Characterizing the lone pair···π-hole interaction in complexes of ammonia with perfluorinated arenes

*Weixing Li,[a], [b], † Imanol Usabiaga,[a], † Camilla Calabrese,[c], [d], [e], * Luca Evangelisti,[a] Assimo Maris,[a] Laura B. Favero[f] and Sonia Melandri[a], **

[a] Department of Chemistry "Giacomo Ciamician", University of Bologna, via Selmi, 2, 40126, Bologna (Italy).

[b] Present address of Dr. W. Li: Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany

[c] Department of Physical Chemistry, University of the Basque Country (UPV/EHU), Barrio Sarriena, S/N, 48940, Leioa (Spain).

[d] Biofisika Institute, (CSIC, UPV/EHU), Barrio Sarriena, S/N, 48940, Leioa (Spain).

[e] Fundación Biofisika Bizkaia/Biofisika Bizkaia Fundazioa (FBB), Barrio Sarriena, S/N, 48940, Leioa (Spain).

[c] Istituto per lo studio dei materiali nanostrutturati CNR – ISMN Via Gobetti 101, 40129, Bologna (Italy).

[†] These authors contributed equally to this work.

Corresponding Authors

* Camilla Calabrese: calabrese.cami@gmail.com

* Sonia Melandri: sonia.melandri@unibo.it

ELECTRONIC SUPPLEMENTARY INFORMATION

Table of Contents

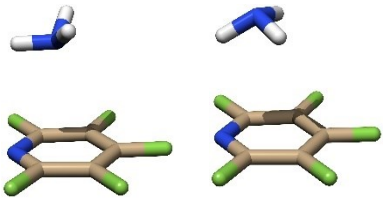
Table S1: Theoretical (B3LYP-D3(BJ)/def2-TZVP) equilibrium structure for $C_6F_6 \cdot NH_3$.

	a/Å	*b*/Å	*c*/Å
C	-1.20037	0.69304	-0.28484
C	0.00000	1.38611	-0.28524
C	1.20037	0.69304	-0.28484
C	1.20041	-0.69306	-0.28524
C	0.00000	-1.38607	-0.28484
C	-1.20041	-0.69306	-0.28524
F	-2.35515	1.35975	-0.26675
F	0.00000	2.71967	-0.26696
F	2.35515	1.35975	-0.26675
F	2.35530	-1.35983	-0.26696
F	0.00000	-2.71950	-0.26675
F	-2.35530	-1.35983	-0.26696
N	0.00000	0.00000	2.924971
H	-0.81534	-0.47074	3.301832
H	0.00000	0.94147	3.301832
H	0.81534	-0.47074	3.301832

Table S2: Theoretical (B3LYP-D3(BJ)/def2-TZVP) equlibrium structure for the observed **I** complex of $C_5F_5N \cdot NH_3$.

	a/Å	*b*/Å	*c*/Å
N	-1.49128	-0.62763	0.00000
C	-0.83698	-0.50834	1.12589
C	0.52638	-0.27317	1.19763
C	1.21651	-0.15402	0.00000
C	0.52638	-0.27317	-1.19763
C	-0.83698	-0.50834	-1.12589
F	-1.53110	-0.61451	2.25789
F	1.16223	-0.14441	2.36185
F	2.51943	0.08961	0.00000
F	1.16223	-0.14441	-2.36185
F	-1.53110	-0.61451	-2.25789
N	-0.85437	2.65950	0.00000
H	-0.66835	3.23164	-0.81646
H	-1.84809	2.45476	0.00000
H	-0.66835	3.23164	0.81646
N	-1.49128	-0.62763	0.00000

Table S3: Theoretical (B3LYP-GD3(BJ)/def2-TZVP) spectroscopic parameters of the two plausible conformers of $C_5F_5N{\cdot}NH_3$.

		
	I	**II**
A/MHz	1005.8	955.3
B/MHz	807.4	782.9
C/MHz	616.1	610.7
χ_{aa}/MHz[c]	2.022/2.225	2.026/2.312
χ_{bb}/MHz[c]	-4.013/0.522	-3.948/1.360
χ_{cc}/MHz[c]	1.991/-2.747	1.922/-3.672
$\mu_a/\mu_b/\mu_c$/D	0/0.2/2	0/1.5/1.2
ΔE (kJ/mol)	0[a]	11.3
ΔE_{+ZPE} (kJ/mol)	0[b]	10.6

[a] Absolute energy -801.3807718 Hartrees

[b] Absolute energy -801.296826 Hartrees

[c]The first value refers to C_5F_5N while the second one to NH_3.

Table S4: Experimental transition frequencies of $C_6F_6 \cdot {}^{14}NH_3$. Assignments, measured transition frequencies (ν/MHz), and observed-calculated residuals ($\Delta\nu$/MHz) from the fit for m = 0, 1, -1.

