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

Electronic Supplementary Information

Electronic and Structural Features of octa-coordinated Yttrium-ammonia complexes: The first Neutral Solvated Electron Precursor with Eight Ligands and Three Outer Electrons

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Table S1. Cartesian coordinates (Å) for the $Y(NH_3)_{n=1-8}^{0,+}$ and $Y(NH_3)_8^-$ species optimized at MP2/cc-pVTZ-PP (Y) cc-pVTZ (N) aug-cc-pVTZ (H).

$Y(NH_3)$				**$Y(NH_3)^+$**			
Y	0.00000	0.00000	-0.40264	Y	-0.50313	0.00000	0.00001
N	0.00000	0.00000	2.03605	N	1.84412	-0.00006	0.00005
H	0.94926	0.00000	2.40711	H	2.23703	0.47185	-0.81633
H	-0.47463	0.82208	2.40711	H	2.23807	0.47132	0.81621
H	-0.47463	-0.82208	2.40711	H	2.23804	-0.94265	-0.00051

$Y(NH_3)_2$				**$Y(NH_3)_2^+$**			
Y	0.00000	0.00000	0.00000	Y	0.00000	0.00000	0.00000
N	0.00000	2.43784	0.00000	N	0.00000	2.40378	0.00000
H	-0.94808	2.81061	0.00000	H	-0.93853	2.80329	0.00000
H	0.47809	2.79689	-0.82453	H	0.47174	2.79784	-0.81416
N	0.00000	-2.43784	0.00000	N	0.00000	-2.40378	0.00000
H	-0.47809	-2.79689	-0.82453	H	-0.47174	-2.79784	-0.81416
H	0.94808	-2.81061	0.00000	H	0.93853	-2.80329	0.00000
H	-0.47809	-2.79689	0.82453	H	-0.47174	-2.79784	0.81416
H	0.47809	2.79689	0.82453	H	0.47174	2.79784	0.81416

$Y(NH_3)_3$				**$Y(NH_3)_3^+$**			
Y	0.23469	-0.00019	-0.02930	Y	0.22884	-0.00005	-0.00287
N	2.64190	-0.00011	0.04728	N	2.62076	0.00005	0.00333
H	3.02100	0.83477	-0.40078	H	3.01927	0.82322	-0.44790
H	2.95149	-0.01774	1.01954	H	2.98921	-0.01731	0.95496
N	-1.75727	1.50792	0.02857	N	-1.72262	1.47545	0.00215
H	-2.37391	1.46725	-0.78206	H	-2.32713	1.36240	-0.81265
H	-2.32296	1.46058	0.87497	H	-2.31242	1.36359	0.82793
N	-1.75898	-1.50680	0.02830	N	-1.72293	-1.47520	0.00205
H	-1.31450	-2.42132	0.01386	H	-1.44927	-2.45490	-0.00352
H	-2.32024	-1.46324	0.87783	H	-2.31031	-1.36493	0.82979
H	-2.37994	-1.46439	-0.77890	H	-2.32983	-1.36064	-0.81073
H	-1.31400	2.42306	0.01947	H	-1.44898	2.45516	-0.00081
H	3.02044	-0.81876	-0.43041	H	3.01842	-0.80655	-0.47769

$Y(NH_3)_4$				$Y(NH_3)_4^+$			
Y	0.37526	-0.00026	0.03044	Y	0.39286	0.00005	-0.00012
N	-1.57918	-0.01803	1.75053	N	-1.40087	0.94757	1.45780
H	-2.15097	0.80418	1.93047	H	-2.39023	0.80926	1.24427
H	-2.14326	-0.84784	1.91928	H	-1.26475	0.60171	2.40646
N	2.75942	-0.00041	0.06483	N	2.77174	-0.00002	-0.00001
H	3.14804	0.00887	-0.88141	H	3.15294	-0.53292	-0.78264
H	3.10284	0.82205	0.56891	H	3.15244	0.94441	-0.07032
N	-1.30898	1.60550	-0.96517	N	-1.40140	0.78853	-1.54932
H	-1.22537	1.64195	-1.97755	H	-1.26494	0.34687	-2.45727
H	-2.29727	1.63692	-0.71478	H	-2.39069	0.67213	-1.32274
N	-1.30807	-1.58610	-0.99669	N	-1.40090	-1.73636	0.09199
H	-0.87417	-2.44252	-0.65532	H	-1.26402	-2.30141	0.92868
H	-2.29770	-1.61837	-0.75177	H	-2.39035	-1.48260	0.07938
H	-0.85260	-0.01952	2.46685	H	-1.26429	1.95479	1.52801
H	3.10284	-0.83254	0.55280	H	3.15290	-0.41115	0.85292
H	-0.87054	2.45397	-0.60997	H	-1.26564	1.78329	-1.72289
H	-1.21950	-1.60389	-2.00916	H	-1.26476	-2.38430	-0.68244

$Y(NH_3)_5$				$Y(NH_3)_5^+$			
Y	0.00019	-0.03271	-0.51196	Y	0.01749	-0.00894	0.00870
N	0.00070	-0.17620	1.95365	N	-2.31607	0.31091	0.75399
H	0.81404	0.25849	2.38453	H	-3.04442	0.40463	0.04137
H	-0.81445	0.25498	2.38464	H	-2.58894	-0.46568	1.35395
N	-1.61526	1.77307	0.02875	N	-1.13998	-2.10673	-0.59222
H	-1.45177	2.41439	-0.75078	H	-0.60038	-2.56749	-1.32329
H	-2.57873	1.46089	-0.08551	H	-1.26140	-2.78348	0.16515
N	-1.84608	-1.63747	-0.05434	N	1.77189	-1.73528	0.20434
H	-2.41866	-1.50238	-0.89035	H	2.46825	-1.65719	-0.53897
H	-1.51886	-2.60235	-0.10985	H	2.25096	-1.58173	1.09287
N	1.85473	-1.62805	-0.05499	N	2.14376	1.23012	0.18968
H	2.42767	-1.48924	-0.89011	H	2.54626	1.32740	-0.74737
H	2.48123	-1.56228	0.75548	H	2.03565	2.17188	0.56113
N	1.60532	1.78216	0.02933	N	-0.53534	2.32579	-0.58084
H	1.43872	2.42196	-0.75080	H	0.12539	2.68014	-1.27031
H	1.55844	2.33768	0.89173	H	-1.44326	2.39480	-1.03716
H	-2.47383	-1.57346	0.75528	H	1.49018	-2.71241	0.21953
H	-1.57261	2.32837	0.89155	H	-2.06041	-1.96149	-1.00249
H	0.00282	-1.14715	2.25982	H	-2.38214	1.13194	1.35304
H	2.57072	1.47562	-0.08376	H	-0.54633	2.99275	0.19543
H	1.53194	-2.59433	-0.11217	H	2.85862	0.80106	0.77329

