Characterizing the Tautomers of Protonated Aniline using Differential Mobility Spectrometry and Mass Spectrometry

Supporting Information

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Table S1. The calculated electronic energy (E_{elec}), zero-point corrected energy (E_{ZPE}), standard enthalpy (H^o), standard Gibbs' energy (G^o), and standard total entropy (S^o) of the lowest energy structures for $(C_6H_5NH_2 + H)^+•(H_2O)_n$ (n = 0–5). Calculations were conducted at the B3LYP/6-311++G(d,p) level of theory and energies are reported in hartree. N-protonated tautomers are labeled as "N-prot", *p*-protonated tautomers are labeled as "p-prot", and solvent-bridged structures are labeled as "bridge". The number of water molecules is given in the form "_xw" where x = 1 – 5.

Cluster	E_{elec} (hartree)	E_{ZPE} (hartree)	H^o (hartree)	G^o (hartree)	S^o_{total} (cal/mol*K)
N-prot	-288.0426705	-287.9116145	-287.9044115	-287.9426275	80.432
N-prot_1w	-364.5327898	-364.3773238	-364.3679628	-364.4103168	89.142
N-prot_2w	-441.019005	-440.839485	-440.826572	-440.877753	107.72
N-prot_3w	-517.5022565	-517.2989675	-517.2813065	-517.3456715	135.468
N-prot_4w	-593.9824178	-593.7543218	-593.7338888	-593.8044648	148.539
N-prot_5w	-670.4659171	-670.2110401	-670.1889041	-670.2626461	155.204
p-prot	-288.043686	-287.914738	-287.907785	-287.944246	76.738
p-prot_1w	-364.5173774	-364.3653394	-364.3543584	-364.4021464	100.58
p-prot_2w	-440.9945312	-440.8170022	-440.8033872	-440.8564772	111.736
p-prot_3w	-517.4762402	-517.2724932	-517.2568572	-517.3144252	121.163
p-prot_4w	-593.9496717	-593.7219467	-593.7026027	-593.7706737	143.268
p-prot_5w	-670.4305447	-670.1764557	-670.1552097	-670.2257267	148.415
bridge_3w	-517.4949065	-517.2902415	-517.2744445	-517.3331835	123.627
bridge_4w	-593.966023	-593.739598	-593.721689	-593.78719	137.857
bridge_5w	-670.4331987	-670.1810137	-670.1583097	-670.2351297	161.681

Table S2. The calculated electronic energy (E_{elec}), zero-point corrected energy (E_{ZPE}), standard enthalpy (H^o), and standard Gibbs' energy (G^o) of the lowest energy structures for $(C_6H_5NH_2 + H)^+•(H_2O)_n$ (n = 0–3). Electronic energies were calculated at the CCSD(T)/6-311++G(d,p) level of theory and thermodynamic corrections were calculated at the B3LYP/6-311++G(d,p) level of theory. N-protonated tautomers are labeled as "N-prot" and *p*-protonated tautomers are labeled as "p-prot". Energies are reported in hartree. The number of water molecules is given in the form "_xw" where x = 1 – 3.

Cluster	E_{elec} (hartree)	E_{ZPE} (hartree)	H^o (hartree)	G^o (hartree)
N-prot	-287.2530863	-287.1220303	-287.1148273	-287.1530433
N-prot_1w	-363.5696899	-363.4142239	-363.4048629	-363.4472169
N-prot_2w	-439.8829263	-439.7034063	-439.6904933	-439.7416743
N-prot_3w	-516.1942516	-515.9909626	-515.9733016	-516.0376666
p-prot	-287.2496277	-287.1206797	-287.1137267	-287.1501877
p-prot_1w	-363.5498244	-363.3977864	-363.3868054	-363.4345934
p-prot_2w	-439.8538746	-439.6763456	-439.6627306	-439.7158206
p-prot_3w	-516.160307	-515.95656	-515.940924	-515.998492

Table S3. The relative zero-point corrected energies ($ZPE_{rel.}$), standard enthalpy ($\Delta_{rel.}H^o$), and standard Gibbs' energies ($\Delta_{rel.}G^o$) of the *p*-protonated and solvent-bridged isomers of $(C_6H_5NH_2 + H)^+•(H_2O)_n$ (n = 0–5). Energies are reported in kJ/mol and are relative to the analogous N-protonated species. Calculations were conducted at the B3LYP/6-311++G(d,p) level of theory.

Cluster	ZPE_{rel}	$\Delta_{rel}H^o$	$\Delta_{rel}G^o$
p-prot	-8.2	-8.9	-4.2
p-prot_1w	31.5	35.7	21.5
p-prot_2w	59.0	60.9	55.9
p-prot_3w	69.5	64.2	82.0
p-prot_4w	85.0	82.1	88.7
p-prot_5w	90.8	88.5	96.9
bridge_3w	22.9	18.0	32.8
bridge_4w	38.7	32.0	45.4
bridge_5w	78.8	80.3	72.2

Table S4. The relative zero-point corrected energies ($ZPE_{rel.}$), standard enthalpy ($\Delta_{rel.}H^o$), and standard Gibbs' energies ($\Delta_{rel.}G^o$) of the *p*-protonated isomers of $(C_6H_5NH_2 + H)^+\bullet(H_2O)_n$ (n = 0–5). Energies are reported in kJ/mol and are relative to the analogous N-protonated species. Electronic energies were calculated at the CCSD(T)/6-311++G(d,p) level of theory and thermodynamic corrections were calculated at the B3LYP/6-311++G(d,p) level of theory. The number of water molecules is given in the form "_xw" where x = 1 – 5.

Cluster	ZPE_{rel}	$\Delta_{rel}H^o$	$\Delta_{rel}G^o$
p-prot	3.5	2.9	7.5
p-prot_1w	43.2	47.4	33.1
p-prot_2w	71.0	72.9	67.9
p-prot_3w	90.3	85.0	102.9

Table S5. The calculated electronic energy (E_{elec}), zero-point corrected energy (E_{ZPE}), standard enthalpy (H^o), standard Gibbs' energy (G^o), and standard total entropy (S^o) of the lowest energy structures for $(C_6H_5NH_2 + H)^+\bullet(CH_3OH)_n$ (n = 0–5). Calculations were conducted at the B3LYP/6-311++G(d,p) level of theory and energies are reported in hartree. N-protonated tautomers are labeled as "N-prot", *p*-protonated tautomers are labeled as "p-prot", and solvent-bridged structures are labeled as "bridge". The number of methanol molecules is given in the form "_xm" where x = 1 – 5.

Cluster	E_{elec} (hartree)	E_{ZPE} (hartree)	H^o (hartree)	G^o (hartree)	S^o_{total} (cal/mol*K)
N-prot	-288.042671	-287.9116145	-287.9044115	-287.9426255	80.432
N-prot_1m	-403.844878	-403.6608638	-403.6492918	-403.6999368	106.592
N-prot_2m	-519.640891	-519.4035343	-519.3872553	-519.4504583	133.021
N-prot_3m	-635.433062	-635.1427827	-635.1215557	-635.1979377	160.76
N-prot_4m	-751.223929	-750.8795729	-750.8543819	-750.9400879	180.384
N-prot_5m	-867.007265	-866.6103138	-866.5801158	-866.6803908	211.046
p-prot	-288.043686	-287.914738	-287.907785	-287.944246	76.738
p-prot_1m	-403.826046	-403.6452484	-403.6329754	-403.6871254	113.969
p-prot_2m	-519.611777	-519.3769947	-519.3604047	-519.4235567	132.914
p-prot_3m	-635.402681	-635.1136187	-635.0931767	-635.1649517	151.063
p-prot_4m	-751.18765	-750.8455973	-750.8202753	-750.9058413	180.088
p-prot_5m	-866.981533	-866.5856984	-866.5565734	-866.6507384	198.185
bridge_3m	-635.425025	-635.1355883	-635.1152673	-635.1883733	153.863
bridge_4m	-751.215796	-750.8747903	-750.8503513	-750.9347743	177.682
bridge_5m	-866.980231	-866.584745	-866.554855	-866.652302	205.094

Table S6. The calculated electronic energy (E_{elec}), zero-point corrected energy (E_{ZPE}), standard enthalpy (H^o), and standard Gibbs' energy (G^o) of the lowest energy structures for $(C_6H_5NH_2 + H)^+•(CH_3OH)_n$ (n = 0–2). Electronic energies were calculated at the CCSD(T)/6-311++G(d,p) level of theory and thermodynamic corrections were calculated at the B3LYP/6-311++G(d,p) level of theory. N-protonated tautomers are labeled as "N-prot" and *p*-protonated tautomers are labeled as "p-prot". Energies are reported in hartree. The number of water molecules is given in the form "_xm" where x = 1,2.