						m = 0		m = 1		m= - 1	
J'	K'	F'	J"	K"	F"	ν/MHz	$\Delta\nu$/MHz	ν/MHz	$\Delta\nu$/MHz	ν/MHz	$\Delta\nu$/MHz
5	0	6	4	0	5	7596.2580	-0.0042	7595.5898	-0.0019	7595.5898	-0.0019
5	1	6	4	1	5	7596.2343	0.0019	7595.4672	-0.0005	7595.7140	0.0106
5	2	6	4	2	5	7596.2343	-0.0104	7595.3301	-0.0018	7595.7997	-0.0036
5	0	5	4	0	4	7596.2580	0.0125	7595.5719	-0.0031	7595.5719	-0.0031
5	1	5	4	1	4	7596.1868	0.0003	7595.3938	-0.0042	7595.6321	-0.0017
5	2	5	4	2	4	7596.0106	-0.0004	7595.1041	0.0004	7595.5719	-0.0032
5	0	4	4	0	3			7595.5345	-0.0024	7595.5345	-0.0024
6	0	7	5	0	6	9115.4828	0.0000	9114.6762	-0.0018	9114.6762	-0.0018
6	1	7	5	1	6	9115.4653	-0.0026	9114.5184	-0.0032	9114.8009	-0.0037
6	2	7	5	2	6	9115.4233	-0.0005	9114.3324	-0.0037	9114.9057	0.0038
6	3	7	5	3	6	9115.3647	0.0124			9114.9698	-0.0020
6	4	7	5	4	6	9115.2524	-0.0041	9113.8837	-0.0020	9115.0237	0.0063
6	0	6	5	0	5	9115.4653	-0.0050	9114.6608	-0.0049	9114.6608	-0.0049
6	1	6	5	1	5	9115.4233	-0.0015	9114.4757	-0.0029	9114.8009	-0.0036
6	2	6	5	2	5	9115.2897	0.0013	9114.2012	0.0004	9114.9057	0.0039
6	3	6	5	3	5	9115.0679	0.0048	9113.8436	0.0096	9114.9698	-0.0019
6	4	6	5	4	5	9114.7606	0.0039	9113.3857	0.0041	9115.0237	0.0063
6	0	5	5	0	4	9115.4458	-0.0005	9114.6444	0.0026	9114.6444	0.0026
6	1	5	5	1	4	9115.4458	0.0054	9114.4931	-0.0012	9114.7775	0.0002
6	2	5	5	2	4	9115.4233	-0.0001	9114.3324	-0.0031	9114.9057	0.0042
7	0	8	6	0	7	10634.6901	-0.0010	10633.7521	-0.0007	10633.7521	-0.0007
7	1	8	6	1	7	10634.6672	-0.0026	10633.5632	-0.0031	10633.8981	0.0016
7	2	8	6	2	7	10634.6080	0.0017	10633.3399	0.0020	10633.9914	-0.0067
7	3	8	6	3	7	10634.4912	-0.0118	10633.0659	-0.0036	10634.0615	0.0017
7	0	7	6	0	6	10634.6901	0.0083	10633.7521	-0.0006	10633.7521	-0.0006
7	1	7	6	1	6	10634.6387	-0.0025	10633.5356	-0.0021	10633.8599	-0.0079
7	2	7	6	2	6	10634.6080	0.0014	10633.2506	-0.0008	10633.9067	-0.0049
7	3	7	6	3	6			10632.8899	0.0032	10633.8730	-0.0039
7	4	7	6	4	6			10632.4551	0.0081		
7	5	7	6	5	6			10631.9322	-0.0052		
7	0	6	6	0	5	10634.6672	0.0019	10633.7249	-0.0018	10633.7249	-0.0018
7	1	6	6	1	5	10634.6515	0.0028				
7	2	6	6	2	5	10634.5965	-0.0031				
7	3	6	6	3	5	10634.5188	-0.0014				
8	0	9	7	0	8	12153.8882	0.0025	12152.8142	0.0011	12152.8142	0.0011
8	1	9	7	1	8	12153.8578	-0.0012	12152.5957	-0.0021	12152.9651	-0.0099
8	2	9	7	2	8	12153.7805	0.0008	12152.3295	-0.0004	12153.0958	0.0114
8	3	9	7	3	8	12153.6515	0.0012	12152.0119	-0.0001	12153.1440	0.0005
8	4	9	7	4	8	12153.4745	-0.0003	12151.6503	0.0025		
8	0	8	7	0	7	12153.8882	0.0101	12152.8142	0.0085	12152.8142	0.0085
8	1	8	7	1	7	12153.8347	-0.0039	12152.5816	0.0042	12152.9616	0.0070
8	2	8	7	2	7	12153.7199	-0.0004	12152.2725	0.0020		
8	3	8	7	3	7	12153.5308	0.0050	12151.8904	0.0030		
8	4	8	7	4	7			12151.4321	-0.0001		
8	0	7	7	0	6	12153.8578	-0.0081	12152.7975	0.0040	12152.7975	0.0040
8	1	7	7	1	6	12153.8347	-0.0073	12152.5815	0.0006	12152.9616	0.0035
8	2	7	7	2	6	12153.7805	0.0095	12152.3295	0.0082		
8	3	7	7	3	6			12152.0119	-0.0052		
9	0	10	8	0	9	13673.0612	-0.0019	13671.8546	-0.0020	13671.8546	-0.0018
9	1	10	8	1	9	13673.0293	-0.0023	13671.6140	0.0009	13672.0251	-0.0119
9	2	10	8	2	9	13672.9384	0.0005	13671.3037	-0.0038	13672.1586	0.0033
9	3	10	8	3	9	13672.7834	-0.0015	13670.9437	0.0013	13672.2172	0.0030
9	4	10	8	4	9	13672.5726	-0.0045	13670.5189	-0.0038	13672.2172	-0.0011
9	5	10	8	5	9	13672.3207	-0.0003	13670.0623	0.0076		
9	6	10	8	6	9	13672.0249	-0.0001				
9	7	10	8	7	9	13671.7002	0.0010				
9	0	9	8	0	8	13673.0612	0.0040	13671.8546	0.0042	13671.8546	0.0042
9	1	9	8	1	8	13673.0140	-0.0023	13671.5956	-0.0020	13672.0251	0.0032
9	2	9	8	2	8	13672.8917	-0.0036	13671.2682	0.0038	13672.1185	0.0059
9	3	9	8	3	8	13672.6973	0.0008	13670.8568	0.0033	13672.1185	-0.0071
9	4	9	8	4	8	13672.4182	-0.0065	13670.3685	-0.0010	13672.0666	0.0011
9	0	9	8	0	8			13671.8379	-0.0034	13671.8379	-0.0034
9	1	8	8	1	7	13673.0140	-0.0040	13671.5956	-0.0039	13672.0251	0.0017
9	2	8	8	2	7	13672.9268	-0.0026	13671.3037	0.0047	13672.1586	0.0119
9	3	8	8	3	7	13672.7834	-0.0014	13670.9437	0.0013	13672.2183	0.0041
9	4	8	8	4	7	13672.5868	-0.0020	13670.5316	-0.0029	13672.2183	-0.0119

Table S5: Experimental transition frequencies of C_6F_6·$^{15}NH_3$. Assignments, measured transition frequencies (ν/MHz), and observed-calculated residuals ($\Delta\nu$/MHz) from the fit for m = 0, 1, -1.

				m = 0		m = 1		m = -1	
J'	K'	J"	K"	ν	$\Delta\nu$	ν	$\Delta\nu$	ν	$\Delta\nu$
6	0	5	0	8996.9833	-0.0028	8996.2062	-0.0007	8996.2062	-0.0007
6	1	5	1	8996.9625	-0.0004	8996.0426	0.0002	8996.3257	0.0008
6	2	5	2	8996.8967	0.0030	8995.8336	0.0017	8996.3933	-0.0036
6	3	5	3	8996.7854	0.0055	8995.5826	0.0057		
6	4	5	4	8996.6210	-0.0030	8995.2771	-0.0026		
6	5	5	5	8996.4283	-0.0009	8994.9352	-0.0085		
7	0	6	0	10496.4469	-0.0031	10495.5396	-0.0013	10495.5396	-0.0013
7	1	6	1	10496.4217	-0.0012	10495.3471	-0.0019	10495.6788	0.0003
7	2	6	2	10496.3456	0.0035	10495.1068	0.0034	10495.7590	-0.0036
7	3	6	3	10496.2114	0.0020	10494.8120	0.0061		
7	4	6	4	10496.0284	0.0010				
7	5	6	5	10495.7975	-0.0027				
7	6	6	6	10495.5390	0.0064				
8	0	7	0	11995.8929	-0.0053	11994.8585	0.0008	11994.8585	0.0008
8	1	7	1	11995.8664	-0.0008	11994.6416	0.0017	11995.0166	0.0000
8	2	7	2	11995.7747	-0.0002	11994.3632	0.0040	11995.1108	-0.0018
8	3	7	3	11995.6231	-0.0001	11994.0227	0.0035		
8	4	7	4	11995.4130	-0.0023	11993.6258	0.0029		
8	5	7	5	11995.1520	-0.0036	11993.1664	-0.0085		
8	6	7	6	11994.8585	0.0084				
8	7	7	7	11994.5026	-0.0024				

