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Hydrogen versus tetrel bonds in complexes of 3-oxetanone with water and formaldehyde

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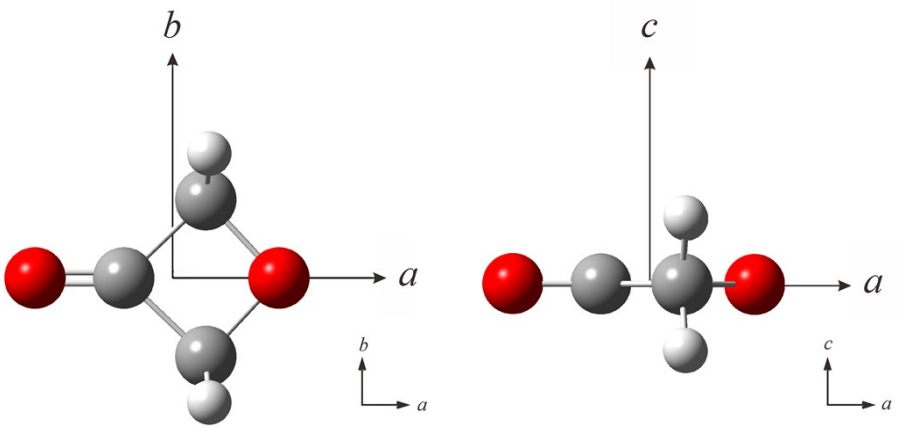
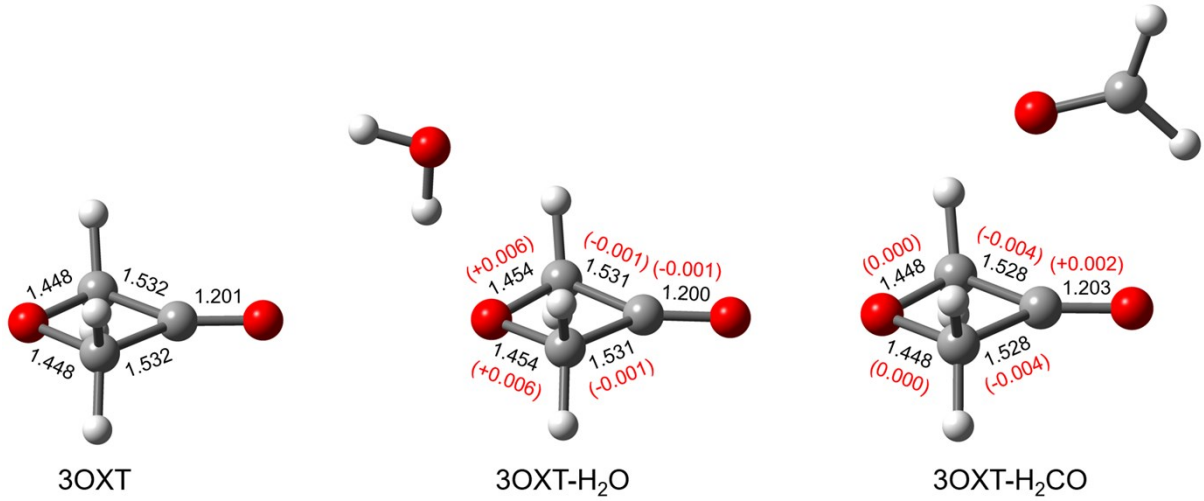
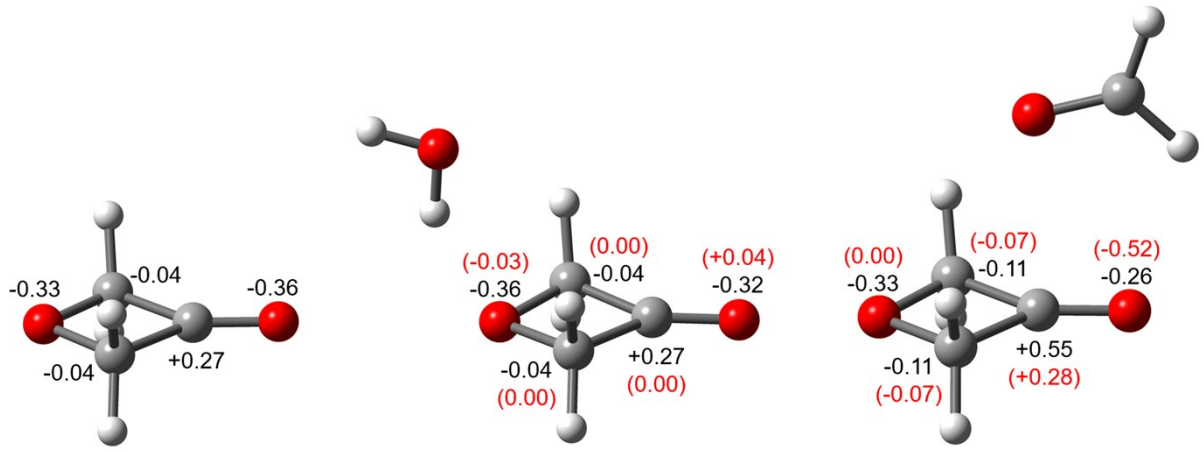


Figure S1. Geometry and principal axes of the 3OXT monomer with two views.



3OXT 3OXT-H_2O 3OXT-H_2CO

Figure S2 Comparison of theoretically optimized geometries of 3OXT, 3OXT-H_2O and 3OXT-H_2CO at MP2/6-311++g(d,p) level. Values in parentheses are the changes upon complexation.



3OXT 3OXT-H_2O 3OXT-H_2CO

Figure S3 Atomic charges of 3OXT and of the 3OXT moiety in 3OXT-H_2O and 3OXT-H_2C according to Hirshfeld population analysis. Values in parentheses are the changes upon complexation.

Table S1. Shapes and spectroscopic parameters of three predicted isomers of 3OXT-H_2O.

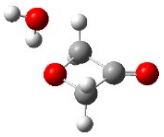
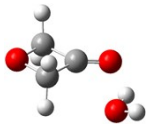
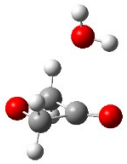
	W-I	W-II	W-III
			
ΔE[cm^{-1}]	0	207	613
ΔE_{ZPE}[cm^{-1}]	0	201	438
$\Delta E_{ZPE,BSSE}$[cm^{-1}]	0	157	427
A [MHz]	6235	6363	4187
B [MHz]	1827	2133	2690
C [MHz]	1796	1634	2172
μ_a,μ_b,μ_c[D]	-1.0,-2.1,0.3	0.3,1.0,0.8	-0.3,1.7,0.3

Table S2. Shapes and spectroscopic parameters of four predicted isomers of 3OXT-H_2CO.

