Electronic Supplementary Information for manuscript:

The N-atom in $[N(PR_3)_2]^+$ cations (R = Ph, Me) can act as electron donor for (pseudo) anti-electrostatic interactions

by

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1. Figures S1–S

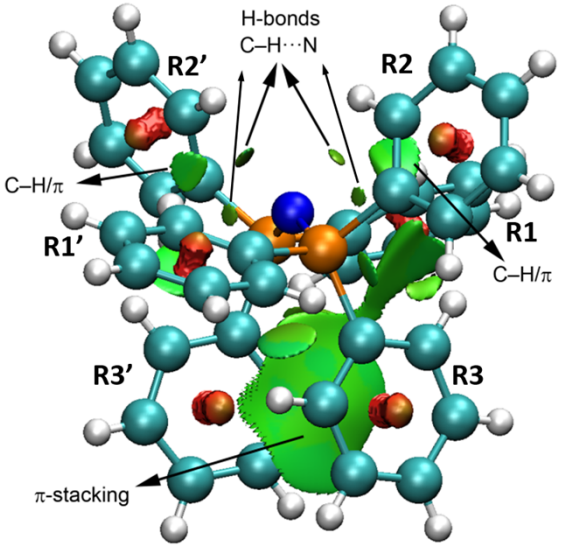

Figure S1. NCI plot of compound **1** with indication of several intramolecular interactions.

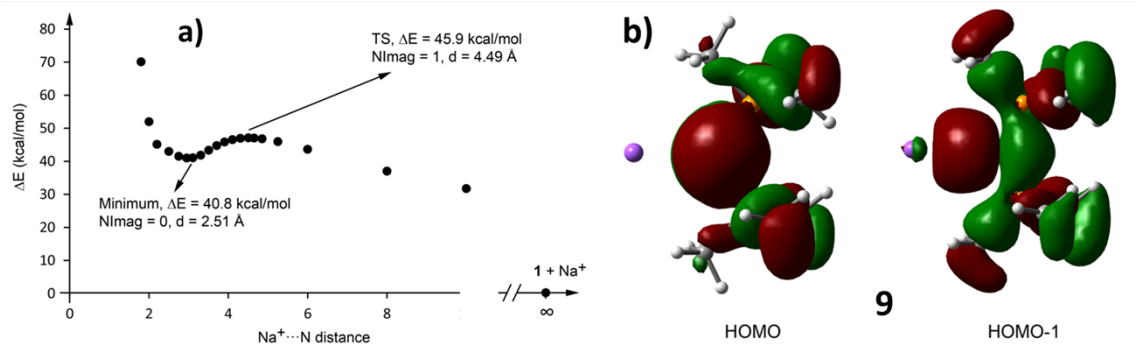

Figure S2. Scan potential energy curve of complex **9** at the BP86-D3/def2-TZVP (a) and graphical renderings of the HOMO and HOMO-1 in complex **9**.

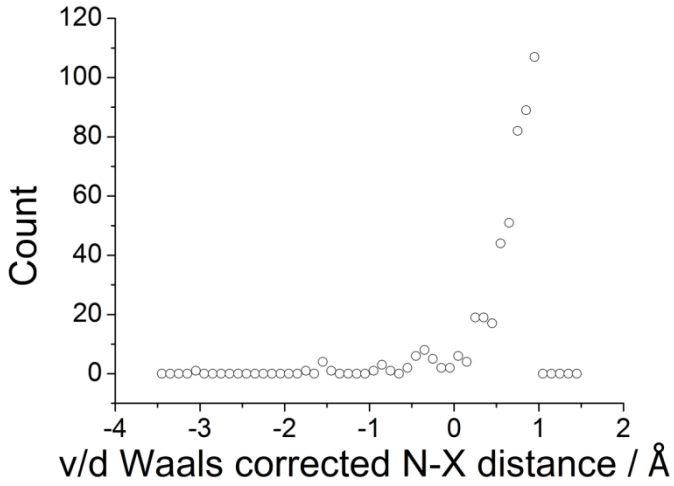

Figure S3. Plot of the amount of hits (count) as a function of the van der Waals corrected N···X distance found in the CSD for intermolecular N(**1**)···X interactions (X can be any atom and the N···X distance was set to the sum of the van der Waals radii of interacting atoms +1 Å).