$Y(NH_3)_6$				$Y(NH_3)_6^+$			
Y	0.00000	0.00000	0.01721	Y	0.00000	-0.00005	0.00007
N	-2.44428	0.00000	-0.07605	N	1.80149	0.73663	1.55833
N	0.00000	1.47021	-1.92756	H	1.70797	0.26243	2.45647
N	0.00000	1.45045	1.97047	H	2.77392	0.59580	1.26056
N	0.00000	-1.45045	1.97047	N	-1.80154	0.98164	-1.41696
N	0.00000	-1.47021	-1.92756	H	-1.70747	0.66147	-2.38074
N	2.44428	0.00000	-0.07605	H	-2.77418	0.79425	-1.14692
H	-2.82091	0.00000	-1.02701	N	-1.80148	0.73641	1.55845
H	2.82091	0.00000	-1.02701	H	-2.77391	0.59596	1.26051
H	-2.83969	-0.81830	0.39585	H	-1.70813	0.26159	2.45630
H	-2.83969	0.81830	0.39585	N	-1.80142	-1.71790	-0.14172
H	2.83969	0.81830	0.39585	H	-1.70835	-2.25944	-1.00098
H	2.83969	-0.81830	0.39585	H	-1.70794	-2.39186	0.61810
H	0.00000	2.47540	-1.74498	N	1.80154	0.98142	-1.41711
H	0.00000	-2.47540	-1.74498	H	1.70754	1.99626	-1.45584
H	0.81892	1.29219	-2.53379	H	2.77418	0.79433	-1.14686
H	-0.81892	1.29219	-2.53379	N	1.80140	-1.71793	-0.14147
H	-0.81892	-1.29219	-2.53379	H	2.77384	-1.38962	-0.11484
H	0.81892	-1.29219	-2.53379	H	1.70810	-2.39140	0.61882
H	0.00000	2.45818	1.80326	H	-2.77385	-1.38961	-0.11467
H	0.00000	-2.45818	1.80326	H	-1.70768	1.99652	-1.45509
H	-0.82290	1.26169	2.57047	H	-1.70826	1.73108	1.76381
H	0.82290	-1.26169	2.57047	H	1.70845	1.73147	1.76303
H	0.82290	1.26169	2.57047	H	1.70816	-2.26003	-1.00035
H	-0.82290	-1.26169	2.57047	H	1.70762	0.66068	-2.38071

	$Y(NH_3)_7$				$Y(NH_3)_7^+$		
H	-1.70378	-1.75681	-1.83011	H	-1.91981	-1.36276	-2.01631
N	-2.02951	-0.98486	-1.24965	N	-1.98223	-0.49986	-1.47955
H	1.36787	2.45861	-1.35792	H	1.36112	2.58602	-0.88600
H	-2.45067	-0.33164	-1.90727	H	-1.95711	0.23605	-2.18611
H	-2.77099	-1.36200	-0.65657	H	-2.92633	-0.48818	-1.07084
H	1.69434	-1.77197	-1.82449	H	1.91991	-1.36286	-2.01619
H	2.45286	-0.35294	-1.90111	H	1.95708	0.23593	-2.18615
N	1.49576	2.02228	-0.44670	N	1.52243	2.04705	-0.03161
N	2.02453	-1.00196	-1.24398	N	1.98226	-0.49990	-1.47952
H	-1.34601	2.47324	-1.35451	H	-1.36109	2.58607	-0.88595
H	1.26591	2.72336	0.26267	H	1.32954	2.67028	0.75450
H	2.49515	1.85300	-0.34872	H	2.52618	1.85382	-0.00031
H	2.76124	-1.38435	-0.64832	H	2.92636	-0.48811	-1.07080
Y	0.00024	0.01753	-0.20582	Y	0.00000	0.07629	-0.01298
N	-1.47809	2.03491	-0.44484	N	-1.52241	2.04707	-0.03158
H	-0.01038	-3.03166	-0.32118	H	0.00005	-2.75502	-1.04432
H	-2.47897	1.87377	-0.34804	H	-2.52616	1.85382	-0.00031
N	-0.01005	-2.39130	0.48335	N	-0.00005	-2.45243	-0.06939
H	-1.24289	2.73186	0.26695	H	-1.32954	2.67027	0.75456
H	-0.82779	-2.66882	1.03949	H	-0.81261	-2.89244	0.35835
H	-2.49939	0.13047	1.64719	H	-2.84109	-0.60487	1.20840
H	0.80311	-2.67441	1.04338	H	0.81240	-2.89250	0.35853
N	-1.49155	0.12894	1.80826	N	-1.88797	-0.48424	1.57650
H	-1.28571	1.00960	2.29853	H	-1.91891	0.31529	2.21003
N	1.48805	0.12125	1.81129	N	1.88796	-0.48426	1.57652
H	2.49629	0.11706	1.65276	H	2.84108	-0.60486	1.20842
H	1.28585	1.00367	2.30000	H	1.91887	0.31528	2.21004
H	-1.32992	-0.61128	2.49341	H	-1.71748	-1.28035	2.18848
H	1.32060	-0.61726	2.49689	H	1.71748	-1.28037	2.18849

