Supporting Information Available:

"Table 1. Energetic and geometric parameters for the 1:1-Complexes obtained in the present work and reported in ref.52 (see also Figure 15)."

Parameter	B3LYP/6-311++G**[a]	B3LYP/6-311+G**[b]
Dipole moment(debye)	3.24	3.17
BSSE corrected binding energy (kcal/mol)	-6.01	-6.17
H-bonded distance[c] (Å)	1.886	1.84
H-bond angle[d](degree)	171.23	173.09

"*a*. present work ; *b*. reference 54 ; *c*. Hw···O(I) distance ; *d*. O_w–H_w–O(I) angle

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