2. Computational methods

The geometries of all the species included in this study were optimized at the BP86-D3/def2-TZVP level of theory within the program TURBOMOLE version 6.4.[1] The interaction energies were calculated at the same level with correction for the basis set superposition error (BSSE) by using the Boys-Bernardi counterpoise technique.[2] For the calculations we have used the BP86 functional with the latest available correction for dispersion (D3). The H-bonded complexes where optimized using either C_s or C_{2v} symmetry constrain. The antielectrostatic complexes of **1** with H^+, Li^+, Na^+ and CH_3Hg^+ were optimized without symmetry constrains and they correspond to true minima (NImag = 0). The "atoms-in-molecules" (AIM)[3] analysis was performed at the BP86/def2-TZVP level of theory. The calculation of AIM properties was done using the AIMAll program.[4] We have used the NCI method[5] to study the different intramolecular noncovalent interactions observed in compound **1**. This method relies on two scalar fields to map local bonding properties: the electron density (ρ) and the reduced-density gradient (RDG, σ). It is able of mapping real-space regions where non-covalent interactions are important and is based exclusively on the electron density and its gradient. The information provided by NCI plots is essentially qualitative, i.e. which molecular regions interact. The color scheme is a red-blue scale with red for ρ^+_{cut} (repulsive) and blue for ρ^-_{cut} (attractive). Moreover, green and yellow isosurfaces correspond to weakly attractive and weakly repulsive interactions, respectively.

3. Cartesian Coordinates:

1.

C	0.5023416	2.7635845	-1.1392914
C	-0.7638581	3.3545878	-1.2731905
H	-1.6173088	2.9264054	-0.7464050
C	-0.9221212	4.4762695	-2.0880197
H	-1.9065208	4.9325818	-2.1954610
C	0.1778107	5.0130257	-2.7639921
H	0.0508907	5.8899249	-3.3994862
C	1.4391597	4.4243575	-2.6330177
H	2.2946321	4.8370733	-3.1682571
C	1.6050099	3.2996120	-1.8239897
H	2.5854841	2.8277533	-1.7450526
C	1.9617234	0.2779752	-0.7633109
C	1.8544699	-0.0534956	-2.1256786
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C	2.7569307	-0.9491248	-2.6963578
H	2.6762922	-1.1995872	-3.7544230
C	3.7656729	-1.5190653	-1.9130024
H	4.4736301	-2.2164879	-2.3620002
C	3.8682111	-1.1983727	-0.5573248
H	4.6483829	-1.6505763	0.0550328
C	2.9694732	-0.3014174	0.0213923
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C	1.3152996	1.9369273	1.5595570
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C	1.0780697	2.0673054	3.9654674

H	0.5225305	1.8299132	4.8731780
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H	2.6222507	3.1601412	5.0060708
C	2.9627189	3.1303552	2.8732615
H	3.8779608	3.7200168	2.9307259
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C	-2.8871936	-2.2766036	1.9137037
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C	-3.9218452	-2.3856392	2.8430747
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C	-4.6066078	-1.2423694	3.2659598
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C	-4.2544736	0.0140277	2.7641593
H	-4.7846257	0.9056237	3.1000325
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H	-3.5502464	-3.7886913	-3.1122104
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H	0.2340259	-2.8497055	-1.4710446
N	-0.7339861	0.6602093	0.1632935
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P	-1.2460510	-0.8535424	0.1510033
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P	0.0911863	-0.2688501	-1.4843722
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H	-0.0735529	2.1150719	1.4742677