$Y(NH_3)_8$				$Y(NH_3)_8^+$				$Y(NH_3)_8^-$		
Y	0.00001	-0.00004	-0.00020	Y	0.00000	0.00000	0.00000	Y	-0.00001	0.00000	-0.00002
H	1.57827	-2.36796	1.13737	H	1.80200	-2.20027	1.21105	H	-2.36857	-1.61357	1.10033
N	0.66128	-1.98022	1.37892	N	0.81686	-1.95447	1.34658	N	-1.98861	-0.69587	1.35714
H	-0.02351	-2.76249	-1.33626	H	-0.27689	-2.82946	-1.21358	H	-2.78114	0.07810	-1.27977
H	0.00438	-2.76237	1.33636	H	0.29763	-2.82736	1.21354	H	-2.78179	-0.05250	1.27971
H	0.72784	-1.72426	2.36743	H	0.72456	-1.72921	2.34226	H	-1.78972	-0.76044	2.35991
H	2.45515	-1.55298	-1.00932	H	2.21354	-1.78572	-1.21093	H	-1.63494	-2.35192	-1.10167
H	1.84438	-0.81016	-2.33266	H	1.73482	-0.71180	-2.34230	H	-0.77593	-1.78191	-2.36144
N	-0.67520	-1.97592	-1.37838	N	-0.80251	-1.96040	-1.34660	N	-1.98210	0.71418	-1.35717
N	2.01820	-0.67818	-1.33096	N	1.96051	-0.80243	-1.34657	N	-0.71353	-1.98106	-1.35860
H	-2.46566	-1.53669	1.00953	H	-2.20036	-1.80191	1.21096	H	-1.61324	2.36684	1.10180
H	-1.59451	-2.35739	-1.13528	H	-1.78582	-2.21342	-1.21104	H	-2.35362	1.63529	-1.10022
H	-0.74151	-1.72046	-2.36706	H	-0.71189	-1.73445	-2.34228	H	-1.78267	0.77705	-2.35993
H	2.77048	0.01953	-1.28075	H	2.82945	-0.27670	-1.21323	H	-0.07807	-2.78058	-1.28071
N	-2.02293	-0.66455	1.33029	N	-1.95457	-0.81679	1.34658	N	-0.69524	1.98752	1.35861
H	2.77268	-0.03751	1.27732	H	2.82736	0.29744	1.21323	H	0.05246	-2.78130	1.28049
H	-1.84989	-0.79699	2.33203	H	-1.72952	-0.72449	2.34230	H	-0.75936	1.78892	2.36145
N	2.02443	0.66431	1.32846	N	1.95459	0.81678	1.34656	N	0.69521	-1.98763	1.35846
H	-2.77099	0.03758	1.28009	H	-2.82734	-0.29745	1.21325	H	-0.05247	2.78117	1.28068
H	1.85184	0.79609	2.33037	H	1.72954	0.72449	2.34228	H	0.75928	-1.78906	2.36132
H	-0.72665	1.72428	2.36801	H	-0.72454	1.72920	2.34228	H	1.78971	0.76035	2.35997
H	2.46669	1.53680	1.00802	H	2.20039	1.80190	1.21093	H	1.61323	-2.36693	1.10169
N	-0.65979	1.98007	1.37953	N	-0.81684	1.95447	1.34660	N	1.98860	0.69574	1.35720
H	-1.57647	2.36847	1.13796	H	-1.80198	2.20027	1.21107	H	2.36861	1.61342	1.10036
N	0.67359	1.97626	-1.37847	N	0.80249	1.96040	-1.34660	N	1.98214	-0.71405	-1.35717
H	0.73989	1.72108	-2.36717	H	0.71187	1.73446	-2.34228	H	1.78273	-0.77694	-2.35994
H	0.02131	2.76223	-1.33593	H	0.27686	2.82946	-1.21358	H	2.78114	-0.07792	-1.27977
H	-0.00228	2.76162	1.33690	H	-0.29761	2.82736	1.21356	H	2.78174	0.05234	1.27978
H	1.59267	2.35826	-1.13549	H	1.78580	2.21343	-1.21105	H	2.35371	-1.63513	-1.10021
N	-2.01963	0.67832	-1.32898	N	-1.96053	0.80244	-1.34654	N	0.71354	1.98116	-1.35843
H	-2.77218	-0.01896	-1.27791	H	-2.82947	0.27670	-1.21321	H	0.07811	2.78070	-1.28050
H	-1.84603	0.80945	-2.33083	H	-1.73484	0.71181	-2.34227	H	0.77588	1.78204	-2.36129
H	-2.45603	1.55354	-1.00786	H	-2.21356	1.78572	-1.21090	H	1.63499	2.35198	-1.10156

Table S2. Cartesian coordinates (Å) for the $Y(NH_3)_{6,7,8}^{0,+}$ and $Y(NH_3)_8^-$ species optimized at B3LYP/cc-pVTZ-PP (Y), cc-pVTZ (N) and aug-cc-pVTZ (H).

$Y(NH_3)_6$				$Y(NH_3)_6^+$			
Y	0.00000	-0.00038	0.03885	Y	0.00000	-0.00006	0.00001
N	-1.63538	1.62986	-0.93354	N	-1.78560	-1.78169	0.04911
H	-1.48167	1.84565	-1.92114	H	-1.69056	-2.36570	0.88032
H	-2.63087	1.40286	-0.83251	H	-2.76056	-1.45394	0.03795
N	1.85442	0.00365	1.77544	N	1.78671	0.84805	-1.56692
H	1.76239	-0.81786	2.37000	H	1.69124	1.85324	-1.71333
H	2.81436	0.00354	1.41372	H	2.76147	0.69120	-1.27825
N	1.63542	1.62977	-0.93362	N	1.78560	-1.78168	0.04936
H	2.63090	1.40274	-0.83260	H	2.76055	-1.45395	0.03804
H	1.48170	1.84553	-1.92123	H	1.69059	-2.36540	0.88080
N	1.63646	-1.63281	-0.92808	N	1.78631	0.93366	1.51747
H	1.47217	-2.49712	-0.39991	H	1.69105	1.94548	1.60778
H	1.48324	-1.85246	-1.91487	H	1.68967	0.56041	2.46204
N	-1.85442	0.00357	1.77544	N	-1.78672	0.84828	-1.56678
H	-1.76166	0.82676	2.36754	H	-1.69083	0.42326	-2.48933
H	-2.81436	0.00355	1.41372	H	-2.76148	0.69133	-1.27816
N	-1.63650	-1.63272	-0.92816	N	-1.78629	0.93345	1.51762
H	-2.63181	-1.40474	-0.82762	H	-2.76109	0.76031	1.23861
H	-1.48328	-1.85233	-1.91496	H	-1.68966	0.55990	2.46208
H	2.63178	-1.40487	-0.82753	H	2.76110	0.76042	1.23852
H	1.76170	0.82694	2.36742	H	1.69081	0.42277	-2.48935
H	1.47104	2.49616	-0.40885	H	1.68816	-2.41333	-0.74588
H	-1.47095	2.49622	-0.40873	H	-1.68821	-2.41305	-0.74637
H	-1.47226	-2.49706	-0.40002	H	-1.69102	1.94524	1.60824
H	-1.76243	-0.81803	2.36988	H	-1.69127	1.85351	-1.71291

