Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Table S1 The change (Δθ, deg) of angle C–T–Y (T = C, Si and Ge; Y = H, F and Cl) in the dyads relative to that in the monomers

dyads	Δθ
$PhCF_3$···PyI	-0.58
$PhSiF_3$···PyI	-12.66
$PhGeF_3$···PyI	-13.73
$PhSiH_3$···PyI	-4.50
$PhSiCl_3$···PyI	-11.78
$PhSiF_3$···PyBr	-12.65

Table S2 The increased/decreased percentage of binding energies of both interactions in the triads

triads	$\Delta\Delta E_{TB}$%	$\Delta\Delta E_{XB}$%
$PhCF_3$···PyI···NH_3	-41.3%	-6.1%
$PhSiF_3$···PyI···NH_3	14.7%	30.8%
$PhGeF_3$···PyI···NH_3	9.5%	34.3%
$PhSiH_3$···PyI···NH_3	20.3%	11.7%
$PhSiCl_3$···PyI···NH_3	15.5%	35.1%
$PhSiF_3$···PyI···NCH	12.9%	37.0%
$PhSiF_3$···PyI···$NHCH_2$	14.7%	28.3%
$PhSiF_3$···PyI···NH_2CH_3	16.1%	26.6%
$PhSiF_3$···PyBr···NH_3	12.3%	43.1%

Table S3. Change of electron density (Δρ, au) in the triads relative to the dyads.

triads	$\Delta\rho_{TB/HB}$	$\Delta\rho_{XB}$
$PhCF_3$···PyI···NH_3	-0.0001	-0.0001
$PhSiF_3$···PyI···NH_3	0.0041	0.0021
$PhGeF_3$···PyI···NH_3	0.0032	0.0023
$PhSiH_3$···PyI···NH_3	0.0030	0.0010
$PhSiCl_3$···PyI···NH_3	0.0047	0.0023
$PhSiF_3$···PyI···HCN	0.0036	0.0014
$PhSiF_3$···PyI···$NHCH_2$	0.0041	0.0023
$PhSiF_3$···PyI···NH_2CH_3	0.0044	0.0025
$PhSiF_3$···PyBr···NH_3	0.0035	0.0011

Table S4. Change of second-order perturbation energies ($\Delta E^{(2)}$, kJ/mol) in the triads relative to the dyads.

triads	$\Delta E_1^{(2)}$	$\Delta E_2^{(2)}$	$\Delta E_3^{(2)}$
$PhCF_3$···PyI···NH_3	0.00	---	-0.14
$PhSiF_3$···PyI···NH_3	17.90	0.52	6.94
$PhGeF_3$···PyI···NH_3	40.13	0.17	7.82
$PhSiH_3$···PyI···NH_3	12.75	7.44	3.26
$PhSiCl_3$···PyI···NH_3	26.88	3.01	8.03
$PhSiF_3$···PyI···HCN	51.12	1.08	3.39
$PhSiF_3$···PyI···$NHCH_2$	19.95	1.21	7.74
$PhSiF_3$···PyI···NH_2CH_3	62.62	1.29	9.03
$PhSiF_3$···PyBr···NH_3	51.37	1.01	2.67

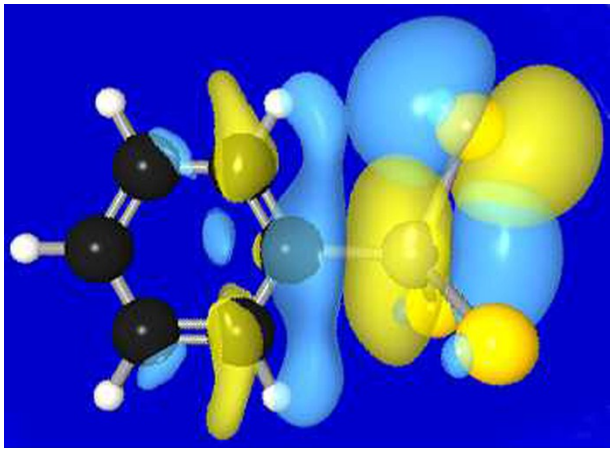

Figure S1 Diagram of Lp(Cl)→σ*(C–Si) orbital interaction in $PhSiCl_3$