Cluster	E_{elec} (hartree)	E_{ZPE} (hartree)	H^o (hartree)	G^o (hartree)
N-prot	-287.253086	-287.1220303	-287.1148273	-287.1530413
N-prot_1m	-402.765295	-402.5812814	-402.5697094	-402.6203544
N-prot_2m	-518.27121	-518.0338527	-518.0175737	-518.0807767
p-prot	-287.249628	-287.1206797	-287.1137267	-287.1501877
p-prot_1m	-402.74135	-402.5605518	-402.5482788	-402.6024288
p-prot_2m	-518.237376	-518.0025943	-517.9860043	-518.0491563

Table S7. The relative zero-point corrected energies ($ZPE_{rel.}$), standard enthalpy ($\Delta_{rel.}H^o$), and standard Gibbs' energies ($\Delta_{rel.}G^o$) of the *p*-protonated and solvent-bridged isomers of $(C_6H_5NH_2 + H)^+•(CH_3OH)_n$ (n = 0–5). Energies are reported in kJ/mol and are relative to the analogous N-protonated species. Calculations were conducted at the B3LYP/6-311++G(d,p) level of theory.

Cluster	ZPE_{rel}	$\Delta_{rel}H^o$	$\Delta_{rel}G^o$
p-prot	-8.2	-8.9	-4.3
p-prot_1m	41.0	42.8	33.6
p-prot_2m	69.7	70.5	70.6
p-prot_3m	76.6	74.5	86.6
p-prot_4m	89.2	89.5	89.9
p-prot_5m	64.6	61.8	77.9
bridge_3m	18.9	16.5	25.1
bridge_4m	12.6	10.6	14.0
bridge_5m	9.5	5.9	21.7

Table S8. The relative zero-point corrected energies ($ZPE_{rel.}$), standard enthalpy ($\Delta_{rel.}H^o$), and standard Gibbs' energies ($\Delta_{rel.}G^o$) of the *p*-protonated isomers of $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_n$ (n = 0–2). Energies are reported in kJ/mol and are relative to the analogous N-protonated species. Electronic energies were calculated at the CCSD(T)/6-311++G(d,p) level of theory and thermodynamic corrections were calculated at the B3LYP/6-311++G(d,p) level of theory. The number of water molecules is given in the form "_xm" where x = 1,2.

Cluster	ZPE_{rel}	$\Delta_{rel}H^o$	$\Delta_{rel}G^o$
p-prot	3.5	2.9	7.5
p-prot_1m	54.4	56.3	47.1
p-prot_2m	82.1	82.9	83.0

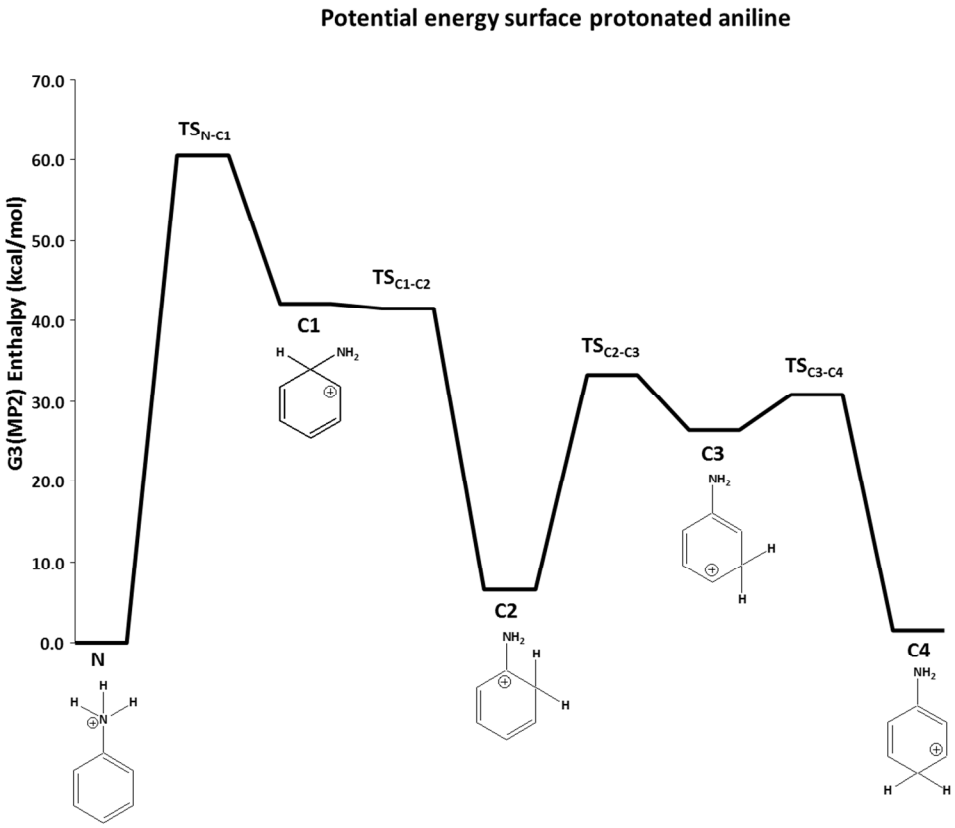


Figure S1. The potential energy surface of protonated aniline as calculated at the G3MP2 level of theory. Energies are given as relative standard enthalpy ($\Delta_{rel.}H^o$) in kcal/mol.

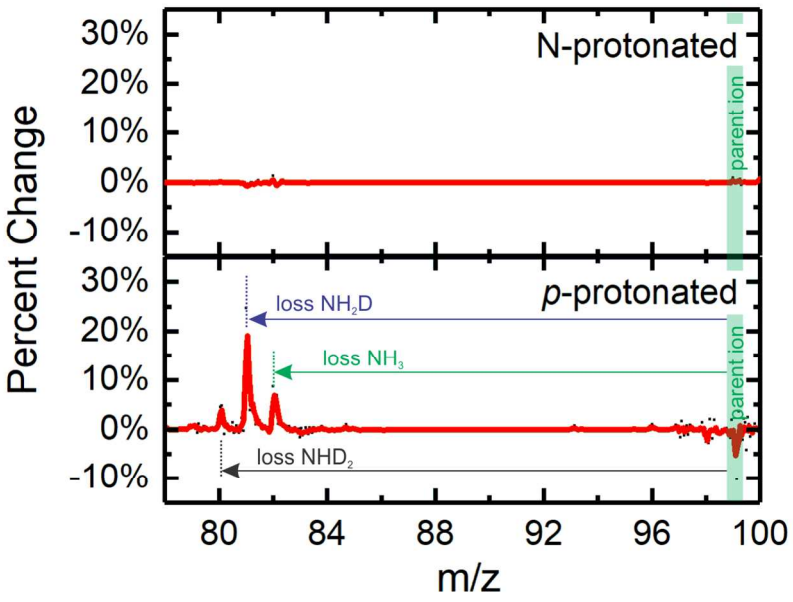
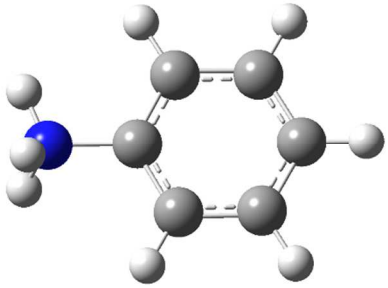


Figure S2. (**Top panel**) The percent difference fragmentation spectrum observed for N-protonated d_5-aniline, $(C_6D_5NH_2 + H)^+$, determined by subtracting the fragmentation spectrum measured following exposure to a dry N_2 environment from that observed following exposure to an N_2 environment saturated with water vapor. For the N-protonated tautomer, no change is observed from one condition to the other. (**Bottom panel**) The percent difference fragmentation spectrum observed for *p*-protonated d_5-aniline, $(C_6D_5NH_2 + H)^+$. Water-clustering enhances H/D scrambling for the *p*-protonated species.

