Dissecting Halide-Receptor Interactions in "Four Wall" Aryl-Extended Calix[4]pyrrole Complexes: The Role of the Aromatic Walls – Supplementary Information

Lane M. Terry,[a] River A. Leversee,[b] Gemma Aragay,[c] Pablo Ballester,[c,d] Anne B. McCoy,[e] and J. Mathias Weber[a],*

[a] JILA and Department of Chemistry, University of Colorado, 440 UCB, Boulder, CO 80309-0440, USA.

[b] JILA and Department of Physics, University of Colorado, 440 UCB, Boulder, CO 80309-0440, USA.

[c] Institute of Chemical Research of Catalonia (ICIQ)-CERCA, The Barcelona Institute of Science and Technology (BIST), Av. Països Catalans, 16, 43007- Tarragona, Spain.

[d] ICREA, Passeig Lluís Companys 23, 08010 Barcelona, Spain.

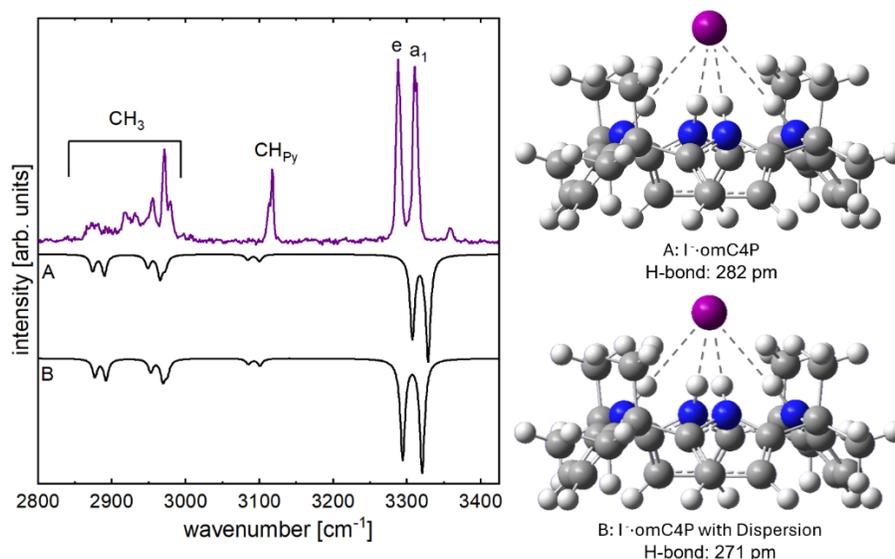[e] Department of Chemistry, University of Washington, Seattle, WA 98195, USA.

Figure S1. Experimental (upright, purple) and calculated (inverted, black) photodissociation spectrum of I⁻·omC4P. The calculated spectrum is from a scaled (0.9529) harmonic calculation. Calculated geometry of I⁻·omC4P in the gas-phase with NH···I⁻ H-bond represented by dashed gray lines and quantified below the structure. All calculations were performed using the B3LYP functional. A cc-pVDZ basis was employed for the oxygen and carbon atoms, while an aug-cc-pVDZ basis was used to describe the hydrogen and nitrogen atoms. For iodine, we used the aug-cc-pVDZ-pp basis and associated effective core potential (ECP). See main text for additional details. Calculations with Grimme's dispersion correction (D3) are shown below, labeled B.

Table S1. Selected experimental and calculated scaled harmonic vibrational frequencies in I⁻·omC4P in cm^{-1}.