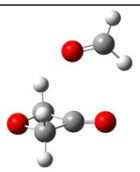
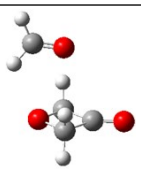
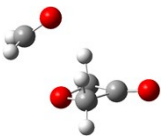
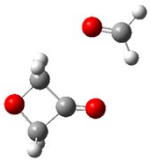
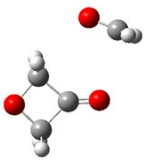
	FA-I	FA-II	FA-III	FA-IV	FA-V
					
ΔE[cm^{-1}]	0	83	49	338	265
ΔE_{ZPE}[cm^{-1}]	0	48	51	200	207
$\Delta E_{ZPE,BSSE}$[cm^{-1}]	30	74	92	0	111
A [MHz]	4068	3975	4806	5568	5431
B [MHz]	1732	1688	1496	1310	1431
C [MHz]	1487	1444	1391	1075	1165
μ_a,μ_b,μ_c[D]	1.9,0.8,0	2.0,-2.2,0	1.3,-2.4,0	-1.1,1.5,0	-0.3,1.7,0.3

Table S3. Experimental spectroscopic parameters of 8 isoptopologues of 3OXT-H_2O.

	Parent	^{13}C4/C5	^{13}C2	$^{18}O_{3OXT}$
A [MHz]	5907.7955(9)[a]	5817.610(3)	5905.455(2)	5815.688(1)
B [MHz]	1873.7304(2)	1866.1540(8)	1864.2452(4)	1811.2126(4)
C [MHz]	1810.2588(2)	1808.7814(1)	1801.1548(5)	1743.4268(4)
D_J [kHz]	8.228(2)	[8.228][b]	[8.228]	7.687(3)
D_{JK} [kHz]	-61.20(1)	[-61.20]	[-61.20]	-60.19(2)
d_1 [kHz]	-1.738(3)	[-1.738]	[-1.738]	-1.642(6)
d_2 [kHz]	0.058(1)	[0.058]	[0.058]	0.048(2)
P_{aa}[uÅ^2]	231.674(6)	231.67(2)	233.05(1)	241.00(1)
P_{bb}[uÅ^2]	47.500(6)	47.73(2)	47.54(1)	48.87(1)
P_{cc}[uÅ^2]	38.044(6)	39.14(2)	38.04(1)	38.02(1)
N [c]	28	10	10	28
σ [kHz] [d]	1.1	3.8	2.5	2.0
	$^{18}O_{H2O}$	DOH	HOD	D_2O
A [MHz]	5828.357(1)	5936.959(2)	5867.498(1)	5895.811(1)
B [MHz]	1782.2747(4)	1836.695(1)	1795.4846(7)	1762.4220(6)
C [MHz]	1717.7815(4)	1778.550(1)	1733.9712(7)	1705.7386(6)
χ_{aa}(D11) [MHz]	-	0.020(4)	-	-0.009(2)
χ_{bb}-χ_{cc}(D11) [MHz]	-	0.208(8)	-	0.256(8)
χ_{aa}(D12) [MHz]	-	-	0.245(3)	0.299(2)
χ_{bb}-χ_{cc}(D12) [MHz]	-	-	0.009(2)	0.029(2)
D_J [kHz]	7.727(3)	7.63(1)	7.322(8)	6.860(6)
D_{JK} [kHz]	-58.95(2)	-58.14(8)	-57.80(6)	-55.19(7)
d_1 [kHz]	-1.586(6)	-1.65(2)	-1.55(1)	-1.472(9)
d_2 [kHz]	0.039(2)	0.004(1)	0.051(9)	0.047(8)
P_{aa}[uÅ^2]	245.52(1)	237.09(3)	243.40(2)	248.66(2)
P_{bb}[uÅ^2]	48.68(1)	47.06(3)	48.06(2)	47.62(2)
P_{cc}[uÅ^2]	38.03(1)	38.06(3)	38.07(2)	38.09(2)
N [c]	28	62	57	126
σ [kHz] [d]	1.9	4.5	3.4	4.4

[a] Numbers in parentheses are standard errors in units of the least significant digit;
[b] Values of centrifugal distortion constants are fixed at those of the parent species;
[c] Number of lines in the fit;
[d] Relative standard deviation of the fit.

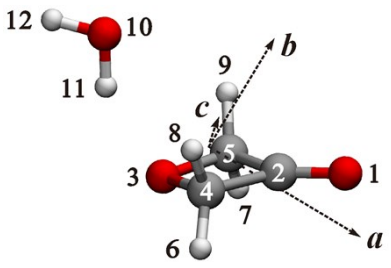


Table S4. Experimental spectroscopic parameters of 6 isoptopologues of 3OXT-H_2CO.

	Parent		$^{18}O_{3OXT}$	
	v =0	v = 1	v = 0	v = 1
A [MHz]	4077.9047(4)[a]	4077.8392(4)	3896.978(2)	3896.913(2)
B [MHz]	1683.3473(2)	1683.3402(2)	1683.3584(6)	1683.3518(6)
C [MHz]	1452.3693(2)	1452.3728(2)	1428.5852(5)	1428.5881(5)
D_J [kHz]	2.710(2)		2.624(4)	
D_{JK} [kHz]	-4.488(8)		-4.35(3)	
D_K [kHz]	14.84(4)		13.5(4)	
d_1 [kHz]	-0.559(1)		-0.594(5)	
P_{aa}[uÅ^2]	262.130(1)	262.130(1)	262.15(2)	262.15(2)
P_{bb}[uÅ^2]	85.838(1)	85.838(1)	91.61(2)	91.61(2)
P_{cc}[uÅ^2]	38.092(1)	38.094(1)	38.07(2)	38.07(2)
N [b]	52	55	30	30
σ [kHz] [c]	3.1		2.9	

	$^{18}O_{H2CO}$		^{13}C2	^{13}C4/5	^{13}C11
	v = 0	v = 1			
A [MHz]	4023.864(4)	4023.817(4)	4061.0986(8)	4040.664(1)	4077.836(1)
B [MHz]	1647.0611(5)	1647.0554(5)	1681.5588(4)	1669.4795(5)	1643.8501(5)
C [MHz]	1418.6143(4)	1418.6165(4)	1448.8865(3)	1446.4646(3)	1422.8853(4)
D_J [kHz]	[2.710][d]		[2.710]	[2.710]	[2.710]
D_{JK} [kHz]	[-4.488]		[-4.488]	[-4.488]	[-4.488]
D_K [kHz]	[14.84]		[14.84]	[14.84]	[14.84]
d_1 [kHz]	[-0.559]		[-0.559]	[-0.559]	[-0.559]
P_{aa}[uÅ^2]	268.74(2)	268.74(2)	262.45(2)	263.51(2)	269.34(2)
P_{bb}[uÅ^2]	87.50(2)	87.50(2)	86.35(2)	85.87(2)	85.84(2)
P_{cc}[uÅ^2]	38.09(2)	38.09(2)	38.09(2)	39.20(2)	38.09(2)
N [b]	14	16	16	17	15
σ [kHz] [c]	3.8		3.2	3.9	3.8

[a] Numbers in parentheses are standard errors in units of the least significant digit;
[b] Number of lines in the fit;
[c] Relative standard deviation of the fit;
[d] Centrifugal distortion constants are fixed at the values of the parent species.