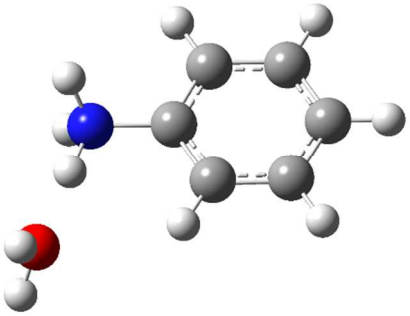
The atomic coordinates and structures of $(C_6H_5NH_2 + H)^+ \bullet (H_2O)_n$ (n = 0–5)

N-protonated $(C_6H_5NH_2 + H)^+$



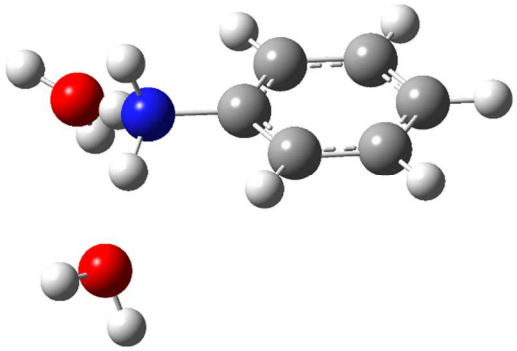
C	0.82544800	0.00257200	-0.00020300
C	0.16577100	1.22166200	-0.00017800
C	-1.22907800	1.20930600	-0.00003900
C	-1.91738500	-0.00204900	0.00012100
C	-1.22283700	-1.21246500	0.00010400
C	0.17012200	-1.22093600	-0.00005300
H	0.70597700	2.16278800	-0.00029000
H	-1.77006400	2.14718100	-0.00010200
H	-3.00043400	-0.00460100	0.00019800
H	-1.76149900	-2.15173700	0.00016000
H	0.71626200	-2.15833500	-0.00007100
N	2.32348500	0.00054200	0.00015200
H	2.70095300	-0.46754000	0.83147500
H	2.70119700	-0.47706600	-0.82560000
H	2.69097200	0.95698100	-0.00534500

N-protonated ($C_6H_5NH_2 + H)^+ \bullet (H_2O)$



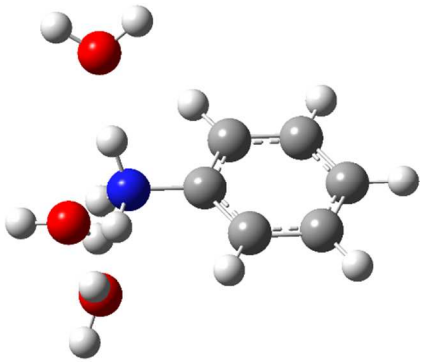
C	0.03399800	0.51333600	0.00012400
C	-1.12655200	1.27678200	0.00008800
C	-2.35124600	0.61380700	-0.00003200
C	-2.39236600	-0.78103000	-0.00010800
C	-1.21236100	-1.52138900	-0.00006700
C	0.02342100	-0.87375000	0.00005100
H	-1.08747700	2.36113100	0.00014800
H	-3.26960000	1.18754800	-0.00006600
H	-3.34819800	-1.29045800	-0.00019900
H	-1.24676600	-2.60372100	-0.00012600
H	0.94833600	-1.43818300	0.00008800
N	1.34789200	1.21716400	0.00026700
H	1.44827600	1.81617400	0.82468600
H	2.15128800	0.54330400	-0.00001600
H	1.44815600	1.81671700	-0.82377100
O	3.46811800	-0.56771200	-0.00027300
H	3.96304600	-0.86874400	-0.77212400
H	3.96339000	-0.86875200	0.77135400

N-protonated $(C_6H_5NH_2 + H)^+ \bullet (H_2O)_2$



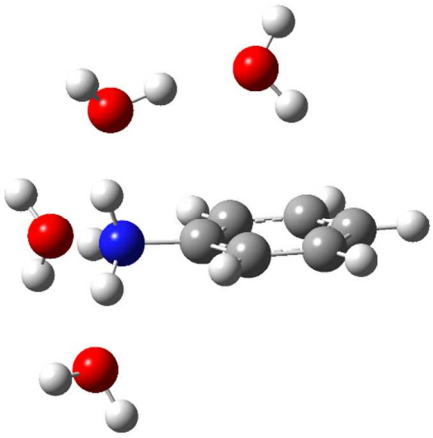
C	0.15522100	0.00001100	0.34002900
C	0.80659000	1.21770300	0.18959800
C	2.16465700	1.20906500	-0.12472500
C	2.84057900	-0.00030300	-0.28138400
C	2.16421600	-1.20951000	-0.12540100
C	0.80615200	-1.21783300	0.18896000
H	0.26954000	2.15125000	0.31244700
H	2.69106200	2.14772100	-0.24624100
H	3.89586200	-0.00042700	-0.52564600
H	2.69028300	-2.14829100	-0.24741800
H	0.26875900	-2.15124900	0.31128700
N	-1.28430700	0.00019000	0.69623400
H	-1.76186800	0.84529800	0.31751400
H	-1.76205400	-0.84491300	0.31774100
H	-1.40907100	0.00033500	1.71160600
O	-2.41848400	-2.34000800	-0.34453800
H	-3.10141700	-2.90056900	0.04200200
H	-2.31279800	-2.63579200	-1.25635300
O	-2.41781300	2.34040700	-0.34510200
H	-3.10131500	2.90075700	0.04073600
H	-2.31093100	2.63655400	-1.25666100

N-protonated $(C_6H_5NH_2 + H)^+ \bullet (H_2O)_3$



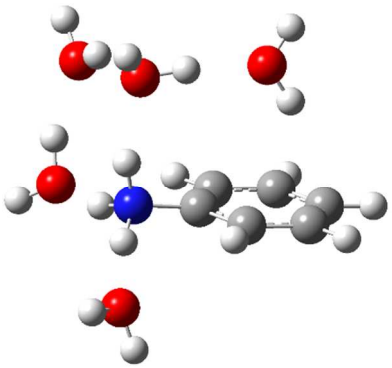
C	-0.30467800	-0.03716200	-0.00000400
C	-0.90014400	-1.29154000	0.00099500
C	-2.29313900	-1.36965100	0.00075800
C	-3.06188000	-0.20773300	-0.00042500
C	-2.44312600	1.04283100	-0.00144800
C	-1.05322000	1.13534700	-0.00125600
H	-0.29144200	-2.18809400	0.00182200
H	-2.77341700	-2.34049800	0.00152600
H	-4.14302700	-0.27499000	-0.00056200
H	-3.04043400	1.94649200	-0.00243500
H	-0.56069100	2.10149900	-0.00209200
N	1.16682000	0.07263900	0.00020500
H	1.61562100	-0.86029200	0.00178800
H	1.48268700	0.58764900	-0.84445700
H	1.48211100	0.59026300	0.84343300
O	1.72167800	1.47389300	-2.36976900
H	2.51854100	1.88476600	-2.72296800
H	1.03485800	1.59975100	-3.03426000
O	2.31225900	-2.53803700	0.00413400
H	2.63495000	-3.01855100	0.77521300
H	2.63995900	-3.01851500	-0.76484900
O	1.71890800	1.48241800	2.36630200
H	1.03033700	1.61317500	3.02800600
H	2.51656400	1.89012300	2.72134400

N-protonated $(C_6H_5NH_2 + H)^+ \bullet (H_2O)_4$



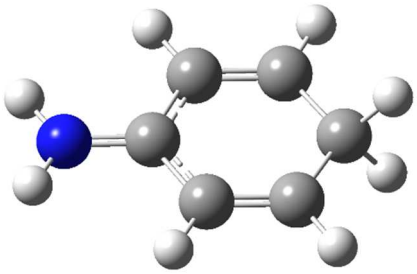
C	-0.06284200	-0.43431400	-0.13732000
C	0.44277200	-0.41539100	-1.43118900
C	1.74005800	-0.87704800	-1.65161200
C	2.51005400	-1.34486600	-0.58690700
C	1.98215000	-1.35953400	0.70603200
C	0.68647000	-0.89957600	0.93803200
H	-0.16310700	-0.04389400	-2.24912100
H	2.14606800	-0.87176800	-2.65581000
H	3.51568800	-1.70704300	-0.76416300
H	2.57503100	-1.73073500	1.53333000
H	0.26883700	-0.89679900	1.93812000
N	-1.40025700	0.11806000	0.12717500
H	-1.94431400	0.22982300	-0.74563100
H	-1.92603700	-0.48819400	0.78210200
H	-1.27557700	1.06975200	0.55860800
O	-2.60410400	-1.64846900	1.98559900
H	-3.28875400	-1.46978800	2.64008200
H	-2.49777000	-2.60621800	1.96435400
O	-2.71838000	0.54109900	-2.36513000
H	-2.93926200	1.42136100	-2.69100200
H	-3.24690800	-0.07515500	-2.88502300
O	-0.56708900	2.51579500	1.02995500
H	0.41132400	2.51263400	0.96021500
H	-0.81325300	3.18844700	1.67153900
O	2.12952000	2.16494100	0.72917800
H	2.82355600	2.76762900	0.44305900
H	2.44472400	1.27097800	0.55008400

