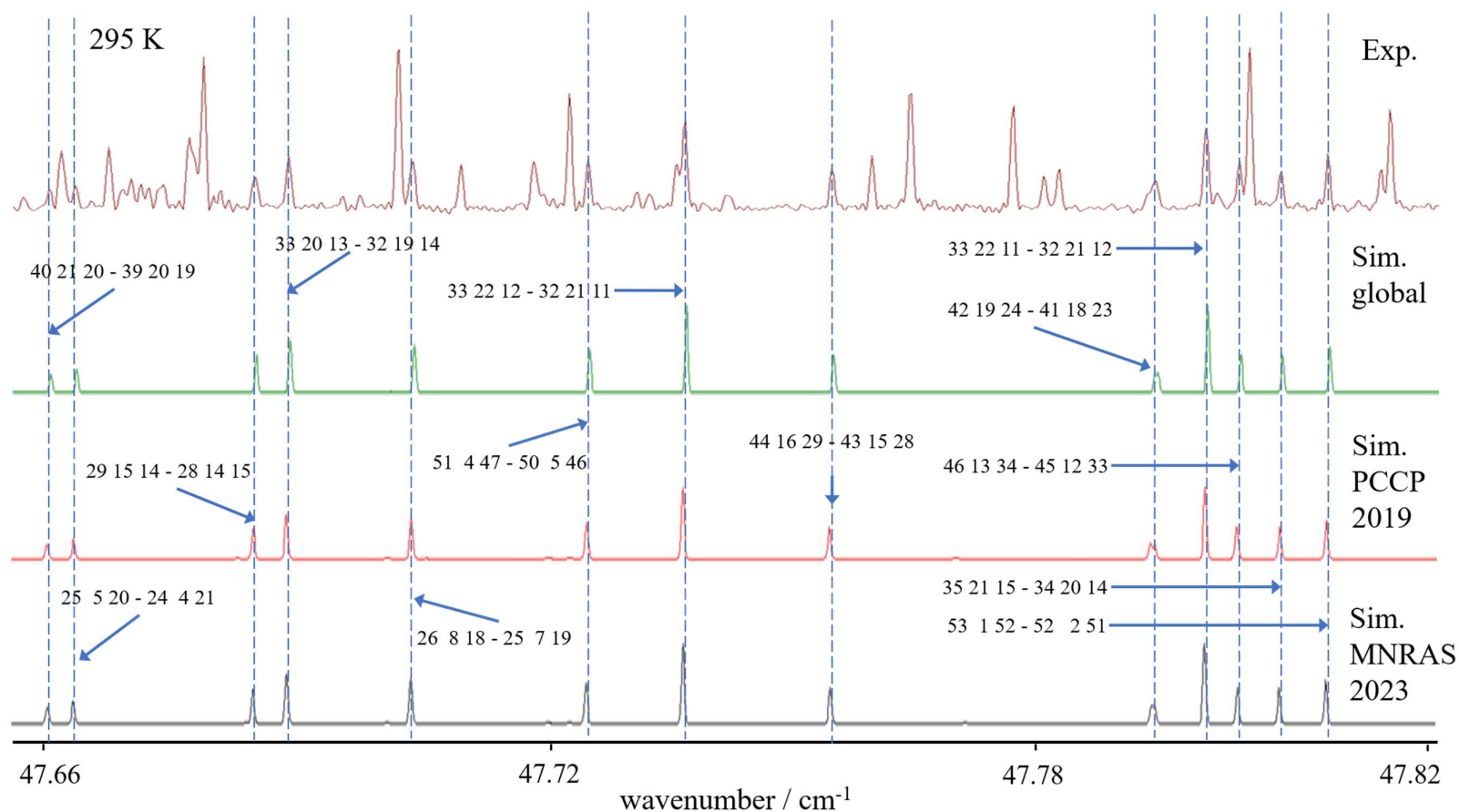


Figure S_1: A comparison of the THz spectrum of monodeutero-oxirane near 47.7 cm^{-1} (from top to bottom): 1) observed spectrum; 2) simulated spectrum based on the global analysis of this study (Table 4, column 4); 3) simulated spectrum reproduced using data in [14] (Table 4, column 1); 4) simulated spectrum reproduced using data in [16] (Table 4, column 2). Quantum numbers of transitions are arranged in the form of $J'K_a'K_c' - J''K_a''K_c''$.