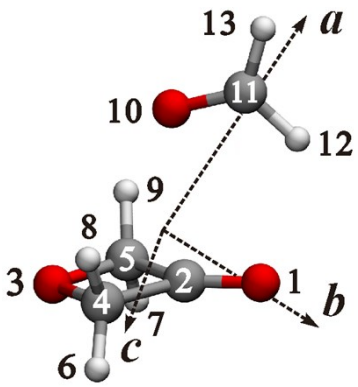

13
a
11
10
12
9
8
5
3
2
1
b
4
7
c
6

Table S5. Experimental transition frequencies (MHz) of the parent species of 3OXT-H_2O.

J'	K_a'	K_c'	←	J''	K_a''	K_c''	ν_{obs}	$\Delta\nu_{obs-calc}$
2	0	2		1	0	1	7366.9737	0.0006
2	1	2		1	1	1	7304.5462	0.0023
2	1	1		1	1	0	7431.3782	0.0022
3	0	3		2	0	2	11048.1167	0.0000
3	1	3		2	1	2	10955.9659	-0.0002
3	1	2		2	1	1	11146.0007	0.0005
3	2	2		2	2	1	11052.5425	0.0002
3	2	1		2	2	0	11055.5157	-0.0001
4	0	4		3	0	3	14726.4670	-0.0003
4	1	4		3	1	3	14606.3798	0.0001
4	1	3		3	1	2	14859.3434	-0.0003
4	2	3		3	2	2	14735.2185	-0.0014
4	2	2		3	2	1	14742.6309	0.0001
4	3	2		3	3	1	14739.7165	-0.0026
4	3	1		3	3	0	14739.7527	0.0008
5	0	5		4	0	4	18401.1293	-0.0013
5	1	5		4	1	4	18255.4666	-0.0005
5	1	4		4	1	3	18570.9719	-0.0012
5	2	4		4	2	3	18416.6167	0.0025
5	2	3		4	2	2	18431.3726	0.0017
1	1	1		0	0	0	7718.1497	-0.0010
2	1	2		1	0	1	11338.7379	-0.0004
3	0	3		2	1	2	7076.3503	-0.0012
3	1	3		2	0	2	14927.7318	0.0005
4	0	4		3	1	3	10846.8526	-0.0001
4	1	4		3	0	3	18485.9942	-0.0001
5	0	5		4	1	4	14641.6037	0.0001
6	0	6		5	1	5	18457.3922	0.0003

Table S6. Experimental transition frequencies (MHz) of the ^{13}C isotopologues of 3OXT-H_2O.

J'	K_a'	K_c'	←	J''	K_a''	K_c''	$^{13}C4/5$		$^{13}C1$	
							ν_{obs}	$\Delta\nu_{obs-calc}$	ν_{obs}	$\Delta\nu_{obs-calc}$
2	0	2		1	0	1	7348.9915	0.0033	7329.8047	0.0000
2	1	2		1	1	1	7292.5351	-0.0002	7267.7503	0.0036
2	1	1		1	1	0	7407.1734	0.0042	7393.8104	-0.0058
3	0	3		2	0	2	11021.4524	0.0067	10992.3890	-0.0005
3	1	3		2	1	2	10938.0272	-0.0020	10900.7753	-0.0011
3	1	2		2	1	1	11109.7595	-0.0078	11089.6700	0.0031
1	1	1		0	0	0	7626.4903	0.0025	7706.7077	0.0014
2	1	2		1	0	1	11244.1194	-0.0013	11309.0857	-0.0002
3	0	3		2	1	2	7126.3129	-0.0003		
3	1	3		2	0	2	14833.1602	-0.0015	14880.0567	-0.0009
4	0	4		3	1	3			10764.5435	0.0004

Table S7. Experimental transition frequencies (MHz) of the $^{18}O_{3OXT}$ isotopologue of 3OXT-H_2O.

J'	K_a'	K_c'	←	J''	K_a''	K_c''	ν_{obs}	$\Delta\nu_{obs-calc}$
2	0	2		2	0	2	10659.6816	-0.0036
2	1	2		2	1	2	10561.4170	-0.0020
2	1	1		2	1	1	10764.4146	-0.0006
3	0	3		2	2	1	10664.5283	0.0003
3	1	3		2	2	0	10667.9397	-0.0002
3	1	2		3	0	3	14208.1062	-0.0010
3	2	2		3	1	3	14080.2406	-0.0005
3	2	1		3	1	2	14350.5043	0.0007
4	0	4		3	2	2	14217.8440	0.0006
4	1	4		3	2	1	14226.3488	0.0001
4	1	3		3	3	1	14222.6003	-0.0018
4	2	3		3	3	0	14222.6459	0.0034
4	2	2		4	0	4	17752.4618	0.0012
4	3	2		4	1	4	17597.6775	0.0014
4	3	1		4	1	3	17934.8218	-0.0009
5	0	5		4	2	3	17769.8535	-0.0016
5	1	5		4	2	2	17786.7920	-0.0014
5	1	4		0	0	0	7559.2110	-0.0002
5	2	4		1	0	1	11046.1444	0.0016
5	2	3		2	1	2	6721.7226	-0.0003
1	1	1		2	0	2	14499.3811	-0.0001
2	1	2		3	1	3	10368.4098	-0.0014
3	0	3		3	0	3	17919.9362	-0.0010
3	1	3		4	1	4	14040.6320	0.0013
4	0	4		5	1	5	17734.7654	0.0008
4	1	4		2	0	2	10659.6816	-0.0036
5	0	5		2	1	2	10561.4170	-0.0020
6	0	6		2	1	1	10764.4146	-0.0006

Table S8. Experimental transition frequencies (MHz) of the $^{18}O_{H2O}$ isotopologue of 3OXT-H_2O.

J'	K_a'	K_c'	←	J''	K_a''	K_c''	ν_{obs}	$\Delta\nu_{obs-calc}$
2	0	2		1	0	1	6999.1015	0.0002
2	1	2		1	1	1	6935.6596	0.0011
2	1	1		1	1	0	7064.5446	0.0012
3	0	3		2	0	2	10496.2829	-0.0012
3	1	3		2	1	2	10402.6444	-0.0009
3	1	2		2	1	1	10595.7763	-0.0004
3	2	2		2	2	1	10500.7448	-0.0004
3	2	1		2	2	0	10503.8043	0.0015
4	0	4		3	0	3	13990.6429	-0.0004
4	1	4		3	1	3	13868.6330	0.0006
4	1	3		3	1	2	14125.7606	0.0014
4	2	3		3	2	2	13999.5319	0.0006
4	2	2		3	2	1	14007.1507	-0.0030
4	3	2		3	3	1	14004.0032	0.0065
4	3	1		3	3	0	14004.0266	-0.0042
5	0	5		4	0	4	17481.2730	-0.0004
5	1	5		4	1	4	17333.3079	0.0027
5	1	4		4	1	3	17654.0687	0.0022
5	2	4		4	2	3	17497.0661	-0.0030
5	2	3		4	2	2	17512.2495	-0.0015
1	1	1		0	0	0	7546.2306	-0.0012
2	1	2		1	0	1	10981.8652	0.0003
3	0	3		2	1	2	6513.5199	-0.0006
3	1	3		2	0	2	14385.4092	0.0002
4	0	4		3	1	3	10101.5181	-0.0004
4	1	4		3	0	3	17757.7568	-0.0005
5	0	5		4	1	4	13714.1589	-0.0006
6	0	6		5	1	5	17348.1663	0.0004

