Table 1S. Experimental and calculated Raman data of H_2O…CO complex and H_2O, CO monomers.

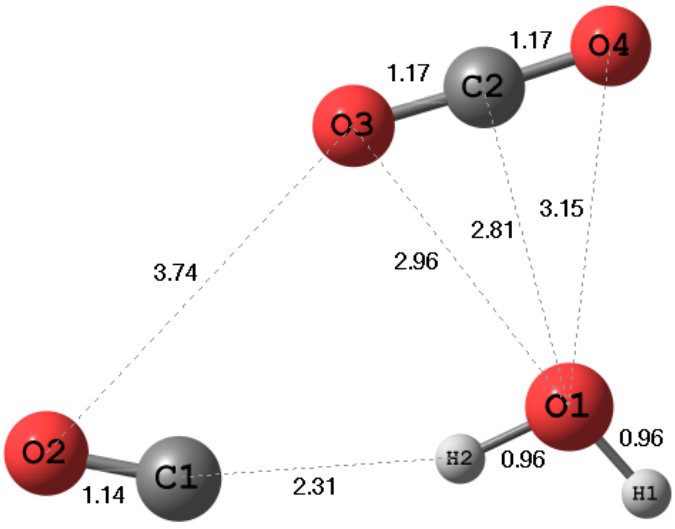
Theoretical						**Experimental**		
Frequency	Raman intensities	Freq shift				Ar matrix (IR data)	Ar matrix (this work)	Assignment
MP2/6-311++G(2d,2p)			**MP2/aug-cc-pVTZ**					
H_2O								
3982 (26)*	313	-	3948 (23)	280	-	3734.3[a]	n.o.	ν_{as}OH
3862 (81)	1049	-	3822 (106)	1399	-	3638.0[a]	3641.2	ν_{s}OH
1661 (5)	247	-	1628 (1)	58	-	1589.1[a]		δH_2O
CO								
2114	811	-	2110 (25)	941	-	2138.5[b]	2141.0	νCO
H_2O…CO								
3967 (35)	432	-15	3931 (33)	410	-17	3723.5 (-8.1)[c]	3726.8	ν_{as}OH
3843 (132)	1713	-19	3801 (155)	2067	-21	3627.8 (-8.8)[c]	3631.0 (-10.2)	ν_{s}OH
2125 (29)	1047	+11	2124 (32)	1155	+14	2149.2 (+10.2)[c]	2151.0 (+9.8)	νCO
1671 (4)	193	+10	1637 (0.5)	29	+9	1595.4 (+5.4)[c]	-	δH_2O
375 (0.03)	11	-	357 (0.01)	4	-	-	-	
233 (0.1)	71	-	234 (0.04)	22	-	-	-	
101 (0.1)	187	-	102 (0.13)	156	-	-	-	inter-molecula vibrations
74 (0.5)	820	-	70 (0.27)	470	-	-	-	
69 (0.6)	1110	-	65 (0.4)	822	-	-	-	
H_2O…OC								
3982 (34)	409	0	3945 (29)	353	-3	-	-	ν_{as}OH
3865 (103)	1327	+3	3823 (131)	1723	+1	-	-	ν_{s}OH
2110 (29)	1051	-4	2109 (32)	1191	-1	2130.3 (-5.7) (Kr matrix)[c]	-	νCO
1666 (4.5)	231	+5	1631 (1)	54	+3	1593.5 (+6.5) (Kr matrix)[c]	-	δH_2O
221 (0.1)	61	-	212 (0.2)	108	-	-	-	
139 (0.3)	264	-	145 (0.08)	68	-	-	-	
71 (0.1)	166	-	78 (0.13)	204	-	-	-	inter-molecular vibrations
49 (1)	2832	-	46 (0.2)	594	-	-	-	
49 (1)	2668	-	27 (0.6)	2871	-	-	-	

[a] From ref [1] [b] From ref. [2] [c] From ref. [3] * the calculated Raman scattering activities [Å/a.m.u.] are presented in the parentheses

Table 2S. Experimental and calculated Raman data of the ternary complexes .

Calculated				Experimental	
Harmonic	Raman activities	Raman intensities	Freq shift	Ar matrix (this work)	
3961	34	422	-21	-	$\nu_{as}OH$
3828	119	1563	-34	3615.5 (-27.0)	$\nu_{s}OH$
2400	0.1	4	+3	-	$\nu_{as}CO_2$
2129	29	1064	+15	2158.1 (+17.8)	νCO
1662	3	157	+1	-	δH_2O
1320	33	2313	+3	- ν_+ 1287.2 ν_- ?	$\nu_{s}CO_2$
666	0.01	1	+3	-	δCO_2
650	0.1	24	-13	-	δCO_2
409	0.1	26	-	-	inter-molecular vibrations
266	0.2	101	-	-	
145	0.7	606	-	-	
121	0.7	742	-	-	
111	0.3	331	-	-	
104	0.2	277	-	-	
73	1.7	2907	-	-	
66	1.2	2295	-	-	
28	0.2	826	-	-	
24	1.6	8422	-	-	

Figure 1S. BSSE-optimized structures of the most stable $CO_2…H_2O…CO$ complex. All presented geometrical parameters were calculated at MP2 level using 6-311++G(2d,2p) basis set.



[1] A. Engdahl, B. Nelander, J. Mol. Struct., 193 (1989) 101
[2] A.Schriver, L. Schriver-Mazzuoli, A.A. Vigasin, Vib. Spectr. 23 (2000) 83
[3] J. Lundell, M. Räsänen, J. Mol. Struct. 436 (1997) 349