[14] S. Albert, Z. Chen, K. Keppler, P. Lerch, M. Quack, V. Schurig and O. Trapp, *Phys. Chem. Chem. Phys.* 2019, **21**, 3669.

[17] H. S. P. Müller, J. K. Jørgensen, J.-C. Guillemin, F. Lewen, S. Schlemmer, *Monthly Notices of the Royal Astronomical Society* 2023, **518**(1), 185.

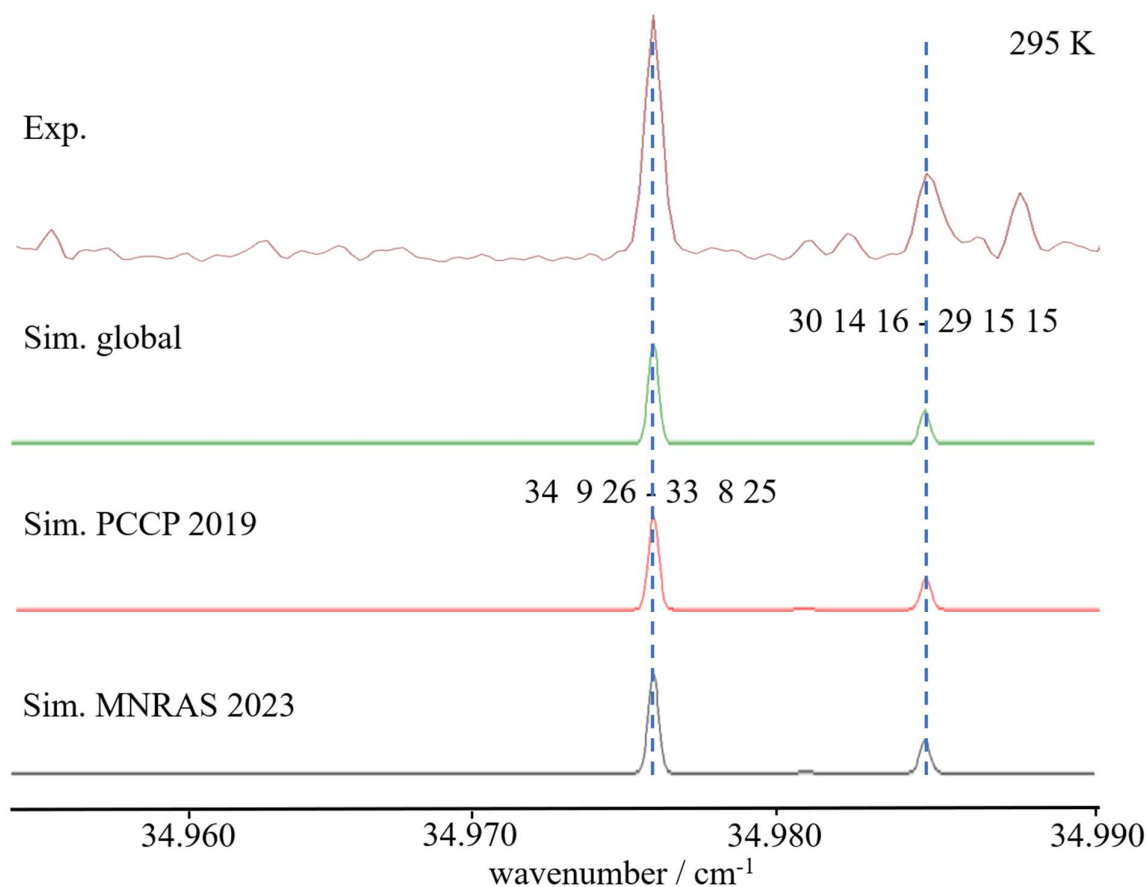


Figure S_2: A comparison of the THz spectrum of monodeutero-oxirane near 35 cm^{-1} (from top to bottom): 1) observed spectrum; 2) simulated spectrum based on the global analysis of this study (Table 4, column 4); 3) simulated spectrum reproduced using data in [14] (Table 4, column 1); 4) simulated spectrum reproduced using data in [16] (Table 4, column 2). Quantum numbers of transitions are arranged in the form of $J'K_a'K_c' - J''K_a''K_c''$.

[14] S. Albert, Z. Chen, K. Keppler, P. Lerch, M. Quack, V. Schurig and O. Trapp, *Phys. Chem. Chem. Phys.* 2019, **21**, 3669.

