Supporting Information

Substituent Effects in Cation/π Interactions and Electrostatic Potentials above the Center of Substituted Benzenes Are Due Primarily to through-Space Effects of the Substituents

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Complete Citations for refs 10 and 12.

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MOLPRO, version 2006.1, is a package of ab initio programs written by H.-J. Werner, P. J. Knowles, R. Lindh, F. R. Manby, M. Schütz, P. Celani, T. Korona, G. Rauhut, R. D. Amos, A. Bernhardsson, A. Berning, D. L. Cooper, M. J. O. Deegan, A. J. Dobbyn, F. Eckert, C. Hampel, G. Hetzer, A. W. Lloyd, S. J. McNicholas, W. Meyer, M. E. Mura, A. Nicklaß, P. Palmieri, R. Pitzer, U. Schumann, H. Stoll, A. J. Stone, R. Tarroni, and T. Thorsteinsson.

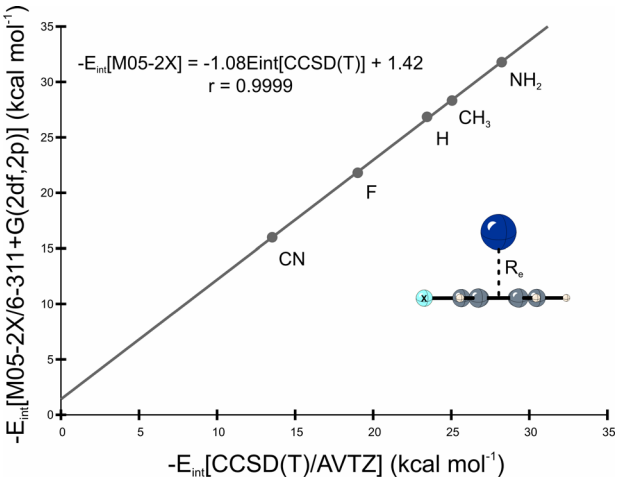

Figure S1. M05-2X/6-311+G(2df,2p) versus CCSD(T)/AVTZ interaction energies (kcal mol^{-1})for $C_6H_5X\cdots Na^+$ (X = H, CH_3, CN, F, NH_2).

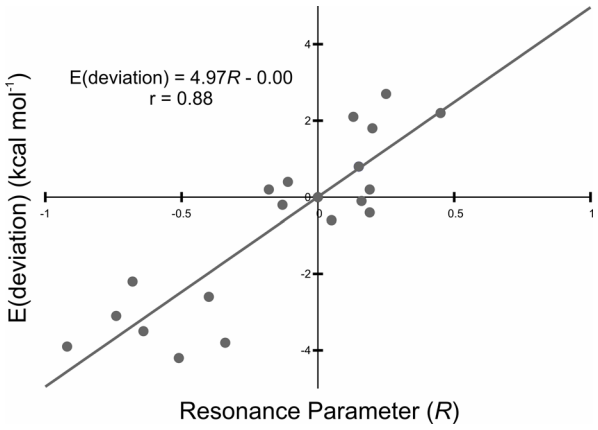

Figure S2. Deviations in interaction energies from additive model compared to intact $C_6H_5X\cdots Na^+$ dimers [E(deviation)] versus resonance parameter *R*. E(deviation) = $E_{int}(C_6H_5\text{-}X\cdots Na^+)$ – [E_{int}(H-$X\cdots Na^+$) + $E_{int}(C_6H_6\cdots Na^+)$ – Eint($HH\cdots Na^+$)]

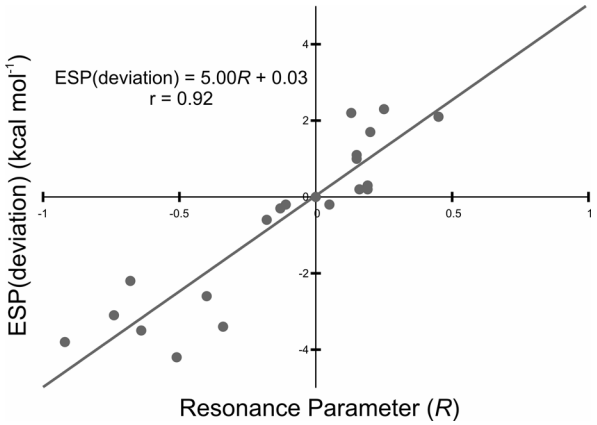

Figure S3. Deviations in electrostatic potentials (ESPs) from additive model compared to intact $C_6H_5X\cdots Na^+$ dimers [E(deviation)] versus resonance parameter *R*. ESP(deviation) = ESP(C_6H_5) – [ESP (H-X) + ESP(C_6H_6) – ESP(HH)]

Table S1. M05-2X/6-311+G(2df,2p) energies (hartree) of $C_6H_5X\cdots Na^+$ and $HX\cdots Na^+$. Asterisks (*) denote presence of basis functions but not the associated nuclei or electrons (for Counterpoise-corrections).