	$Y(NH_3)_7$				$Y(NH_3)_7^+$		
H	-1.78760	-1.54920	-2.06386	H	-1.85367	-1.41108	-2.04916
N	-1.94106	-0.66447	-1.57974	N	-1.95103	-0.52778	-1.54992
H	1.41430	2.51372	-1.05689	H	1.39057	2.63666	-0.89498
H	-2.00825	0.04528	-2.30933	H	-1.98303	0.18247	-2.28186
H	-2.85943	-0.73364	-1.12829	H	-2.88866	-0.54554	-1.12153
H	1.78517	-1.55393	-2.06263	H	1.85367	-1.41115	-2.04912
H	2.00834	0.04007	-2.30906	H	1.98302	0.18240	-2.28187
N	1.56244	2.07537	-0.14505	N	1.54163	2.08368	-0.04785
N	1.93998	-0.66914	-1.57905	N	1.95102	-0.52784	-1.54991
H	-1.40863	2.51740	-1.05606	H	-1.39051	2.63670	-0.89497
H	1.36464	2.78285	0.56583	H	1.36390	2.70783	0.74187
H	2.56210	1.86698	-0.07274	H	2.54375	1.87335	-0.02144
H	2.85823	-0.73945	-1.12750	H	2.88866	-0.54558	-1.12152
Y	0.00010	0.06497	-0.10294	Y	0.00000	0.07753	-0.01808
N	-1.55783	2.07880	-0.14451	N	-1.54158	2.08372	-0.04784
H	-0.00190	-2.99465	-0.74283	H	-0.00001	-2.84869	-0.98823
H	-2.55794	1.87252	-0.07246	H	-2.54371	1.87341	-0.02143
N	-0.00365	-2.47424	0.13844	N	-0.00005	-2.50446	-0.02512
H	-1.35861	2.78542	0.56683	H	-1.36384	2.70786	0.74188
H	-0.81802	-2.81486	0.66235	H	-0.81246	-2.93123	0.42043
H	-2.57489	-0.36157	1.59664	H	-2.81506	-0.54894	1.26278
H	0.80690	-2.81703	0.66690	H	0.81230	-2.93127	0.42051
N	-1.58053	-0.29330	1.83970	N	-1.86313	-0.45647	1.64731
H	-1.50282	0.48284	2.50605	H	-1.90151	0.31023	2.32023
N	1.58031	-0.29658	1.83937	N	1.86312	-0.45651	1.64731
H	2.57456	-0.36616	1.59623	H	2.81505	-0.54898	1.26278
H	1.50377	0.47943	2.50601	H	1.90150	0.31018	2.32024
H	-1.36914	-1.14093	2.38308	H	-1.70559	-1.29119	2.21124
H	1.36775	-1.14410	2.38247	H	1.70558	-1.29124	2.21123

$Y(NH_3)_8$				$Y(NH_3)_8^+$				$Y(NH_3)_8^-$			
Y	0.00000	0.00001	0.00002	Y	0.00000	0.00000	-0.00003	Y	-0.00001	0.00000	-0.00002
H	1.74801	-2.28024	1.16903	H	-1.95621	-2.13248	-1.21289	H	-2.36857	-1.61357	1.10033
N	0.78645	-1.99817	1.38472	N	-0.95902	-1.95131	-1.36150	N	-1.98861	-0.69587	1.35714
H	-0.21341	-2.84090	-1.29249	H	0.12264	-2.89070	1.21428	H	-2.78114	0.07810	-1.27977
H	0.21507	-2.84102	1.29191	H	-0.49264	-2.85118	-1.21309	H	-2.78179	-0.05250	1.27971
H	0.78484	-1.76480	2.38124	H	-0.86050	-1.75053	-2.35976	H	-1.78972	-0.76044	2.35991
H	2.36447	-1.70020	-1.12945	H	-2.36612	-1.66644	1.21171	H	-1.63494	-2.35192	-1.10167
H	1.84350	-0.77503	-2.37764	H	-1.84608	-0.63058	2.35982	H	-0.77593	-1.78191	-2.36144
N	-0.78540	-1.99842	-1.38490	N	0.70102	-2.05819	1.36155	N	-1.98210	0.71418	-1.35717
N	2.01897	-0.76176	-1.36751	N	-2.05820	-0.70100	1.36155	N	-0.71353	-1.98106	-1.35860
H	-2.36330	-1.70151	1.12959	H	2.13248	-1.95619	-1.21288	H	-1.61324	2.36684	1.10180
H	-1.74669	-2.28124	-1.16890	H	1.66646	-2.36611	1.21173	H	-2.35362	1.63529	-1.10022
H	-0.78435	-1.76486	-2.38137	H	0.63057	-1.84605	2.35981	H	-1.78267	0.77705	-2.35993
H	2.83291	-0.14777	-1.23848	H	-2.89069	-0.12262	1.21428	H	-0.07807	-2.78058	-1.28071
N	-2.01837	-0.76285	1.36773	N	1.95130	-0.95901	-1.36152	N	-0.69524	1.98752	1.35861
H	2.83254	0.14940	1.23917	H	-2.85118	0.49262	-1.21308	H	0.05246	-2.78130	1.28049
H	-1.84283	-0.77611	2.37785	H	1.75054	-0.86053	-2.35978	H	-0.75936	1.78892	2.36145
N	2.01821	0.76291	1.36796	N	-1.95132	0.95900	-1.36150	N	0.69521	-1.98763	1.35846
H	-2.83272	-0.14939	1.23881	H	2.85117	-0.49262	-1.21311	H	-0.05247	2.78117	1.28068
H	1.84258	0.77630	2.37806	H	-1.75056	0.86052	-2.35976	H	0.75928	-1.78906	2.36132
H	-0.78511	1.76483	2.38110	H	0.86048	1.75053	-2.35977	H	1.78971	0.76035	2.35997
H	2.36318	1.70151	1.12973	H	-2.13250	1.95619	-1.21286	H	1.61323	-2.36693	1.10169
N	-0.78668	1.99819	1.38458	N	0.95900	1.95131	-1.36152	N	1.98860	0.69574	1.35720
H	-1.74827	2.28013	1.16885	H	1.95619	2.13248	-1.21292	H	2.36861	1.61342	1.10036
N	0.78564	1.99836	-1.38487	N	-0.70100	2.05820	1.36155	N	1.98214	-0.71405	-1.35717
H	0.78463	1.76476	-2.38134	H	-0.63055	1.84605	2.35981	H	1.78273	-0.77694	-2.35994
H	0.21377	2.84093	-1.29253	H	-0.12262	2.89070	1.21428	H	2.78114	-0.07792	-1.27977
H	-0.21541	2.84112	1.29180	H	0.49262	2.85118	-1.21311	H	2.78174	0.05234	1.27978
H	1.74696	2.28105	-1.16883	H	-1.66644	2.36612	1.21174	H	2.35371	-1.63513	-1.10021
N	-2.01882	0.76172	-1.36778	N	2.05821	0.70101	1.36153	N	0.71354	1.98116	-1.35843
H	-2.83271	0.14765	-1.23889	H	2.89070	0.12262	1.21424	H	0.07811	2.78070	-1.28050
H	-1.84326	0.77515	-2.37788	H	1.84611	0.63058	2.35980	H	0.77588	1.78204	-2.36129
H	-2.36441	1.70010	-1.12960	H	2.36613	1.66645	1.21168	H	1.63499	2.35198	-1.10156

Table S3. Cartesian coordinates (Å) for the $Y(NH_3)_8^{0,\pm}$ species optimized at MP2/cc-pVTZ-PP (Y), cc-pVTZ (N) and aug-cc-pVTZ (H) under D_{4d} symmetry constraints.