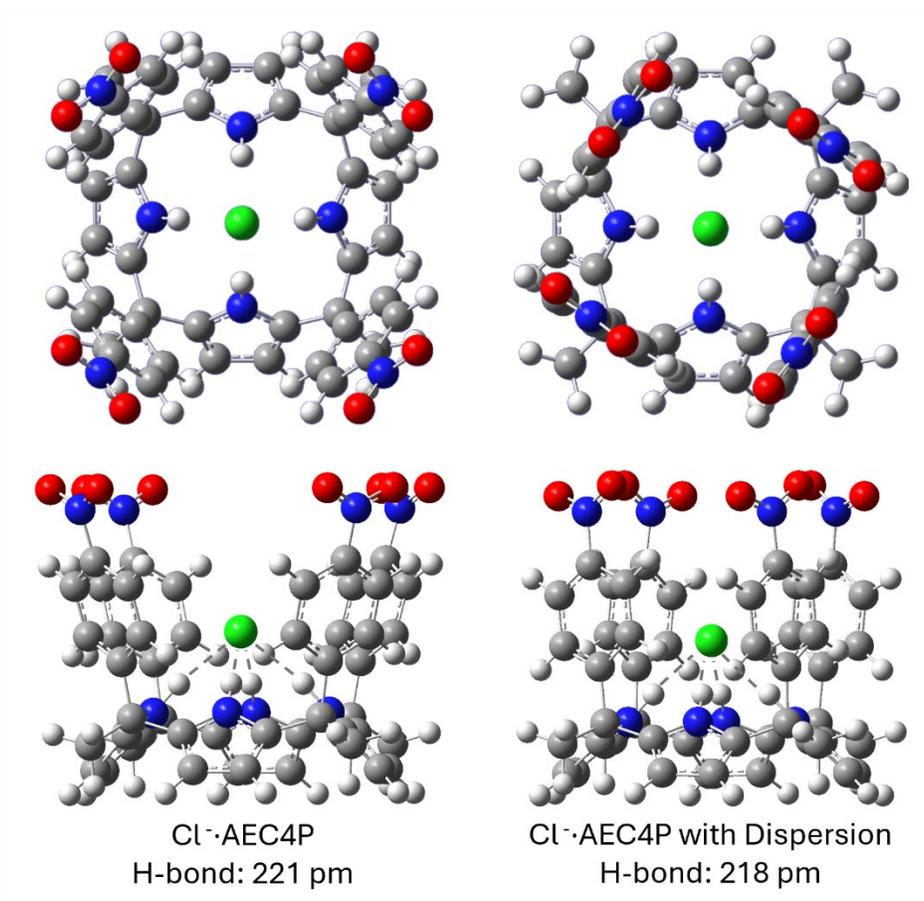| Experimental	Scaled Harmonic[a]	Characterization
2875, 2891	2873, 2889	CH$_3$ symmetric stretching
2955, 2971	2948, 2965	CH$_3$ asymmetric stretching
3113	3084	CH$_{Py}$ antisymmetric stretching
3117	3100	CH$_{Py}$ symmetric stretching
3288	3307	degenerate NH stretching (e)
3311	3328	symmetric NH stretching (a$_1$)

[a] Scaling factor (0.9529)

Figure S2. Calculated geometry of Cl$^-$·AEC4P without (left) and with Grimme's dispersion correction (D3, right). A top view along the C$_4$ symmetry axis (top) and a side view (bottom) of the complex is shown. The H-bond length is given below each structure.

Table S2. Selected experimental and anharmonic vibrational frequencies of NH stretching modes and NH bending overtones/combination bands in halide-AEC4P complexes in cm^{-1}.

Halide	Label	Experimental	Calculated[a]	Characterization and Symmetry[b]
Cl$^-$	CH$_{Py}$, e	3110	3121	$\nu_{2/3}$; e
	α	3132	3168	$2\nu_{52}$ (65%) + ν_1 (26%); a
	α'	3171	3190	$2\nu_{52}$ (33%) + ν_1 (22%)+ $2\nu_{50}$ (22%); a
	ε	3192	3200	$\nu_{52}/\nu_{50/51}$; e
	α''	3210	3248	$2\nu_{49}$ (48%) + ν_1 (31%) + $2\nu_{51}$ (11%); a
Br$^-$	CH$_{Py}$, e	3118	3125	$\nu_{2/3}$ (80%) + $\nu_{52}/\nu_{50/51}$ (10%); e
	ε	3140	3188	$\nu_{52}/\nu_{50/51}$; e
	ε'	3168	3197	$\nu_{50/51}$ (46%) + $2\nu_{50}$ (27%) + $2\nu_{51}$ (24%); e
	ε''	3186	3222	ν_{49}/ν_{50}; e
	α	3207	3233	$2\nu_{49}$ (47%) + ν_1 (37%); a
I$^-$	e	3153	3133	$\nu_{2/3}$ (82%) + $\nu_{52}/\nu_{50/51}$ (12%); e
	ε	3168	3185	$\nu_{52}/\nu_{50/51}$ (57%) + $2\nu_{52}$ (15%); e
	ε'	3187	3213	$\nu_{49}/\nu_{50/51}$; e
	α	3212	3230	$2\nu_{49}$ (60%) + ν_1 (33%); a

[a] These calculations were performed under C$_1$, rather than C$_4$ symmetry, and the reported energies for doubly degenerate states reflect the average of the calculated values, which differ by at most 4 cm^{-1}.

