SUPPORTING INFORMATION

An insight into characteristics of nonconventional hydrogen bonds in the complexes of haloforms with carbon monoxide

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Table S1. Results of AIM analysis of complexes $X_3CH\cdots OC$ (X = F, Cl, Br) at the MP2/6-311++G(3df,2pd) when $R_{C\cdots O}$ = 2.7 ÷ 4.5 Å

Complexes	$R_{C\cdots O}$ (Å)	ρ(r) (au)	$\nabla^2\rho(r)$ (au)	H(r) (au)
$F_3CH\cdots OC$	2.7	0.0495	0.1852	-0.0057
	2.9	0.0313	0.1306	0.0012
	3.1	0.0199	0.0859	0.0026
	3.3	0.0128	0.0534	0.0021
	3.5	0.0082	0.0330	0.0014
	3.7	0.0053	0.0209	0.0010
	3.9	0.0034	0.0136	0.0007
	4.1	0.0021	0.0091	0.0005
	4.3	0.0013	0.0060	0.0004
	4.5	0.0008	0.0040	0.0003
$Cl_3CH\cdots OC$	2.7	0.0496	0.2459	-0.0065
	2.9	0.0313	0.1766	0.0007
	3.1	0.0199	0.1258	0.0023
	3.3	0.0127	0.0833	0.0019
	3.5	0.0082	0.0521	0.0013
	3.7	0.0053	0.0322	0.0009
	3.9	0.0033	0.0205	0.0007
	4.1	0.0021	0.0133	0.0005
	4.3	0.0013	0.0089	0.0004
	4.5	0.0008	0.0059	0.0003
$Br_3CH\cdots OC$	2.7	0.0496	0.1755	-0.0066
	2.9	0.0313	0.1253	0.0007
	3.1	0.0198	0.0831	0.0023
	3.3	0.0127	0.0520	0.0019
	3.5	0.0081	0.0322	0.0013
	3.7	0.0052	0.0205	0.0009
	3.9	0.0033	0.0134	0.0007
	4.1	0.0021	0.0089	0.0005
	4.3	0.0013	0.0059	0.0004
	4.5	0.0008	0.0039	0.0003

Table S2. Interaction energy (kJ.mol^{-1}), the change in C-H bond length (Δr, Å), and their stretching frequency (Δν, cm^{-1}) when fixing C···O distance ($R_{C...O}$, Å) in X_3CH···OC complexes (X = F, Cl, Br),

Complexes	$R_{C...O}$ (Å)	Δr (Å)	Δν (cm^{-1})	ΔE* (kJ.mol^{-1})
F_3CH···OC	2.7	-0.03747	503.51	57.25
	2.9	-0.02059	293.12	21.58
	3.1	-0.01014	159.75	8.54
	3.3	-0.00417	78.79	2.48
	3.5	-0.00116	34.56	-0.07
	3.7	-0.00005	15.39	-0.71
	3.9	0.00075	3.33	-0.85
	4.1	0.00093	-0.62	-0.74
	4.3	0.00096	-2.02	-0.56
	4.5	0.00092	-2.29	-0.36
Cl_3CH···OC	2.7	-0.03264	287.63	24.39
	2.9	-0.01720	227.07	15.47
	3.1	-0.00741	110.26	4.56
	3.3	-0.00224	38.29	-0.27
	3.5	0.00030	-4.97	-2.02
	3.7	0.00137	-24.08	-2.27
	3.9	0.00176	-24.09	-2.06
	4.1	0.00188	-35.13	-1.70
	4.3	0.00188	-35.98	-1.70
	4.5	0.00182	-35.87	-1.01
Br_3CH···OC	2.7	-0.03157	271.89	22.52
	2.9	-0.01589	185.70	20.83
	3.1	-0.00702	100.31	3.59
	3.3	-0.00205	32.70	-0.90
	3.5	0.00033	-4.82	-2.47
	3.7	0.00141	-23.93	-2.63
	3.9	0.00178	-31.57	-2.37
	4.1	0.00188	-32.52	-1.93
	4.3	0.00188	-35.12	-1.51
	4.5	0.00182	-34.98	-1.17

Table S3. Selected data from SAPT2+ analysis in $X_3CH\cdots OC$ (X = F, Cl, Br) complexes upon $R_{C\cdots O}$ = 2.7÷4.5 Å

