Supporting information for "Accurate intermolecular interactions at dramatically reduced cost: XPol+SAPT with empirical dispersion"

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Optimized values of the range separation parameter, ω, for use with the LRC-ωPBEh functional are provided in Table S1 for each monomer unit consider in this work. Figure S1 shows some Ar$\cdots$Ne potential energy curves computed at various levels of theory.

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Table S1: Optimized range separation parameters (ω) for monomers.

Monomer	ω/bohr^{-1}	Ionization potential/eV
adenine[a]	0.05	9.8587
2-aminopyridine	0.10	8.2416
benzene	0.10	9.2163
ethyne	0.15	11.1043
ethene	0.15	10.2657
methane	0.20	14.2371
formamide[a]	0.05	10.1339
formic acid[a]	0.05	11.3846
water	0.10	12.3393
HCN	0.35	13.9377
indole	0.10	7.8064
ammonia	0.10	10.6694
phenol	0.10	8.5962
pyrazine	0.20	10.4075
2-pyridoxine	0.10	8.3881
thymine	0.25	10.0360
uracil	0.20	10.0986
acetate	0.05	3.9296
formaldehyde	0.10	10.7603
guanidinium	0.05	16.1640
imidazolium[a]	0.05	17.1969
methylamine	0.10	9.5708
methylammonium	0.20	20.6299
methanol	0.10	10.9272
$AcNH_2$[a]	0.05	9.6747
AcOH[a]	0.05	10.7562
cyclopentane	0.20	11.7103
neopentane	0.10	11.3508
pentane	0.10	11.3075
peptide[a]	0.05	9.4611
pyridine	0.10	9.6925

[a]This monomer does not meet the condition $\varepsilon_{\mathrm{HOMO}} = -\mathrm{IP}$, so we set $\omega = 0.05$ bohr^{-1} to approximate this condition as best as possible.

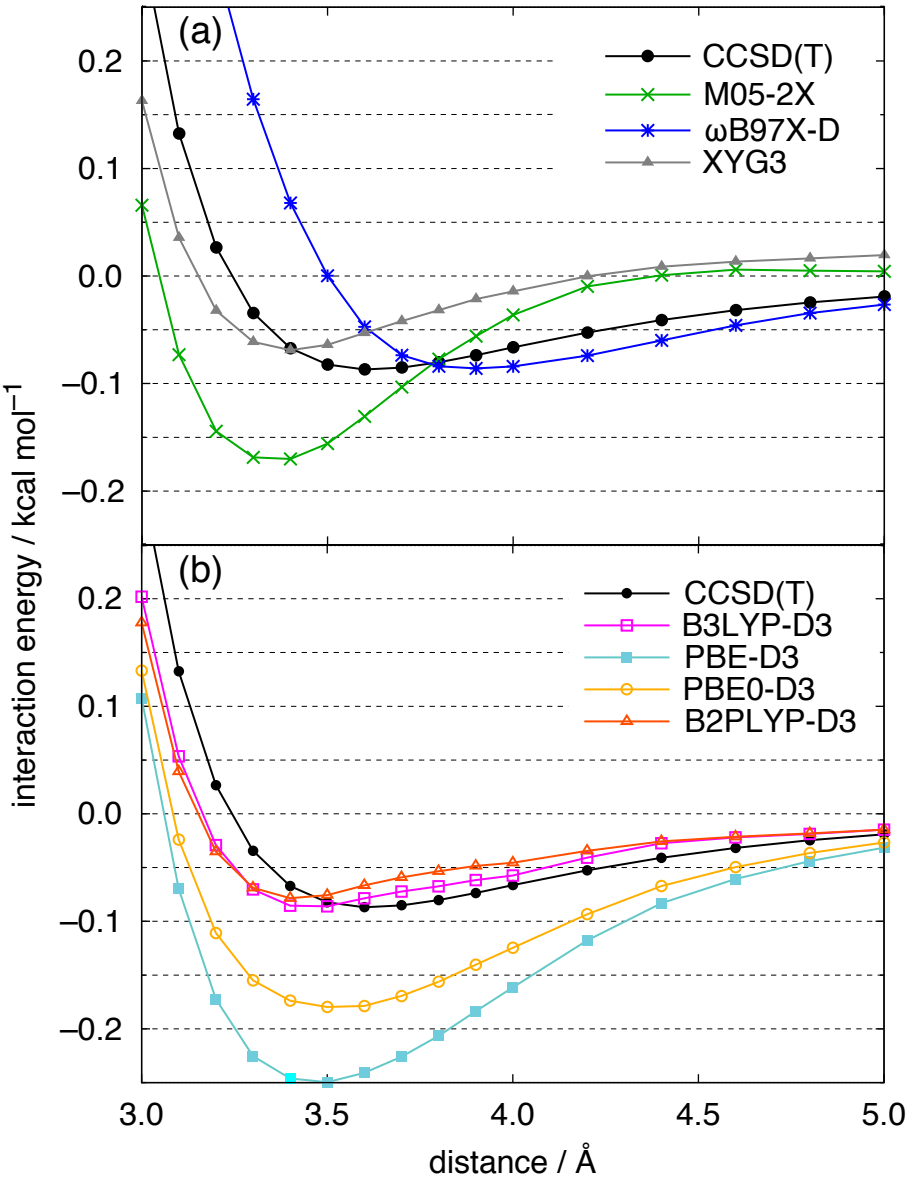

Figure S1: Potential energy curves for Ar···Ne, computed using the aug-cc-pVTZ basis set with counterpoise correction.