[b] notation $\nu_{i/j}$ indicates degenerate e modes, notation $2\nu_k$ indicates an overtone, notation ν_l/ν_m indicates a combination band with one quantum of excitation in both modes l and m; contributing states with 10% or more are listed.
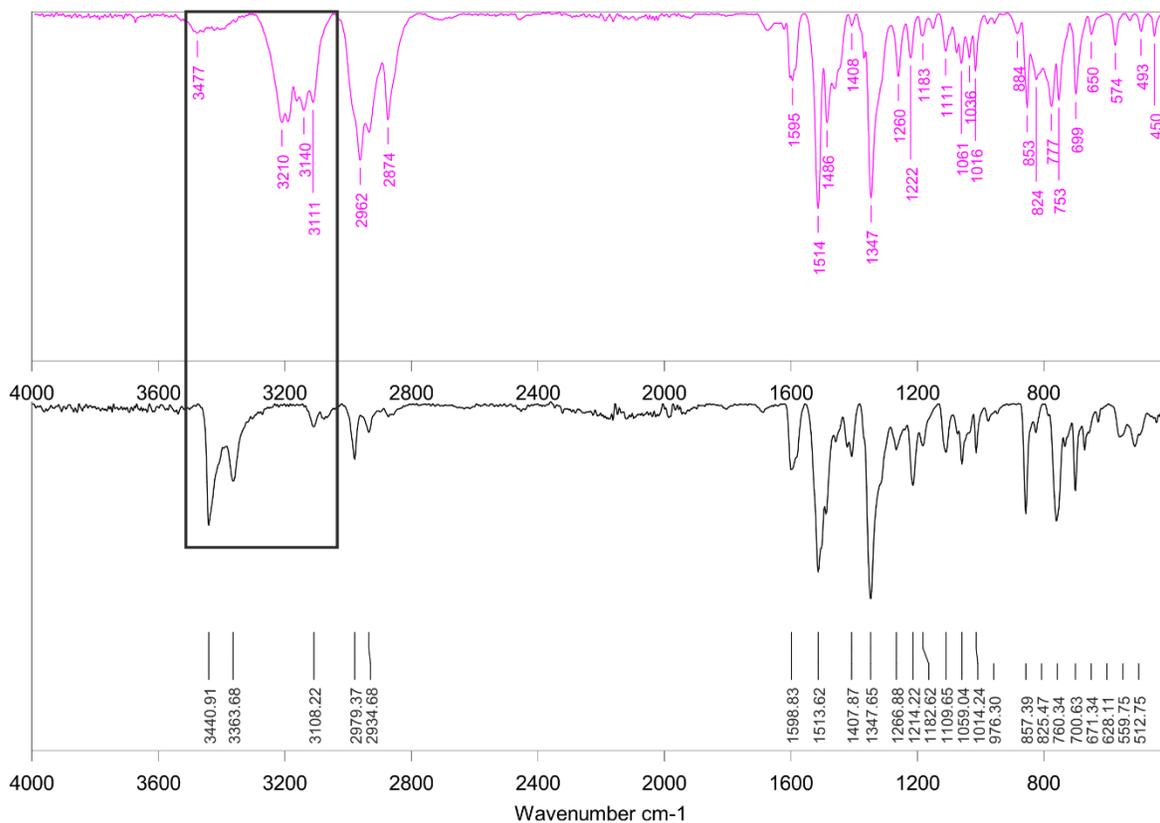
Figure S3. Attenuated total reflection Fourier-Transform IR spectra of the solid AEC4P receptor (black) and the solid obtained after assembling the complex with tetrabutylammonium chloride and removing the solvent (pink). FT-IR measurements were carried out on a Bruker Optics FT-IR Alpha spectrometer equipped with a DTGS detector, and a KBr beam splitter, using a single-reflection ATR accessory with diamond crystal. Due to the limited solubility of the receptor and its chloride complexes (< 2 mM), solution-phase IR spectra could not be acquired at analyzable concentrations. The NH stretching region shows a clear red shift upon chloride binding, with similar IR signatures as in the gas phase $Cl^- \cdot AEC4P$ complex. We note, however, that solvation effects cannot be captured using this approach.