	$R_{C\text{-}O}$ (Å)	ΔE^{SAPT2+} *(kJ.mol^{-1})*	E_{ele} *(kJ.mol^{-1})*	$\%E_{ele}$	E_{ind} *(kJ.mol^{-1})*	$\%E_{ind}$	E_{disp} *(kJ.mol^{-1})*	$\%E_{disp}$	E_{ex} *(kJ.mol^{-1})*	δ_{int}^{HF}	E_{ind}/E_{disp}
$F_3CH\cdots OC$	2.7	31.9	-32.4	33.0	-38.7	39.5	-19.2	19.6	130.0	-7.8	2.02
	2.9	12.0	-17.7	33.6	-18.2	34.5	-12.6	23.9	64.7	-4.2	1.44
	3.1	2.2	-9.6	33.1	-8.5	29.3	-8.3	29.1	31.1	-2.1	0.96
	3.3	-1.2	-5.3	33.8	-3.9	24.8	-5.5	35.0	14.5	-1.0	0.72
	3.5	-2.4	-3.0	33.3	-1.9	21.1	-3.7	41.1	6.7	-0.4	0.51
	3.7	-2.5	-1.8	33.3	-0.9	16.7	-2.5	46.3	3.0	-0.2	0.38
	3.9	-2.1	-1.2	34.3	-0.5	14.3	-1.7	48.6	1.4	-0.1	0.29
	4.1	-1.8	-0.8	34.8	-0.3	13.0	-1.2	52.2	0.6	0.0	0.24
	4.3	-1.4	-0.6	35.3	-0.2	11.8	-0.9	52.9	0.3	0.0	0.20
	4.5	-1.1	-0.4	36.4	-0.1	9.1	-0.6	54.6	0.1	0.0	0.18
$Cl_3CH\cdots OC$	2.7	50.9	-8.0	10.1	-40.1	50.6	-22.0	27.7	130.2	-9.2	1.82
	2.9	7.7	-18.2	32.1	-18.9	33.3	-14.7	25.9	64.4	-4.9	1.28
	3.1	-0.2	-10.0	32.2	-8.8	28.3	-9.9	31.8	30.9	-2.4	0.89
	3.3	-3.0	-5.6	32.0	-4.1	23.4	-6.7	38.3	14.4	-1.1	0.61
	3.5	-3.7	-3.2	31.4	-1.9	18.6	-4.6	45.1	6.6	-0.5	0.42
	3.7	-3.4	-2.0	31.7	-0.9	14.3	-3.2	50.8	3.0	-0.2	0.29
	3.9	-2.8	-1.3	30.9	-0.5	11.9	-2.3	54.8	1.4	-0.1	0.21
	4.1	-2.2	-0.9	31.0	-0.3	10.3	-1.7	58.6	0.6	0.0	0.16
	4.3	-1.8	-0.6	31.6	-0.1	5.3	-1.2	63.2	0.3	0.0	0.12
	4.5	-1.4	-0.5	33.3	-0.1	6.7	-0.9	60.0	0.1	0.0	0.10
$Br_3CH\cdots OC$	2.7	23.9	-33.4	31.6	-39.8	37.7	-23.0	21.8	129.5	-9.5	1.73
	2.9	6.6	-18.3	31.9	-18.6	32.4	-15.5	27.0	63.9	-5.0	1.20
	3.1	-1.0	-10.0	31.7	-8.6	27.3	-10.5	33.3	30.4	-2.4	0.82
	3.3	-3.6	-5.5	31.3	-3.9	22.2	-7.1	40.3	14.1	-1.1	0.55
	3.5	-4.1	-3.2	30.5	-1.8	17.1	-5.0	47.6	6.4	-0.5	0.37
	3.7	-3.2	-1.9	29.2	-0.9	13.8	-3.5	53.8	3.3	-0.2	0.25
	3.9	-3.0	-1.3	30.2	-0.4	9.3	-2.5	58.1	1.3	-0.1	0.17
	4.1	-2.4	-0.9	30.0	-0.2	6.7	-1.9	63.3	0.6	0.0	0.12
	4.3	-1.9	-0.6	28.6	-0.1	4.8	-1.4	66.7	0.3	0.0	0.09
	4.5	-1.5	-0.5	29.4	-0.1	5.9	-1.1	64.7	0.1	0.0	0.07

Table S4. Selected data obtained from NBO analysis upon $R_{C...O}$ are in the range of 2.7-4.5 Å at MP2/6-311++G(3df,2pd)