[17] H. S. P. Müller, J. K. Jørgensen, J.-C. Guillemin, F. Lewen, S. Schlemmer, *Monthly Notices of the Royal Astronomical Society* 2023, **518**(1), 185.

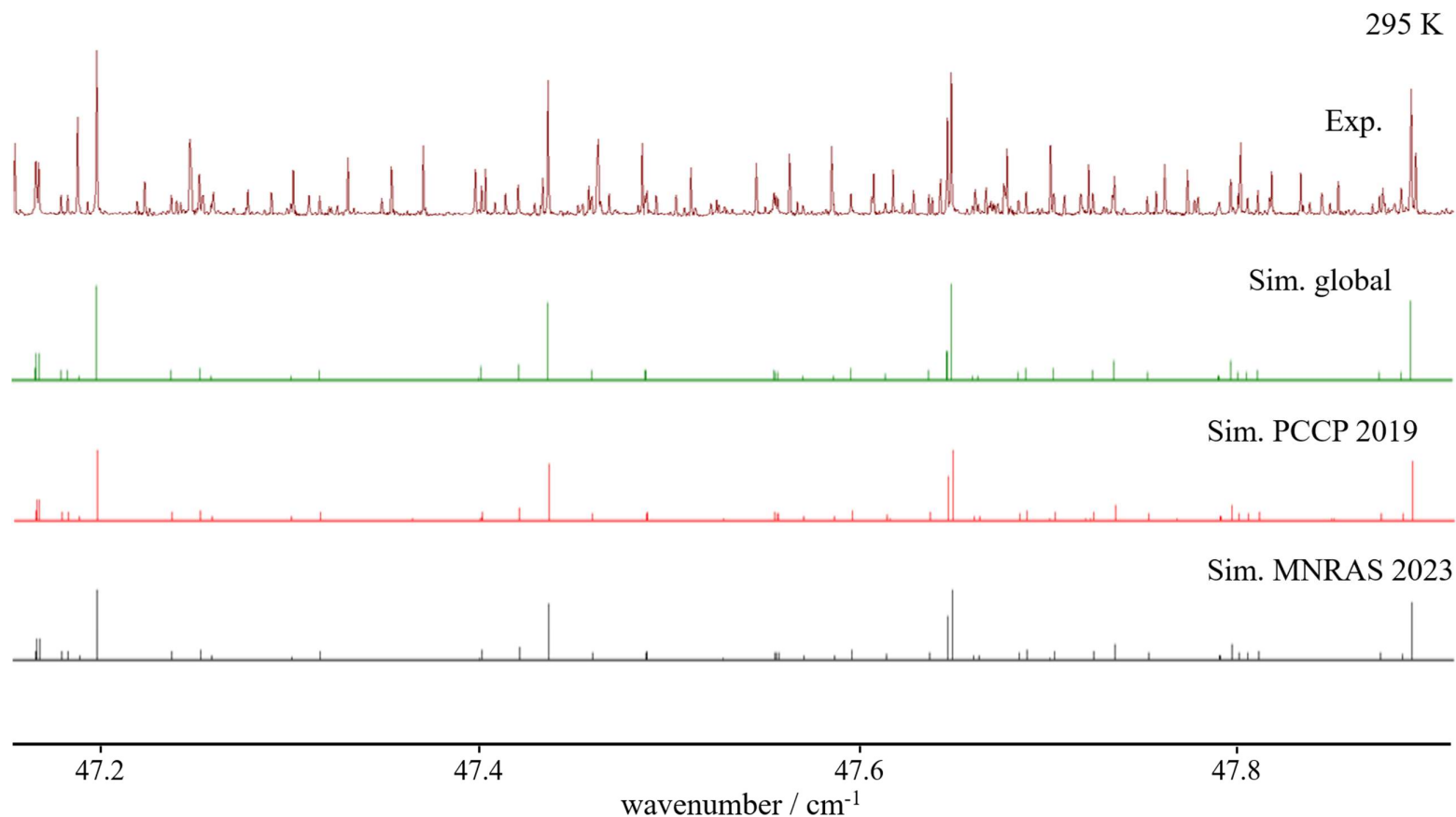


Figure S_3: A comparison of the THz spectrum of monodeutero-oxirane near 47.5 cm^{-1} (from top to bottom): 1) observed spectrum; 2) simulated spectrum based on the global analysis of this study (Table 4, column 4); 3) simulated spectrum reproduced using data in [14] (Table 4, column 1); 4) simulated spectrum reproduced using data in [16] (Table 4, column 2).

