Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

SUPPORTING INFORMATION

Nature of Anion-templated π^+-π^+ Interactions

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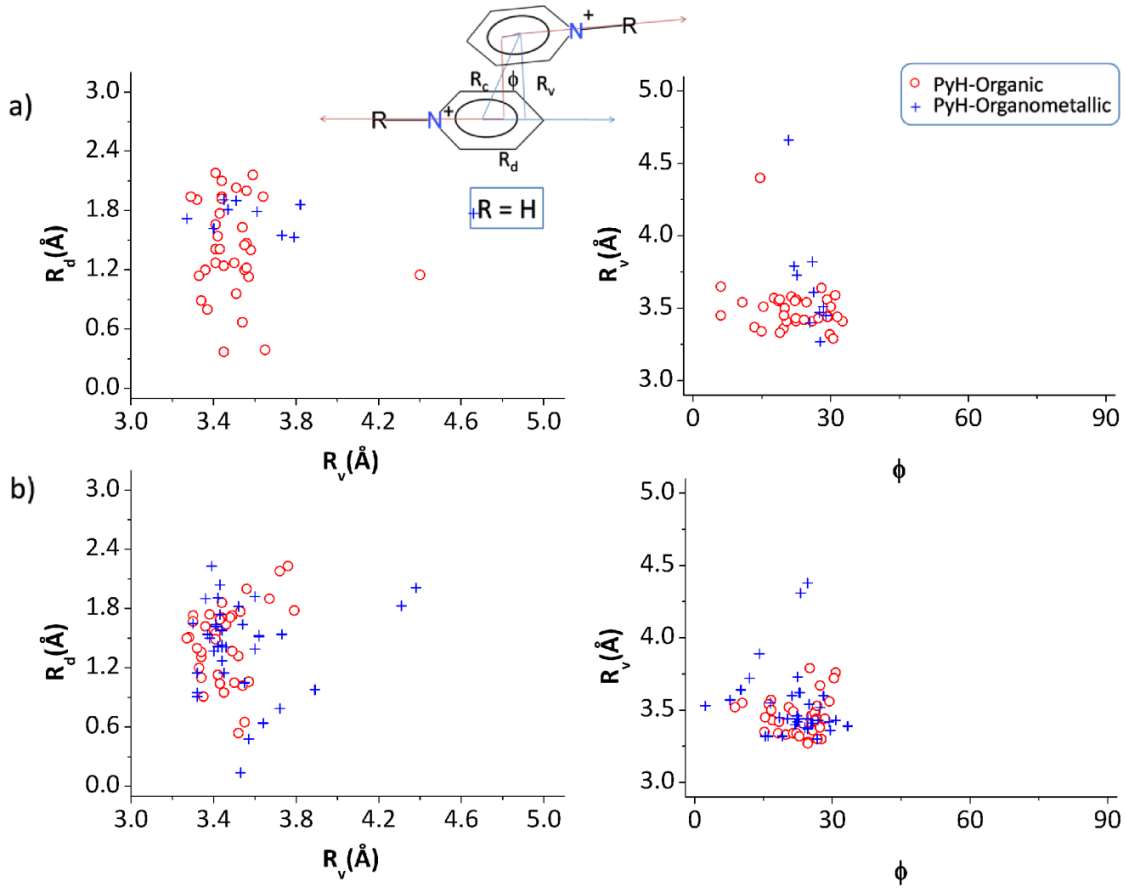

Fig. S1 Scatter plots of R_v vs. R_d and ϕ vs. R_v of pyridinium (R=H, PyH) dimer complexes in the presence of a) halide and b) water. Search results are restricted to $R_v < 5$ Å and $R_d < 3.5$ Å. Contact distance and angle with halide or water are 1.5-2.2 Å and 140-180°. Organic and organometallic complexes are searched separately.

Table S1 MP2 binding energies (kcal/mol) of PyH dimers using aug-cc-pVDZ (aVDZ), aug-cc-pVTZ (aVTZ) and aug-cc-pVQZ (aVQZ) basis sets. The complete basis set limit (CBS) is determined using both aVDZ-aVTZ and aVTZ-aVQZ extrapolation.

Complex	aVDZ	aVTZ	aVQZ	CBS	
				aVDZ-aVTZ	aVTZ-aVQZ
PyH-De	18.7	20.1	20.6	20.6	20.9
PyH-T	18.8	19.5	20.0	19.8	20.2
PyH-Ds	17.8	18.8	19.3	19.2	19.6

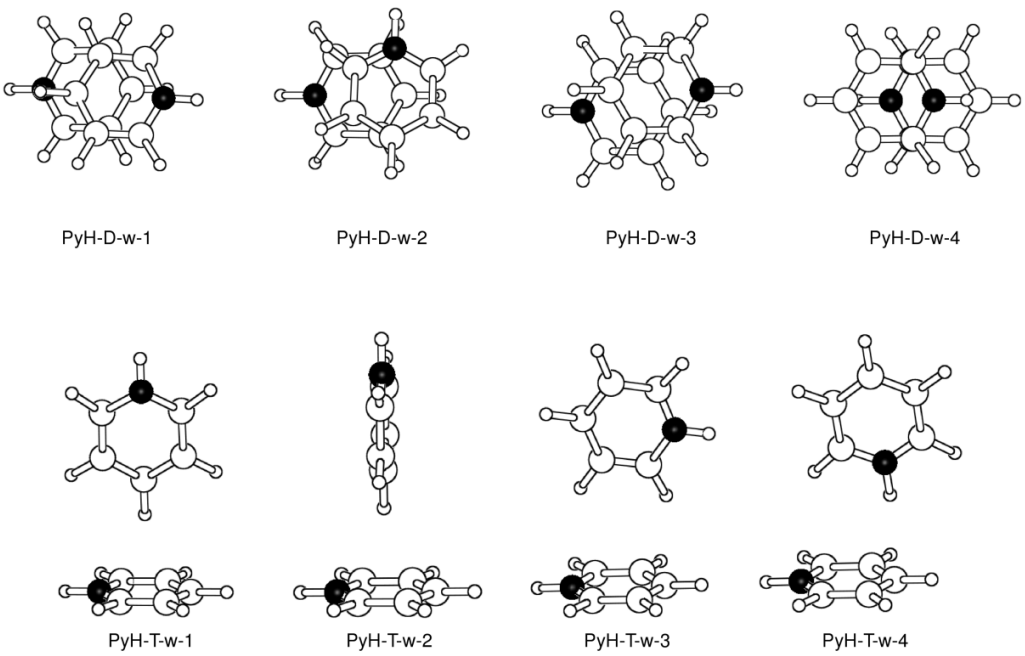

Fig. S2 PyH dimers optimized at the MP2/aug-cc-pVDZ level using the polarizable continuum model (PCM) of water. Energies and geometric parameters are summarized in Table S2.

Table S2 MP2/aug-cc-pVDZ binding energies and geometric parameters of PyH dimers. R_c, R_v and R_d are the centroid, vertical and off-center distances, respectively.

Complex	-E (kcal/mol)	R_c, Å	R_v, Å	R_d, Å
PyH-D-w-1	27.3	3.4	3.2	1.0
PyH-D-w-2	26.8	3.5	3.4	1.1
PyH-D-w-3	7.1	3.4	3.3	0.9
PyH-D-w-4	5.1	3.6	3.4	1.4
PyH-T-w-1	2.9	4.9	4.9	0.1
PyH-T-w-2	2.9	4.9	4.9	0.0
PyH-T-w-3	2.5	5.1	5.1	0.5
PyH-T-w-4	2.0	5.1	5.0	1.1