X	$C_6H_5X\cdots Na^+$	$[C_5H_6X]^*\cdots Na^+$	$C_5H_6X\cdots[Na^+]^*$	$HX\cdots Na^+$	$[HX]^*\cdots Na^+$	$HX\cdots[Na^+]^*$
$N(CH_3)_2$	-528.42793	-162.07936	-366.29447	-297.26413	-162.07931	-135.17749
$NHCH_3$	-489.11670	-162.07935	-326.98462	-257.95724	-162.07931	-95.87066
NH_2	-449.80417	-162.07935	-287.67416	-218.65288	-162.07931	-56.56721
CH_2OH	-508.98461	-162.07935	-346.85831	-277.83053	-162.07931	-115.74647
NHOH	-524.98134	-162.07935	-362.85564	-293.82614	-162.07931	-131.74533
SCH_3	-831.94837	-162.07935	-669.82342	-600.79748	-162.07931	-438.71300
OCH_3	-508.97611	-162.07935	-346.85139	-277.82247	-162.07931	-115.74528
CH_3	-433.74777	-162.07935	-271.62328	-202.60016	-162.07931	-40.51674
H	-394.42155	-162.07935	-232.29941	-163.25119	-162.07931	-1.16979
OH	-469.66785	-162.07935	-307.54615	-238.52161	-162.07931	-76.44625
SH	-792.62338	-162.07935	-630.50220	-561.47755	-162.07931	-399.39642
SiH_3	-685.11035	-162.07935	-522.98953	-453.95482	-162.07931	-291.86864
CCH	-470.58544	-162.07935	-308.46568	-239.42369	-162.07931	-77.34568
$COOCH_3$	-622.35565	-162.07935	-460.23862	-391.19343	-162.07931	-229.11591
$COCH_3$	-547.09725	-162.07935	-384.98257	-315.93557	-162.07931	-153.85882
F	-493.68427	-162.07935	-331.57017	-262.54116	-162.07931	-100.47375
COOH	-583.04591	-162.07935	-420.93223	-351.88294	-162.07931	-189.80864
OCF_3	-806.80899	-162.07935	-644.69669	-575.66552	-162.07931	-413.59899
BF_2	-618.56496	-162.07935	-456.45339	-387.39599	-162.07931	-225.32113
CHO	-507.76259	-162.07935	-345.65192	-276.59721	-162.07931	-114.52382
CF_3	-731.56654	-162.07935	-569.45634	-500.41095	-162.07931	-338.34110
SiF_3	-983.16934	-162.07935	-821.06049	-752.00454	-162.07931	-589.93204
NO	-523.72706	-162.07935	-361.61997	-292.56522	-162.07931	-130.49533
CN	-486.67213	-162.07935	-324.56729	-255.50845	-162.07931	-93.44486
NO_2	-598.95405	-162.07935	-436.85235	-367.79687	-162.07931	-205.73577

Table S2. CCSD(T)/AVTZ energies (hartree) of $C_6H_5X\cdots Na^+$ and $HX\cdots Na^+$. Asterisks (*) denote presence of basis functions but not the associated nuclei or electrons (for Counterpoise corrections).

X	$C_6H_5X\cdots Na^+$	$[C_5H_6X]^*\cdots Na^+$	$C_5H_6X\cdots[Na^+]^*$	$HX\cdots Na^+$	$[HX]^*\cdots Na^+$	$HX\cdots[Na^+]^*$
H	-393.80333	-161.94472	-231.82124	-163.11880	-161.94413	-1.17266
CH_3	-433.04467	-161.94482	-271.05993	-202.38890	-161.94417	-40.44072
CN	-485.88889	-161.94473	-323.92260	-255.21023	-161.94417	-93.28074
F	-492.93776	-161.94469	-330.96278	-262.28265	-161.94412	-100.34965
NH_2	-449.09292	-161.94477	-287.10317	-218.42791	-161.94416	-56.47773

Optimized Cartesian Coordinates (Angstrom)

C_6H_5-X$^{\cdots}$Na$^+$ Dimer geometries

13
C6H5-H...Na+

C	0.98556382	-0.98556382	-0.48773585
C	-0.36074140	-1.34630522	-0.48773585
C	1.34630522	0.36074140	-0.48773585
C	-0.98556382	0.98556382	-0.48773585
C	0.36074140	1.34630522	-0.48773585
C	-1.34630522	-0.36074140	-0.48773585
H	1.75154749	-1.75154749	-0.48773585
H	-0.64111088	-2.39265837	-0.48773585
H	-2.39265837	-0.64111088	-0.48773585
H	-1.75154749	1.75154749	-0.48773585
H	0.64111088	2.39265837	-0.48773585
H	2.39265837	0.64111088	-0.48773585
Na	0.00000000	0.00000000	1.86226415