Table S3. Electrostatic force analysis. Forces originating from the charge distributions on different functional groups acting on an anion at the binding site in AEC4P and omC4P along the C_4 symmetry axis (in nN). A negative sign represents forces pushing into the pocket.

Ion	Receptor	Total force	C4P macrocycle	Phenyl group	Nitro group	Methyl group
Cl	AEC4P	−1.74	−1.51	+0.12	−0.35	N/A
	omC4P	−1.12	−1.35	N/A	N/A	+0.23
	Tetra-phenyl-AEC4P[a]	−1.68	−1.46	−0.21	N/A	N/A
Br	AEC4P	−1.47	−1.26	+0.34	−0.55	N/A
	omC4P	−0.97	−1.10	N/A	N/A	+0.13
I	AEC4P	−1.16	−0.96	+0.31	−0.52	N/A
	omC4P	−0.81	−0.84	N/A	N/A	+0.03

[a] From calculations where the nitro groups were replaced with hydrogen atoms.

Table S4. Atomic coordinates for I⁻·omC4P (in Å) from a DFT calculation using the B3LYP functional. A cc-pVDZ basis was employed for the oxygen and carbon atoms, while an aug-cc-pVDZ basis was used to describe the hydrogen and nitrogen atoms. For iodine, we used the aug-cc-pVDZ-pp basis and associated effective core potential (ECP). See main text for additional details.

Element	X	Y	Z
C	-1.13865	2.91925	-0.79567
C	-0.71292	3.72611	-1.83940
C	0.71292	3.72611	-1.83940
C	1.13865	2.91925	-0.79567
N	0.00000	2.44055	-0.17425
H	-1.35269	4.25999	-2.53508
H	1.35269	4.25999	-2.53508
C	-2.55175	2.55175	-0.35073
C	-3.54176	3.54176	-0.99880
H	-3.30543	4.56872	-0.68587
H	-3.50335	3.50335	-2.09578
H	-4.56872	3.30543	-0.68587
C	-2.69195	2.69195	1.18554
H	-2.02219	2.02219	1.74204
H	-2.45923	3.72340	1.49146
H	-3.72340	2.45923	1.49146
C	2.55175	2.55175	-0.35073
C	3.54176	3.54176	-0.99880
H	3.30543	4.56872	-0.68587
H	4.56872	3.30543	-0.68587
H	3.50335	3.50335	-2.09578
C	2.69195	2.69195	1.18554
H	3.72340	2.45923	1.49146
H	2.45923	3.72340	1.49146
H	2.02219	2.02219	1.74204
C	2.91925	1.13865	-0.79567
C	3.72611	0.71292	-1.83940
N	2.44055	0.00000	-0.17425
C	3.72611	-0.71292	-1.83940
H	4.25999	1.35269	-2.53508
C	2.91925	-1.13865	-0.79567
H	1.83078	0.00000	0.64148
H	4.25999	-1.35269	-2.53508
C	1.13865	-2.91925	-0.79567
C	0.71292	-3.72611	-1.83940
C	-0.71292	-3.72611	-1.83940

