Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Expanded ensemble predictions of absolute binding free energies in the SAMPL9 host–guest challenge

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Supporting Tables

Table S1. SMILES strings for all host (WP6) and guest microstates

Index	Guest	Microstate	Isomeric SMILES
0	G1	1	C1CCCCC(CCCCC1)N
1	G1	2	C1CCCCC(CCCCC1)[NH3+]
2	G2	1	C[N+]1(CCC(CC1)C2CC[N+](CC2)(C)C)C
3	G3	1	[NH3+][C@@H]1C[C@H]2CC[C@@H]1C2
4	G3	2	N[C@@H]1C[C@H]2CC[C@@H]1C2
5	G3	3	[NH2]C1CC2CCC1C2
6	G3	4	[NH3+]C1CC2CCC1C2
7	G4	1	C[Si](C)(C)C[NH3+]
8	G4	2	C[Si](C)(C)CN
9	G5	1	CC12CC3(CC(C1)(CC(C2)(C3)[N+](C)(C)C)[N+](C)(C)C)C
10	G6	1	C1CCCC(CCC1)[NH3+]
11	G6	2	C1CCCC(CCC1)N
12	G7	1	C1CCC(CC1)N
13	G7	2	C1CCC(CC1)[NH3+]
14	G8	1	C[N+](C)(CCCS(=O)(=O)[O-])Cc1ccccc1
15	G9	1	[NH3+]C12CC3CC(C1)CC(O)(C3)C2
16	G9	2	[NH2]C12CC3CC(C1)CC(O)(C3)C2
17	G10	1	C[N+](C)(C)Cc1ccc(cc1)C[N+](C)(C)C
18	G11	1	CC(C)(C)C[NH3+]
19	G11	2	CC(C)(C)CN
20	G12	1	C[N+](C)(C)[C@H]1[C@@H]2C[C@@H]3C[C@H]1C[C@H](C2)[C@H]3[N+](C)(C)C
21	G12	2	C[N+](C)(C)[C@H]1[C@H]2C[C@H]3C[C@@H]1C[C@@H](C2)[C@H]3[N+](C)(C)C
22	G13	1	C[n+]1ccc(cc1)c2cc[n+](cc2)C

	Host	Net charge	
1	WP6	-8	O=C([O-])COc1cc2c(OCC(=O)[O-])cc1Cc1cc(OCC(=O)O)c(cc1OCC(=O)[O-])Cc1cc(OCC(=O)[O-

			])c(cc1OCC(=O)O)Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)[O-])Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)O)Cc1cc(OCC(=O)O)c(cc1OCC(=O)[O-])C2
2	WP6	-10	O=C([O-])COc1cc2c(OCC(=O)[O-])cc1Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)[O-])Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)O)Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)[O-])Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)[O-])Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)O)C2
3	WP6	-12	O=C([O-])COc1cc2c(OCC(=O)[O-])cc1Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)[O-])Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)[O-])Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)[O-])Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)[O-])Cc1cc(OCC(=O)[O-])c(cc1OCC(=O)[O-])C2

Supporting Figures

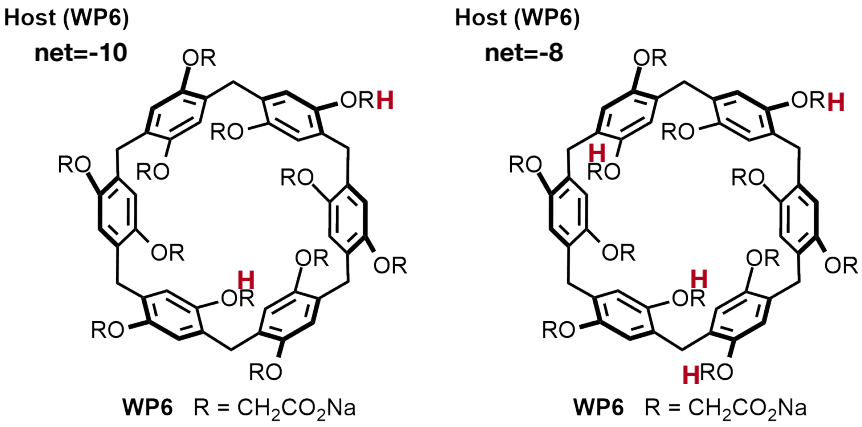

Figure S1. Protonation states used for WP6 microstates with net charge -10e (left) and -8e (right).