Table S9. Experimental transition frequencies (MHz) of the DOH isotopologue of 3OXT-H_2O.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	$\Delta\nu_{obs-calc}$
2	0	2	3		1	0	1	2	7229.6330	0.0000
2	0	2	2		1	0	1	1	7229.6330	0.0000
2	0	2	1		1	0	1	0	7229.6205	-0.0069
2	1	2	3		1	1	1	2	7172.3937	0.0080
2	1	2	2		1	1	1	1	7172.3729	-0.0089
2	1	2	1		1	1	1	0	7172.4199	0.0000
2	1	1	3		1	1	0	2	7288.5694	-0.0039
2	1	1	2		1	1	0	1	7288.5694	0.0044
2	1	1	1		1	1	0	0	7288.5534	0.0019
3	0	3	4		2	0	2	3	10842.4629	-0.0006
3	0	3	3		2	0	2	2	10842.4629	-0.0011
3	0	3	2		2	0	2	1	10842.4629	0.0008
3	1	3	4		2	1	2	3	10757.8447	0.0046
3	1	3	3		2	1	2	2	10757.8447	0.0049
3	1	3	2		2	1	2	1	10757.8531	0.0067
3	1	2	4		2	1	1	3	10931.9110	-0.0043
3	1	2	3		2	1	1	2	10931.9110	-0.0015
3	1	2	2		2	1	1	1	10931.9120	0.0032
3	2	2	4		2	2	1	3	10846.3065	0.0027
3	2	2	3		2	2	1	2	10846.2994	0.0019
3	2	2	2		2	2	1	1	10846.3065	-0.0008
3	2	1	4		2	2	0	3	10848.7535	-0.0062
3	2	1	3		2	2	0	2	10848.7535	0.0008
3	2	1	2		2	2	0	1	10848.7535	-0.0099
4	0	4	5		3	0	3	4	14452.9236	-0.0028
4	0	4	4		3	0	3	3	14452.9236	-0.0037
4	0	4	3		3	0	3	2	14452.9256	-0.0001
4	1	4	5		3	1	3	4	14342.4156	-0.0005
4	1	4	4		3	1	3	3	14342.4156	-0.0008
4	1	4	3		3	1	3	2	14342.4166	-0.0022
4	1	3	5		3	1	2	4	14574.1275	0.0015
4	1	3	4		3	1	2	3	14574.1275	0.0028
4	1	3	3		3	1	2	2	14574.1150	-0.0077
4	2	3	5		3	2	2	4	14460.4021	-0.0009
4	2	3	4		3	2	2	3	14460.4021	0.0017
4	2	3	3		3	2	2	2	14460.4021	-0.0015
4	2	2	5		3	2	1	4	14466.5266	0.0025
4	2	2	4		3	2	1	3	14466.5266	0.0060
4	2	2	3		3	2	1	2	14466.5266	0.0017
5	0	5	6		4	0	4	5	18060.2626	0.0009
5	0	5	5		4	0	4	4	18060.2626	-0.0003

5	0	5	4	4	0	4	3	18060.2626	0.0014
1	1	1	2	0	0	0	1	7715.5995	0.0039
1	1	1	1	0	0	0	1	7715.6259	-0.0036
1	1	1	0	0	0	0	1	7715.5448	0.0000
2	1	2	3	1	0	1	2	11272.7632	-0.0027
2	1	2	2	1	0	1	1	11272.8004	-0.0014
2	1	2	1	1	0	1	0	11272.7514	0.0110
3	0	3	4	2	1	2	3	6799.3277	-0.0028
3	0	3	3	2	1	2	2	6799.2983	0.0032
3	1	3	4	2	0	2	3	14800.9641	-0.0090
3	1	3	3	2	0	2	2	14801.0095	0.0009
3	1	3	2	2	0	2	1	14800.9641	0.0046
4	0	4	5	3	1	3	4	10494.4236	0.0068
4	0	4	4	3	1	3	3	10494.3793	-0.0034
4	0	4	3	3	1	3	2	10494.4236	-0.0047
4	1	4	5	3	0	3	4	18300.9243	-0.0015
4	1	4	4	3	0	3	3	18300.9650	0.0040
4	1	4	3	3	0	3	2	18300.9125	-0.0038
5	0	5	6	4	1	4	5	14212.2627	0.0003
5	0	5	5	4	1	4	4	14212.2229	-0.0063
5	0	5	4	4	1	4	3	14212.2802	0.0095

Table S10. Experimental transition frequencies (MHz) of the HOD isotopologue of 3OXT-H_2O.

J'	K_a'	K_c'	F'	←	J''	K_a''	K_c''	F''	ν_{obs}	$\Delta\nu_{obs-calc}$
2	0	2	3		1	0	1	2	7057.9821	0.0009
2	0	2	2		1	0	1	1	7057.9821	-0.0044
2	0	2	1		1	0	1	0	7058.0447	-0.0031
2	1	2	3		1	1	1	2	6997.4282	-0.0016
2	1	2	2		1	1	1	1	6997.5097	0.0036
2	1	2	1		1	1	1	0	6997.3527	-0.0012
2	1	1	3		1	1	0	2	7120.3574	0.0000
2	1	1	2		1	1	0	1	7120.4311	-0.0025
3	0	3	4		2	0	2	3	10584.8157	0.0001
3	0	3	3		2	0	2	2	10584.8157	-0.0029
3	0	3	2		2	0	2	1	10584.8332	0.0024
3	1	3	4		2	1	2	3	10495.3844	-0.0012
3	1	3	3		2	1	2	2	10495.4114	0.0038
3	1	3	2		2	1	2	1	10495.3844	-0.0019
3	1	2	4		2	1	1	3	10679.5871	0.0014
3	1	2	3		2	1	1	2	10679.6119	0.0043
3	1	2	2		2	1	1	1	10679.5871	0.0012
3	2	2	4		2	2	1	3	10588.9399	-0.0016
3	2	2	3		2	2	1	2	10589.0223	0.0019
3	2	2	2		2	2	1	1	10588.8912	-0.0065
3	2	1	4		2	2	0	3	10591.7067	-0.0026
3	2	1	3		2	2	0	2	10591.7860	-0.0022
3	2	1	2		2	2	0	1	10591.6662	0.0007
4	0	4	5		3	0	3	4	14109.0701	-0.0011
4	0	4	4		3	0	3	3	14109.0701	-0.0030
4	0	4	3		3	0	3	2	14109.0780	-0.0003
4	1	4	5		3	1	3	4	13992.4137	-0.0023
4	1	4	4		3	1	3	3	13992.4329	0.0071
4	1	4	3		3	1	3	2	13992.4227	0.0034
4	1	3	5		3	1	2	4	14237.6454	-0.0004
4	1	3	4		3	1	2	3	14237.6603	0.0048
4	1	3	3		3	1	2	2	14237.6534	0.0046
4	2	3	5		3	2	2	4	14117.2453	0.0035
4	2	3	4		3	2	2	3	14117.2735	-0.0018
4	2	3	3		3	2	2	2	14117.2324	-0.0008
1	1	1	2		0	0	0	1	7601.5647	-0.0027
1	1	1	1		0	0	0	1	7601.5343	0.0023
1	1	1	0		0	0	0	1	7601.6231	0.0026
2	1	2	3		1	0	1	2	11069.5804	-0.0025
2	1	2	2		1	0	1	1	11069.5539	0.0036
2	1	2	1		1	0	1	0	11069.6650	-0.0056