C	-1.13865	-2.91925	-0.79567
N	0.00000	-2.44055	-0.17425
H	0.00000	-1.83078	0.64148
H	1.35269	-4.25999	-2.53508
H	-1.35269	-4.25999	-2.53508
C	2.55175	-2.55175	-0.35073
C	3.54176	-3.54176	-0.99880
H	3.30543	-4.56872	-0.68587
H	3.50335	-3.50335	-2.09578
H	4.56872	-3.30543	-0.68587
C	2.69195	-2.69195	1.18554
H	2.02219	-2.02219	1.74204
H	2.45923	-3.72340	1.49146
H	3.72340	-2.45923	1.49146
C	-2.55175	-2.55175	-0.35073
C	-3.54176	-3.54176	-0.99880
H	-3.30543	-4.56872	-0.68587
H	-4.56872	-3.30543	-0.68587
H	-3.50335	-3.50335	-2.09578
C	-2.69195	-2.69195	1.18554
H	-3.72340	-2.45923	1.49146
H	-2.45923	-3.72340	1.49146
H	-2.02219	-2.02219	1.74204
C	-2.91925	-1.13865	-0.79567
C	-3.72611	-0.71292	-1.83940
N	-2.44055	0.00000	-0.17425
C	-3.72611	0.71292	-1.83940
H	-4.25999	-1.35269	-2.53508
C	-2.91925	1.13865	-0.79567
H	-1.83078	0.00000	0.64148
H	-4.25999	1.35269	-2.53508
H	0.00000	1.83078	0.64148
I	0.00000	0.00000	2.79214

Table S5. Atomic coordinates for Cl⁻·AEC4P (in Å) from a DFT calculation using the B3LYP functional using a modified cc-pVDZ basis, with a cc-pVDZ basis for the oxygen and carbon atoms as well as for most of the hydrogen atoms, while an aug-cc-pVDZ basis was used to describe the halogen and nitrogen atoms, as well as the hydrogen atoms in the NH groups.

Element	X	Y	Z
C	1.16467	2.87668	-2.55968
C	2.15227	3.30478	-3.43287
C	3.20356	2.33727	-3.39863
C	2.83172	1.34455	-2.50373
C	2.87742	-1.16443	-2.55875
C	3.30586	-2.15195	-3.43188
C	2.33834	-3.20323	-3.39811
C	1.34527	-2.83149	-2.50356
C	-1.16369	-2.87716	-2.55953
C	-2.15087	-3.30547	-3.43311
C	-3.20217	-2.33795	-3.39960
C	-2.83077	-1.34502	-2.50476
C	-2.87645	1.16395	-2.56041
C	-3.30446	2.15124	-3.43400
C	-2.33695	3.20253	-3.40004
C	-1.34432	2.83101	-2.50491
H	2.13311	4.21624	-4.02306
H	4.12592	2.37031	-3.97062
H	4.21754	-2.13272	-4.02170
H	2.37160	-4.12554	-3.97018
H	-2.13142	-4.21707	-4.02306
H	-4.12425	-2.37113	-3.97204
H	-4.21586	2.13187	-4.02427
H	-2.36994	4.12469	-3.97237
C	-0.09465	3.56609	-2.05785
C	0.09538	-3.56645	-2.05692
C	-3.56590	-0.09520	-2.05821
C	3.56663	0.09484	-2.05652
N	1.58682	1.68197	-2.02087
H	1.09458	1.17494	-1.27543
N	1.68250	-1.58664	-2.02044
H	1.17518	-1.09448	-1.27515
N	-1.58611	-1.68232	-2.02121
H	-1.09423	-1.17511	-1.27566
N	-1.68179	1.58629	-2.02164
H	-1.17483	1.09432	-1.27597
C	-0.14096	5.00395	-2.61804

H	0.74637	5.56645	-2.29891
H	-0.16837	4.99061	-3.71685
H	-1.03762	5.52079	-2.24967
C	5.00470	0.14122	-2.61616
H	5.56709	-0.74614	-2.29692
H	4.99178	0.16874	-3.71498
H	5.52139	1.03784	-2.24751
C	0.14196	-5.00445	-2.61673
H	-0.74552	-5.56687	-2.29790
H	0.16991	-4.99138	-3.71553
H	1.03844	-5.52120	-2.24780
C	-5.00370	-0.14172	-2.61853
H	-4.99025	-0.16951	-3.71733
H	-5.52057	-1.03825	-2.24990
H	-5.56625	0.74572	-2.29977
Cl	-0.00018	0.00010	0.19156
C	0.00728	3.66956	-0.51740
C	-1.07300	3.42260	0.33786
C	1.24800	4.01046	0.05057
C	-0.91720	3.44996	1.72442
H	-2.04110	3.15715	-0.07856
C	1.42304	4.05174	1.42749
H	2.09538	4.21317	-0.60622
C	0.33574	3.75126	2.25050
H	-1.73863	3.20580	2.39616
H	2.38380	4.29365	1.87765
C	-3.66953	0.00727	-0.51780
C	-4.01047	1.24819	0.04970
C	-3.42268	-1.07273	0.33785
C	-4.05189	1.42370	1.42656
H	-4.21310	2.09534	-0.60740
C	-3.45018	-0.91645	1.72436
H	-3.15720	-2.04097	-0.07821
C	-3.75151	0.33667	2.24997
H	-4.29383	2.38461	1.87636
H	-3.20611	-1.73765	2.39640
C	-0.00731	-3.66954	-0.51649
C	-1.24831	-4.01035	0.05094
C	1.07253	-3.42232	0.33925
C	-1.42404	-4.05127	1.42778
H	-2.09535	-4.21326	-0.60623
C	0.91603	-3.44932	1.72574
H	2.04083	-3.15692	-0.07675