15
C6H5-BF2...Na+

C	-0.73054303	2.34517561	0.00000000
C	-0.62132084	1.66046523	-1.20980600
C	-0.62132084	1.66046523	1.20980600
C	-0.29022765	-0.41514734	0.00000000
C	-0.40217926	0.28667372	1.20800000
C	-0.40217926	0.28667372	-1.20800000
H	-0.31671190	-0.24911840	-2.14609300
H	-0.70685168	2.19665532	-2.14674300
H	-0.70685168	2.19665532	2.14674300
H	-0.31671190	-0.24911840	2.14609300
F	0.06347266	-2.63248314	-1.13455100
F	0.06347266	-2.63248314	1.13455100
B	-0.04673879	-1.94157116	0.00000000
H	-0.90121389	3.41510576	0.00000000
Na	1.85874113	1.34877598	0.00000000

17
C6H5-CH2OH...Na+

C	0.08221119	-2.05677228	-0.79451855
C	-0.85419979	-1.11054505	-1.20004731
C	1.17749113	-1.65709079	-0.02882296
C	0.38930569	0.63188917	-0.08148476
C	1.32781373	-0.32025168	0.32421823
C	-0.70363177	0.23062043	-0.84601508
H	1.91209176	-2.38554592	0.29198641
H	-1.70725458	-1.41376908	-1.79484637
C	0.58674007	2.07266959	0.32127017
H	0.61685834	2.13907828	1.41449085
H	1.54832059	2.42572082	-0.06753107
H	2.18156977	-0.01304287	0.92022875
H	-1.42805508	0.96994496	-1.15832565
H	-0.03777848	-3.09692308	-1.07111185
O	-0.47546155	2.86020199	-0.19401265
H	-0.34309402	3.77784899	0.06666638
Na	-0.99757704	-1.09345858	1.52572230

15
C6H5-CCH...Na+

C	-0.28579743	0.77470604	0.00000000
C	-0.39053414	0.07735854	1.21067500
C	-0.39053414	0.07735854	-1.21067500
C	-0.70072410	-1.98791718	0.00000000
C	-0.59705084	-1.29765026	-1.20665700
C	-0.59705084	-1.29765026	1.20665700
H	-0.30885864	0.62116220	-2.14301400
H	-0.30885864	0.62116220	2.14301400
H	-0.67714482	-1.83092403	-2.14584400
H	-0.67714482	-1.83092403	2.14584400
C	-0.07259508	2.19422858	0.00000000
C	0.10678913	3.38858658	0.00000000
H	0.26507225	4.44245136	0.00000000
H	-0.86159381	-3.05900380	0.00000000
Na	1.83031937	-0.95800431	0.00000000

16
C6H5-CF3...Na+

C	0.77349943	2.53436605	0.11467377
C	0.85758197	1.84464342	-1.09309851
C	0.45496588	1.85446782	1.28846259
C	0.30662161	-0.19924450	0.04702211
C	0.21948027	0.48312485	1.25822137
C	0.62338237	0.47326906	-1.13094696
H	0.39280629	2.38935616	2.22754087
H	1.10828724	2.37189744	-2.00468464
C	0.00189571	-1.66644556	0.00155990
F	0.31284126	-2.28520597	1.15767392
F	-1.31130537	-1.89904104	-0.21948447
F	0.67474957	-2.29403687	-0.98309787
H	-0.02351587	-0.05372690	2.16586037
H	0.69151189	-0.07117449	-2.06368680
H	0.95869417	3.60093618	0.14158271
Na	-1.78535602	1.64747088	-0.27070931

16
C6H5-CH3...Na+

C	0.76107951	1.68685138	0.07922316
C	0.77139588	0.99241616	-1.12844088
C	0.48510224	1.00224683	1.26072842
C	0.22481894	-1.07192817	0.02631532
C	0.22124767	-0.36529143	1.23154179
C	0.50678622	-0.37509615	-1.15132720
H	0.47932529	1.53117260	2.20627719
H	0.98969591	1.51364746	-2.05284474
C	-0.09430415	-2.54607973	-0.00586029
H	0.20608634	-3.03379724	0.92285033
H	-1.16830754	-2.70658869	-0.13389726
H	0.41652763	-3.04102334	-0.83331739
H	0.01068345	-0.89263913	2.15589896
H	0.52006244	-0.91013009	-2.09495370
H	0.97038692	2.74936718	0.09993291
Na	-1.78920166	0.80466163	-0.19482075

15
C6H5-CHO...Na+

C	0.30629423	0.72184903	0.17786454
C	0.18976073	0.25964206	-1.13638744
C	0.61316939	-0.16275634	1.21238081
C	0.68865153	-1.97348196	-0.37236277
C	0.80508268	-1.51419972	0.93782711
C	0.38136411	-1.08832590	-1.40900499
H	0.70080766	0.20859401	2.22817445
H	-0.04928941	0.96876476	-1.91913151
H	1.04335944	-2.20414846	1.73752578
H	0.29300531	-1.45488457	-2.42409372
C	0.10502850	2.15605148	0.48530786
O	-0.16376397	3.00107759	-0.33978550
H	0.21694896	2.42879470	1.54993023
H	0.83739501	-3.02432879	-0.58908579
Na	-1.84256566	-1.02946220	0.25101944