3	0	3	4	2	1	2	3	6573.2192	0.0053
3	0	3	3	2	1	2	2	6573.2470	-0.0078
3	0	3	2	2	1	2	1	6573.2132	0.0052
3	1	3	4	2	0	2	3	14506.9875	0.0002
3	1	3	3	2	0	2	2	14506.9636	-0.0077
3	1	3	2	2	0	2	1	14507.0159	0.0068
4	0	4	5	3	1	3	4	10186.8944	-0.0051
4	0	4	4	3	1	3	3	10186.9241	0.0038
4	0	4	3	3	1	3	2	10186.8985	-0.0015
4	1	4	5	3	0	3	4	17914.5804	-0.0072
4	1	4	4	3	0	3	3	17914.5804	0.0019
4	1	4	3	3	0	3	2	17914.5982	0.0006
5	0	5	6	4	1	4	5	13824.4040	-0.0007
5	0	5	5	4	1	4	4	13824.4149	-0.0022
5	0	5	4	4	1	4	3	13824.4040	-0.0021

Table S11. Experimental transition frequencies (MHz) of the D_2O isotopologue of 3OXT-H_2O.

J'	K_a'	K_c'	F'	F_1'	←	J''	K_a''	K_c''	F''	F_1''	ν_{obs}	$\Delta\nu_{obs-calc}$
2	1	2	3	2		1	1	1	2	1	6879.6319	-0.0063
2	1	2	2	3		1	1	1	1	2	6879.6590	-0.0019
2	1	2	3	4		1	1	1	2	3	6879.6590	-0.0068
2	1	2	2	3		1	1	1	2	2	6879.7379	0.0076
2	1	2	3	3		1	1	1	2	2	6879.7716	0.0080
2	0	2	2	3		1	0	1	1	2	6935.5176	0.0007
2	0	2	3	4		1	0	1	2	3	6935.5176	0.0006
2	0	2	3	3		1	0	1	2	2	6935.5204	-0.0036
2	0	2	3	3		1	0	1	2	2	6935.5204	-0.0036
2	1	1	3	2		1	1	0	2	1	6992.8693	0.0062
2	1	1	2	3		1	1	0	2	3	6992.9038	-0.0003
2	1	1	3	4		1	1	0	2	3	6992.9456	0.0017
2	1	1	2	2		1	1	0	1	2	6992.9675	-0.0036
2	1	1	3	3		1	1	0	2	2	6992.9961	-0.0097
2	1	1	3	3		1	1	0	1	2	6993.0452	-0.0048
3	1	3	4	5		2	1	2	3	4	10318.8371	-0.0006
3	1	3	4	3		2	1	2	3	2	10318.8371	-0.0023
3	1	3	3	4		2	1	2	2	3	10318.8482	0.0046
3	1	3	4	4		2	1	2	3	3	10318.8717	0.0123
3	1	3	3	3		2	1	2	2	2	10318.8717	0.0024
3	0	3	4	5		2	0	2	3	4	10401.4282	-0.0002
3	0	3	3	4		2	0	2	2	3	10401.4282	-0.0008
3	0	3	4	4		2	0	2	3	3	10401.4282	-0.0040
3	0	3	3	2		2	0	2	2	1	10401.4448	-0.0021
3	0	3	4	3		2	0	2	3	2	10401.4448	-0.0024
3	1	2	3	4		2	1	1	2	3	10488.5652	-0.0007
3	1	2	4	5		2	1	1	3	4	10488.5652	-0.0037
3	1	2	3	3		2	1	1	3	2	10488.6081	-0.0035
3	1	2	4	3		2	1	1	2	2	10488.5724	-0.0030
3	1	2	4	4		2	1	1	3	3	10488.6010	0.0047
4	1	4	5	6		3	1	3	4	5	13757.1885	-0.0029
4	1	4	4	5		3	1	3	3	4	13757.1885	-0.0054
4	1	4	3	2		3	1	3	2	1	13757.1954	-0.0038
4	1	4	3	3		3	1	3	2	2	13757.1954	-0.0069
4	1	4	4	4		3	1	3	3	3	13757.1954	-0.0108
4	0	4	5	6		3	0	3	4	5	13865.1285	0.0008
4	0	4	4	5		3	0	3	3	4	13865.1285	-0.0003
4	0	4	5	5		3	0	3	4	4	13865.1321	0.0019
4	0	4	4	4		3	0	3	3	3	13865.1321	0.0012
4	0	4	5	4		3	0	3	4	3	13865.1397	0.0032
4	0	4	4	3		3	0	3	3	2	13865.1397	0.0024

4	2	3	4	5	3	2	2	3	4	13872.1877	0.0067
4	2	3	5	6	3	2	2	4	5	13872.1877	0.0054
4	2	3	5	5	3	2	2	4	4	13872.2210	-0.0022
4	2	2	4	5	3	2	1	3	4	13877.9630	0.0043
4	2	2	5	6	3	2	1	4	5	13877.9630	0.0019
4	2	2	5	5	3	2	1	4	4	13878.0024	0.0006
4	1	3	4	5	3	1	2	3	4	13983.1467	-0.0022
4	1	3	3	2	3	1	2	2	1	13983.1467	-0.0035
4	1	3	4	3	3	1	2	3	2	13983.1467	-0.0044
4	1	3	5	6	3	1	2	4	5	13983.1579	0.0074
4	1	3	4	4	3	1	2	2	3	13983.1860	-0.0059
4	1	3	5	4	3	1	2	4	3	13983.1579	0.0013
4	1	3	3	3	3	1	2	2	2	13983.1621	0.0017
4	1	3	5	5	3	1	2	4	4	13983.1621	-0.0009
5	1	5	6	7	4	1	4	5	6	17194.4713	-0.0033
5	1	5	4	5	4	1	4	3	4	17194.4713	-0.0047
5	1	5	5	6	4	1	4	4	5	17194.4779	0.0017
5	1	5	6	6	4	1	4	5	5	17194.4853	0.0049
5	1	5	4	4	4	1	4	3	3	17194.4853	0.0041
5	1	5	5	5	4	1	4	4	4	17194.4853	0.0023
5	0	5	6	7	4	0	4	5	6	17325.9062	0.0018
5	0	5	5	6	4	0	4	4	5	17325.9062	0.0004
5	0	5	4	4	4	0	4	3	3	17325.9110	0.0051
5	0	5	6	6	4	0	4	5	5	17325.9110	0.0048
5	0	5	5	5	4	0	4	4	4	17325.9110	0.0035
5	0	5	6	5	4	0	4	5	4	17325.9110	0.0014
5	1	4	6	5	4	1	3	5	4	17476.3427	-0.0044
5	1	4	6	6	4	1	3	5	5	17476.3427	-0.0069
1	1	1	0	1	0	0	0	1	1	7601.5642	0.0037
1	1	1	0	1	0	0	0	1	2	7601.5642	0.0037
1	1	1	2	3	0	0	0	1	2	7601.6507	0.0130
1	1	1	2	1	0	0	0	1	0	7601.6507	0.0132
1	1	1	1	2	0	0	0	1	2	7601.6696	-0.0023
2	1	2	3	2	1	0	1	2	2	11013.0669	-0.0009
2	1	2	2	1	1	0	1	1	0	11013.1520	-0.0033
2	1	2	3	3	1	0	1	2	2	11013.1656	0.0075
2	1	2	2	2	1	0	1	1	1	11013.1797	0.0031
2	1	2	3	4	1	0	1	2	3	11013.1797	-0.0052
2	1	2	2	3	1	0	1	1	2	11013.2178	0.0013
2	1	2	3	3	1	0	1	2	3	11013.2515	0.0041
2	1	2	3	2	1	0	1	2	1	11013.2952	0.0025
3	0	3	3	4	2	1	2	2	3	6323.7265	-0.0029
3	0	3	3	2	2	1	2	1	1	6323.7468	0.0066
3	0	3	4	3	2	1	2	3	2	6323.7590	0.0059
3	0	3	4	5	2	1	2	3	4	6323.7590	-0.0016