Table S6: Experimental frequencies of $C_5F_5N\cdot{}^{14}NH_3$. Assignements, measured transition frequencies (ν/MHz), and observed-calculated residuals ($\Delta\nu$/MHz)) from the fit.

J'	K_a'	K_c'	F_1'	F'	J''	K_a''	K_c''	F_1''	F''	ν/MHz	$\Delta\nu$/MHz
5	3	3	4	4	4	2	3	3	3	8878.5270	-0.0017
5	3	3	6	6	4	2	3	5	5	8878.5795	0.0003
5	3	3	5	5	4	2	3	4	4	8878.8458	-0.0016
5	3	3	4	5	4	2	3	3	4	8878.8603	0.0001
5	3	3	6	7	4	2	3	5	6	8878.9158	0.0033
5	3	3	4	3	4	2	3	3	2	8878.9480	-0.0005
5	3	3	6	5	4	2	3	5	4	8878.9846	-0.0030
5	3	3	5	6	4	2	3	4	5	8879.1664	-0.0012
5	3	3	5	4	4	2	3	4	3	8879.2510	-0.0032
5	4	1	5	5	4	3	1	4	4	9093.0790	0.0009
5	4	1	5	5	4	3	1	5	4	9093.3300	-0.0017
5	4	1	5	6	4	3	1	4	5	9093.2918	-0.0011
5	4	1	5	4	4	3	1	4	3	9093.2918	0.0025
5	4	1	5	5	4	3	1	3	4	9093.5734	-0.0006
5	4	1	6	5	4	3	1	4	4	9093.5477	-0.0003
5	4	1	6	6	4	3	1	5	5	9093.6590	0.0000
5	4	1	4	5	4	3	1	5	4	9093.6773	0.0089
5	4	1	6	7	4	3	1	5	6	9093.7263	-0.0011
5	4	1	4	4	4	3	1	3	3	9093.7757	0.0022
5	4	1	6	5	4	3	1	5	4	9093.7992	-0.0025
5	4	1	4	3	4	3	1	3	2	9093.8373	-0.0010
5	4	1	4	5	4	3	1	3	4	9093.9108	0.0002
5	4	2	5	5	4	3	2	4	4	9197.4642	-0.0014
5	4	2	6	6	4	3	2	5	5	9197.5491	-0.0024
5	4	2	4	4	4	3	2	3	3	9197.5761	0.0029
5	4	2	5	6	4	3	2	4	5	9197.6130	-0.0029
5	4	2	5	4	4	3	2	4	3	9197.6327	-0.0025
5	4	2	6	7	4	3	2	5	6	9197.7153	0.0010
5	4	2	6	5	4	3	2	5	4	9197.7235	-0.0016
5	4	2	4	5	4	3	2	3	4	9197.7326	0.0008
5	4	2	4	3	4	3	2	3	2	9197.7526	-0.0024
4	2	2	5	5	3	1	2	4	4	6792.1297	-0.0005
4	2	2	3	3	3	1	2	2	2	6792.1697	-0.0018
4	2	2	5	6	3	1	2	4	5	6792.3684	0.0002
4	2	2	3	4	3	1	2	2	3	6792.3843	-0.0002
4	2	2	4	4	3	1	2	3	3	6792.4348	0.0012
4	2	2	5	4	3	1	2	4	3	6792.4160	0.0002
4	2	2	4	5	3	1	2	3	4	6792.6366	-0.0014
4	2	2	4	3	3	1	2	3	2	6792.6938	-0.0008
4	1	3	3	3	3	0	3	2	2	6920.8261	0.0021
4	1	3	5	5	3	0	3	4	4	6921.1303	-0.0006
4	1	3	3	4	3	0	3	2	3	6921.5673	0.0055
4	1	3	3	2	3	0	3	2	1	6921.7372	0.0012
4	1	3	5	6	3	0	3	4	5	6921.7920	-0.0057
4	1	3	4	4	3	0	3	3	3	6922.0737	-0.0017
4	1	3	5	4	3	0	3	4	3	6922.1173	0.0009
4	1	3	4	5	3	0	3	3	4	6922.8911	0.0044
4	1	3	4	4	3	0	3	4	3	6923.0772	0.0022
4	1	3	4	3	3	0	3	3	2	6923.1336	0.0017
4	2	3	3	3	3	1	3	2	2	7073.3486	0.0009
4	2	3	5	5	3	1	3	4	4	7073.5415	-0.0018
4	2	3	3	4	3	1	3	3	3	7073.5804	0.0012
4	2	3	4	4	3	1	3	3	3	7073.9705	-0.0016
4	2	3	3	4	3	1	3	2	3	7074.0855	0.0077
4	2	3	5	6	3	1	3	4	5	7074.1637	-0.0024
4	2	3	3	2	3	1	3	2	1	7074.1861	0.0007
4	2	3	5	4	3	1	3	4	3	7074.5148	0.0013
4	2	3	4	5	3	1	3	3	4	7074.8369	0.0022
4	2	3	4	3	3	1	3	3	2	7075.0508	0.0013
4	3	1	4	4	3	2	1	3	3	7089.2089	0.0014
4	3	1	4	5	3	2	1	3	4	7089.2562	-0.0019
4	3	1	4	3	3	2	1	3	2	7089.2562	-0.0010
4	3	1	5	5	3	2	1	4	4	7089.6312	-0.0004
4	3	1	5	4	3	2	1	4	3	7089.6762	-0.0015
4	3	1	5	6	3	2	1	4	5	7089.7092	-0.0029
4	3	1	3	3	3	2	1	2	2	7089.8333	-0.0010
4	3	1	3	4	3	2	1	2	3	7089.9169	-0.0015
4	3	1	3	2	3	2	1	2	1	7089.9169	0.0028
4	3	2	3	3	3	2	2	2	2	7273.6974	-0.0037
4	3	2	5	5	3	2	2	4	4	7273.7211	0.0032
4	3	2	4	4	3	2	2	3	3	7273.7771	-0.0010
4	3	2	3	4	3	2	2	2	3	7273.9986	-0.0042
4	3	2	5	6	3	2	2	4	5	7274.0166	0.0006
4	3	2	3	2	3	2	2	2	1	7274.0697	-0.0044
4	3	2	4	5	3	2	2	3	4	7274.0836	-0.0031
4	3	2	5	4	3	2	2	4	3	7274.0981	0.0004
4	3	2	4	3	3	2	2	3	2	7274.1602	-0.0015
4	4	0	4	4	3	3	0	3	3	7688.6636	0.0116
4	4	0	4	5	3	3	0	3	4	7688.7767	0.0000
4	4	0	5	5	3	3	0	4	4	7688.8578	-0.0005
4	4	0	5	4	3	3	0	4	3	7688.9242	-0.0001