N-protonated $(C_6H_5NH_2 + H)^+ \bullet (H_2O)_5$



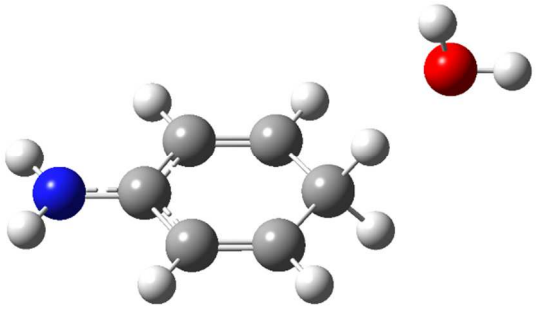
C	0.52253800	0.49721200	0.33661000
C	0.46342500	-0.43643600	1.36438000
C	1.62826900	-1.11738600	1.71647300
C	2.82371600	-0.86327400	1.04313600
C	2.86240500	0.08282200	0.01636000
C	1.70402800	0.77065400	-0.34456500
H	-0.47132600	-0.62522200	1.87807100
H	1.59975400	-1.84341000	2.51977700
H	3.72703100	-1.39077500	1.32559600
H	3.79189300	0.29009700	-0.50004800
H	1.71974900	1.50637700	-1.14050300
N	-0.71381700	1.16913000	-0.09503500
H	-1.44920400	1.14306800	0.65124500
H	-0.52855400	2.14965900	-0.37109600
H	-1.09894800	0.64569800	-0.90603400
O	0.07167000	3.78541800	-0.86323100
H	-0.33906500	4.37912000	-1.50206800
H	0.63282900	4.34002400	-0.30899000
O	-2.67729600	0.61889800	1.70528500
H	-3.06297100	-0.19546300	1.31688200
H	-3.34302800	1.04242600	2.25473800
O	-1.43464100	-0.84849600	-1.92921300
H	-0.61549000	-1.39909700	-1.92013800
H	-1.71872800	-0.79413300	-2.84846000
O	0.88833600	-2.22899700	-1.77259200
H	1.03155800	-3.17519500	-1.88006200
H	1.57094000	-1.91201400	-1.16749200
O	-3.10785800	-1.59156700	0.22686300
H	-3.72893800	-2.32341900	0.16992400
H	-2.66875100	-1.50525700	-0.63735600

p-protonated ($C_6H_5NH_2 + H)^+$



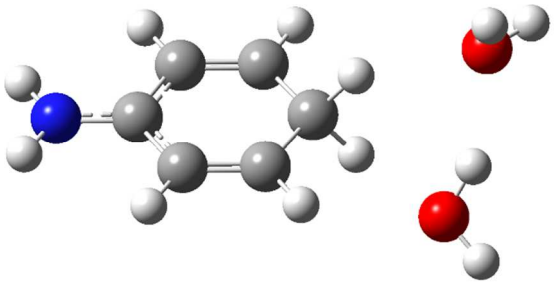
C	-1.08054200	-1.25060900	0.00000200
C	-1.08054300	1.25060500	0.00000700
C	0.26706300	1.24951200	-0.00000800
C	0.98539000	0.00000600	0.00001900
C	0.26705700	-1.24951000	-0.00001700
H	-1.62025600	-2.19148100	0.00001700
H	-1.62024600	2.19148300	0.00000700
H	0.82841300	2.17734100	-0.00003600
H	0.82842900	-2.17732700	-0.00003800
N	2.30674000	-0.00000300	0.00000300
H	2.83748900	-0.86105700	-0.00002300
H	2.83750400	0.86104200	0.00002600
C	-1.87699200	0.00000100	0.00000700
H	-2.56352200	0.00000600	-0.86180600
H	-2.56358100	-0.00000600	0.86176600

p-protonated ($C_6H_5NH_2 + H)^+ \bullet (H_2O)$



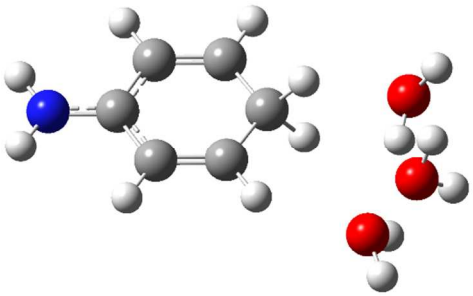
C	0.26338300	-1.24714400	-0.56911400
C	0.26466700	1.24503200	-0.57101700
C	-0.99099000	1.24735000	-0.07523500
C	-1.65843400	0.00052400	0.18931400
C	-0.99227200	-1.24740300	-0.07332500
H	0.76505100	-2.18784900	-0.76837400
H	0.76734100	2.18490000	-0.77168200
H	-1.51397800	2.17567900	0.12584400
H	-1.51622400	-2.17487900	0.12917700
C	1.00894300	-0.00164600	-0.83768100
H	1.94040600	-0.00156200	-0.23146000
H	1.40423900	-0.00262400	-1.86543300
N	-2.89133400	0.00153700	0.67483300
H	-3.38549000	-0.85925400	0.86726100
H	-3.38460300	0.86314200	0.86589200
O	3.67641700	0.00118300	0.79907100
H	3.82429600	0.00109000	1.75110300
H	4.55518300	0.00084400	0.40362300

p-protonated $(C_6H_5NH_2 + H)^+ \bullet (H_2O)_2$



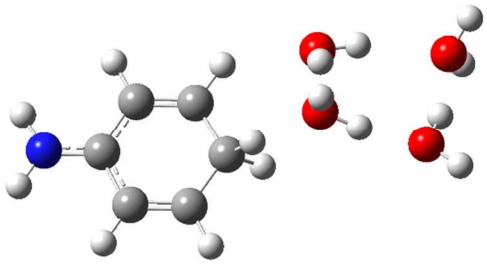
C	0.00464000	-0.91820300	0.06323500
C	-0.55870700	1.41569800	-0.61957100
C	-1.85857100	1.18316300	-0.34197900
C	-2.26729000	-0.10866000	0.14695300
C	-1.29707000	-1.14977900	0.34153200
H	0.75616000	-1.68965200	0.18421800
H	-0.25341600	2.38897300	-0.98857900
H	-2.61013200	1.95228300	-0.48167200
H	-1.62985500	-2.11577500	0.70508200
C	0.48370100	0.38510800	-0.43902200
H	1.29102200	0.75987400	0.21462400
H	1.04161700	0.21346600	-1.37429600
N	-3.54593500	-0.33481500	0.41502300
H	-3.86330600	-1.23171200	0.75658700
H	-4.24944600	0.37873700	0.28269600
O	3.61447800	0.93843500	0.90014500
H	3.87622900	0.82535100	1.82140100
H	4.17340300	1.64764600	0.56156000
O	2.91883600	-1.31949600	-0.68375900
H	3.41222600	-0.65464800	-0.17715800
H	3.57031200	-1.92631100	-1.04760500

p-protonated ($C_6H_5NH_2 + H)^+ \bullet (H_2O)_3$



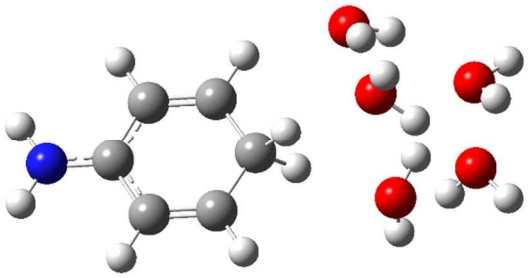
C	0.33612200	0.79583100	-0.00464400
C	1.06600200	-1.58924300	-0.00702500
C	2.35749400	-1.19579800	-0.00519800
C	2.67746900	0.20735900	-0.00365900
C	1.62930100	1.18918500	-0.00326100
H	-0.47006600	1.52263800	-0.00617200
H	0.82522700	-2.64688200	-0.00884200
H	3.16615400	-1.91824000	-0.00533500
H	1.89598300	2.24037100	-0.00218300
C	-0.05183600	-0.62752300	-0.00642700
H	-0.73521100	-0.82165300	0.84075300
H	-0.73453400	-0.82304300	-0.85324300
N	3.94709900	0.59268700	-0.00254700
H	4.20229300	1.57057000	-0.00163200
H	4.70375600	-0.07720800	-0.00287700
O	-2.90526800	-0.54594500	1.45779900
H	-2.99616800	0.40616700	1.26971200
H	-3.41022500	-0.72898300	2.25635300
O	-2.98922900	-0.78159100	-1.30146700
H	-3.57848000	-1.24003800	-1.90891500
H	-3.21242000	-1.07718600	-0.40059300
O	-2.74674600	1.72294900	-0.13680300
H	-3.27120200	2.51485900	-0.29244500
H	-2.97217500	1.08765600	-0.84170400