14
C6H5-CN...Na+

C	-0.72515765	-1.95079368	0.00000000
C	-0.61493727	-1.26555249	1.20898600
C	-0.61493727	-1.26555249	-1.20898600
C	-0.28421738	0.79053637	0.00000000
C	-0.39416619	0.10698348	-1.21523800
C	-0.39416619	0.10698348	1.21523800
C	-0.05556880	2.21204685	0.00000000
N	0.12804317	3.35356424	0.00000000
H	-0.70084926	-1.79966818	2.14648100
H	-0.70084926	-1.79966818	-2.14648100
H	-0.30649239	0.65205239	-2.14582200
H	-0.30649239	0.65205239	2.14582200
H	-0.89711869	-3.01987711	0.00000000
Na	1.86494586	-0.96070455	0.00000000

18
C6H5-COCH3...Na+

C	-0.05411738	0.42881609	-0.27958267
C	-1.24833866	-0.29368905	-0.36770986
C	1.16685324	-0.23761751	-0.41326203
C	0.00069580	-2.32626573	-0.71959497
C	1.19363310	-1.61275973	-0.63287202
C	-1.22119420	-1.66524234	-0.58675650
H	2.10003314	0.30713203	-0.34755570
H	-2.18296754	0.24142878	-0.26140324
H	2.14238046	-2.12431733	-0.73574491
H	-2.14826052	-2.22067253	-0.65430175
C	-0.13496373	1.90602958	-0.04249711
O	-1.21403781	2.45602872	0.06943792
C	1.14904409	2.69879204	0.05479388
H	1.72826116	2.60892367	-0.86703481
H	1.76759762	2.33120773	0.87674897
H	0.89572197	3.74229032	0.22669644
H	0.02199396	-3.39557166	-0.89037365
Na	0.02526079	-1.32063917	1.82021391

19
C6H5-COOCH3...Na+

C	-0.15127839	-0.02422634	-0.30042867
C	-1.27182047	0.80801421	-0.32857965
C	1.12797633	0.50926078	-0.46999876
C	0.16349017	2.70998807	-0.69604438
C	1.28170689	1.87821758	-0.66778093
C	-1.11317707	2.17494726	-0.52645933
H	1.98877381	-0.14484021	-0.44636434
H	-2.25138610	0.36766864	-0.19440590
H	2.27228786	2.29537336	-0.79963740
H	-1.98102159	2.82217844	-0.54862519
C	-0.37634491	-1.48004036	-0.08542635
O	-1.46545367	-1.98775177	0.06621576
O	0.76506252	-2.18828594	-0.07571626
C	0.60056484	-3.59857406	0.12850199
H	1.60418311	-4.01195041	0.10857422
H	0.12241947	-3.78221571	1.08883060
H	-0.01075409	-4.02090779	-0.66679776
H	0.28676228	3.77508271	-0.85020356
Na	0.18228728	1.65839907	1.82381180

16
C6H5-COOH...Na+

C	0.01446744	-2.29864164	-0.74143045
C	1.21247973	-1.59499972	-0.62878807
C	-1.20589163	-1.63326178	-0.62499268
C	-0.02796323	0.44065381	-0.28307030
C	-1.22882542	-0.26262956	-0.39564069
C	1.19529209	-0.22265432	-0.39917376
H	2.15800907	-2.11425654	-0.71962634
H	-2.13471302	-2.18226338	-0.71290437
H	2.11801357	0.33397874	-0.30995990
H	-2.16116766	0.27848087	-0.30120273
C	-0.10236912	1.90277681	-0.03819835
O	-1.12783702	2.53528900	0.07192029
O	1.11029080	2.48962435	0.05484696
H	0.95004984	3.43359034	0.21341256
H	0.03141126	-3.36663199	-0.92013656
Na	0.00323887	-1.32451513	1.85491320

13
C6H5-F...Na+

C	-0.19801494	1.07370703	0.00000000
C	-0.34573765	0.42890614	1.21658000
C	-0.34573765	0.42890614	-1.21658000
C	-0.81284602	-1.60999427	0.00000000
C	-0.65686721	-0.92915601	-1.20644900
C	-0.65686721	-0.92915601	1.20644900
F	0.10428797	2.39324134	0.00000000
H	-0.21846413	0.98444752	2.13600000
H	-0.21846413	0.98444752	-2.13600000
H	-0.77729061	-1.45479702	-2.14537100
H	-0.77729061	-1.45479702	2.14537100
H	-1.05451171	-2.66485069	0.00000000
Na	1.83671396	-0.79208187	0.00000000