4	4	0	3	2	3	3	0	2	1	7688.9242	-0.0035
4	4	0	5	6	3	3	0	4	5	7688.9681	-0.0006
4	4	0	3	4	3	3	0	2	3	7688.9849	-0.0016
4	4	1	4	4	3	3	1	3	3	7708.5202	0.0003
4	4	1	4	3	3	3	1	3	2	7708.6731	0.0021
4	4	1	4	5	3	3	1	3	4	7708.6597	-0.0013
4	4	1	5	5	3	3	1	4	4	7708.6332	0.0014
4	4	1	3	3	3	3	1	2	2	7708.5429	-0.0030
4	4	1	3	2	3	3	1	2	1	7708.6731	-0.0019
4	4	1	5	4	3	3	1	4	3	7708.7086	-0.0018
4	4	1	3	4	3	3	1	2	3	7708.7376	0.0000
4	4	1	5	6	3	3	1	4	5	7708.7567	0.0056
5	2	3	4	4	4	1	3	3	3	8517.2331	-0.0030
5	2	3	6	6	4	1	3	5	5	8517.3095	0.0007
5	2	3	4	5	4	1	3	3	4	8517.5143	-0.0004
5	2	3	6	7	4	1	3	5	6	8517.6114	-0.0023
5	2	3	4	3	4	1	3	3	2	8517.6057	0.0013
5	2	3	6	5	4	1	3	5	4	8517.6796	0.0021
5	2	3	5	5	4	1	3	4	4	8517.9279	-0.0003
5	2	3	5	6	4	1	3	4	5	8518.2068	-0.0006
5	2	3	5	4	4	1	3	4	3	8518.2703	-0.0005
5	3	2	5	5	4	2	2	4	4	8567.3498	-0.0016
5	3	2	5	6	4	2	2	4	5	8567.4482	-0.0021
5	3	2	6	6	4	2	2	5	5	8567.4878	0.0003
5	3	2	5	4	4	2	2	4	3	8567.4666	0.0051
5	3	2	4	4	4	2	2	3	3	8567.5873	-0.0004
5	3	2	6	7	4	2	2	5	6	8567.5873	-0.0013
5	3	2	6	5	4	2	2	5	4	8567.6004	0.0038
5	3	2	4	5	4	2	2	3	4	8567.6874	-0.0022
5	3	2	4	3	4	2	2	3	2	8567.7002	0.0002
5	1	4	4	4	4	0	4	3	3	8737.1268	0.0009
5	1	4	6	6	4	0	4	5	5	8737.3180	0.0010
5	1	4	4	5	4	0	4	3	4	8737.7774	-0.0020
5	1	4	4	3	4	0	4	3	2	8737.8605	-0.0011
5	1	4	6	7	4	0	4	5	6	8737.8908	-0.0069
5	1	4	5	5	4	0	4	4	4	8738.0178	0.0031
5	1	4	6	5	4	0	4	5	4	8738.1460	-0.0005
5	1	4	5	6	4	0	4	4	5	8738.7647	0.0027
5	1	4	5	4	4	0	4	4	3	8738.9168	0.0000
5	2	4	4	4	4	1	4	3	3	8797.8479	0.0000
5	2	4	6	6	4	1	4	5	5	8798.0200	0.0060
5	2	4	5	5	4	1	4	4	4	8798.5381	0.0026
5	2	4	4	5	4	1	4	3	4	8798.5156	-0.0001
5	2	4	6	7	4	1	4	5	6	8798.5881	-0.0045
5	2	4	6	5	4	1	4	5	4	8798.8407	-0.0021
5	2	4	5	6	4	1	4	4	5	8799.2891	-0.0035
5	2	4	5	4	4	1	4	4	3	8799.4550	0.0014
5	5	0	5	5	4	4	0	4	4	9688.9051	0.0000
5	5	0	5	4	4	4	0	4	3	9689.0274	-0.0010
5	5	0	4	4	4	4	0	3	3	9688.9454	0.0014
5	5	0	4	3	4	4	0	3	2	9689.0560	0.0002
5	5	0	6	5	4	4	0	5	4	9689.0769	0.0014
5	5	0	4	5	4	4	0	3	4	9689.0907	-0.0036
5	5	0	6	7	4	4	0	5	6	9689.1032	0.0008
5	5	1	5	5	4	4	1	4	4	9694.3088	0.0003
5	5	1	5	4	4	4	1	4	3	9694.4177	0.0002
5	5	1	5	6	4	4	1	4	5	9694.4177	0.0001
5	5	1	4	4	4	4	1	3	3	9694.3332	-0.0017
5	5	1	6	6	4	4	1	5	5	9694.3879	0.0004
5	5	1	4	3	4	4	1	3	2	9694.4385	0.0070
5	5	1	6	5	4	4	1	5	4	9694.4551	-0.0012
5	5	1	4	5	4	4	1	3	4	9694.4697	-0.0020
5	5	1	6	7	4	4	1	5	6	9694.4842	0.0000
6	3	3	7	7	5	2	3	6	6	10166.0118	-0.0004
6	3	3	5	5	5	2	3	4	4	10166.0280	0.0013
6	3	3	7	8	5	2	3	6	7	10166.1600	-0.0016
6	3	3	5	6	5	2	3	4	5	10166.1709	-0.0005
6	3	3	7	6	5	2	3	6	5	10166.1830	0.0027
6	3	3	6	6	5	2	3	5	5	10166.2069	0.0012
6	3	3	5	4	5	2	3	4	3	10166.1949	-0.0029
6	3	3	6	7	5	2	3	5	6	10166.3466	-0.0006
6	3	3	6	5	5	2	3	5	4	10166.3673	-0.0018
6	2	4	5	5	5	1	4	4	4	10340.9821	-0.0021
6	2	4	7	7	5	1	4	6	6	10341.1074	0.0021
6	2	4	5	6	5	1	4	4	5	10341.3699	0.0011
6	2	4	5	4	5	1	4	4	3	10341.4432	-0.0071
6	2	4	7	8	5	1	4	6	7	10341.4859	0.0021
6	2	4	7	6	5	1	4	6	5	10341.5596	0.0021
6	2	4	6	6	5	1	4	5	5	10341.8323	0.0009
6	2	4	6	7	5	1	4	5	6	10342.2000	-0.0019
6	2	4	6	5	5	1	4	5	4	10342.2923	0.0027
6	4	2	6	6	5	3	2	5	5	10480.3122	0.0004
6	4	2	6	7	5	3	2	5	6	10480.3567	-0.0009
6	4	2	6	5	5	3	2	5	4	10480.3567	0.0004
6	4	2	7	7	5	3	2	6	6	10480.6932	0.0013
6	4	2	7	6	5	3	2	6	5	10480.7399	0.0054