p-protonated $(C_6H_5NH_2 + H)^+ \bullet (H_2O)_4$



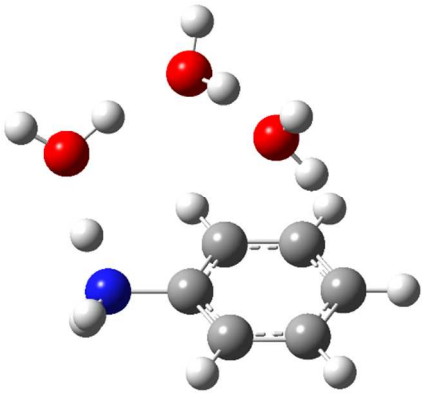
C	1.71087000	1.36792200	-0.69539300
C	1.13056400	-0.93723600	0.06069600
C	2.44389400	-1.20567900	0.24094500
C	3.42593100	-0.19731600	-0.03598800
C	3.02147900	1.09892800	-0.51358700
H	1.40602700	2.34472100	-1.05528500
H	0.36548700	-1.68075500	0.25714600
H	2.77406300	-2.17797700	0.59000800
H	3.78327100	1.84178500	-0.72289600
C	0.65612800	0.38080800	-0.39993500
H	-0.04452400	0.79748900	0.35340100
H	-0.02585500	0.25201500	-1.25457800
N	4.71537400	-0.45786900	0.14497200
H	5.42696100	0.23383200	-0.04441300
H	5.02928600	-1.35879000	0.47779700
O	-3.90113500	1.44826200	-0.28484400
H	-4.29609700	0.57598900	-0.45522900
H	-4.56889300	2.10956500	-0.48835300
O	-4.69038300	-1.27973700	-0.63228800
H	-4.86988100	-1.62550400	-1.51474400
H	-5.35217100	-1.67871900	-0.05471000
O	-1.79527000	1.21509800	1.42862200
H	-1.95278100	1.54667500	2.31799600
H	-2.56657300	1.48350500	0.88484000
O	-1.83836600	-1.42016100	0.34337800
H	-2.73101500	-1.58073000	0.01171100
H	-1.91688800	-0.63027500	0.90313300

p-protonated $(C_6H_5NH_2 + H)^+ \bullet (H_2O)_5$



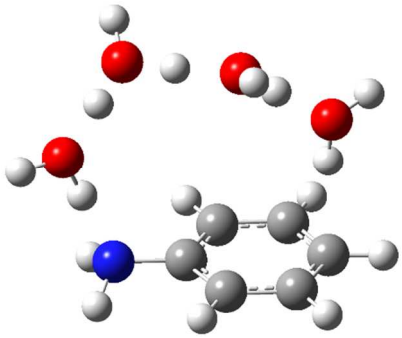
C	-1.63870600	-1.44162300	0.02066400
C	-1.32717900	1.03006300	0.04331600
C	-2.66590800	1.19761600	-0.06334900
C	-3.52749600	0.05404800	-0.12769000
C	-2.97480300	-1.27433000	-0.08448700
H	-1.22372900	-2.44325300	0.05560800
H	-0.64696700	1.87327100	0.10157400
H	-3.10506600	2.18867500	-0.09807600
H	-3.64733400	-2.12360200	-0.13534400
C	-0.70551300	-0.30429500	0.09739900
H	-0.07611000	-0.38390200	1.00437200
H	0.07473400	-0.38448000	-0.68252700
N	-4.84270600	0.21598300	-0.22668600
H	-5.47171600	-0.57312300	-0.27055400
H	-5.25881600	1.13614500	-0.25572100
O	3.58653600	-1.40710900	0.32319700
H	3.01869700	-1.50513700	-0.46818700
H	4.13594200	-2.19581500	0.38095800
O	3.84744100	1.13106000	-0.94398400
H	4.59363000	1.64946000	-1.26284100
H	4.20418500	0.43112400	-0.37219100
O	1.98545200	-0.75841600	-1.83130900
H	1.99491200	-1.06953800	-2.74270400
H	2.50299700	0.06924300	-1.81998800
O	1.76924400	-0.39131800	2.20189200
H	1.96744500	-0.48024100	3.13945700
H	2.48104200	-0.85030600	1.71661700
O	1.48871300	1.95967700	0.57800400
H	2.30745000	1.97950100	0.06421900
H	1.66618300	1.33007800	1.29462000

Solvent-bridged protonated $(C_6H_5NH_2 + H)^+ \bullet (H_2O)_3$



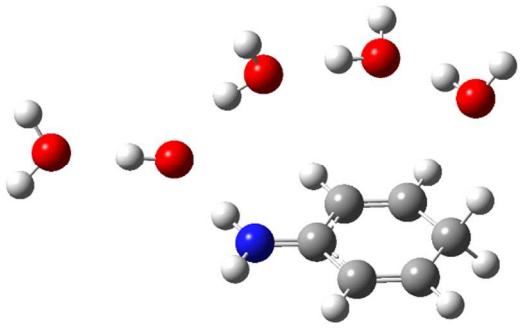
C	-1.22325000	0.70435700	1.35275500
C	-2.60195300	-0.12441100	-0.45572300
C	-1.65154200	-1.10471400	-0.73678200
C	-0.50139300	-1.15737200	0.03928700
C	-0.26281300	-0.26751800	1.07846800
H	-1.05429700	1.40481700	2.16125500
H	-3.50755100	-0.07210900	-1.04738900
H	-1.81617900	-1.80881800	-1.54560200
H	0.65587500	-0.30998100	1.65041800
N	0.52156200	-2.19020800	-0.24304000
H	0.47941500	-2.95079200	0.44035200
H	0.38501300	-2.60065300	-1.16830600
C	-2.38969500	0.77581200	0.58948400
H	-3.13777300	1.52675900	0.81471100
H	-0.59732500	2.06843500	-0.98168600
O	0.29434300	2.11966400	-1.34626000
H	1.67213800	1.89188200	-0.22974900
H	0.25651300	2.75044000	-2.07344500
O	2.34126500	1.54311200	0.39394500
H	2.79508900	-0.02541200	0.11809800
H	2.92235800	2.26925400	0.64025100
O	2.84406900	-1.00881500	-0.01727000
H	3.72787500	-1.23807200	-0.32036600
H	1.51438400	-1.76289800	-0.20551600

Solvent-bridged protonated $(C_6H_5NH_2 + H)^+ \bullet (H_2O)_4$



C	-2.37304900	0.40272400	1.18655500
C	-2.16356300	0.61391500	-1.20805200
C	-1.46077500	-0.58760700	-1.25532700
C	-1.22768700	-1.30643100	-0.07944600
C	-1.67284100	-0.80041900	1.14476000
H	-2.73813300	0.77363200	2.13717800
H	-2.36393700	1.15144600	-2.12748400
H	-1.11660100	-0.97746800	-2.20766800
H	-1.49555700	-1.35612000	2.05973200
N	-0.49585400	-2.53610900	-0.12734500
H	-0.73582800	-3.14452700	0.65059900
H	-0.68393300	-3.04677600	-0.98589900
C	-2.62636800	1.11522000	0.01167300
H	-3.21036200	2.02802600	0.04030100
H	-0.65126600	2.22438600	0.16934400
O	0.15112600	2.75872600	0.27625000
H	1.65253500	2.33044400	-0.16291200
H	-0.07333700	3.50289800	0.84435500
O	3.49958000	-0.08432100	0.33357000
H	3.86084400	-0.02452600	1.22666000
H	2.91442900	-0.95426500	0.20042600
O	2.20715800	-2.15674400	0.02499500
H	2.64390400	-2.88541300	-0.42840500
H	1.21069800	-2.28268800	-0.03988700
O	2.57714100	2.04281400	-0.39311200
H	3.07091800	0.85128900	-0.00080500
H	2.85227000	2.45421800	-1.21872300

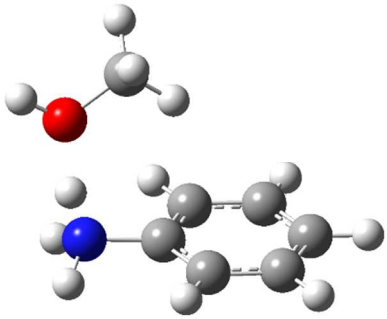
Solvent-bridged protonated $(C_6H_5NH_2 + H)^+ \bullet (H_2O)_5$