21
C6H5-NCH3_2...Na+

C	0.16674153	0.41363130	0.00000000
C	0.33712789	-0.29734315	1.20480793
C	0.33712789	-0.29734315	-1.20480793
C	0.78423994	-2.35350912	0.00000000
C	0.63461238	-1.65568208	-1.19537793
C	0.63461238	-1.65568208	1.19537793
H	0.23611128	0.20327502	2.15666636
H	0.75469544	-2.16966241	2.14181038
H	0.75469544	-2.16966241	-2.14181038
H	0.23611128	0.20327502	-2.15666636
N	-0.16663527	1.76239103	0.00000000
C	-0.00013440	2.50422019	-1.23492805
H	-0.27325821	3.54273206	-1.05913561
H	-0.66461075	2.11704988	-2.00861254
H	1.03148169	2.46963891	-1.61084506
C	-0.00013440	2.50422019	1.23492805
H	-0.66461075	2.11704988	2.00861254
H	-0.27325821	3.54273206	1.05913561
H	1.03148169	2.46963891	1.61084506
H	1.01858486	-3.41008147	0.00000000
Na	-1.76237602	-1.47525411	0.00000000

15
C6H5-NH2...Na+

C	0.21335916	-1.08296565	0.00000000
C	0.35108808	-0.38326701	-1.20529550
C	0.35108808	-0.38326701	1.20529550
C	0.76406558	1.67529025	0.00000000
C	0.62429574	0.98020399	1.19985750
C	0.62429574	0.98020399	-1.19985750
H	0.23669323	-0.91197430	2.14520650
H	0.73011936	1.50169020	2.14355150
H	0.73011936	1.50169020	-2.14355150
H	0.23669323	-0.91197430	-2.14520650
H	0.14949527	-2.94176826	0.83449000
H	0.14949527	-2.94176826	-0.83449000
N	-0.11411218	-2.44073126	0.00000000
H	0.97833962	2.73608226	0.00000000
Na	-1.81648403	0.75781363	0.00000000

18
C6H5-NHCH3...Na+

C	-0.25860192	-0.65183135	-0.22533118
C	1.07266642	-0.21301427	-0.20158507
C	-1.26842058	0.28461976	-0.50855968
C	0.37230582	2.04934147	-0.72615628
C	-0.95379155	1.61216379	-0.75612469
C	1.37378446	1.12618681	-0.44665237
H	-2.30328497	-0.04083140	-0.52208798
H	-1.75116873	2.31311395	-0.97268461
H	2.40964861	1.44317990	-0.42050896
H	1.87425101	-0.90789026	0.00971584
N	-0.60439540	-1.96724215	0.05252332
H	-1.49999280	-2.24252316	-0.31611017
C	0.40234484	-3.00803065	0.05308779
H	-0.09308596	-3.96887128	0.18183736
H	1.08579695	-2.87172891	0.89314016
H	0.98945416	-3.03212874	-0.87357725
H	0.61517084	3.08635463	-0.91836501
Na	-0.13979512	1.16321881	1.76717330

16
C6H5-NHOH...Na+

C	0.80533908	2.00577902	0.28471228
C	-0.14582012	1.58297710	1.21386700
C	1.33321633	1.08203993	-0.61205396
C	-0.02653012	-0.66393720	0.33736101
C	0.92551142	-0.25112358	-0.59333196
C	-0.56335703	0.25858369	1.24226641
H	-1.31364060	-0.06328790	1.95649370
H	-0.56710799	2.28808875	1.92019652
H	2.07663936	1.39470075	-1.33551185
H	1.34884117	-0.97022108	-1.27936643
N	-0.53442614	-1.98525390	0.36278375
H	-0.62449230	-2.31800555	1.31557823
O	0.31813450	-2.89936748	-0.28493553
H	-0.23099081	-3.26967549	-0.98730873
H	1.12918799	3.03852380	0.26379344
Na	-1.32660792	1.17324364	-1.21370924

14
C6H5-NO...Na+

C	0.29709857	0.74390576	0.17932342
C	0.61547549	-0.12133145	1.22277152
C	0.17681677	0.29192403	-1.13700077
C	0.70220773	-1.93285178	-0.35860454
C	0.38182714	-1.05472333	-1.39980401
C	0.81962718	-1.47116005	0.95062492
H	-0.07207831	0.99631764	-1.91959872
H	0.69666210	0.28019283	2.22544001
H	0.29406940	-1.42839608	-2.41217719
H	1.06780954	-2.15762923	1.74981490
N	0.10605011	2.11800334	0.56530638
O	-0.16945155	2.86373932	-0.34115198
H	0.86033142	-2.98231683	-0.57409141
Na	-1.83562270	-1.01624413	0.26898366

15
C6H5-NO2...Na+

C	-0.28106830	-0.46446783	0.00000000
C	-0.39950020	0.18953641	-1.21951500
C	-0.39950020	0.18953641	1.21951500
C	-0.77079300	2.23988837	0.00000000
C	-0.64732494	1.55807345	-1.21000200
C	-0.64732494	1.55807345	1.21000200
H	-0.74377202	2.09067322	-2.14716400
H	-0.29871563	-0.36701580	-2.13988900
H	-0.29871563	-0.36701580	2.13988900
H	-0.74377202	2.09067322	2.14716400
O	0.08142926	-2.46625072	-1.07799600
O	0.08142926	-2.46625072	1.07799600
N	-0.01900837	-1.91161436	0.00000000
H	-0.96369198	3.30511448	0.00000000
Na	1.88653884	1.31500376	0.00000000