$Y(NH_3)_8$ / Doublet				$Y(NH_3)_8^+$ / Singlet				$Y(NH_3)_8^-$ / Quintet			
Y	0.00000	0.00000	0.00000	Y	0.00000	0.00000	0.00000	Y	0.00000	0.00000	0.00000
N	0.00000	2.10066	1.36526	N	0.00000	2.11855	1.34693	N	0.00000	2.08656	1.39148
N	-2.10066	0.00000	1.36526	N	-2.11855	0.00000	1.34693	N	-2.08656	0.00000	1.39148
N	0.00000	-2.10066	1.36526	N	0.00000	-2.11855	1.34693	N	0.00000	-2.08656	1.39148
N	-1.48539	1.48539	-1.36526	N	-1.49804	1.49804	-1.34693	N	-1.47542	1.47542	-1.39148
N	1.48539	-1.48539	-1.36526	N	1.49804	-1.49804	-1.34693	N	1.47542	-1.47542	-1.39148
N	1.48539	1.48539	-1.36526	N	1.49804	1.49804	-1.34693	N	1.47542	1.47542	-1.39148
N	2.10066	0.00000	1.36526	N	2.11855	0.00000	1.34693	N	2.08656	0.00000	1.39148
N	-1.48539	-1.48539	-1.36526	N	-1.49804	-1.49804	-1.34693	N	-1.47542	-1.47542	-1.39148
H	-0.81406	2.70355	1.20927	H	-0.81495	2.72434	1.21239	H	-0.81094	2.69415	1.25390
H	0.00000	1.89737	2.37018	H	0.00000	1.87524	2.34262	H	0.00000	1.86647	2.39218
H	0.81406	2.70355	1.20927	H	0.81495	2.72434	1.21239	H	0.81094	2.69415	1.25390
H	-2.70355	-0.81406	1.20927	H	-2.72434	-0.81495	1.21239	H	-2.69415	-0.81094	1.25390
H	-1.89737	0.00000	2.37018	H	-1.87524	0.00000	2.34262	H	-1.86647	0.00000	2.39218
H	-2.70355	0.81406	1.20927	H	-2.72434	0.81495	1.21239	H	-2.69415	0.81094	1.25390
H	0.81406	-2.70355	1.20927	H	0.81495	-2.72434	1.21239	H	0.81094	-2.69415	1.25390
H	0.00000	-1.89737	2.37018	H	0.00000	-1.87524	2.34262	H	0.00000	-1.86647	2.39218
H	-0.81406	-2.70355	1.20927	H	-0.81495	-2.72434	1.21239	H	-0.81094	-2.69415	1.25390
H	2.70355	0.81406	1.20927	H	2.72434	0.81495	1.21239	H	2.69415	0.81094	1.25390
H	1.89737	0.00000	2.37018	H	1.87524	0.00000	2.34262	H	1.86647	0.00000	2.39218
H	2.70355	-0.81406	1.20927	H	2.72434	-0.81495	1.21239	H	2.69415	-0.81094	1.25390
H	-1.33607	2.48732	-1.20927	H	-1.35014	2.50266	-1.21239	H	-1.33163	2.47847	-1.25390
H	-1.34164	1.34164	-2.37018	H	-1.32600	1.32600	-2.34262	H	-1.31979	1.31979	-2.39218
H	-2.48732	1.33607	-1.20927	H	-2.50266	1.35014	-1.21239	H	-2.47847	1.33163	-1.25390
H	1.33607	-2.48732	-1.20927	H	1.35014	-2.50266	-1.21239	H	1.33163	-2.47847	-1.25390
H	1.34164	-1.34164	-2.37018	H	1.32600	-1.32600	-2.34262	H	1.31979	-1.31979	-2.39218
H	2.48732	-1.33607	-1.20927	H	2.50266	-1.35014	-1.21239	H	2.47847	-1.33163	-1.25390
H	2.48732	1.33607	-1.20927	H	2.50266	1.35014	-1.21239	H	2.47847	1.33163	-1.25390
H	1.34164	1.34164	-2.37018	H	1.32600	1.32600	-2.34262	H	1.31979	1.31979	-2.39218
H	1.33607	2.48732	-1.20927	H	1.35014	2.50266	-1.21239	H	1.33163	2.47847	-1.25390
H	-2.48732	-1.33607	-1.20927	H	-2.50266	-1.35014	-1.21239	H	-2.47847	-1.33163	-1.25390
H	-1.34164	-1.34164	-2.37018	H	-1.32600	-1.32600	-2.34262	H	-1.31979	-1.31979	-2.39218
H	-1.33607	-2.48732	-1.20927	H	-1.35014	-2.50266	-1.21239	H	-1.33163	-2.47847	-1.25390

Table S4. Cartesian coordinates (Å) for the $Y(NH_3)_8^-$ species optimized at MP2/cc-pVTZ-PP (Y), cc-pVTZ (N) and aug-cc-pVTZ (H).