C	-1.93890000	-0.11713700	1.03689500
C	-2.54664500	-2.10498800	-0.34067400
C	-1.23902700	-2.35513700	-0.55221900
C	-0.23687100	-1.48274000	0.00984800
C	-0.63199900	-0.36371600	0.81889400
H	-2.22796100	0.75422900	1.61090500
H	-3.29742300	-2.75939000	-0.77036800
H	-0.91830800	-3.20270000	-1.14814400
H	0.13194400	0.29090200	1.21623100
N	1.04544600	-1.70938600	-0.21715600
H	1.77376600	-1.08688700	0.14439300
H	1.33525200	-2.48717300	-0.79294800
C	-3.01208400	-0.94174600	0.44435100
H	-3.74610100	-1.24694700	1.20359100
H	-3.58360800	-0.25959700	-0.21451600
O	-3.26744400	1.78932400	-0.89686000
H	-2.52747400	2.28423500	-0.49827200
H	-3.79590600	2.43129700	-1.37914600
O	3.06512600	0.18887400	0.68761500
H	3.16997100	0.41397300	1.61923800
H	3.97633700	0.04518900	0.34702900
O	5.58496500	-0.21655500	-0.29401700
H	6.14130300	0.46061200	-0.69437800
H	6.16495600	-0.95893700	-0.09231000
O	-1.02306100	2.82093700	0.46076000
H	-0.18479200	2.57246300	0.02444000
H	-0.92225200	3.73464300	0.74491300
O	1.28597700	1.85651600	-0.76001400
H	2.03110300	1.42267900	-0.30902600
H	1.62971700	2.23711800	-1.57398300

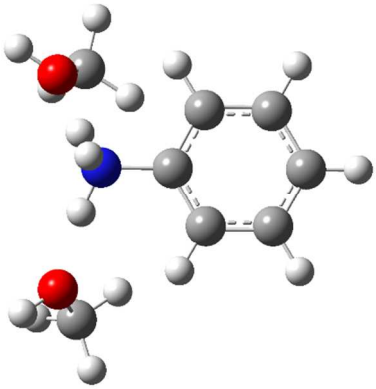
The atomic coordinates and structures of $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_n$ (n = 0–5)

N-protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)$



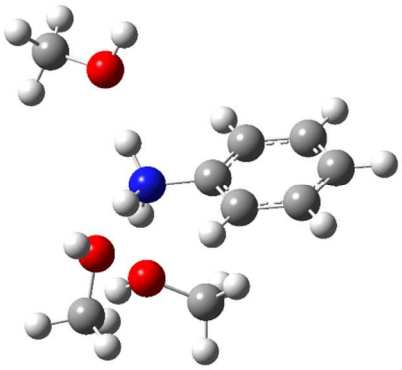
C	0.31633400	-0.82530400	0.00074600
C	0.84837800	-0.42480300	-1.21719400
C	1.96393200	0.41108300	-1.20976500
C	2.51810600	0.82919000	-0.00057700
C	1.96322500	0.41395500	1.20928800
C	0.84768600	-0.42192700	1.21804600
H	0.41262000	-0.75127900	-2.15557100
H	2.39879000	0.72907300	-2.14915400
H	3.38691300	1.47592400	-0.00109800
H	2.39754700	0.73418000	2.14816600
H	0.41136800	-0.74615500	2.15694300
N	-0.90831000	-1.66366200	0.00140200
H	-0.94406400	-2.26706000	0.82595500
H	-1.77016000	-1.03651100	0.00080400
H	-0.94396000	-2.26849300	-0.82208500
C	-2.56915100	1.54069700	-0.00169600
H	-1.48281500	1.61564600	-0.00173400
H	-2.96698600	2.02039300	0.89431100
H	-2.96692800	2.01836500	-0.89881000
O	-2.88341300	0.12401100	-0.00009300
H	-3.83790400	-0.00788500	0.00011100

N-protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_2$



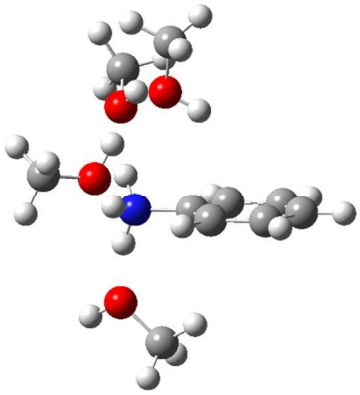
C	-0.61786800	-0.09651500	-0.62315600
C	-1.42409400	1.01746700	-0.42174100
C	-2.67809200	0.83589500	0.15875800
C	-3.10254500	-0.44085200	0.52562600
C	-2.27732700	-1.54385300	0.31195600
C	-1.02052400	-1.37805200	-0.26866600
H	-1.08117700	2.00464500	-0.70938700
H	-3.32100000	1.69207000	0.32224600
H	-4.07821600	-0.57623800	0.97628300
H	-2.60911000	-2.53547300	0.59430900
H	-0.36958900	-2.22708900	-0.44157000
N	0.71202100	0.09153900	-1.24575600
H	1.12936400	1.00494200	-0.94504500
H	1.36596300	-0.67868000	-0.96870200
H	0.64174300	0.09532100	-2.26579300
O	2.28273400	-1.99397900	-0.37309100
H	2.96339600	-2.46524600	-0.86569000
O	1.59839100	2.51578100	-0.30577100
H	2.21265300	3.12737400	-0.72595500
C	1.38957000	2.89850100	1.07340500
H	0.65655800	2.20313100	1.48062500
H	2.31822800	2.82417300	1.64372200
H	0.99093400	3.91333300	1.13504400
C	2.38970300	-2.30541500	1.03506200
H	3.34110900	-1.95502400	1.44151600
H	1.57021800	-1.78606100	1.53093100
H	2.28283400	-3.37943100	1.20119200

N-protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_3$



C	-0.65503600	0.43178700	-0.31008600
C	-1.50368200	-0.34016800	-1.09370300
C	-2.84277200	0.03541900	-1.20099800
C	-3.31174400	1.16329900	-0.52993400
C	-2.44280100	1.92557400	0.25109500
C	-1.10277100	1.56152300	0.36600100
H	-1.12455900	-1.21362800	-1.61124400
H	-3.51595600	-0.55399400	-1.81160400
H	-4.35255900	1.45061900	-0.61722100
H	-2.80587800	2.80423100	0.77031000
H	-0.41687400	2.14574800	0.96909900
N	0.75104400	0.02512500	-0.14813200
H	1.02012300	-0.69394100	-0.84862500
H	1.38296400	0.84925300	-0.23089900
H	0.86950600	-0.41932200	0.78645200
O	2.24063000	2.36330400	-0.34899800
H	1.93310800	3.07261800	-0.92340400
O	1.28217100	-2.20968800	-1.70987700
H	1.62070300	-2.36355300	-2.59797400
O	0.59433900	-1.43997600	2.19721500
H	1.24431000	-1.66182000	2.87225900
C	3.58829500	2.63865400	0.08797200
H	3.87917800	1.81722300	0.74203900
H	4.27558600	2.68191800	-0.76050000
H	3.63032900	3.57351000	0.65168700
C	-0.73719600	-1.54676100	2.75189000
H	-0.86978400	-0.85783600	3.58961900
H	-1.42746400	-1.27620700	1.95415700
H	-0.94022800	-2.57084200	3.07350800
C	1.27516700	-3.44278300	-0.95898400
H	2.27887700	-3.87043400	-0.89608900
H	0.93024700	-3.19104900	0.04448300
H	0.58918600	-4.16676500	-1.40537300

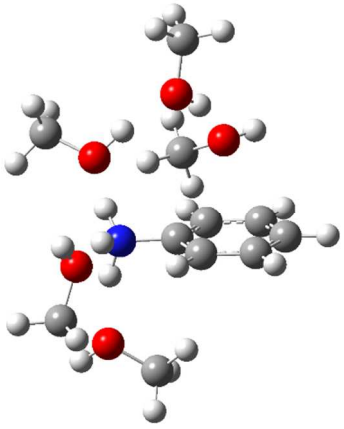
N-protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_4$