3	0	3	3	3	2	1	2	2	2	6323.7756	-0.0007
3	0	3	4	4	2	1	2	3	3	6323.7904	-0.0077
3	0	3	2	2	2	1	2	2	1	6323.8067	0.0028
4	0	4	4	5	3	1	3	3	4	9870.0107	-0.0038
4	0	4	4	4	3	1	3	3	3	9870.0322	-0.0057
4	0	4	5	4	3	1	3	4	3	9870.0503	0.0000
4	0	4	5	5	3	1	3	4	4	9870.0733	0.0044
4	0	4	3	3	3	1	3	2	2	9870.0809	0.0034
5	0	5	5	6	4	1	4	4	5	13438.7290	0.0026
5	0	5	5	5	4	1	4	4	4	13438.7359	-0.0033
5	0	5	6	7	4	1	4	5	6	13438.7649	0.0012
5	0	5	6	5	4	1	4	5	4	13438.7649	0.0001
5	0	5	6	6	4	1	4	5	5	13438.7727	-0.0006
5	0	5	4	4	4	1	4	3	3	13438.7851	0.0040
5	0	5	4	3	4	1	4	3	2	13438.7727	-0.0037

Table S12. Experimental transition frequencies (MHz) of the parent species of 3OXT-H_2CO.

J'	K_a'	K_c'	v	←	J''	K_a''	K_c''	v	ν_{obs}	$\Delta\nu_{obs-calc}$
2	0	2	1		1	0	1	1	6255.4272	0.0011
2	0	2	0		1	0	1	0	6255.4272	-0.0049
2	1	2	1		1	1	1	1	6040.4082	0.0004
2	1	2	0		1	1	1	0	6040.4082	0.0040
2	1	1	1		1	1	0	1	6502.3069	0.0000
2	1	1	0		1	1	0	0	6502.3311	0.0067
3	0	3	1		2	0	2	1	9343.7006	0.0006
3	0	3	0		2	0	2	0	9343.7006	-0.0058
3	1	3	1		2	1	2	1	9050.8586	-0.0001
3	1	3	0		2	1	2	0	9050.8586	0.0059
3	1	2	1		2	1	1	1	9742.9546	0.0015
3	1	2	0		2	1	1	0	9742.9804	0.0017
3	2	2	1		2	2	1	1	9406.9568	0.0026
3	2	2	0		2	2	1	0	9406.9600	-0.0047
3	2	1	1		2	2	0	1	9470.1000	-0.0008
3	2	1	0		2	2	0	0	9470.1201	0.0047
4	0	4	1		3	0	3	1	12387.4414	0.0014
4	0	4	0		3	0	3	0	12387.4414	-0.0025
4	1	4	1		3	1	3	1	12050.5481	0.0014
4	1	4	0		3	1	3	0	12050.5366	-0.0011
4	1	3	1		3	1	2	1	12970.0225	0.0011
4	1	3	0		3	1	2	0	12970.0503	-0.0039
4	2	3	1		3	2	2	1	12529.9127	-0.0004
4	2	3	0		3	2	2	0	12529.9279	0.0016
4	2	2	1		3	2	1	1	12684.6038	-0.0033
4	2	2	0		3	2	1	0	12684.6327	0.0024
4	3	2	1		3	3	1	1	12572.3316	-0.0059
4	3	2	0		3	3	1	0	12572.3565	0.0031
4	3	1	1		3	3	0	1	12576.4420	-0.0045
4	3	1	0		3	3	0	0	12576.4630	0.0002
5	0	5	1		4	0	4	1	15379.6710	0.0017
5	0	5	0		4	0	4	0	15379.6710	0.0031
5	1	5	1		4	1	4	1	15037.3706	0.0037
5	1	5	0		4	1	4	0	15037.3522	-0.0018
5	1	4	1		4	1	3	1	16177.3632	0.0004
5	1	4	0		4	1	3	0	16177.3976	-0.0038
5	2	4	1		4	2	3	1	15642.0599	0.0011
5	2	4	0		4	2	3	0	15642.0779	0.0040
5	2	3	1		4	2	2	1	15939.3987	-0.0049
5	2	3	0		4	2	2	0	15939.4306	-0.0070
5	3	3	1		4	3	2	1	15725.4114	-0.0067

