Electronic Supplementary Information (ESI) for: Resonance-Assisted Hydrogen Bonds Revisited. Resonance Stabilization vs. Charge Delocalization

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Table 1 Interaction energy components and the basis set extension effects estimated at MP2 level of approximation. All energies are in kJ/mol

dimer of	ΔE^{HL}	$\varepsilon_{el}^{(1)}$	ε_{ex}^{HL}	ΔE_{del}^{HF}	ΔE^{HF}	$\varepsilon_{MP}^{(2)}$	$\varepsilon_{el,r}^{(12)}$	$\varepsilon_{disp}^{(2)}$	$\Delta E_{ex}^{(2)}$	ΔE^{MP2}
					AUG-cc-pVDZ					
formic acid	8.4	-137.2	146.0	-73.2	-64.4	-4.2	5.0	-39.7	30.5	-68.6
acetic acid	8.8	-144.8	153.6	-75.3	-66.5	-5.4	4.6	-42.3	32.2	-72.0
trifluoroacetic acid	15.5	-123.8	139.3	-74.1	-58.6	-6.7	4.2	-39.3	28.5	-64.9
formamide	-7.5	-111.3	103.8	-46.0	-53.6	-7.5	3.8	-33.5	22.2	-61.1
acetamide	-5.4	-115.9	110.5	-48.5	-54.0	-9.2	2.9	-35.6	23.4	-63.2
trifluoroacetamide	-7.5	-106.3	98.7	-45.2	-53.1	-7.9	5.0	-32.6	20.1	-61.1
					AUG-cc-pVTZ					
formic acid	14.2	-144.8	159.0	-79.9	-65.7	-9.6	5.9	-46.9	31.4	-75.3
acetic acid	14.2	-151.9	166.1	-82.0	-67.8	-11.3	5.4	-49.4	33.1	-78.7
trifluoroacetic acid	20.1	-130.1	150.2	-78.7	-58.6	-7.1	3.8	-41.0	30.1	-65.3
formamide	-4.6	-112.5	107.9	-47.3	-51.9	-12.1	4.2	-37.7	21.8	-64.0
acetamide	-3.3	-116.3	113.4	-49.0	-52.3	-13.8	3.3	-39.7	22.6	-66.1
trifluoroacetamide	-5.4	-107.9	102.5	-46.4	-51.9	-12.1	5.4	-36.8	19.2	-64.0
					AUG-cc-pVQZ					
formic acid	13.0	-143.5	156.5	-78.7	-65.3	-11.7	6.3	-48.1	30.1	-77.4
acetic acid	13.4	-150.6	164.0	-80.8	-67.4	-13.4	5.4	-50.6	31.8	-80.8
formamide	-5.9	-110.9	105.4	-46.0	-51.9	-13.8	4.2	-38.5	20.9	-65.3
acetamide	-3.3	-116.3	113.4	-49.0	-52.3	-15.5	3.4	-41.1	22.2	-67.7

Table 2 The selected AIM descriptors (in a.u.), estimated for various substituted MDA derivatives using MP2/6-31+G(d,p) method.

R_1	R_2	$\rho(\mathbf{r}_{BCP})$	$\nabla^2\rho(\mathbf{r}_{BCP})$	$H(\mathbf{r}_{BCP})$
-	-	0.0543	0.1522	-0.0051
-	-F	0.0361	0.1053	-0.0018
-	-Cl	0.0405	0.1193	-0.0020
-	-OH	0.0295	0.0901	-0.0013
-	$-CF_3$	0.0499	0.1418	-0.0038
-	$-OCH_3$	0.0485	0.1418	-0.0032
-F	-F	0.0331	0.0970	-0.0016
-Cl	-Cl	0.0544	0.1536	-0.0049
-OH	-OH	0.0371	0.1126	-0.0015