C	-0.89775300	-0.37289400	0.11457300
C	-0.66511500	-0.89909700	1.38127300
C	-1.00573500	-2.23008100	1.63058100
C	-1.57111500	-3.01129800	0.62381900
C	-1.79936800	-2.46477500	-0.63962100
C	-1.46056000	-1.13904700	-0.90117100
H	-0.22484900	-0.28147300	2.15530500
H	-0.83465900	-2.64936300	2.61489900
H	-1.83712300	-4.04241000	0.82306100
H	-2.24022700	-3.06958400	-1.42280100
H	-1.63151800	-0.70674100	-1.88046500
N	-0.54643500	1.02469500	-0.16917000
H	0.07827500	1.40109000	0.57641100
H	0.02880200	1.06030000	-1.04164400
H	-1.40855300	1.60189100	-0.26534100
O	1.42841900	0.70506200	-1.99032400
H	1.98450200	0.13159300	-1.43551600
O	1.50530000	1.45174800	1.60500300
H	2.09738200	0.77935200	1.22673700
O	-3.03495400	2.20042400	-0.40093000
H	-3.30272900	3.08018400	-0.68577800
C	1.72774200	0.52495800	-3.38203400
H	1.07781700	1.19758200	-3.94094600
H	2.76776400	0.78681700	-3.59513500
H	1.53512600	-0.50409900	-3.70138700
C	-4.16792800	1.49360100	0.14733600
H	-4.95192200	1.37374100	-0.60431700
H	-3.80549300	0.50973600	0.44331600
H	-4.56590200	2.00970700	1.02453200
C	2.26009700	2.56254800	2.11694900
H	2.83431200	3.05265200	1.32488500
H	1.54503700	3.27315100	2.53011500
H	2.93440500	2.23988500	2.91476800

C	3.86914500	-1.33737800	0.24143300
H	4.55883200	-0.54571000	-0.04744300
H	3.98008800	-2.18080400	-0.44382100
H	4.09095800	-1.65505500	1.26285600
O	2.53752600	-0.77549900	0.15569600
H	1.88794700	-1.44839300	0.39751700

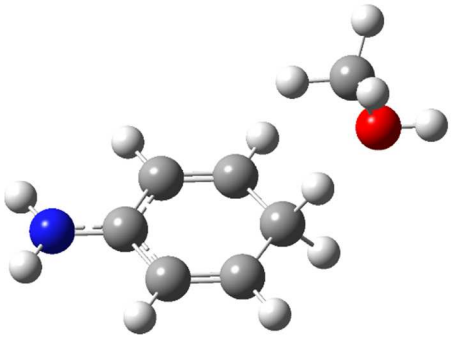
N-protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_5$



C	0.81500600	-0.59159900	-0.40088700
C	1.65525100	-1.24720600	-1.29347800
C	1.35579700	-2.55988800	-1.65632100
C	0.23137700	-3.19430700	-1.12965800
C	-0.60176200	-2.51595600	-0.24081400
C	-0.31190400	-1.20591200	0.13081700
H	2.52153800	-0.73786900	-1.69922900
H	1.99963300	-3.08248600	-2.35347200
H	0.00226600	-4.21356000	-1.41693100
H	-1.48503700	-2.99503300	0.16277900
H	-0.96351600	-0.67309800	0.81077600
N	1.13889600	0.77881900	0.02441100
H	1.80496600	1.22688900	-0.63093000
H	0.26077300	1.35824500	0.10361800
H	1.61859300	0.74209300	0.94440300
O	-1.26248300	1.99996100	0.25103500
H	-1.93147700	1.53038200	-0.30755200
O	3.31363400	1.72620100	-1.45500300
H	3.43504600	2.23633500	-2.26224500
O	2.76337100	0.23218100	2.23014000
H	2.98188700	0.73669400	3.02063900
C	-1.64666600	3.36757300	0.43114000
H	-0.91236900	3.83829000	1.08616400
H	-1.66880700	3.90640700	-0.52154700

H	-2.63065800	3.43625000	0.90506200
C	2.92061100	-1.17895900	2.49828300
H	2.25659600	-1.50300900	3.30377100
H	2.64938200	-1.70042800	1.58148400
H	3.95745300	-1.41181900	2.75296600
C	4.54354500	1.68751000	-0.70228500
H	4.87212200	2.69437200	-0.43133500
H	4.33095800	1.12398200	0.20689700
H	5.33063300	1.17952300	-1.26540300
C	-3.97247700	0.78316600	-2.09295900
H	-3.56386900	1.54892300	-2.75253700
H	-4.90212800	1.15657800	-1.65061500
H	-4.18571600	-0.11062200	-2.68685100
O	-2.98554900	0.50909200	-1.09316400
H	-3.30686300	-0.16491100	-0.46528800
C	-3.58696200	-0.19062300	2.21843200
H	-2.84796900	0.58547300	2.01648400
H	-4.56811300	0.27627900	2.34399000
H	-3.31176800	-0.72116800	3.13417200
O	-3.56582000	-1.07679300	1.08303900
H	-4.23195700	-1.76238600	1.19785800

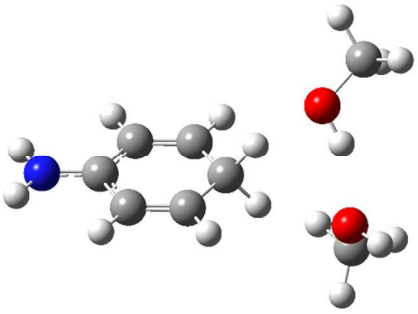
p-protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)$



C	-0.31805300	1.24782500	0.83057500
C	-0.31577200	-1.24182400	0.83681200
C	-1.43156100	-1.24654700	0.07568500
C	-2.02427900	-0.00148000	-0.33274000
C	-1.43386300	1.24669500	0.06948200
H	0.12547400	2.18940300	1.13560500
H	0.12958800	-2.18103800	1.14640700
H	-1.89757400	-2.17590800	-0.23238600
H	-1.90163900	2.17365300	-0.24310400
C	0.35333800	0.00465600	1.25281900
H	1.39282500	0.00426800	0.84571300
H	0.53666400	0.00757200	2.33805700

N	-3.11943400	-0.00429000	-1.08006200
H	-3.55971200	0.85579400	-1.37722200
H	-3.55820300	-0.86658900	-1.37299800
O	3.19117900	-0.00365500	0.11316600
H	3.99449100	-0.00404000	0.64383200
C	3.54043700	-0.00025900	-1.28105900
H	2.60315000	0.00071600	-1.83841800
H	4.10977900	0.89483000	-1.54785800
H	4.11028200	-0.89378700	-1.55196500

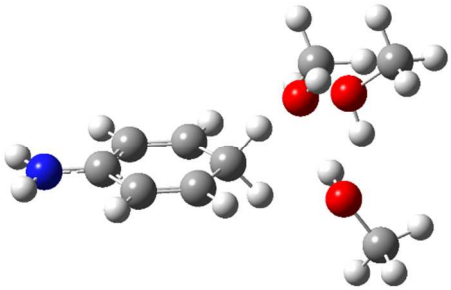
p-protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_2$



C	0.62711700	0.66854500	0.43738700
C	1.45403000	-0.83435900	-1.37453500
C	2.71061800	-0.72054000	-0.89532700
C	2.96397700	0.09211900	0.26635800
C	1.88534300	0.78167500	0.91715600
H	-0.20572200	1.19236000	0.89246100
H	1.26599800	-1.44585800	-2.25052700
H	3.54238600	-1.22871400	-1.37059600
H	2.10228600	1.39441800	1.78524400
C	0.30592500	-0.15256500	-0.74595900
H	-0.48641300	-0.87917100	-0.48847200
H	-0.23347200	0.48067900	-1.46994400
N	4.20068400	0.20483900	0.73218400
H	4.40977900	0.77083300	1.54306600
H	4.97850500	-0.26485300	0.28965100
O	-2.72279400	-1.49489200	-0.15181100
H	-3.19518900	-1.97918700	-0.83761600
C	-3.11973900	-1.99777500	1.14042800
H	-2.58776900	-1.40165600	1.88139400
H	-4.19534800	-1.88157800	1.29816300
H	-2.84050800	-3.04836600	1.25630400
C	-3.29793700	2.25863500	-0.29485700
H	-2.82417300	3.24056900	-0.27718400
H	-3.88711900	2.17461600	-1.21474000
H	-3.96859000	2.18048000	0.56825500

O	-2.25440700	1.28199900	-0.24473500
H	-2.63783900	0.39028400	-0.26228200

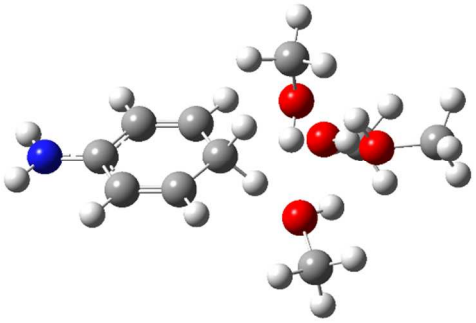
p-protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_3$