H	0.9087588	1.5387416	2.8675315
H	1.6252401	1.5857171	1.2335596
C	0.7009366	1.4056446	-1.7970921
H	-0.0735529	2.1150719	-1.4742677
H	1.6252401	1.5857171	-1.2335596
H	0.9087588	1.5387416	-2.8675315
C	1.4208197	-1.4153714	-1.9304896
H	2.2996080	-1.2325657	-1.2983785
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H	0.8892559	2.4321654	2.0070434
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H	-0.8892559	-2.4321654	2.0070434
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H	-2.3611065	1.6628937	-0.4493392
H	-1.4490480	2.9427799	-1.3071414
H	-1.4482541	1.2741483	-1.9406372
C	-1.4530857	-1.8808934	-1.0260907
H	-2.3611065	-1.6628937	-0.4493392
H	-1.4482541	-1.2741483	-1.9406372
H	-1.4490480	-2.9427799	-1.3071414
C	1.4530857	-1.8808934	-1.0260907
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H	2.3611065	-1.6628937	-0.4493392
H	1.4490480	-2.9427799	-1.3071414
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H	0.8938253	-2.4752026	-1.7964731
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H	0.8938253	2.4752026	-1.7964731
H	-0.8938253	2.4752026	-1.7964731
C	1.4518418	-1.8780366	1.2199749
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H	1.4445858	-2.9395684	1.5021120
H	2.3622661	-1.6628459	0.6459161

C	-1.4518418	-1.8780366	1.2199749
H	-2.3622661	-1.6628459	0.6459161
H	-1.4445858	-2.9395684	1.5021120
H	-1.4475124	-1.2704467	2.1339544
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H	-2.3622661	1.6628459	0.6459161
H	-1.4475124	1.2704467	2.1339544
H	-1.4445858	2.9395684	1.5021120
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H	-1.4495033	-1.3108312	2.3466631
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H	0.8892187	2.3741001	0.5138575
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H	0.0000000	-3.6371149	-0.4019344
H	0.8892187	-2.3741001	0.5138575
H	-0.8892187	-2.3741001	0.5138575

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H	1.4396110	3.0203692	-2.7797984
H	2.3607904	1.7199560	-1.9641437
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H	-2.3607904	1.7199560	-1.9641437
H	-1.4396110	3.0203692	-2.7797984
H	-1.4539628	1.3710018	-3.4670294
C	-1.4515316	-1.9498573	-2.5342898
H	-2.3607904	-1.7199560	-1.9641437
H	-1.4539628	-1.3710018	-3.4670294
H	-1.4396110	-3.0203692	-2.7797984
C	1.4515316	-1.9498573	-2.5342898
H	1.4539628	-1.3710018	-3.4670294
H	2.3607904	-1.7199560	-1.9641437
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H	-2.1554361	0.0000000	5.0831019
H	-2.1582886	0.0000000	2.5938894

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N	0.3751641	-0.0078205	0.0000000
P	-0.3516047	-0.0185570	-1.4785931
P	-0.3516047	-0.0185570	1.4785931
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H	1.6096204	0.8270959	-2.6139778
H	1.5599553	-0.9824819	-2.5983092
C	0.9710809	-0.0616701	2.7051702
H	0.5273769	-0.0570308	3.7102495
H	1.5599553	-0.9824819	2.5983092
H	1.6096204	0.8270959	2.6139778
C	-1.3981614	-1.4595625	-1.7744379
H	-2.3095890	-1.4108516	-1.1660370
H	-1.6945332	-1.4735759	-2.8330031
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H	-0.7592243	2.3574521	-1.6232538
H	-1.6645074	1.4393847	-2.8653475
H	-2.2463681	1.4586253	-1.1845429
C	-1.3469933	1.4500172	1.8129225
H	-0.7592243	2.3574521	1.6232538
H	-2.2463681	1.4586253	1.1845429
H	-1.6645074	1.4393847	2.8653475
C	-1.3981614	-1.4595625	1.7744379
H	-2.3095890	-1.4108516	1.1660370
H	-0.8491866	-2.3812668	1.5424771
H	-1.6945332	-1.4735759	2.8330031
H	1.9920935	0.0688581	0.0000000
N	3.1117362	0.1274317	0.0000000
H	3.5008813	-0.3355105	-0.8315654
H	3.4235125	1.1073944	0.0000000

H	3.5008813	-0.3355105	0.8315654

8.