6	4	2	7	8	5	3	2	6	7	10480.7399	0.0016
6	4	2	5	5	5	3	2	4	4	10480.7999	0.0020
6	4	2	5	6	5	3	2	4	5	10480.8448	-0.0013
6	4	2	5	4	5	3	2	4	3	10480.8448	0.0019
6	1	5	5	5	5	0	5	4	4	10529.6547	0.0009
6	1	5	7	7	5	0	5	6	6	10529.7947	-0.0014
6	1	5	5	6	5	0	5	4	5	10530.2667	0.0005
6	1	5	5	4	5	0	5	4	3	10530.3243	0.0088
6	1	5	6	6	5	0	5	5	5	10530.3788	0.0007
6	1	5	7	8	5	0	5	6	7	10530.3378	0.0038
6	1	5	7	6	5	0	5	6	5	10530.5209	-0.0045
6	1	5	6	7	5	0	5	5	6	10531.0616	0.0034
6	1	5	6	5	5	0	5	5	4	10531.1832	0.0012
6	3	4	5	5	5	2	4	4	4	10548.8693	0.0015
6	3	4	7	7	5	2	4	6	6	10548.9318	-0.0010
6	2	5	5	5	5	1	5	4	4	10549.3085	0.0087
6	3	4	5	6	5	2	4	4	5	10549.2153	-0.0002
6	3	4	6	6	5	2	4	5	5	10549.3085	-0.0013
6	3	4	7	8	5	2	4	6	7	10549.2760	-0.0010
6	3	4	5	4	5	2	4	4	3	10549.2760	-0.0119
6	2	5	7	7	5	1	5	6	6	10549.4352	0.0018
6	3	4	7	6	5	2	4	6	5	10549.3526	0.0004
6	3	4	6	7	5	2	4	5	6	10549.6598	0.0028
6	3	4	6	5	5	2	4	5	4	10549.7334	0.0004
6	2	5	5	6	5	1	5	4	5	10549.9100	0.0022
6	2	5	6	6	5	1	5	5	5	10549.9594	0.0000
6	2	5	7	8	5	1	5	6	7	10549.9723	0.0062
6	2	5	5	4	5	1	5	4	3	10549.9519	-0.0040
6	2	5	7	6	5	1	5	6	5	10550.1567	0.0005
6	2	5	6	7	5	1	5	5	6	10550.6293	-0.0048
6	2	5	6	5	5	1	5	5	4	10550.7558	-0.0016
6	4	3	7	7	5	3	3	6	6	10736.3430	0.0000
6	4	3	5	5	5	3	3	4	4	10736.3528	-0.0001
6	4	3	6	6	5	3	3	5	5	10736.3863	-0.0001
6	4	3	5	6	5	3	3	4	5	10736.5221	-0.0031
6	4	3	7	8	5	3	3	6	7	10736.5221	-0.0049
6	4	3	7	6	5	3	3	6	5	10736.5493	0.0080
6	4	3	6	7	5	3	3	5	6	10736.5493	0.0049
6	5	1	6	6	5	4	1	5	5	11117.7681	0.0006
6	5	1	6	5	5	4	1	5	4	11117.8184	-0.0002
6	5	1	6	7	5	4	1	5	6	11117.8184	-0.0019
6	5	1	7	7	5	4	1	6	6	11118.0223	-0.0003
6	5	1	5	5	5	4	1	4	4	11118.0712	-0.0005
6	5	1	7	6	5	4	1	6	5	11118.0831	0.0013
6	5	1	7	8	5	4	1	6	7	11118.0968	-0.0007
6	5	1	5	6	5	4	1	4	5	11118.1360	-0.0029
6	5	1	5	4	5	4	1	4	3	11118.1481	0.0031
6	5	2	6	6	5	4	2	5	5	11158.1410	-0.0013
6	5	2	6	7	5	4	2	5	6	11158.2428	0.0001
6	5	2	6	5	5	4	2	5	4	11158.2428	-0.0032
6	5	2	7	7	5	4	2	6	6	11158.2804	-0.0003
6	5	2	5	5	5	4	2	4	4	11158.2991	-0.0030
6	5	2	7	6	5	4	2	6	5	11158.3866	0.0017
6	5	2	7	8	5	4	2	6	7	11158.3866	0.0005
6	5	2	5	6	5	4	2	4	5	11158.4071	-0.0001
6	5	2	5	4	5	4	2	4	3	11158.4071	-0.0038
6	6	0	6	6	5	5	0	5	5	11683.7063	0.0006
6	6	0	6	5	5	5	0	5	4	11683.7893	0.0034
6	6	0	6	7	5	5	0	5	6	11683.7893	-0.0003
6	6	0	5	5	5	5	0	4	4	11683.7301	0.0000
6	6	0	7	7	5	5	0	6	6	11683.7656	-0.0005
6	6	0	5	4	5	5	0	4	3	11683.8017	-0.0008
6	6	0	7	6	5	5	0	6	5	11683.8017	0.0046
6	6	0	5	6	5	5	0	6	5	11683.8198	-0.0024
6	6	0	7	6	5	5	0	4	5	11683.8295	-0.0010
6	6	0	7	8	5	5	0	6	7	11683.8423	0.0000
6	6	1	6	6	5	5	1	5	5	11685.0058	0.0015
6	6	1	6	5	5	5	1	5	4	11685.0837	0.0017
6	6	1	6	7	5	5	1	5	6	11685.0837	-0.0023
6	6	1	5	5	5	5	1	4	4	11685.0233	-0.0024
6	6	1	7	7	5	5	1	6	6	11685.0630	0.0005
6	6	1	5	6	5	5	1	6	5	11685.1150	-0.0007
6	6	1	7	6	5	5	1	4	5	11685.1245	0.0005
6	6	1	7	8	5	5	1	6	7	11685.1343	-0.0020
7	3	4	6	6	6	2	4	5	5	11902.5797	0.0010
7	3	4	8	8	6	2	4	7	7	11902.6201	0.0015
7	3	4	6	7	6	2	4	5	6	11902.7804	0.0015
7	3	4	6	5	6	2	4	5	4	11902.8134	-0.0019
7	3	4	8	9	6	2	4	7	8	11902.8288	0.0037
7	3	4	8	7	6	2	4	7	6	11902.8519	-0.0004
7	3	4	7	7	6	2	4	6	6	11903.0791	0.0026
7	3	4	7	8	6	2	4	6	7	11903.2744	0.0005
7	3	4	7	6	6	2	4	6	5	11903.3042	0.0001
7	4	3	7	7	6	3	3	6	6	11938.9705	0.0025
7	4	3	7	8	6	3	3	6	7	11939.0331	-0.0006
7	4	3	7	6	6	3	3	6	5	11939.0331	-0.0049