17
C6H5-OCF3...Na+

C	0.31948820	-0.25219554	0.37191705
C	0.45006383	-1.21951786	1.36092323
C	0.38644652	-0.57366499	-0.97763757
C	0.72421232	-2.89371713	-0.35683900
C	0.59068192	-1.90818355	-1.32910488
C	0.65297925	-2.54344155	0.99077586
H	0.28490711	0.17843197	-1.74543054
H	0.39070159	-0.91960613	2.39877850
H	0.64438722	-2.16914165	-2.37839104
H	0.75524568	-3.30035230	1.75799055
C	-0.02507832	2.08631700	0.03911492
O	0.11955556	1.03990655	0.86808945
F	-1.08819967	1.96067646	-0.77596048
F	1.05034120	2.28005161	-0.74593298
F	-0.19835124	3.17683681	0.78064474
H	0.88225553	-3.92490276	-0.64480145
Na	-1.85280150	-1.91957671	-0.02332007

14
C6H5-OH...Na+

C	0.20639797	-1.08305918	0.00394661
C	0.35113081	-0.40713753	1.21453495
C	0.34534863	-0.40285968	-1.20433396
C	0.77747205	1.64694607	0.00543787
C	0.63071959	0.96125962	-1.19681584
C	0.63569963	0.95333324	1.20795113
H	0.23170909	-0.93371414	-2.14403693
H	0.73763491	1.48480321	-2.13905683
H	0.74757696	1.47572891	2.15026846
H	0.23800907	-0.96010369	2.13803793
O	-0.07301777	-2.41959106	0.06323234
H	-0.15064260	-2.77890474	-0.82889407
H	0.99908484	2.70634306	0.00733255
Na	-1.80907657	0.75924370	0.01146960

17
C6H5-OMe...Na+

C	0.36873113	0.65903438	0.08094942
C	-0.27377803	0.21982609	-1.07682669
C	1.05914893	-0.25189011	0.88752150
C	0.46525543	-2.04519496	-0.62159165
C	1.10463318	-1.59231203	0.53554560
C	-0.21805564	-1.13436644	-1.41692508
H	-0.81286521	0.90606751	-1.71452484
H	-0.71901991	-1.46913789	-2.31721325
H	1.64187510	-2.28959128	1.16682548
H	1.54778043	0.11854274	1.77953684
O	0.37976629	1.95292903	0.50782613
C	-0.30667106	2.91103084	-0.27750767
H	-1.37158133	2.67362892	-0.34165172
H	0.11963081	2.97117209	-1.28207611
H	-0.17553030	3.86201297	0.23132317
H	0.50198644	-3.09197242	-0.89454049
Na	-1.54236272	-1.08190195	0.96751994

17
C6H5-SCH3...Na+

C	-0.25940179	-0.35394311	-0.25577099
C	1.03167761	0.12723266	-0.48106587
C	-1.33655499	0.54237358	-0.27524044
C	0.16799459	2.37472306	-0.74104046
C	-1.12219594	1.89287462	-0.51574022
C	1.23707755	1.48625730	-0.72189838
H	1.88291969	-0.53967249	-0.47230145
H	2.24467861	1.84499500	-0.89504261
H	-1.96621607	2.57188385	-0.52726937
H	-2.34138478	0.17435498	-0.10093127
S	-0.65509640	-2.05135207	0.06101931
C	0.96441440	-2.85438369	0.00324487
H	1.62756515	-2.46962284	0.77756940
H	1.42574527	-2.75030456	-0.97845247
H	0.77680573	-3.91030378	0.19358454
H	0.33427476	3.42800990	-0.92850794
Na	0.21809867	1.38013514	1.80728284

14
C6H5-SH...Na+

C	0.25778244	-0.70453212	-0.01008510
C	0.38300801	-0.02547823	1.20500248
C	0.37321737	0.00093936	-1.20931162
C	0.73686260	2.05168166	0.01989331
C	0.61172135	1.37291006	-1.18927189
C	0.62118188	1.34492450	1.21535966
H	0.27809931	-0.51397252	-2.15792035
H	0.69928372	1.90897743	-2.12626647
H	0.71644185	1.86069189	2.16283664
H	0.29419758	-0.56860490	2.13838909
S	-0.04553769	-2.45234412	0.05172967
H	-0.08653652	-2.64282145	-1.27501881
H	0.92219479	3.11793384	0.03117757
Na	-1.81797450	1.07569366	0.01905515

16
C6H5-SiF3...Na+

C	0.31389910	0.12063197	0.01080432
C	0.38371798	0.82141451	1.22251085
C	0.47550320	0.81956018	-1.19321134
C	0.75287145	2.88115489	0.02533281
C	0.69232072	2.19430500	-1.18561831
C	0.60059300	2.19618715	1.22923633
Si	0.00830915	-1.68430770	0.00053410
F	-1.54051576	-2.07163167	-0.06621209
F	0.58160879	-2.36839414	1.32526962
F	0.69385013	-2.37324385	-1.26713276
H	0.43981177	0.29001970	-2.13832921
H	0.27635069	0.29330250	2.16297298
H	0.81746720	2.72688686	-2.11981232
H	0.65456297	2.73021658	2.16940885
H	0.92295246	3.95063055	0.03095792
Na	-1.83230858	1.88265059	-0.06312060