C	-0.33716	-3.75053	2.25126
H	-2.38501	-4.29311	1.87752
H	1.73711	-3.20496	2.39783
C	3.66952	-0.00726	-0.51604
C	4.01020	-1.24805	0.05192
C	3.42226	1.07293	0.33924
C	4.05096	-1.42325	1.42883
H	4.21315	-2.09536	-0.60489
C	3.44910	0.91697	1.72580
H	3.15697	2.04108	-0.07717
C	3.75018	-0.33603	2.25184
H	4.29268	-2.38405	1.87898
H	3.20470	1.73833	2.39753
N	0.53058	3.74829	3.70624
N	3.74665	-0.53104	3.70757
N	-0.53275	-3.74719	3.70690
N	-3.74870	0.53202	3.70565
O	-3.59028	-0.45342	4.41760
O	-3.91036	1.67618	4.12669
O	-0.45510	3.58978	4.41784
O	1.67460	3.90992	4.12770
O	3.58791	0.45457	4.41921
O	3.90807	-1.67511	4.12895
O	-1.67698	-3.90872	4.12781
O	0.45257	-3.58848	4.41896

Table S6. Atomic coordinates for Br⁻·AEC4P (in Å) from a DFT calculation using the B3LYP functional using a modified cc-pVDZ basis, with a cc-pVDZ basis for the oxygen and carbon atoms as well as for most of the hydrogen atoms, while an aug-cc-pVDZ basis was used to describe the halogen and nitrogen atoms, as well as the hydrogen atoms in the NH groups.

Element	X	Y	Z
C	1.16573	2.87683	-2.58243
C	2.14032	3.29078	-3.47629
C	3.18977	2.32119	-3.44696
C	2.83048	1.34050	-2.53459
C	2.87691	-1.16584	-2.58223
C	3.29090	-2.14047	-3.47603
C	2.32130	-3.18992	-3.44670
C	1.34057	-2.83059	-2.53439
C	-1.16578	-2.87702	-2.58214
C	-2.14039	-3.29106	-3.47593
C	-3.18983	-2.32147	-3.44669
C	-2.83052	-1.34068	-2.53443
C	-2.87696	1.16567	-2.58231
C	-3.29099	2.14025	-3.47614
C	-2.32139	3.18970	-3.44692
C	-1.34062	2.83043	-2.53462
H	2.11320	4.19383	-4.07884
H	4.10288	2.34482	-4.03400
H	4.19397	-2.11338	-4.07855
H	2.34496	-4.10306	-4.03371
H	-2.11328	-4.19417	-4.07839
H	-4.10296	-2.34516	-4.03372
H	-4.19408	2.11313	-4.07862
H	-2.34508	4.10281	-4.03397
C	-0.09362	3.56976	-2.08676
C	0.09358	-3.56990	-2.08643
C	-3.56985	-0.09367	-2.08656
C	3.56981	0.09354	-2.08660
N	1.59357	1.68693	-2.03597
H	1.11914	1.19801	-1.26885
N	1.68698	-1.59366	-2.03581
H	1.19803	-1.11919	-1.26873
N	-1.59360	-1.68705	-2.03580
H	-1.11916	-1.19806	-1.26873
N	-1.68700	1.59352	-2.03596
H	-1.19803	1.11910	-1.26887
C	-0.13764	5.00377	-2.65798