7	4	3	8	8	6	3	3	7	7	11939.1001	0.0011
7	4	3	6	6	6	3	3	5	5	11939.1525	-0.0014
7	4	3	8	9	6	3	3	7	8	11939.1694	0.0043
7	4	3	8	7	6	3	3	7	6	11939.1694	0.0006
7	4	3	6	7	6	3	3	5	6	11939.2214	0.0011
7	4	3	6	5	6	3	3	5	4	11939.2214	-0.0030
7	2	5	8	8	6	1	5	7	7	12179.5814	-0.0052
7	2	5	6	7	6	1	5	5	6	12179.8633	-0.0027
7	2	5	6	5	6	1	5	5	4	12179.9221	-0.0063
7	2	5	8	9	6	1	5	7	8	12179.9474	-0.0030
7	2	5	8	7	6	1	5	7	6	12180.0242	0.0029
7	2	5	7	7	6	1	5	6	6	12180.1889	-0.0005
7	2	5	7	8	6	1	5	6	7	12180.5607	-0.0010
7	2	5	7	6	6	1	5	6	5	12180.6311	0.0003
7	3	5	6	6	6	2	5	5	5	12269.6481	-0.0018
7	3	5	8	8	6	2	5	7	7	12269.7193	-0.0018
7	3	5	6	7	6	2	5	5	6	12270.0173	0.0001
7	3	5	8	9	6	2	5	7	8	12270.0749	-0.0020
7	3	5	6	5	6	2	5	5	4	12270.0749	-0.0008
7	3	5	7	7	6	2	5	6	6	12270.1575	-0.0008
7	3	5	8	7	6	2	5	7	6	12270.1438	-0.0038
7	3	5	7	8	6	2	5	6	7	12270.5284	0.0021
7	3	5	7	6	6	2	5	6	5	12270.5959	-0.0003
7	1	6	6	6	6	0	6	5	5	12306.1943	-0.0016
7	1	6	8	8	6	0	6	7	7	12306.3006	-0.0037
7	1	6	6	7	6	0	6	5	6	12306.7464	-0.0025
7	1	6	7	7	6	0	6	6	6	12306.8224	0.0021
7	1	6	8	9	6	0	6	7	8	12306.7984	0.0034
7	1	6	6	5	6	0	6	5	4	12306.7855	0.0019
7	1	6	8	7	6	0	6	7	6	12306.9449	0.0009
7	1	6	7	8	6	0	6	6	7	12307.4234	-0.0018
7	1	6	7	6	6	0	6	6	5	12307.5220	-0.0002
7	2	6	6	6	6	1	6	5	5	12311.8026	-0.0033
7	2	6	8	8	6	1	6	7	7	12311.9130	0.0007
7	2	6	6	7	6	1	6	5	6	12312.3573	0.0002
7	2	6	7	7	6	1	6	6	6	12312.4141	0.0006
7	2	6	8	9	6	1	6	7	8	12312.4043	0.0031
7	2	6	6	5	6	1	6	5	4	12312.3905	-0.0012
7	2	6	8	7	6	1	6	7	6	12312.5517	0.0020
7	2	6	7	8	6	1	6	6	7	12313.0160	0.0000
7	2	6	7	6	6	1	6	6	5	12313.1111	-0.0018
7	4	4	6	6	6	3	4	5	5	12339.3903	-0.0036
7	4	4	8	8	6	3	4	7	7	12339.4069	0.0036
7	4	4	7	7	6	3	4	6	6	12339.5567	-0.0018
7	4	4	6	7	6	3	4	5	6	12339.5908	0.0017
7	4	4	8	9	6	3	4	7	8	12339.6038	-0.0010
7	4	4	6	5	6	3	4	5	4	12339.6220	-0.0036
7	4	4	8	7	6	3	4	7	6	12339.6357	0.0028
7	4	4	7	8	6	3	4	6	7	12339.7514	-0.0001
7	4	4	7	6	6	3	4	6	5	12339.7799	-0.0017
7	5	2	7	7	6	4	2	6	6	12501.9715	0.0065
7	5	2	7	8	6	4	2	6	7	12501.9715	-0.0010
7	5	2	7	6	6	4	2	6	5	12501.9715	0.0005
7	5	2	8	8	6	4	2	7	7	12502.3165	-0.0007
7	5	2	8	7	6	4	2	7	6	12502.3347	-0.0002
7	5	2	8	9	6	4	2	7	8	12502.3590	-0.0008
7	5	2	6	6	6	4	2	5	5	12502.3945	0.0012
7	5	2	6	7	6	4	2	5	6	12502.4227	-0.0014
7	5	2	6	5	6	4	2	5	4	12502.4338	-0.0004
7	5	3	8	8	6	4	3	7	7	12648.4184	-0.0025
7	5	3	6	6	6	4	3	5	5	12648.4433	-0.0001
7	5	3	7	8	6	4	3	6	7	12648.4433	0.0007
7	5	3	7	7	6	4	3	5	6	12648.4998	0.0022
7	5	3	8	7	6	4	3	6	6	12648.4433	0.0026
7	5	3	7	6	6	4	3	6	5	12648.4564	0.0023
7	5	3	6	7	6	4	3	7	6	12648.4998	0.0021
7	5	3	8	9	6	4	3	7	8	12648.5395	0.0011
7	5	3	6	5	6	4	3	5	4	12648.5691	-0.0032
7	5	3	8	7	6	4	3	7	6	12648.5841	0.0012
7	5	3	6	7	6	4	3	5	6	12648.6006	0.0036
7	6	1	7	7	6	5	1	6	6	13126.6743	0.0011
7	6	1	7	6	6	5	1	6	5	13126.7391	0.0008
7	6	1	7	8	6	5	1	6	7	13126.7391	-0.0015
7	6	1	8	8	6	5	1	7	7	13126.8446	-0.0013
7	6	1	6	6	6	5	1	5	5	13126.8671	0.0004
7	6	1	8	7	6	5	1	7	6	13126.9055	-0.0047
7	6	1	8	9	6	5	1	7	8	13126.9170	0.0008
7	6	1	6	5	6	5	1	5	4	13126.9364	0.0019
7	6	1	6	7	6	5	1	5	6	13126.9364	-0.0012
7	6	2	7	7	6	5	2	6	6	13139.1358	-0.0008
7	6	2	7	6	6	5	2	6	5	13139.2127	0.0011
7	6	2	7	8	6	5	2	6	7	13139.2127	-0.0005
7	6	2	8	8	6	5	2	7	7	13139.2712	-0.0008
7	6	2	6	6	6	5	2	5	5	13139.2900	0.0036
7	6	2	8	7	6	5	2	7	6	13139.3457	-0.0003
7	6	2	8	9	6	5	2	7	8	13139.3457	-0.0040