$Y(NH_3)_8^-$ / Singlet				$Y(NH_3)_8^-$ / Triplet				$Y(NH_3)_8^-$ / Quintet			
Y	0.00000	-0.00329	0.00000	Y	-0.00001	0.00000	-0.00002	Y	0.00000	0.00000	0.00000
H	1.93450	-2.16925	0.98912	H	-2.36857	-1.61357	1.10033	N	0.00000	2.08656	1.39148
N	0.98449	-1.91385	1.28306	N	-1.98861	-0.69587	1.35714	N	-2.08656	0.00000	1.39148
H	-0.45867	-2.79114	-1.31440	H	-2.78114	0.07810	-1.27977	N	0.00000	-2.08656	1.39148
H	0.46007	-2.79098	1.31426	H	-2.78179	-0.05250	1.27971	N	-1.47542	1.47542	-1.39148
H	1.09816	-1.62061	2.26253	H	-1.78972	-0.76044	2.35991	N	1.47542	-1.47542	-1.39148
H	2.11662	-1.67420	-1.42830	H	-1.63494	-2.35192	-1.10167	N	1.47542	1.47542	-1.39148
H	1.40177	-0.78941	-2.60388	H	-0.77593	-1.78191	-2.36144	N	2.08656	0.00000	1.39148
N	-0.98353	-1.91427	-1.28314	N	-1.98210	0.71418	-1.35717	N	-1.47542	-1.47542	-1.39148
N	1.73917	-0.74807	-1.64166	N	-0.71353	-1.98106	-1.35860	H	-0.81094	2.69415	1.25390
H	-2.11570	-1.67527	1.42838	H	-1.61324	2.36684	1.10180	H	0.00000	1.86647	2.39218
H	-1.93340	-2.17017	-0.98919	H	-2.35362	1.63529	-1.10022	H	0.81094	2.69415	1.25390
H	-1.09738	-1.62104	-2.26260	H	-1.78267	0.77705	-2.35993	H	-2.69415	-0.81094	1.25390
H	2.55770	-0.13608	-1.64518	H	-0.07807	-2.78058	-1.28071	H	-1.86647	0.00000	2.39218
N	-1.73871	-0.74895	1.64173	N	-0.69524	1.98752	1.35861	H	-2.69415	0.81094	1.25390
H	2.96705	0.11949	0.81858	H	0.05246	-2.78130	1.28049	H	0.81094	-2.69415	1.25390
H	-1.40124	-0.79013	2.60393	H	-0.75936	1.78892	2.36145	H	0.00000	-1.86647	2.39218
N	2.16490	0.72772	1.03825	N	0.69521	-1.98763	1.35846	H	-0.81094	-2.69415	1.25390
H	-2.55756	-0.13739	1.64530	H	-0.05247	2.78117	1.28068	H	2.69415	0.81094	1.25390
H	2.10225	0.69695	2.06846	H	0.75928	-1.78906	2.36132	H	1.86647	0.00000	2.39218
H	-0.28009	1.67953	2.46820	H	1.78971	0.76035	2.35997	H	2.69415	-0.81094	1.25390
H	2.50377	1.67638	0.82441	H	1.61323	-2.36693	1.10169	H	-1.33163	2.47847	-1.25390
N	-0.47204	1.94134	1.49807	N	1.98860	0.69574	1.35720	H	-1.31979	1.31979	-2.39218
H	-1.42894	2.29346	1.46888	H	2.36861	1.61342	1.10036	H	-2.47847	1.33163	-1.25390
N	0.47104	1.94151	-1.49816	N	1.98214	-0.71405	-1.35717	H	1.33163	-2.47847	-1.25390
H	0.27923	1.67955	-2.46828	H	1.78273	-0.77694	-2.35994	H	1.31979	-1.31979	-2.39218
H	-0.13893	2.74048	-1.31611	H	2.78114	-0.07792	-1.27977	H	2.47847	-1.33163	-1.25390
H	0.13751	2.74061	1.31597	H	2.78174	0.05234	1.27978	H	2.47847	1.33163	-1.25390
H	1.42776	2.29411	-1.46898	H	2.35371	-1.63513	-1.10021	H	1.31979	1.31979	-2.39218
N	-2.16532	0.72664	-1.03815	N	0.71354	1.98116	-1.35843	H	1.33163	2.47847	-1.25390
H	-2.96714	0.11799	-0.81844	H	0.07811	2.78070	-1.28050	H	-2.47847	-1.33163	-1.25390
H	-2.10271	0.69590	-2.06837	H	0.77588	1.78204	-2.36129	H	-1.31979	-1.31979	-2.39218
H	-2.50468	1.67512	-0.82431	H	1.63499	2.35198	-1.10156	H	-1.33163	-2.47847	-1.25390

Table S5. Harmonic vibrational frequencies (cm^{-1}) for the $Y(NH_3)_{n=1\text{-}5}^{0,+}$ species at MP2/cc-pVTZ-PP(Y), cc-pVTZ(N) and aug-cc-pVTZ(H), and for $Y(NH_3)_{6,7,8}^{0,+}$ and $Y(NH_3)_8^-$ at DFT(B3LYP)/cc-pVTZ-PP (Y), cc-pVTZ (N) and aug-cc-pVTZ (H).

$Y(NH_3)$	**$Y(NH_3)^+$**
197.5	363.7
270.7	505.2
271.2	506.0
1132.0	1295.2
1667.5	1633.6
1667.5	1633.7
3471.4	3403.1
3614.2	3523.7
3614.2	3524.0

$Y(NH_3)_2$	**$Y(NH_3)_2^+$**
45.3	30.5
55.4	54.1
75.6	54.3
298.0	338.2
310.0	343.0
327.1	466.6
360.0	467.2
363.1	467.4
443.2	468.1
1137.1	1269.6
1145.4	1275.2
1504.4	1639.4
1614.5	1639.4
1615.9	1641.1
1627.0	1641.1
3401.7	3420.0
3521.7	3420.0
3552.8	3541.0
3555.0	3542.0
3560.0	3542.4

$Y(NH_3)_3$	$Y(NH_3)_3^+$
17.9	10.0 *i*
23.5	73.1
61.9	75.1
63.6	76.8
128.3	127.3
149.9	152.0
227.4	283.6
284.8	308.2
316.1	347.4
329.9	423.8
350.8	434.3
356.6	441.4
369.6	445.0
380.1	451.6
526.0	538.3
1120.0	1242.1
1133.6	1248.6
1167.2	1262.9
1594.4	1619.3
1606.8	1631.0
1609.8	1632.7
1619.9	1636.5
1626.8	1651.8
1639.4	1672.7
3360.2	3406.5
3392.2	3409.5
3398.1	3410.5
3517.7	3530.3
3521.7	3531.1
3533.5	3537.3
3540.7	3543.2
3564.3	3562.6
3567.9	3564.8

$Y(NH_3)_4$	$Y(NH_3)_4^+$
45.8	8.5
51.9	86.6
57.8	86.6
95.4	92.3
96.7	101.0
106.0	101.1
113.5	154.0
123.7	154.0

155.5	169.9
200.7	266.1
216.2	266.2
266.3	290.6
288.8	357.5
320.6	365.5
341.5	399.5
347.9	399.5
363.2	422.9
379.3	422.9
406.2	468.9
436.3	469.0
791.3	556.9
1109.8	1215.1
1115.9	1232.3
1135.3	1232.3
1270.7	1252.3
1572.9	1621.1
1594.6	1621.1
1604.1	1621.3
1611.0	1635.6
1616.9	1635.6
1625.4	1652.2
1629.4	1652.2
1649.2	1674.4
3301.0	3382.7
3379.0	3393.3
3384.4	3399.8
3397.1	3399.8
3454.8	3527.7
3473.9	3528.9
3527.0	3529.0
3532.0	3531.6
3534.6	3531.6
3553.4	3550.8
3563.4	3550.8
3563.9	3555.8