[14] S. Albert, Z. Chen, K. Keppler, P. Lerch, M. Quack, V. Schurig and O. Trapp, *Phys. Chem. Chem. Phys.* 2019, **21**, 3669.

[17] H. S. P. Müller, J. K. Jørgensen, J.-C. Guillemin, F. Lewen, S. Schlemmer, *Monthly Notices of the Royal Astronomical Society* 2023, **518**(1), 185.

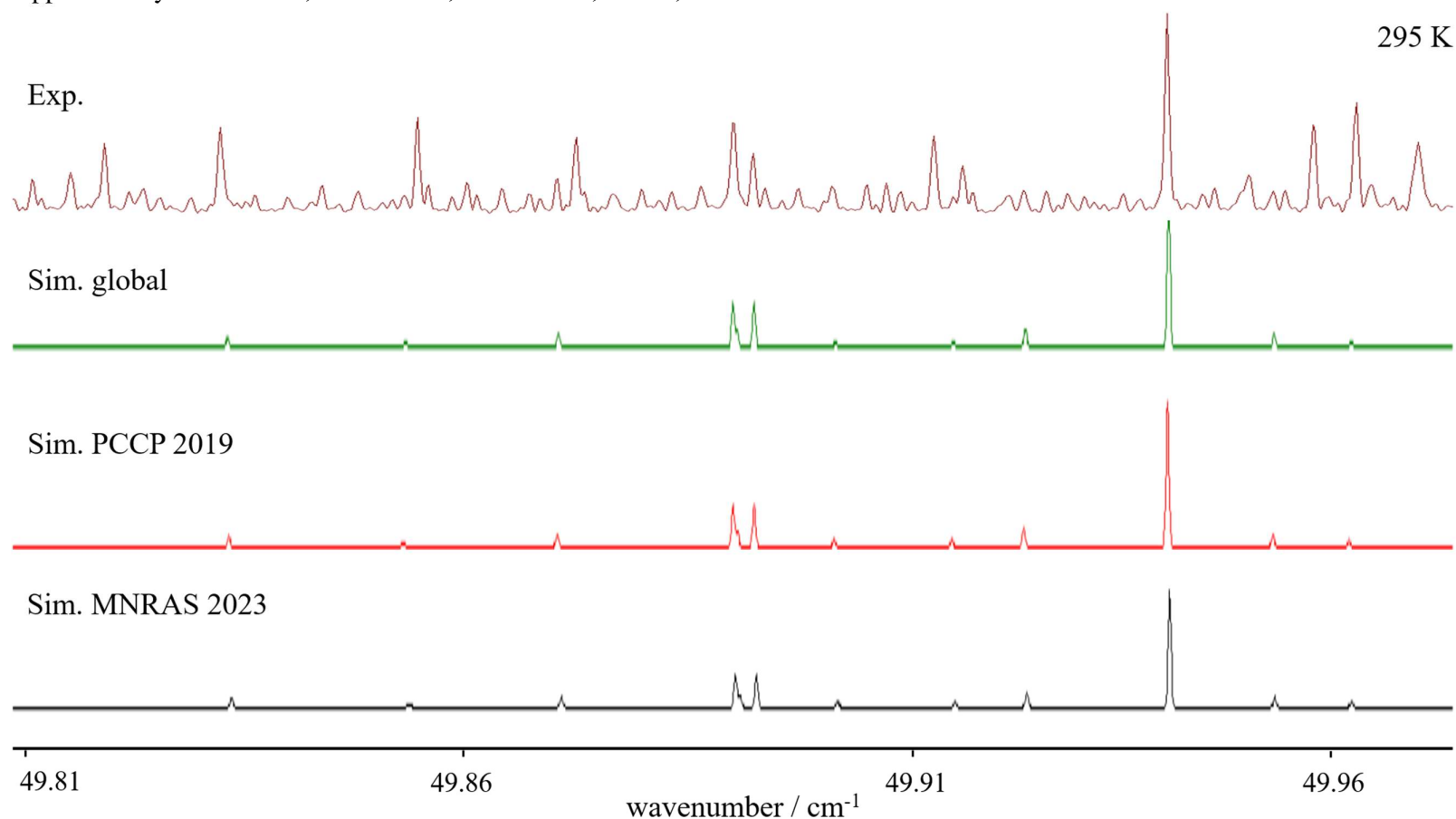


Figure S_4: A comparison of the THz spectrum of monodeutero-oxirane near 49.9 cm⁻¹ (from top to bottom): 1) observed spectrum; 2) simulated spectrum based on the global analysis of this study (Table 4, column 4); 3) simulated spectrum reproduced using data in [14] (Table 4, column 1); 4) simulated spectrum reproduced using data in [16] (Table 4, column 2).