7	6	2	6	5	6	5	2	5	4	13139.3663	0.0038
7	6	2	6	7	6	5	2	5	6	13139.3663	0.0012
8	4	4	9	9	7	3	4	8	8	13532.4104	-0.0004
8	4	4	7	7	7	3	4	6	6	13532.4104	-0.0084
8	4	4	9	10	7	3	4	8	9	13532.5197	0.0011
8	4	4	7	8	7	3	4	6	7	13532.5320	0.0069
8	4	4	9	8	7	3	4	8	7	13532.5320	0.0036
8	4	4	7	6	7	3	4	6	5	13532.5320	-0.0055
8	4	4	8	8	7	3	4	7	7	13532.5517	-0.0035
8	4	4	8	9	7	3	4	7	8	13532.6629	0.0027
8	4	4	8	7	7	3	4	7	6	13532.6757	0.0044
7	7	0	7	7	6	6	0	6	6	13676.7600	0.0009
7	7	0	7	6	6	6	0	6	5	13676.8217	0.0058
7	7	0	7	8	6	6	0	6	7	13676.8217	0.0004
7	7	0	6	6	6	6	0	5	5	13676.7776	0.0008
7	7	0	8	8	6	6	0	7	7	13676.8010	-0.0029
7	7	0	6	5	6	6	0	5	4	13676.8217	-0.0065
7	7	0	8	7	6	6	0	7	6	13676.8417	-0.0077
7	7	0	6	7	6	6	0	5	6	13676.8417	-0.0033
7	7	0	8	9	6	6	0	7	8	13676.8607	-0.0002
7	7	1	7	7	6	6	1	6	6	13677.0482	-0.0010
7	7	1	7	6	6	6	1	6	5	13677.1077	0.0020
7	7	1	7	8	6	6	1	6	7	13677.1147	0.0035
7	7	1	6	6	6	6	1	5	5	13677.0713	0.0050
7	7	1	8	8	6	6	1	7	7	13677.0938	0.0002
7	7	1	6	5	6	6	1	5	4	13677.1147	-0.0026
7	7	1	8	7	6	6	1	7	6	13677.1415	0.0028
7	7	1	6	7	6	6	1	5	6	13677.1415	0.0073
7	7	1	8	9	6	6	1	7	8	13677.1499	-0.0002
7	0	7	7	8	6	1	6	6	7	8920.3790	0.0024
7	0	7	6	7	6	1	6	5	6	8920.4366	0.0009
7	0	7	8	9	6	1	6	7	8	8920.4366	-0.0009
7	0	7	8	7	6	1	6	7	6	8920.4681	0.0012
7	0	7	8	8	6	1	6	7	7	8920.4922	0.0002
7	1	7	7	8	6	0	6	6	7	8920.9936	-0.0003
7	1	7	6	7	6	0	6	5	6	8921.0527	-0.0026
7	1	7	8	9	6	0	6	7	8	8921.0527	-0.0046
7	1	7	8	7	6	0	6	7	6	8921.0876	0.0013
7	1	7	8	8	6	0	6	7	7	8921.1121	0.0001
6	0	6	6	7	5	1	5	5	6	7682.9729	0.0001
6	0	6	6	5	5	1	5	5	4	7683.0015	0.0037
6	0	6	6	6	5	1	5	5	5	7683.0215	0.0000
6	0	6	5	6	5	1	5	4	5	7683.0449	-0.0036
6	0	6	7	8	5	1	5	6	7	7683.0449	-0.0048
6	0	6	7	6	5	1	5	6	5	7683.0886	0.0019
6	1	6	6	7	5	0	5	5	6	7685.6310	-0.0030
6	1	6	6	6	5	0	5	5	5	7685.6913	0.0026
6	1	6	5	6	5	0	5	4	5	7685.7208	0.0001
6	1	6	7	8	5	0	5	6	7	7685.7208	-0.0016
6	1	6	7	6	5	0	5	6	5	7685.7539	-0.0034
6	1	6	7	7	5	0	5	6	6	7685.7946	0.0001