5	3	3	0	4	3	2	0	15725.4439	0.0053
5	3	2	1	4	3	1	1	15739.6936	-0.0064
5	3	2	0	4	3	1	0	15739.7221	0.0004
6	0	6	1	5	0	5	1	18323.1750	0.0045
6	0	6	0	5	0	5	0	18323.1625	0.0011
6	1	6	1	5	1	5	1	18010.2951	0.0048
6	1	6	0	5	1	5	0	18010.2692	-0.0035
6	1	5	1	5	1	4	1	19357.5124	0.0003
6	1	5	0	5	1	4	0	19357.5457	-0.0089
6	2	5	1	5	2	4	1	18740.8437	0.0029
6	2	5	0	5	2	4	0	18740.8644	0.0073
2	1	2	1	1	0	1	1	8434.9044	0.0013
2	1	2	0	1	0	1	0	8434.9561	-0.0020
2	2	1	1	2	1	2	1	7876.2370	-0.0002
2	2	1	0	2	1	2	0	7876.4451	0.0008
2	2	0	1	2	1	1	1	7199.2847	-0.0037
2	2	0	0	2	1	1	0	7199.4629	-0.0020
2	2	0	1	1	1	1	1	13932.5627	0.0045
2	2	0	0	1	1	1	0	13932.7593	-0.0036
2	2	1	1	1	1	0	1	13685.6828	0.0008
2	2	1	0	1	1	0	0	13685.8758	0.0008
3	0	3	1	2	1	2	1	7164.2233	0.0003
3	0	3	0	2	1	2	0	7164.1827	0.0024
3	1	3	1	2	0	2	1	11230.3346	-0.0011
3	1	3	0	2	0	2	0	11230.3745	-0.0042
3	2	2	1	2	1	1	1	16590.3294	0.0001
3	2	2	0	2	1	1	0	16590.5170	0.0017
3	2	2	1	3	1	3	1	8232.3322	-0.0005
3	2	2	0	3	1	3	0	8232.5535	-0.0028
3	2	1	1	2	1	2	1	17362.2499	-0.0013
3	2	1	0	2	1	2	0	17362.4748	0.0008
4	0	4	1	3	1	3	1	10500.8070	0.0027
4	0	4	0	3	1	3	0	10500.7714	-0.0001
4	1	4	1	3	0	3	1	13937.1810	-0.0014
4	1	4	0	3	0	3	0	13937.2158	0.0058
5	0	5	1	4	1	4	1	13829.9313	0.0044
5	0	5	0	4	1	4	0	13829.8985	-0.0033
5	1	5	1	4	0	4	1	16587.1080	-0.0014
5	1	5	0	4	0	4	0	16587.1226	0.0024
6	0	6	0	5	1	5	0	17115.7085	-0.0007
6	1	5	1	5	2	4	1	13485.5471	-0.0010
6	1	5	0	5	2	4	0	13485.4732	-0.0001
3	2	2	1	3	0	3	1	10118.9669	-0.0015
3	3	0	1	3	2	1	1	12480.4748	0.0057
3	3	0	0	3	2	1	0	12480.7852	0.0018

3	3	1	1	3	2	2	1	12558.8393	-0.0024
3	3	1	0	3	2	2	0	12559.1617	0.0005
4	2	3	1	4	1	4	1	8711.7011	0.0020
4	2	3	0	4	1	4	0	8711.9422	-0.0027
4	3	1	1	4	2	2	1	12372.3098	0.0013
4	3	1	0	4	2	2	0	12372.6172	0.0013
4	3	2	1	4	2	3	1	12601.2612	-0.0049
4	3	2	0	4	2	3	0	12601.5873	-0.0010
5	2	4	1	5	1	5	1	9316.3909	-0.0001
5	2	4	0	5	1	5	0	9316.6651	0.0003
5	3	2	1	5	2	3	1	12172.6033	-0.0016
5	3	2	0	5	2	3	0	12172.8977	-0.0024
6	2	5	1	6	1	6	1	10046.9421	0.0006
6	2	5	0	6	1	6	0	10047.2515	0.0024
6	3	3	1	6	2	4	1	11863.3485	-0.0002
6	3	3	0	6	2	4	0	11863.6264	0.0003
7	2	6	1	7	1	7	1	10901.4928	0.0033
7	2	6	0	7	1	7	0	10901.8390	0.0026
7	3	4	1	7	2	5	1	11448.6421	0.0007

Table S13. Experimental transition frequencies (MHz) of the ^{13}C isotopologues of 3OXT-H_2CO.

J'	K_a'	K_c' ←	J''	K_a''	K_c''	$^{13}C11$		$^{13}C2$		$^{13}C4/5$	
						ν_{obs}	$\Delta\nu_{obs-calc}$	ν_{obs}	$\Delta\nu_{obs-calc}$	ν_{obs}	$\Delta\nu_{obs-calc}$
2	0	2	1	0	1	6119.014	-0.0002	6244.5661	0.0019	6216.7973	-0.0037
2	1	2	1	1	1					6008.8245	0.0021
2	1	1	1	1	0	9142.8432	-0.0002	6493.4751	-0.0011	6454.8118	-0.0046
3	0	3	2	0	2	8859.8505	-0.0008	9326.6147	0.0002	9287.9936	-0.0004
3	1	3	2	1	2	9522.0359	0.0025	9032.3002	-0.0046	9004.0218	-0.0042
3	1	2	2	1	1	9200.0165	-0.0003	9729.4933	0.0030	9672.3177	0.0001
3	2	2	2	2	1	9257.0903	-0.0049	9391.1510	0.0001	9347.6426	-0.0047
3	2	1	2	2	0	12126.1310	-0.0007	9455.5774	-0.0022	9407.1964	0.0035
4	0	4	3	0	3	11797.4404	0.0042	12363.3069	0.0006	12317.0584	0.0017
4	1	4	3	1	3	12677.5215	-0.0025	12025.4774	-0.0010	11989.0455	-0.0016
4	1	3	3	1	2	12255.2019	0.0078	12951.6379	0.0045	12877.0427	0.0035
4	2	3	3	2	2	12395.3009	-0.0040	12508.5823	-0.0052	12451.5451	-0.0036
4	2	2	3	2	1	15061.8192	-0.0065	12666.3383	-0.0047	12597.5503	-0.0022
5	0	5	4	0	4	9142.8432	0.0056	15347.7255	0.0073	15297.0869	0.0072
5	1	5	4	1	4					14961.8637	0.0040
2	2	1	1	1	0	13656.1868	0.0009	13631.9731	-0.0008	13568.2504	0.0022
2	2	0	1	1	1			13880.8821	0.0008		
3	1	3	2	0	2	11087.2675	-0.0040	11195.4428	-0.0014	11167.2207	-0.0076

Table S14. Experimental transition frequencies (MHz) of the $^{18}O_{3OXT}$ isotopologue of 3OXT-H_2CO.