16
C6H5-SiH3...Na+

C	0.28081314	-0.66726283	-0.00825691
C	0.43385541	0.04176468	1.19048237
C	0.35671793	0.04340249	-1.21341188
C	0.71352599	2.10956591	-0.02027470
C	0.56918403	1.42027568	-1.22244658
C	0.64654683	1.41867039	1.18771979
Si	-0.03710074	-2.51649064	0.00066864
H	-1.49531259	-2.81807310	0.03956607
H	0.59493099	-3.12630596	1.20246111
H	0.52979048	-3.12748228	-1.23262191
H	0.25353303	-0.48081281	-2.15766250
H	0.39138930	-0.48375457	2.13866799
H	0.62592317	1.95263871	-2.16414629
H	0.76359333	1.94975774	2.12456140
H	0.88131710	3.17964618	-0.02494801
Na	-1.82087403	1.08970519	0.05289897

H-X···Na$^+$ Dimer geometries

```
3
H-H...Na+
H         0.2508900        -2.9100100         0.0000000
Na        0.0037262         0.4954631         0.0000000
H        -0.2970630        -2.4104193         0.0000000


5
H-BF2...Na+
F        -0.1060573         1.5014705         1.1345510
F        -0.1060573         1.5014705        -1.1345510
B         0.2863458         0.9222247         0.0000000
Na       -0.0466091        -2.8654367         0.0000000
H         0.9545187        -0.0640987         0.0000000


5
H-CCH...Na+
C         0.3887913         1.3427951         0.0000000
C        -0.2674724         2.3566924         0.0000000
Na       -0.0437395        -2.3137843         0.0000000
H        -0.8465392         3.2513242         0.0000000
H         0.8823287         0.4204312         0.0000000


6
H-CF3...Na+
C        -0.0000420         0.7156255        -0.1800380
F        -1.0962508         1.4899272        -0.3022441
F         0.0215186         0.2763720         1.0982616
F         1.0745905         1.5148383        -0.3302978
Na        0.0001148        -3.0593118        -0.1970571
H         0.0002438        -0.1056492        -0.8872375


7
H-CH2OH...Na+
C         0.6469806         1.1779491        -0.0133753
H         0.8766917         0.8427691         1.0041393
H         1.4422562         1.8597342        -0.3345516
O        -0.6113077         1.8333659        -0.0470702
H        -0.5862664         2.5948821         0.5420111
Na       -0.1221083        -2.4817724        -0.0047665
H         0.6267609         0.3146588        -0.6777344


6
H-CH3...Na+
C         0.0042713        -1.9684649         0.0000655
H         0.1277161        -2.5850821         0.8917778
H        -1.0325331        -1.6219233        -0.0241296
H         0.1646255        -2.5981168        -0.8765351
Na        0.0006264         1.7913007         0.0000096
H         0.6922124        -1.1247030         0.0082057


5
H-CHO...Na+
C         0.5011022        -1.3271499         0.0317570
O        -0.4880129        -2.0237709        -0.0271315
H         1.3830115        -1.5531589        -0.5939360
Na       -0.0998187         2.3650547        -0.0133093
H         0.6040512        -0.4405426         0.6896457


4
H-CN...Na+
C         0.3450652        -1.4131146         0.0000000
N        -0.3053018        -2.3690424         0.0000000
Na       -0.0487432         2.2746548         0.0000000
H         0.8573697        -0.4996499         0.0000000


8
H-COCH3...Na+
C        -0.1734371         0.9067706        -0.2629960
O        -1.2314474         1.3611136         0.1289430
C         1.1340784         1.5766420         0.0951792
H         1.6681139         1.8861798        -0.8061139
H         1.7795692         0.8907969         0.6486183
H         0.9163899         2.4481234         0.7081582
Na       -0.0134084        -2.8068837         0.0368674
H        -0.1503770        -0.0098904        -0.8919767


9
H-COOCH3...Na+
C         0.4445342         0.3342533        -0.3940206
O         1.4479334         0.7529212         0.1396753
O        -0.7286076         0.9874112        -0.3535230
C        -0.7077558         2.2246837         0.3720107
H        -1.7187581         2.6146738         0.3063687
H        -0.4262003         2.0440092         1.4077044
H         0.0048013         2.9105234        -0.0823731
Na       -0.2187412        -3.2868753         0.1105145
H         0.3893722        -0.6045792        -0.9559287


6
H-COOH...Na+
C        -0.1088487         0.9331897        -0.2629891
O        -1.1301021         1.4565387         0.1203248
O         1.1075597         1.4195836         0.0646741
H         0.9535061         2.2011582         0.6190212
Na       -0.0058802        -2.7962273         0.0391429
H        -0.0610853         0.0413105        -0.8938819
```