$Y(NH_3)_5$	$Y(NH_3)_5^+$
11.3	12.3
45.0	56.5
62.8	76.2
97.2	78.9
106.2	109.8
116.2	122.5
127.5	123.5

141.7	131.0
172.2	162.3
179.0	166.7
193.5	187.0
204.8	200.8
282.8	262.0
298.7	268.7
321.0	298.7
321.1	300.2
359.9	304.6
420.3	374.5
423.2	389.5
427.2	393.0
431.5	404.4
447.4	409.1
456.5	429.1
492.4	446.5
515.1	454.0
555.8	523.2
564.3	527.7
1182.8	1213.0
1191.9	1216.9
1209.1	1220.7
1209.3	1222.8
1234.6	1236.5
1519.0	1618.6
1563.7	1619.3
1574.2	1620.5
1578.2	1625.9
1596.0	1631.3
1603.3	1645.5
1605.4	1648.9
1615.6	1655.4
1618.0	1657.2
1640.7	1664.2
3037.2	3373.2
3148.8	3377.6
3183.9	3381.1
3203.7	3386.3
3298.8	3390.7
3306.4	3516.4
3310.3	3521.9
3323.3	3523.0
3335.4	3524.4
3450.3	3526.6
3470.4	3551.5
3478.8	3553.8

3485.0	3555.9
3503.7	3560.2
3507.1	3563.2

$Y(NH_3)_6$	$Y(NH_3)_6^+$
23.5	36.8
58.1	72.3
63.0	73.5
71.6	89.5
79.8	93.3
83.0	96.9
84.4	104.4
107.4	128.6
119.9	133.2
128.1	136.7
136.8	138.6
152.1	152.1
158.3	153.7
162.0	155.3
163.3	170.2
250.0	250.3
251.7	250.7
261.6	272.3
262.3	272.7
282.9	276.9
305.9	297.8
363.7	383.3
382.9	384.7
396.7	391.1
410.0	392.3
412.3	438.5
434.0	438.8
462.3	473.1
467.1	474.2
471.3	491.2
476.7	492.0
502.2	539.6
526.7	543.9
1169.1	1228.6
1177.9	1229.0
1178.1	1229.1
1181.9	1229.4
1182.8	1241.1
1190.7	1245.9
1586.9	1610.0
1589.2	1610.3
1596.6	1610.7

1597.7	1612.7
1599.4	1613.2
1602.6	1613.5
1604.2	1638.8
1607.1	1638.8
1617.2	1640.2
1618.6	1640.4
1635.9	1653.5
1637.8	1654.7
3210.1	3242.6
3228.8	3267.6
3257.6	3267.7
3264.3	3270.3
3292.4	3271.8
3296.8	3271.9
3326.4	3411.7
3335.1	3422.1
3354.1	3425.9
3356.7	3426.0
3381.7	3429.6
3386.8	3429.6
3403.7	3467.2
3404.7	3467.4
3438.3	3471.4
3442.4	3471.4
3489.9	3479.5
3497.1	3480.3

$Y(NH_3)_7$	$Y(NH_3)_7^+$
31.0 *i*	46.4
53.2	55.3
55.3	58.9
74.6	95.0
75.0	101.5
85.0	102.0
97.7	108.4
114.5	114.3
122.9	122.0
128.1	123.6
137.2	139.3
138.1	141.4
148.2	158.6
151.8	164.0
164.6	166.4
174.4	170.5
175.7	177.3

183.9	187.9
235.9	221.6
236.6	238.1
249.9	241.6
260.5	253.8
273.2	269.5
281.8	285.0
288.2	285.4
396.9	380.5
398.6	394.2
419.5	400.1
442.0	406.1
442.8	433.9
443.3	447.8
453.3	453.5
462.5	469.7
490.3	485.6
491.8	489.2
496.6	501.2
529.2	528.4
541.9	533.5
553.6	550.5
1185.5	1225.2
1186.1	1229.5
1196.5	1234.5
1197.6	1234.8
1217.9	1238.6
1225.3	1249.5
1242.5	1256.7
1581.7	1597.1
1582.6	1599.5
1594.4	1605.1
1600.4	1607.6
1602.5	1622.8
1607.1	1628.1
1607.7	1628.6
1611.3	1633.3
1612.6	1633.5
1616.9	1640.5
1617.3	1642.5
1623.9	1651.5
1631.6	1651.9
1640.5	1654.4
3196.0	3212.2
3213.6	3231.6
3258.4	3242.3
3266.4	3242.6

3279.1	3306.7
3290.9	3310.9
3293.4	3344.8
3305.5	3396.2
3317.2	3411.6
3334.4	3412.4
3335.4	3417.5
3365.0	3418.5
3382.7	3423.3
3390.4	3423.3
3400.6	3431.8
3406.9	3440.9
3416.2	3467.3
3417.4	3468.1
3423.6	3473.7
3454.8	3473.8
3457.3	3476.8

$Y(NH_3)_8$	$Y(NH_3)_8^+$	$Y(NH_3)_8^-$
33.6	38.4	36.5
55.4	82.2	64.4
81.4	82.7	80.1
86.8	114.2	117.1
108.7	114.2	117.2
118.1	121.6	127.1
129.6	122.5	137.1
136.6	132.3	142.0
139.6	132.3	142.0
145.2	142.7	148.3
146.9	142.7	148.3
152.0	151.4	150.7
153.7	152.2	163.6
161.1	153.9	163.6
163.8	159.7	167.8
167.9	169.6	168.6
171.5	169.6	178.8
171.9	172.2	179.0
172.0	175.5	179.4
185.2	175.5	183.6
197.0	177.1	183.8
223.6	227.0	230.7
235.4	227.9	236.3
236.0	233.9	239.5
239.5	233.9	239.6
268.3	259.6	269.2
281.7	276.6	281.7

