Таблица 1: Mol. & vib. params. H_2O

	Values		Freqs	
	Calc.	Exp.	Calc.	Exp.
r(O-H)	0.965	0.958	3931	3657 (asym.)
$\angle$ HOH	105.754	104.478	3809	3756 (sym.)
μ (D)	2.195	1.855	1603	1595
	B3LYP; 6-31+G**	NIST	B3LYP; 6-31+G**	NIST

Таблица 2: Mol. & vib. params. D_2O

	Values		Freqs	
	Calc.	Exp.	Calc.	Exp.
r(O-D)	0.965	0.956	2882	2671 (asym.)
$\angle$ DOD	105.754	105.200	2745	2788 (sym.)
μ (D)	2.195	1.855	1174	1178
	B3LYP; 6-31+G**	NIST	B3LYP; 6-31+G**	NIST

Таблица 3: H_2O F-matrix

$q(OH)_1$	8.3806		
$q(OH)_2$	-0.1159	8.3806	
(HOH)	0.243	0.243	0.6724
	$q(OH)_1$	$q(OH)_2$	(HOH)

Таблица 4: H_2O G-matrix

$q(OH)_1$	1.7902		
$q(OH)_2$	-0.0288	1.7902	
(HOH)	-0.1058	-0.1058	3.906
	$q(OH)_1$	$q(OH)_2$	(HOH)

Таблица 5: D_2O F-matrix

$q(OH)_1$	8.3805		
$q(OH)_2$	-0.1159	8.3805	
(HOH)	0.243	0.243	0.6724
	$q(OH)_1$	$q(OH)_2$	(HOH)

Таблица 6: D_2O G-matrix

$q(OH)_1$	0.9488		
$q(OH)_2$	-0.0288	0.9488	
(HOH)	-0.1058	-0.1058	2.0992
	$q(OH)_1$	$q(OH)_2$	(HOH)

Apostolo				
Exp. ν, cm^{-1}	Calc. ν, cm^{-1}	Desc.	Symm.	Assign.
3534.8/3530.6sh/3529.4/3526.6sh/3525.9/3522.6/3521.0	3525.7	ν(OH)	A′	S1(100)
1796.5/1795.9sh/1794.6sh/1793.7	1802.6	ν(CO)	A′	S2(89)
1350.1/1344.8	1345.0	δ(COH), ν(CO)	A′	S8(44)+S3(28)+S9(16)
1162.0/1160.4sh/1158.6/1155.9sh/1151.2/1149.8sh/1147.5	1170.0	ν(CO), δ(COH)	A′	S8(43)+S3(41)
941.6/940.8/939.2/937.3	943.6	ν(CC)	A′	S4(48)+S3(17)+S13(17)+S7(13)
868-832(d); max.: 865.1/855.9	834.9	ν(CO)	A″	S14(53)+S16(20)+S6(15)
868-832(d); max.: 845.9/833.7	834.1	$\nu(CCl_3)$, as	A′	S5(53)+S10(16)+S15(15)+S11(11)
700.5/699.1sh/696.5/695.7sh/694.9/692.8sh	706.4	$\nu(CCl_3)$, as	A″	S6(53)+S17(32)+S14(11)
658.2/657.3	674.5	δ(OCO)	A′	S9(61)+S7(10)

Calc.; B3LYP, 6-31+G**		
Calc. ν, cm^{-1}	Symm.	Assign.
3762.6	A′	100 $q(OH)_1$
1845.3	A′	89 $q(CO)_1$
1357.3	A′	42 a1+29 $q(CO)_2$ + 11 a2 +10 $q(CC)_1$
1172.1	A′	44 a1+40 $q(CO)_2$ + 6 $q(CO)_1$ + 5 $q(CC)_1$
935.3	A′	48 $q(CC)_1$ + 17 $q(CO)_2$ + 9 $q(CC)_1$
819.8	A″	56 x + 20 a6 + 16 $q(C\text{-}Cl)_2$ + 6 a8
823.5	A′	32 $q(C\text{-}Cl)_1$ + 21 $q(C\text{-}Cl)_2$ + 13 a5 + 10 a10
681.8	A″	53 $q(C\text{-}Cl)_2$ + 23 t2 + 18 x + 7 a8
649.5	A′	44 a2 + 15 a3 + 8 a1 + 8 a4
545.5	A″	75 t2 + 15 $q(C\text{-}Cl)_2$ + 9 x
428.2	A′	60 $q(C\text{-}Cl)_2$ + 14 $q(C\text{-}Cl)_1$ + 13 $q(CC)_1$ + 5 a3