3
H-F...Na+

F	0.0509304	-1.9382085	0.0000000
Na	0.0181998	1.6876035	0.0000000
H	-0.5600930	-1.2586844	0.0000000

11
H-NCH3_2...Na+

N	-0.1043752	-0.6987899	0.0000000
C	0.0481188	-1.4436245	1.2349280
H	0.7232530	-2.2786678	1.0591356
H	0.4952643	-0.8179325	2.0086125
H	-0.9068728	-1.8353115	1.6108451
C	0.0481188	-1.4436245	-1.2349280
H	0.4952643	-0.8179325	-2.0086125
H	0.7232530	-2.2786678	-1.0591356
H	-0.9068728	-1.8353115	-1.6108451
Na	0.0226397	2.9085085	0.0000000
H	-0.7208093	0.0872520	0.0000000

5
H-NH2...Na+

H	-0.0500866	2.4452956	0.8344900
H	-0.0500866	2.4452956	-0.8344900
N	-0.0436366	1.8791814	0.0000000
Na	-0.0196500	-1.7441022	0.0000000
H	0.6239930	1.1367282	0.0000000

8
H-NHCH3...Na+

N	0.5808970	1.0205973	0.0192483
H	1.5030247	1.3849693	0.1944010
C	-0.4757494	2.0106326	0.0094796
H	-0.2060564	2.8116225	0.6957184
H	-1.4092748	1.5699706	0.3640500
H	-0.6482859	2.4384849	-0.9860904
Na	-0.0921519	-2.5153103	0.0140779
H	0.5615293	0.2519421	-0.6174668

6
H-NHOH...Na+

N	0.5742220	1.0704763	-0.0688767
H	1.4266998	1.6074541	0.0387771
O	-0.4810535	1.9914697	0.0731389
H	-0.9341444	1.9568439	-0.7786266
Na	-0.1082290	-2.4817574	0.0010191
H	0.5300026	0.3292797	0.6113241

4
H-NO...Na+

N	-0.5609532	-1.3465312	0.0706492
O	0.4817142	-1.9487862	0.0088122
Na	0.0697095	2.2977267	0.0153665
H	-0.6396537	-0.5225536	-0.5964403

5
H-NO2...Na+

O	-0.1259127	1.4474705	1.0779960
O	-0.1259127	1.4474705	-1.0779960
N	0.2131584	0.9972039	0.0000000
Na	-0.0383067	-2.7416382	0.0000000
H	0.8348283	0.1716626	0.0000000

7
H-OCF3...Na+

C	-0.0188107	0.9111127	0.0045088
O	-0.9071244	0.0215365	0.4763622
F	0.8833352	0.3551001	-0.8245529
F	0.6727043	1.5239677	0.9825559
F	-0.6877804	1.8392731	-0.6738136
Na	0.0174936	-3.4922900	-0.0150124
H	-0.6260654	-0.7271350	0.9933745

4
H-OH...Na+

O	0.0585762	-1.9171631	0.0516276
H	-0.8460316	-2.1968179	-0.1341125
Na	0.0078777	1.7047202	0.0206373
H	0.2982680	-1.1940132	-0.5198924

7
H-OMe...Na+

O	0.6698721	-1.1025034	-0.0420879
C	-0.5036873	-1.8944495	-0.0035628
H	-1.3840678	-1.3020020	-0.2651813
H	-0.6403856	-2.3432956	0.9835333
H	-0.3587682	-2.6774135	-0.7427783
Na	-0.0616935	2.4443388	-0.0134557
H	0.7206566	-0.3576139	0.5488245

7
H-SCH3...Na+

S	-0.6582920	1.0032786	-0.0355717
C	1.0118841	1.6966253	-0.0073730
H	1.7406808	0.9964545	-0.4148096
H	1.2993310	2.0021323	0.9983247
H	0.9758757	2.5782271	-0.6460241
Na	0.0873193	-2.8736825	-0.0198701
H	-0.5457765	-0.0692591	0.7628563

```
4
H-SH...Na+
S         0.0580000       -1.5338008        0.0411719
H        -1.2724425       -1.6885305       -0.0236798
Na        0.0176481        2.4143218        0.0224588
H         0.1214396       -0.4620566       -0.7569510


6
H-SiF3...Na+
Si       -0.0001318        0.6146891       -0.1526802
F         0.0142780        0.2167749        1.3948308
F        -1.3045300        1.5107712       -0.3698281
F         1.2901869        1.5260828       -0.3893610
Na        0.0002615       -3.3988802       -0.2325421
H        -0.0004570       -0.5378265       -1.0551752


6
H-SiH3...Na+
Si        0.0009609       -1.5280657       -0.0002778
H         1.3857535       -1.1513423       -0.3993713
H        -0.5935972       -2.3392260       -1.0976217
H         0.0823503       -2.3430161        1.2426678
Na        0.0008347        2.4955177       -0.0002335
H        -0.8472960       -0.3161822        0.2462948
```