281.8	276.6	281.7
301.7	287.6	303.7
381.3	398.7	452.5
435.0	411.3	452.5
437.8	411.3	460.4
453.7	424.1	465.4
458.6	427.5	470.2
460.2	428.1	477.2
480.8	469.4	497.2
485.5	480.9	521.9
489.5	480.9	521.9
511.2	499.5	528.4
512.7	499.5	528.4
519.2	500.5	535.0
529.7	536.3	535.0
537.6	536.3	555.5
561.2	564.4	587.4
581.5	565.1	594.4
1176.2	1239.7	1166.5
1192.9	1239.7	1166.5
1226.0	1239.8	1219.2
1227.8	1240.4	1225.0
1229.1	1243.3	1228.1
1245.7	1253.8	1248.9
1251.0	1253.8	1249.0
1255.7	1260.2	1257.2
1527.4	1610.9	1544.2
1564.7	1611.2	1544.2
1594.1	1617.1	1599.3
1595.8	1617.7	1601.3
1599.1	1617.7	1601.4
1599.7	1619.0	1601.4
1604.5	1623.3	1604.0
1606.6	1623.3	1606.2
1608.7	1627.1	1607.8
1618.1	1627.1	1607.8
1618.4	1630.3	1607.8
1618.6	1635.5	1613.8
1622.3	1635.5	1619.7
1624.9	1638.2	1619.7
1626.4	1638.4	1621.2
1631.1	1639.3	1625.4
3117.4	3289.9	3196.9
3138.3	3289.9	3197.0
3237.4	3292.5	3245.9
3243.0	3292.5	3252.3
3263.4	3293.0	3257.0

3276.6	3296.5	3257.1
3278.9	3296.6	3265.5
3289.2	3317.9	3286.3
3295.7	3373.8	3318.0
3298.6	3374.0	3318.0
3299.4	3380.0	3327.3
3303.0	3388.6	3330.5
3327.5	3388.6	3340.5
3332.6	3395.2	3346.1
3344.5	3398.6	3346.1
3355.8	3398.7	3355.9
3375.3	3402.4	3356.4
3376.2	3406.9	3358.5
3380.2	3406.9	3358.5
3380.8	3407.7	3369.1
3412.6	3407.7	3369.3
3413.2	3408.7	3369.4
3416.4	3412.7	3371.9
3418.2	3413.1	3379.3

Table S6. Cartesian coordinates (Å) and harmonic vibrational frequencies (cm^{-1}) for the $Y(NH_3)_8^{3+}$ species optimized at MP2 and B3LYP/cc-pVTZ-PP (Y), cc-pVTZ (N) and aug-cc-pVTZ (H).

MP2 - $Y(NH_3)_8^{3+}$				**B3LYP - $Y(NH_3)_8^{3+}$**				**Frequencies - $Y(NH_3)_8^{3+}$**
Y	0.00000	0.00000	0.00000	Y	0.00000	0.00000	0.00004	43.2
H	-2.34868	-1.62819	1.28088	H	-2.34339	1.70239	-1.29901	53.3
N	-2.01781	-0.67275	1.41194	N	-2.04125	0.73865	-1.43828	53.7
H	-2.81254	0.51483	-1.27876	H	-2.86120	-0.45746	1.29769	54.5
H	-2.85720	-0.10955	1.27872	H	-2.89101	0.19297	-1.29830	121.0
H	-1.85829	-0.61784	2.41833	H	-1.88163	0.68025	-2.44430	121.0
H	-1.94521	-2.09280	-1.28269	H	-1.90989	2.17688	1.30099	125.2
H	-0.87437	-1.75113	-2.41918	H	-0.84813	1.81130	2.44498	125.2
N	-1.90156	0.95286	-1.41204	N	-1.96499	-0.92273	1.43833	125.2
N	-0.95231	-1.90120	-1.41287	N	-0.92231	1.96462	1.43902	136.1
H	-1.62778	2.34820	1.28263	H	-1.70211	-2.34280	-1.30044	136.2
H	-2.09311	1.94567	-1.28108	H	-2.17734	-1.91022	1.29971	141.8
H	-1.75147	0.87570	-2.41841	H	-1.81176	-0.84914	2.44435	153.7
H	-0.51431	-2.81212	-1.27918	H	-0.45720	2.86089	1.29819	153.8
N	-0.67227	2.01724	1.41293	N	-0.73827	-2.04073	-1.43911	166.6
H	0.10905	-2.85661	1.27937	H	0.19273	2.89060	-1.29896	168.2
H	-0.61664	1.85752	2.41925	H	-0.67930	-1.88090	-2.44506	170.0
N	0.67225	-2.01727	1.41290	N	0.73825	2.04076	-1.43908	170.2
H	-0.10907	2.85658	1.27941	H	-0.19274	-2.89057	-1.29901	170.3
H	0.61662	-1.85756	2.41921	H	0.67928	1.88094	-2.44503	174.0
H	1.85827	0.61782	2.41836	H	1.88161	-0.68021	-2.44433	174.9
H	1.62776	-2.34824	1.28261	H	1.70210	2.34283	-1.30041	206.5
N	2.01780	0.67272	1.41197	N	2.04124	-0.73862	-1.43831	207.1
H	2.34868	1.62816	1.28091	H	2.34338	-1.70236	-1.29905	218.2
N	1.90157	-0.95283	-1.41204	N	1.96500	0.92270	1.43834	218.3
H	1.75148	-0.87567	-2.41842	H	1.81177	0.84910	2.44435	244.3
H	2.81255	-0.51479	-1.27877	H	2.86121	0.45742	1.29769	253.1
H	2.85718	0.10951	1.27876	H	2.89099	-0.19293	-1.29834	253.1
H	2.09314	-1.94564	-1.28109	H	2.17736	1.91019	1.29972	281.0
N	0.95232	1.90123	-1.41282	N	0.92232	-1.96465	1.43898	426.4
H	0.51432	2.81215	-1.27912	H	0.45721	-2.86091	1.29812	448.7
H	0.87437	1.75117	-2.41914	H	0.84813	-1.81134	2.44494	448.7
H	1.94522	2.09282	-1.28266	H	1.90990	-2.17691	1.30094	455.9
								457.4
								465.5
								518.3
								518.3
								562.5
								562.5

		574.1
		574.2
		574.2
		599.8
		600.3
		606.0
		1336.1
		1336.5
		1340.8
		1340.8
		1351.9
		1353.5
		1353.5
		1376.5
		1646.2
		1658.1
		1658.3
		1665.4
		1665.4
		1665.4
		1675.4
		1675.4
		1677.7
		1677.8
		1685.2
		1685.2
		1690.1
		1694.4
		1694.9
		1698.9
		3424.2
		3424.5
		3426.0
		3426.0
		3426.7
		3426.7
		3428.3
		3431.5
		3494.8
		3495.1
		3496.5
		3496.5
		3496.7
		3496.7
		3499.6

	3500.1
	3501.6
	3503.9
	3503.9
	3504.3
	3505.2
	3505.2
	3505.4
	3505.6