Table S7: Experimental frequencies of $C_5F_5N\cdot{}^{15}NH_3$. Assignements, measured transition frequencies (ν/MHz), and observed-calculated residuals ($\Delta\nu$/MHz) from the fit.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν/MHz	$\Delta\nu$/MHz
4	2	2	5	3	1	2	4	6703.2074	0.0028
4	2	2	3	3	1	2	2	6703.2472	0.0097
4	2	2	4	3	1	2	3	6703.4788	0.0023
4	1	3	3	3	0	3	2	6825.0816	0.0028
4	1	3	5	3	0	3	4	6825.4000	0.0036
4	1	3	4	3	0	3	3	6826.4903	0.0033
4	2	3	3	3	1	3	2	6974.9189	0.0017
4	2	3	5	3	1	3	4	6975.1450	-0.0049
4	2	3	4	3	1	3	3	6975.8452	0.0018
4	3	1	4	3	2	1	3	6993.8045	0.0026
4	3	1	5	3	2	1	4	6994.2695	0.0031
4	3	1	3	3	2	1	2	6994.4869	0.0033
4	3	2	3	3	2	2	2	7169.9427	0.0009
4	3	2	5	3	2	2	4	7169.9634	0.0035
4	3	2	4	3	2	2	3	7170.0331	0.0033
4	4	0	4	3	3	0	3	7571.5892	0.0032
4	4	0	5	3	3	0	4	7571.8211	0.0011
4	4	0	3	3	3	0	2	7571.8407	0.0080
4	4	1	4	3	3	1	3	7590.1890	0.0053
4	4	1	3	3	3	1	2	7590.2654	0.0045
4	4	1	5	3	3	1	4	7590.2974	0.0029
5	1	4	4	4	0	4	3	8614.8845	-0.0021
5	1	4	6	4	0	4	5	8615.1015	-0.0019
5	1	4	5	4	0	4	4	8615.9918	-0.0079
5	2	4	4	4	1	4	3	8675.3569	-0.0056
5	2	4	6	4	1	4	5	8675.5498	0.0051
5	2	4	5	4	1	4	4	8676.2594	0.0003
5	2	3	4	4	1	3	3	8402.2548	0.0001
5	2	3	6	4	1	3	5	8402.3431	0.0026
5	2	3	5	4	1	3	4	8402.9454	0.0019
5	3	3	4	4	2	3	3	8755.0312	0.0005
5	3	3	6	4	2	3	5	8755.0724	-0.0025
5	3	3	5	4	2	3	4	8755.3188	-0.0017
5	3	2	5	4	2	2	4	8456.2193	0.0032
5	3	2	6	4	2	2	5	8456.3631	0.0007
5	3	2	4	4	2	2	3	8456.4718	0.0058
5	4	1	5	4	3	1	4	8966.7885	0.0000
5	4	1	6	4	3	1	5	8967.2282	0.0011
5	4	1	4	4	3	1	3	8967.3472	-0.0005
5	4	2	5	4	3	2	4	9064.8709	-0.0026
5	4	2	6	4	3	2	5	9064.9765	-0.0003
5	4	2	4	4	3	2	3	9064.9984	-0.0031
5	5	0	5	4	4	0	4	9539.4059	0.0019
5	5	0	4	4	4	0	3	9539.5135	-0.0064
5	5	0	6	4	4	0	5	9539.5348	0.0014
5	5	1	5	4	4	1	4	9544.3955	0.0005
5	5	1	4	4	4	1	3	9544.4767	0.0015
5	5	1	6	4	4	1	5	9544.4960	-0.0001
6	3	3	7	5	2	3	6	10032.9514	-0.0022
6	3	3	5	5	2	3	4	10032.9687	0.0000
6	3	3	6	5	2	3	5	10033.1311	-0.0009
6	4	2	6	5	3	2	5	10343.5262	-0.0007
6	4	2	7	5	3	2	6	10343.9104	-0.0032
6	4	2	5	5	3	2	4	10344.0237	0.0018
6	3	4	5	5	2	4	4	10402.7609	0.0007
6	3	4	7	5	2	4	6	10402.8119	-0.0099
6	3	4	6	5	2	4	5	10403.1938	0.0002
6	4	3	7	5	3	3	6	10586.6537	-0.0054
6	4	3	6	5	3	3	5	10586.6716	-0.0030
6	5	1	6	5	4	1	5	10957.9424	-0.0025
6	5	1	7	5	4	1	6	10958.2189	-0.0059
6	5	1	5	5	4	1	4	10958.2764	-0.0008
6	5	2	6	5	4	2	5	10995.3902	-0.0013
6	5	2	7	5	4	2	6	10995.5374	-0.0022
6	5	2	5	5	4	2	4	10995.5606	-0.0028
6	6	0	6	5	5	0	5	11502.0628	0.0018
6	6	0	5	5	5	0	4	11502.1288	-0.0015
6	6	0	7	5	5	0	6	11502.1468	0.0004
6	6	1	6	5	5	1	5	11503.2443	-0.0011
6	6	1	5	5	5	1	4	11503.3113	0.0034
6	6	1	7	5	5	1	6	11503.3233	-0.0017

Table S8: Experimental substitution (r_s) and theoretical equilibrium (r_e, B3LYP-GD3(BJ)/def2-TZVP) coordinates in the principal axis coordinates of ammonia N atom (Å).

$C_5F_5N{\cdot}NH_3$	*a*	*b*	*c*
r_s	[0][a]	±0.803(2)[b]	±2.7738(6)
r_e	[0]	0.729	-2.759
$C_6F_6{\cdot}NH_3$			
r_s	[0]	[0]	±2.9716(5)
r_e	[0]	[0]	2.931

[a] Zero by symmetry. [b] Error in parentheses in units of the last digit.

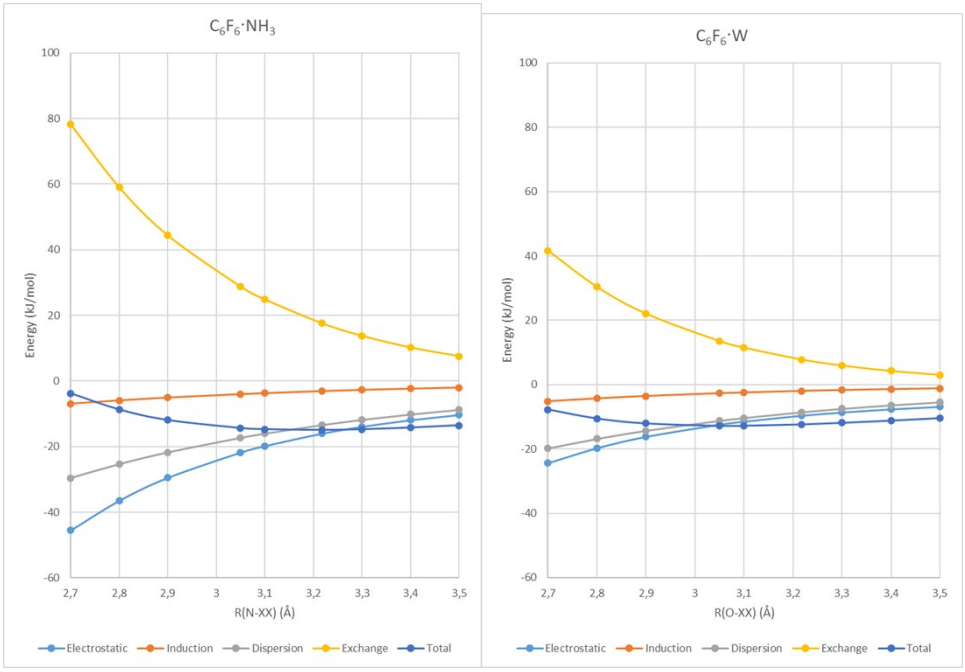


Figure S1. SAPT2+3(CCD)/aug-cc-pVDZ analysis for the complexes of water and ammonia formed with C_6F_6 as a function of the distance of N or O form the center of the ring.