H	0.74925	5.56718	-2.33901
H	-0.16138	4.98344	-3.75675
H	-1.03525	5.52344	-2.29607
C	5.00384	0.13753	-2.65776
H	5.56724	-0.74933	-2.33870
H	4.98357	0.16121	-3.75653
H	5.52350	1.03516	-2.29588
C	0.13760	-5.00395	-2.65751
H	-0.74927	-5.56734	-2.33847
H	0.16132	-4.98373	-3.75629
H	1.03523	-5.52359	-2.29558
C	-5.00388	-0.13772	-2.65770
H	-4.98362	-0.16148	-3.75647
H	-5.52353	-1.03532	-2.29574
H	-5.56729	0.74917	-2.33871
C	-0.00597	3.68921	-0.54781
C	-1.10960	3.49677	0.29163
C	1.23525	3.99871	0.03543
C	-0.97734	3.54706	1.67939
H	-2.07855	3.25686	-0.13890
C	1.38688	4.06252	1.41450
H	2.09942	4.16277	-0.60996
C	0.27520	3.81791	2.22258
H	-1.81715	3.34385	2.34143
H	2.34647	4.28300	1.87782
C	-3.68921	-0.00599	-0.54762
C	-3.99862	1.23526	0.03563
C	-3.49677	-1.10961	0.29183
C	-4.06236	1.38691	1.41470
H	-4.16268	2.09943	-0.60977
C	-3.54700	-0.97733	1.67959
H	-3.25693	-2.07857	-0.13869
C	-3.81777	0.27523	2.22278
H	-4.28277	2.34652	1.87801
H	-3.34380	-1.81714	2.34164
C	0.00598	-3.68920	-0.54747
C	-1.23523	-3.99859	0.03585
C	1.10965	-3.49675	0.29191
C	-1.38681	-4.06230	1.41493
H	-2.09944	-4.16267	-0.60949
C	0.97745	-3.54693	1.67968
H	2.07860	-3.25693	-0.13867
C	-0.27508	-3.81768	2.22295

H	-2.34639	-4.28269	1.87831
H	1.81729	-3.34372	2.34168
C	3.68919	0.00600	-0.54765
C	3.99862	-1.23519	0.03571
C	3.49675	1.10970	0.29170
C	4.06238	-1.38671	1.41479
H	4.16269	-2.09942	-0.60961
C	3.54699	0.97755	1.67947
H	3.25689	2.07862	-0.13891
C	3.81778	-0.27496	2.22278
H	4.28281	-2.34627	1.87819
H	3.34379	1.81741	2.34144
N	0.44031	3.84637	3.68192
N	3.84619	-0.43995	3.68213
N	-0.44013	-3.84603	3.68229
N	-3.84615	0.44036	3.68212
O	-3.71211	-0.56167	4.37603
O	-4.01035	1.57576	4.12412
O	-0.56172	3.71228	4.37582
O	1.57570	4.01067	4.12393
O	3.71208	0.56213	4.37594
O	4.01048	-1.57530	4.12423
O	-1.57550	-4.01026	4.12436
O	0.56194	-3.71194	4.37614
Br	-0.00001	0.00003	0.40452

Table S7. Atomic coordinates for I⁻·AEC4P (in Å) from a DFT calculation using the B3LYP functional using a modified cc-pVDZ basis, with a cc-pVDZ basis for the oxygen and carbon atoms as well as for most of the hydrogen atoms, while an aug-cc-pVDZ basis was used to describe the nitrogen atoms, as well as the hydrogen atoms in the NH groups. For iodine, we used the aug-cc-pVDZ-pp basis and associated effective core potential (ECP). See main text for additional details.