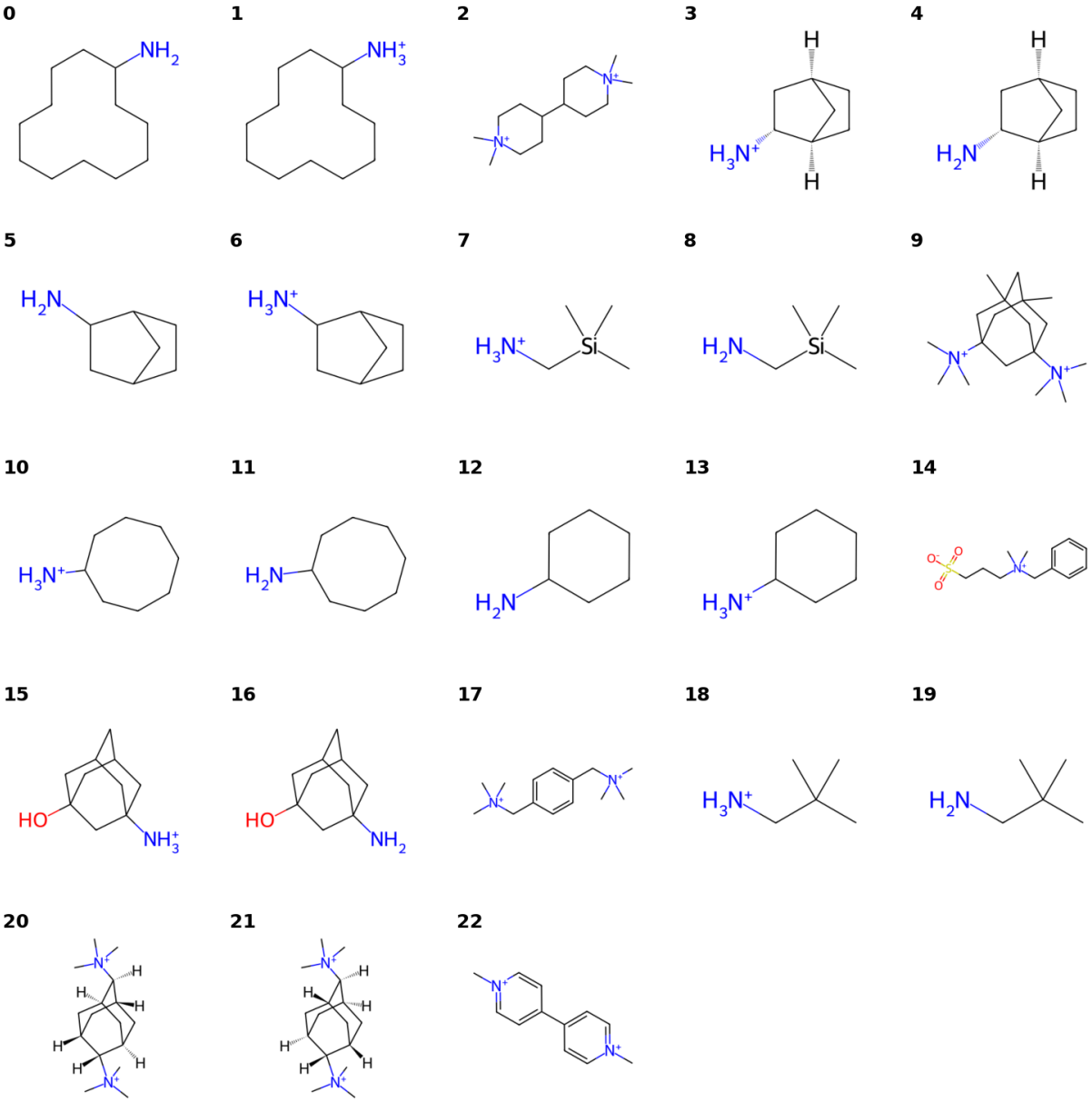

Figure S2. Chemical structures for all microstates. Labels correspond to the indices found in Table S1.