	R_{C-O}(Å)	EDT/e CHX_3	E(2) ($kJ.mol^{-1}$)	Δσ* (C-H)/e	Δ%s(C)
$F_3CH\cdots OC$	2.7	-0.01815	20.86	0.0075	2.85
	2.9	-0.01047	10.55	0.0023	1.92
	3.1	-0.00625	5.32	0.0003	1.25
	3.3	-0.00390	2.79	-0.0003	0.80
	3.5	-0.00243	1.55	-0.0004	0.53
	3.7	-0.00145	0.91	-0.0004	0.37
	3.9	-0.00082	0.56	-0.0118	0.65
	4.1	-0.00048	0.28	-0.0118	0.60
	4.3	-0.00033	0.19	-0.0117	0.56
	4.5	-0.00030	0.13	-0.0116	0.54
$Cl_3CH\cdots OC$	2.7	-0.01695	17.23	0.0045	3.37
	2.9	-0.00952	8.78	0.0000	2.32
	3.1	-0.00561	4.36	-0.0013	1.45
	3.3	-0.00352	2.28	-0.0013	0.86
	3.5	-0.00215	1.17	-0.0009	0.50
	3.7	-0.00116	0.76	-0.0006	0.28
	3.9	-0.00049	0.47	-0.0003	0.16
	4.1	-0.00012	0.54	-0.0002	0.09
	4.3	0.00000	0.17	-0.0001	0.05
	4.5	0.00000	0.10	-0.0001	0.02
$Br_3CH\cdots OC$	2.7	-0.01685	16.52	0.0058	3.77
	2.9	-0.00945	8.50	0.0009	2.61
	3.1	-0.00549	4.20	-0.0009	1.68
	3.3	-0.00341	2.18	-0.0012	1.01
	3.5	-0.00205	1.19	-0.0009	0.60
	3.7	-0.00107	0.69	-0.0006	0.35
	3.9	-0.00044	0.37	-0.0004	0.20
	4.1	-0.00012	0.23	-0.0003	0.12
	4.3	-0.00006	0.14	-0.0002	0.07
	4.5	-0.00011	0.08	-0.0001	0.04

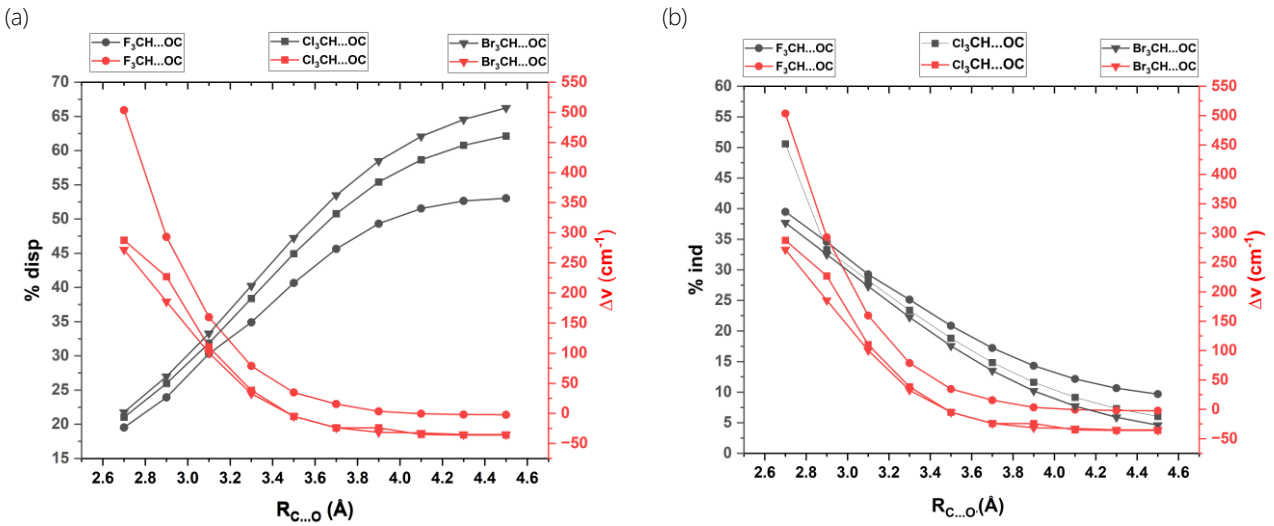

Figure S1. The relationship between percentage of (a) dispersion component (%disp) and (b) induction component (%ind) with the change in the stretching frequency of C-H bond involving C-H···O hydrogen bonds in $X_3CH\cdots OC$ complexes (X= F, Cl, Br)