J'	K_a'	K_c'	v	←	J''	K_a''	K_c''	v	ν_{obs}	$\Delta\nu_{obs-calc}$
2	0	2	0		1	0	1	0	6203.0496	0.0000
2	0	2	1		1	0	1	1	6203.0496	-0.0063
2	1	1	0		1	1	0	0	6478.5606	0.0027
2	1	1	1		1	1	0	1	6478.5704	-0.0044
3	0	3	0		2	0	2	0	9253.4660	0.0028
3	0	3	1		2	0	2	1	9253.4660	-0.0042
3	1	3	0		2	1	2	0	8941.0076	0.0030
3	1	3	1		2	1	2	1	8941.0076	0.0071
3	1	2	0		2	1	1	0	9704.1107	0.0035
3	1	2	1		2	1	1	1	9704.1326	0.0007
3	2	2	0		2	2	1	0	9335.6456	0.0048
3	2	2	1		2	2	1	1	9335.6456	-0.0062
3	2	1	0		2	2	0	0	9417.7132	-0.0009
3	2	1	1		2	2	0	1	9417.7236	-0.0054
4	0	4	0		3	0	3	0	12247.4935	0.0021
4	0	4	1		3	0	3	1	12247.4935	-0.0030
4	1	4	0		3	1	3	0	11899.2653	0.0027
4	1	4	1		3	1	3	1	11899.2653	0.0092
4	1	3	0		3	1	2	0	12911.6840	0.0017
4	1	3	1		3	1	2	1	12911.7184	0.0045
4	2	3	0		3	2	2	0	12431.0734	0.0054
4	2	3	1		3	2	2	1	12431.0734	-0.0084
4	2	2	0		3	2	1	0	12630.6240	0.0043
4	2	2	1		3	2	1	1	12630.6406	-0.0025
4	3	2	0		3	3	1	0	12485.8897	0.0034
4	3	2	1		3	3	1	1	12485.9031	0.0003
4	3	1	0		3	3	0	0	12492.2176	0.0004
4	3	1	1		3	3	0	1	12492.2332	-0.0009
5	0	5	0		4	0	4	0	15179.6440	0.0030
5	0	5	1		4	0	4	1	15179.6440	0.0025
5	1	5	0		4	1	4	0	14841.5185	-0.0031
5	1	5	1		4	1	4	1	14841.5185	0.0065
5	1	4	0		4	1	3	0	16092.7977	-0.0005
5	1	4	1		4	1	3	1	16092.8366	0.0012
5	2	4	0		4	2	3	0	15512.5166	0.0094
5	2	4	1		4	2	3	1	15512.5166	-0.0066
5	2	3	0		4	2	2	0	15890.8928	-0.0031
5	2	3	1		4	2	2	1	15890.9269	-0.0028
6	0	6	0		5	0	5	0	18058.7536	-0.0040
6	0	6	1		5	0	5	1	18058.7536	0.0019
6	1	6	0		5	1	5	0	17767.0053	-0.0083

6	1	6	1	5	1	5	1	17767.0053	0.0051
6	2	5	0	5	2	4	0	18576.7404	0.0087
6	2	5	1	5	2	4	1	18576.7404	-0.0087
2	1	2	0	1	0	1	0	8182.6286	0.0008
2	1	2	1	1	0	1	1	8182.6812	-0.0024
3	0	3	0	2	1	2	0	7273.8815	-0.0034
3	0	3	1	2	1	2	1	7273.8386	-0.0038
3	1	3	0	2	0	2	0	10920.5841	0.0013
3	1	3	1	2	0	2	1	10920.6287	0.0004
3	2	2	0	2	1	1	0	15976.2204	-0.0030
3	2	2	1	2	1	1	1	15976.4115	0.0028
4	0	4	0	3	1	3	0	10580.3702	-0.0015
4	0	4	1	3	1	3	1	10580.3417	0.0034
4	1	4	0	3	0	3	0	13566.3815	-0.0008
4	1	4	1	3	0	3	1	13566.4060	-0.0082
5	0	5	0	4	1	4	0	13860.7453	-0.0048
5	0	5	1	4	1	4	1	13860.7275	0.0038
5	1	5	0	4	0	4	0	16160.4118	-0.0007
5	1	5	1	4	0	4	1	16160.4328	0.0030

Table S15. Experimental transition frequencies (MHz) of the $^{18}O_{H2CO}$ isotopologue of 3OXT-H_2CO.

J'	K_a'	K_c'	v	←	J''	K_a''	K_c''	v	ν_{obs}	$\Delta\nu_{obs-calc}$
2	0	2	1		1	0	1	1	6115.5752	0.0038
2	0	2	0		1	0	1	0	6115.5752	-0.0023
2	1	1	1		1	1	0	1	6359.6977	0.0017
2	1	1	0		1	1	0	0	6359.7089	-0.0019
3	0	3	1		2	0	2	1	9134.4752	-0.0013
3	0	3	0		2	0	2	0	9134.4752	-0.0086
3	1	3	1		2	1	2	1	8844.6611	-0.0034
3	1	3	0		2	1	2	0	8844.6611	-0.0016
3	1	2	1		2	1	1	1	9529.1864	0.0008
3	1	2	0		2	1	1	0	9529.2068	-0.0005
3	2	2	1		2	2	1	1	9196.8256	-0.0051
3	2	2	0		2	2	1	0	9196.8363	-0.0048
3	2	1	1		2	2	0	1	9259.0706	-0.0065
4	0	4	1		3	0	3	1	12109.4652	0.0041
4	0	4	0		3	0	3	0	12109.4652	-0.0022
4	1	4	1		3	1	3	1	11775.8600	0.0001
4	1	4	0		3	0	3	0	13650.1089	-0.0013
4	1	3	1		3	1	2	1	12685.2985	0.0054
4	1	3	0		3	1	2	0	12685.3254	0.0044
4	2	3	1		3	2	2	1	12249.9201	-0.0056
4	2	2	1		3	2	1	1	12402.4317	-0.0026
4	2	2	0		3	2	1	0	12402.4576	0.0024
5	0	5	1		4	0	4	1	15033.6062	0.0079
5	0	5	0		4	0	4	0	15033.6062	0.0048
2	1	2	1		1	0	1	1	8279.6154	0.0033
2	1	2	0		1	0	1	0	8279.6512	-0.0010
3	1	3	1		2	0	2	1	11008.7028	-0.0024
3	1	3	0		2	0	2	0	11008.7395	0.0021
4	1	4	1		3	0	3	1	13650.0863	-0.0023
4	1	4	0		3	1	3	0	11775.8600	0.0034

Table S16. Comparison of the r_s, r_0 coordinates (Å) of C and O atoms in both targeted complexes with those from theoretical coordinates (r_e) calculated at the MP2/6-311++G(d,p) level.

		3OXT-H_2O				3OXT-H_2CO		
		a	b	c		a	b	c
	r_s	±1.177(1)	±0.192(8)	0[a]		±0.569(3)	±0.721(2)	0[b]
C2	r_e	-1.204	0.173	0.000	C2	-0.544	0.727	0.000
	r_0	-1.182	0.187	0.000		-0.561	0.722	0.000
	r_s	0[b]	0.452(3)	±1.064(1)		±1.178(1)	±0.185(8)	±1.059(1)
C4	r_e	-0.263	-0.404	-1.061	C4	-1.187	-0.172	-1.057
	r_0	-0.268	-0.432	-1.061		-1.207	-0.174	1.056
	r_s	0[b]	±0.452(3)	±1.064(1)		±1.178(1)	±0.185(8)	±1.059(1)
C5	r_e	-0.263	-0.404	1.061	C5	-1.187	-0.172	1.057
	r_0	-0.268	-0.432	1.061		-1.207	-0.174	1.056
	r_s	±2.6496(6)	±0.804(2)	0[b]		±1.8258(8)	±0.937(2)	0[b]
O10	r_e	2.686	0.768	0.000	O10	1.768	-0.942	0.000
	r_0	2.658	0.800	0.000		1.826	-0.948	0.000
	r_s	±2.1732(7)	±0.858(2)	0[b]		±0.096(16)	±1.7144(9)	0[b]
O1	r_e	-2.237	0.784	0.000	O1	0.122	1.728	0.000
	r_0	-2.190	0.838	0.000		0.109	1.721	0.000
	r_s					±2.694(6)	0[b]	0[b]
	r_e				C11	2.678	-0.135	0.000
	r_0					2.708	-0.111	0.000

[b] Imaginary: set to zero.