[14] S. Albert, Z. Chen, K. Keppler, P. Lerch, M. Quack, V. Schurig and O. Trapp, *Phys. Chem. Chem. Phys.* 2019, **21**, 3669.

[17] H. S. P. Müller, J. K. Jørgensen, J.-C. Guillemin, F. Lewen, S. Schlemmer, *Monthly Notices of the Royal Astronomical Society* 2023, **518**(1), 185.

Table Sa: Anharmonic constants as calculated ab initio.

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Anharmonic constants χ_{kl} in cm^{-1} : Lower triangular form of the anharmonicities (in cm^{-1}).

Numbering follows the numbers of the fundamentals $i = (k,l)$ from

$i = 1$ (highest wavenumber 3252.318 cm^{-1} , Table 1, column 2) to

$i = 15$ (lowest wavenumber 714.490 cm^{-1} , Table 1, column 2).

D stands for the decadic exponent, i.e. $\text{D}+02 = 10^2$, etc.

	1	2	3	4	5
1	-0.318548D+02				
2	-0.370995D+01	-0.568669D+02			
3	-0.111801D+03	-0.145267D+01	-0.276991D+02		
4	0.370004D+00	-0.232303D+01	0.247123D+00	-0.309809D+02	
5	-0.160141D+02	0.150786D-01	-0.284492D+02	-0.153674D+01	-0.136926D+01
6	-0.183818D+01	-0.793796D+01	-0.144956D+01	-0.601450D+01	-0.208127D+01
7	-0.103097D+01	-0.646084D+01	-0.320538D+00	-0.104795D+01	-0.329955D+01
8	-0.323229D+01	-0.811659D+01	-0.382382D+01	0.199816D+01	-0.811351D+01
9	-0.950500D+01	-0.123647D+01	-0.249665D+01	-0.180611D-01	-0.711784D+01
10	-0.525718D+01	-0.373755D+01	-0.654545D+01	0.271570D+00	-0.399724D+01
11	-0.343331D+01	-0.301256D+01	-0.361405D+01	-0.337564D+01	-0.398373D+01
12	-0.889457D+00	-0.727189D+00	-0.898302D+00	0.843358D+00	-0.225854D+01
13	-0.347153D+00	-0.352604D+01	-0.713369D+00	-0.273137D+01	-0.334157D+01
14	-0.137560D+01	0.123279D+01	-0.904554D+00	-0.227103D+01	-0.437044D+01
15	-0.240431D+01	-0.291543D+01	-0.226681D+01	-0.525310D+01	-0.320051D+01
	6	7	8	9	10
6	-0.573918D+01				
7	-0.558576D+01	-0.235646D+01			
8	-0.153587D+01	-0.225316D+01	-0.168531D+01		
9	-0.114929D+01	-0.443716D+01	0.544700D+00	-0.370861D+01	
10	-0.151149D+01	-0.293428D+01	-0.292612D+01	-0.519490D+01	-0.143238D+01
11	-0.155723D+01	-0.320351D+01	-0.318611D+01	-0.704627D+00	-0.172151D+01
12	-0.450422D+01	-0.725224D+01	-0.266883D+01	-0.218572D+01	-0.339598D+01
13	-0.531677D+01	-0.310476D+01	-0.685599D+00	-0.280239D+01	-0.380105D+01
14	-0.376891D+01	-0.467580D+01	-0.244705D+01	-0.272994D+01	-0.226236D+01
15	-0.751794D+01	-0.226926D+01	0.347592D+00	0.834654D+00	0.260555D+00
	11	12	13	14	15
11	-0.179890D+01				
12	-0.177031D+01	-0.235109D+01			
13	0.228810D+00	-0.255552D+01	-0.153624D+01		
14	-0.321968D+01	-0.476795D+01	-0.328043D+01	-0.277245D+01	
15	-0.136965D+01	-0.698628D+00	0.360389D+01	-0.108673D+01	0.106652D+01