Element	X	Y	Z
C	1.29135	2.845166	-2.592
C	2.252643	3.201565	-3.52463
C	3.244429	2.173252	-3.53861
C	2.86426	1.21337	-2.61477
C	2.84567	-1.29064	-2.59181
C	3.20230	-2.25160	-3.52469
C	2.17399	-3.24337	-3.53930
C	1.21387	-2.86353	-2.61558
C	-1.29016	-2.84494	-2.59322
C	-2.25094	-3.20123	-3.52642
C	-3.24272	-2.17292	-3.54083
C	-2.86307	-1.21315	-2.61667
C	-2.84443	1.29087	-2.59341
C	-3.20049	2.25197	-3.52637
C	-2.17218	3.24377	-3.54015
C	-1.21265	2.86379	-2.61587
H	2.24981	4.10027	-4.13387
H	4.13779	2.14832	-4.15530
H	4.10117	-2.24855	-4.13370
H	2.14922	-4.13651	-4.15632
H	-2.24776	-4.09987	-4.13576
H	-4.13573	-2.14792	-4.15802
H	-4.09896	2.24901	-4.13594
H	-2.14702	4.13700	-4.15701
C	0.04120	3.57637	-2.13874
C	-0.04026	-3.57620	-2.13934
C	-3.57582	0.04082	-2.14014
C	3.57675	-0.04064	-2.13794
N	1.67109	1.62942	-2.06392
H	1.20819	1.17123	-1.27248
N	1.62978	-1.67056	-2.06419
H	1.17138	-1.20795	-1.27269
N	-1.67020	-1.62925	-2.06520
H	-1.20776	-1.17115	-1.27344
N	-1.62889	1.67073	-2.06494

H	-1.17100	1.20800	-1.27322
C	0.06060	5.00371	-2.73025
H	0.95493	5.53977	-2.38482
H	0.07281	4.97014	-3.82882
H	-0.83081	5.55782	-2.40708
C	5.00422	-0.05981	-2.72914
H	5.54022	-0.95426	-2.38391
H	4.97089	-0.07163	-3.82773
H	5.55824	0.83149	-2.40554
C	-0.05930	-5.00344	-2.73113
H	-0.95383	-5.53957	-2.38634
H	-0.07085	-4.96965	-3.82971
H	0.83192	-5.55759	-2.40753
C	-5.00293	0.06009	-2.73223
H	-4.96891	0.07203	-3.83079
H	-5.55717	-0.83123	-2.40907
H	-5.53912	0.95451	-2.38724
C	-0.00178	3.72851	-0.60323
C	-1.23231	3.94083	0.03894
C	1.16322	3.69379	0.17405
C	-1.30966	4.07117	1.42070
H	-2.14278	3.98582	-0.55903
C	1.10663	3.81653	1.56049
H	2.12501	3.53526	-0.30909
C	-0.13381	3.99655	2.16720
H	-2.25823	4.22002	1.93246
H	1.99947	3.75192	2.17879
C	-3.72860	-0.00175	-0.60468
C	-3.69434	1.16349	0.17227
C	-3.94107	-1.23211	0.03775
C	-3.81769	1.10729	1.55866
H	-3.53571	2.12515	-0.31109
C	-4.07200	-1.30907	1.41948
H	-3.98572	-2.14276	-0.55996
C	-3.99784	-0.13299	2.16567
H	-3.75347	2.00033	2.17673
H	-4.22097	-2.25750	1.93145
C	0.00180	-3.72864	-0.60383
C	-1.16366	-3.69408	0.17276
C	1.23195	-3.94111	0.03901
C	-1.10788	-3.81711	1.55920
H	-2.12516	-3.53545	-0.31092
C	1.30849	-4.07173	1.42079

H	2.14277	-3.98599	-0.55843
C	0.13220	-3.99727	2.16661
H	-2.00109	-3.75263	2.17699
H	2.25675	-4.22071	1.93307
C	3.72855	0.00183	-0.60238
C	3.69353	-1.16340	0.17454
C	3.94086	1.23214	0.04020
C	3.81595	-1.10723	1.56102
H	3.53500	-2.12503	-0.30892
C	4.07089	1.30907	1.42201
H	3.98609	2.14279	-0.55748
C	3.99597	0.13301	2.16815
H	3.75108	-2.00025	2.17904
H	4.21974	2.25746	1.93409
N	-0.20795	4.12354	3.62901
N	4.12261	0.20670	3.63001
N	0.20547	-4.12457	3.62844
N	-4.12548	-0.20670	3.62744
O	-4.27381	-1.31629	4.13304
O	-4.08983	0.84432	4.25948
O	-1.31767	4.27180	4.13434
O	0.84287	4.08745	4.26135
O	4.27087	1.31626	4.13570
O	4.08626	-0.84430	4.26204
O	-0.84573	-4.08865	4.26017
O	1.31490	-4.27290	4.13439
I	-0.00046	-0.00013	0.67913