N	-0.3368790	0.0139400	-0.8373374
P	-0.0395857	-1.4676831	-0.1523412
P	-0.0603517	1.4713180	-0.0941959
C	-0.0836894	-2.6868119	-1.4825496
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H	-1.0833137	-2.7445336	-1.9388360
H	0.6829320	-2.4678105	-2.2386349
C	1.6838476	1.9290279	-0.0769934
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H	2.2594941	1.2500166	0.5638749
H	2.0915887	1.8967986	-1.0962186
C	1.5748809	-1.5979766	0.6432614
H	1.6283686	-0.9481089	1.5268059
H	1.7225139	-2.6348295	0.9779945
H	2.3721876	-1.3343740	-0.0635969
C	-1.2915513	-1.9465512	1.0542028
H	-2.2903556	-1.8896165	0.6018308
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H	-1.2551097	-1.2935584	1.9347964
C	-0.9332657	2.7291084	-1.0501934
H	-0.5268107	2.8084688	-2.0698328
H	-2.0132129	2.5266949	-1.0708776
H	-0.7821447	3.7066626	-0.5700067
C	-0.6745016	1.5606951	1.6001864
H	-1.7426915	1.3097717	1.6339866
H	-0.1110128	0.8847572	2.2571787
H	-0.5366755	2.5858727	1.9737277
Li	-1.0688938	0.0473413	-2.6626502

9.

N	-0.3319500	0.0139696	-0.8293921
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H	0.6936849	-2.4654222	-2.2189173
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H	1.7906830	2.9504014	0.3165890
H	2.2706573	1.2511098	0.5604100
H	2.0923015	1.8960895	-1.0975082
C	1.5693500	-1.5950699	0.6719210
H	1.6195285	-0.9383901	1.5504896
H	1.7086739	-2.6298681	1.0153406
H	2.3749345	-1.3397958	-0.0285093
C	-1.2955355	-1.9439892	1.0569898
H	-2.2917201	-1.8840787	0.5994689
H	-1.1107368	-2.9781144	1.3808838
H	-1.2648090	-1.2925161	1.9389141
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H	-2.0077484	2.5205521	-1.0462950
H	-0.7906800	3.7027500	-0.5144686
C	-0.6503299	1.5557472	1.6166821
H	-1.7195477	1.3110261	1.6610100
H	-0.0866943	0.8745468	2.2678729
H	-0.5025604	2.5790867	1.9905152

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TS geometry

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P	-0.0382692	1.4716155	0.0158880
C	-0.1507267	-2.6226293	-1.4358740
H	0.0315578	-3.6481664	-1.0884104
H	-1.1714888	-2.5665231	-1.8373408
H	0.5823368	-2.3754905	-2.2147739
C	1.6987619	1.9669063	0.1184894
H	1.7752340	3.0002762	0.4837325
H	2.2386749	1.3096124	0.8118917
H	2.1633461	1.8987276	-0.8736944
C	1.6637807	-1.7034518	0.6406263
H	1.7744014	-1.1021053	1.5530782
H	1.8067791	-2.7599520	0.9065983
H	2.4313862	-1.4076432	-0.0860103
C	-1.1690613	-1.9754382	1.2021776
H	-2.1920208	-1.8708312	0.8184099
H	-0.9908486	-3.0239944	1.4780252
H	-1.0588063	-1.3540248	2.1000223
C	-0.8663356	2.6845905	-1.0345154
H	-0.4217169	2.6579742	-2.0380285
H	-1.9379123	2.4527505	-1.0868607
H	-0.7392935	3.6940734	-0.6218120
C	-0.7263185	1.6579812	1.6803475
H	-1.7867548	1.3746963	1.6825112
H	-0.1774815	1.0229529	2.3891161
H	-0.6320196	2.7016220	2.0111513
Na	-1.8604754	-0.0457554	-4.8547419

10.

N	-0.0766400	0.0027003	-0.1896146
P	0.1870880	-1.4983743	0.4992681
P	0.1963562	1.4725948	0.5599861
C	0.2269300	-2.7074179	-0.8334977
H	0.4611832	-3.6934477	-0.4069594
H	-0.7544527	-2.7735875	-1.3240323
H	1.0017524	-2.4443974	-1.5655475
C	1.9382938	1.9274946	0.5303007
H	2.0530034	2.9459746	0.9291437
H	2.5342340	1.2414223	1.1446298
H	2.3073025	1.9038610	-0.5040256
C	1.7590655	-1.5978633	1.3775681
H	1.7802662	-0.9225150	2.2424226
H	1.8830338	-2.6254614	1.7493428
H	2.5874527	-1.3634754	0.6965568
C	-1.1375076	-1.9632863	1.6272096
H	-2.1028882	-1.8944187	1.1082419
H	-0.9813957	-2.9999588	1.9596559
H	-1.1499368	-1.3116494	2.5092676
C	-0.7182977	2.7248300	-0.3533123
H	-0.3138826	2.8346988	-1.3696215
H	-1.7846060	2.4650846	-0.3939311
H	-0.6070165	3.6896369	0.1622902
C	-0.3829253	1.5076988	2.2673885
H	-1.4556629	1.2783153	2.3087262
H	0.1771759	0.8052707	2.8977103
H	-0.2203494	2.5202737	2.6655493

Hg	-0.8432645	0.0528663	-2.3018933
C	-1.5582604	0.0993652	-4.2699831
H	-0.8562587	-0.4764390	-4.8837171
H	-2.5574355	-0.3509276	-4.2625813
H	-1.5923570	1.1511319	-4.5765414

11.

N	0.4246212	-0.0019695	-0.0039917
P	-0.2567874	-0.0930607	-1.5436199
P	-0.2530648	0.0632823	1.5390907
C	1.0548663	0.3653248	-2.6759049
H	0.6851515	0.2457124	-3.7043639
H	1.3433902	1.4121093	-2.5143537
H	1.9255468	-0.2869417	-2.5263117
C	1.0575368	-0.4182991	2.6625427
H	0.6946877	-0.3049292	3.6941151
H	1.3354843	-1.4659761	2.4881328
H	1.9335136	0.2272353	2.5122702
C	-0.8239765	-1.7595393	-1.9027856
H	-1.6361163	-2.0493927	-1.2234975
H	-1.2030016	-1.7928490	-2.9350671
H	0.0108539	-2.4661204	-1.8030021
C	-1.6371748	1.0487311	-1.6938348
H	-1.3034242	2.0753095	-1.4936765
H	-2.0222539	0.9922977	-2.7229167
H	-2.4545887	0.7765156	-1.0129189
C	-0.8167127	1.7243611	1.9281593
H	0.0213065	2.4295177	1.8456457
H	-1.6229771	2.0293598	1.2482391
H	-1.2009317	1.7413299	2.9588712
C	-1.6360121	-1.0778934	1.6653537
H	-2.4561970	-0.7874361	0.9955074
H	-1.3063734	-2.1010558	1.4426209
H	-2.0156044	-1.0427304	2.6974399
H	1.4799505	0.0492607	-0.0048114
H	3.7931261	-0.6042759	0.1173010
H	3.7178204	0.9343908	-0.0699513
O	3.1673409	0.1377311	0.0357177

12.

N	-0.2880898	0.0162854	-0.7400181
P	-0.0499691	-1.5592589	-0.1434186
P	-0.0371886	1.5644968	-0.0801414
C	-0.0615780	-2.6182735	-1.5895016
H	0.0853252	-3.6561423	-1.2547523
H	-1.0311619	-2.5547956	-2.1040062
H	0.7522667	-2.3434358	-2.2738187
C	1.7043727	1.9951532	-0.1149156
H	1.8201948	3.0239756	0.2587992
H	2.2867470	1.3228485	0.5284799
H	2.0824804	1.9434637	-1.1451093
C	1.5307266	-1.6486288	0.7028806
H	1.5446310	-1.0010968	1.5899674
H	1.6763637	-2.6854245	1.0422961
H	2.3459710	-1.3795618	0.0185525
C	-1.3712798	-2.0219822	0.9793585
H	-2.3409124	-1.9416216	0.4692315
H	-1.2170292	-3.0654776	1.2941791
H	-1.3668555	-1.3835985	1.8723372
C	-0.9765792	2.6782949	-1.1238602

H	-0.6039249	2.6407506	-2.1573903
H	-2.0447764	2.4246019	-1.0935477
H	-0.8397779	3.7014602	-0.7430170
C	-0.6433250	1.6056503	1.6090434
H	-1.7121671	1.3561432	1.6377458
H	-0.0732317	0.9227171	2.2534473
H	-0.5041294	2.6265677	1.9966695
H	-0.6671034	0.0368884	-1.6894912

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