C	1.18199700	0.77989600	-0.02290700
C	1.93291300	-1.59647200	0.01362900
C	3.22139000	-1.19157600	0.00273700
C	3.52862200	0.21373600	-0.02206000
C	2.47197600	1.18543400	-0.03422800
H	0.36626500	1.49667500	-0.03411800
H	1.70193700	-2.65616400	0.03153300
H	4.03650900	-1.90670700	0.01167700
H	2.72903600	2.23888200	-0.05298400
C	0.80823900	-0.64546600	0.00182400
H	0.12318000	-0.83060500	0.85185700
H	0.11891700	-0.86190600	-0.83653100
N	4.79556800	0.61051400	-0.03400900
H	5.04167000	1.59038800	-0.05211200
H	5.55795900	-0.05255200	-0.02614600
O	-1.99986400	-0.60494600	1.45742900
H	-2.07464900	0.33620700	1.20987300
O	-2.07699900	-0.88484500	-1.28818500
H	-2.26286400	-1.14265300	-0.36656400
O	-1.89433400	1.63046300	-0.16315400
H	-2.06606200	0.95038300	-0.84189500
C	-2.73999900	2.76943100	-0.37791000
H	-2.53136900	3.48203700	0.41990700
H	-2.52687800	3.24442400	-1.34039800
H	-3.79905700	2.49487200	-0.33778200
C	-2.94682100	-1.57938800	-2.19393300
H	-3.99806900	-1.34880900	-1.99422500
H	-2.69721200	-1.24440900	-3.20035200
H	-2.79662100	-2.66158400	-2.13450200
C	-2.76566400	-0.87533800	2.63987600
H	-3.82748000	-0.65838000	2.48568900
H	-2.65272400	-1.93607500	2.86303500

H	-2.39781100	-0.29453700	3.49121800

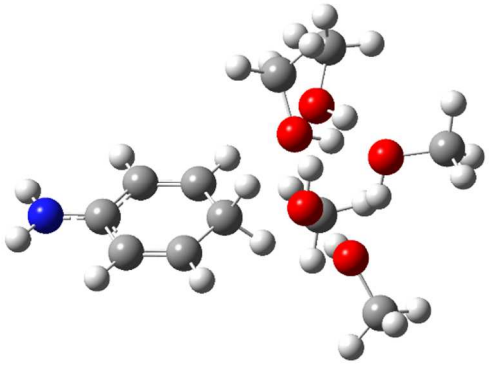
p-protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_4$



C	-1.64834200	-1.00745700	-0.64243400
C	-1.85468500	1.19283200	0.51324300
C	-3.19821400	1.04740100	0.55112000
C	-3.80437900	-0.12895600	-0.00659600
C	-2.99127900	-1.15171900	-0.60792100
H	-1.01258300	-1.76159100	-1.09198500
H	-1.36873900	2.08027600	0.90149400
H	-3.83537400	1.80914400	0.98695300
H	-3.47635600	-2.02547200	-1.02923100
C	-0.97304700	0.17132900	-0.07558400
H	-0.22917900	-0.15931200	0.67368700
H	-0.32488700	0.65383200	-0.82413600
N	-5.12472600	-0.27220600	0.02730300
H	-5.57837800	-1.08576900	-0.36356500
H	-5.72116200	0.43090400	0.44027000
O	1.48252600	-1.33265700	1.50618500
H	1.47100900	-1.86660700	0.69095400
O	2.74981800	0.55807100	0.01424400
H	2.47702000	0.01764600	0.78385600
O	1.48075200	-1.65608000	-1.21534200
H	2.00367600	-0.83859300	-1.13057000
C	2.05956000	-2.49414100	-2.22630100
H	1.47319700	-3.41256700	-2.26043500
H	2.01973700	-2.01358100	-3.20854000
H	3.09766700	-2.74969200	-1.99062100
C	4.15789200	0.84080700	0.08475600
H	4.74406400	-0.08273500	0.11002400
H	4.42025100	1.40217900	-0.81155500
H	4.39383900	1.44497300	0.96542900
C	1.70830500	-2.15280400	2.66156500
H	2.66390800	-2.68208200	2.59524700
H	1.73073400	-1.49025600	3.52625200

H	0.90025100	-2.87877300	2.79316500
C	1.25426100	3.88845100	-0.48448000
H	0.37406700	4.52766200	-0.56705000
H	1.78216200	3.90351200	-1.44517400
H	1.91062000	4.30283800	0.28960900
O	0.80276900	2.57624900	-0.14826200
H	1.57018300	1.98038200	-0.08401700

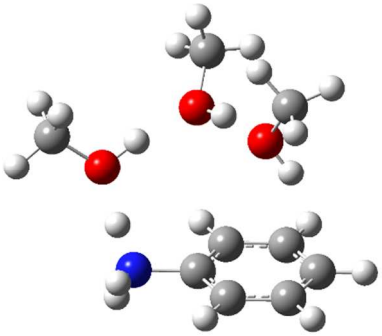
p-protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_5$



C	-1.56959700	-0.16748900	-0.55205800
C	-2.52921700	0.32066900	1.68436000
C	-3.77692600	0.13416500	1.19410600
C	-3.95520200	-0.20549500	-0.18894900
C	-2.81723300	-0.35430300	-1.04631600
H	-0.70281500	-0.27078000	-1.19456700
H	-2.39474600	0.57727600	2.72960300
H	-4.65117000	0.23356500	1.82798100
H	-2.97475800	-0.62079600	-2.08571100
C	-1.33331900	0.22125000	0.84232800
H	-0.54139700	-0.39078500	1.30646400
H	-0.80994800	1.22149200	0.83371800
N	-5.18313400	-0.38239600	-0.67368900
H	-5.33773300	-0.62330000	-1.64190100
H	-6.00062300	-0.28241800	-0.08961600
O	1.09331500	-2.26566800	-0.80698300
H	1.34225800	-1.47671400	-1.33306000
O	2.55296400	1.04821200	0.65234300
H	2.26017600	0.23593900	1.13356700
O	1.57323900	0.22496000	-1.78312900
H	2.02720100	0.61466100	-1.00673900
C	2.17088300	0.70950400	-2.99217300
H	1.63142500	0.26164100	-3.82700100
H	2.08543400	1.79848000	-3.06379800
H	3.22602500	0.42573100	-3.06055500

C	3.91304400	1.36228800	0.99614800
H	4.58171700	0.53381300	0.74440300
H	4.20293700	2.24072300	0.41983800
H	4.00213000	1.59262700	2.06125600
C	1.61954600	-3.45276800	-1.41192800
H	2.71365400	-3.43077200	-1.45809900
H	1.30971000	-4.29848400	-0.79777600
H	1.21929600	-3.58951100	-2.42124400
C	0.25583100	3.39548400	-0.52912800
H	-0.70607800	3.90805400	-0.56743400
H	0.32794400	2.70789800	-1.38143300
H	1.04860400	4.14709300	-0.60680600
O	0.32108200	2.69606300	0.71446100
H	1.18767800	2.25154200	0.77826400
C	1.92468700	-2.04205500	2.72273900
H	2.02179900	-1.40042500	3.59875700
H	1.18581500	-2.82037900	2.93621100
H	2.89259500	-2.51076500	2.51796300
O	1.50001500	-1.21919400	1.62812800
H	1.39489600	-1.76110700	0.81021000

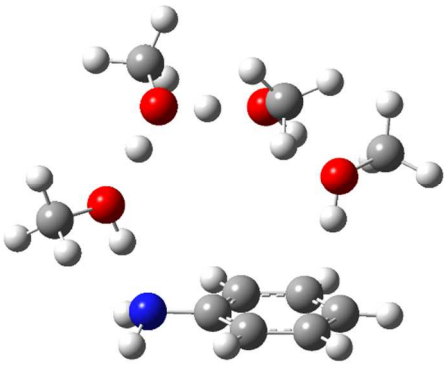
Solvent-bridged protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_3$



C	-1.83371000	0.14891000	1.61391400
C	-3.15792000	-0.26113200	-0.36915700
C	-2.23794200	-1.22081400	-0.78960000
C	-1.12881500	-1.47712800	0.00609800
C	-0.90413400	-0.80266700	1.19997600
H	-1.67391400	0.68009100	2.54407000
H	-4.03132800	-0.05556300	-0.97573200
H	-2.39427700	-1.75604600	-1.72025100
H	-0.01567700	-0.99587700	1.78859900
N	-0.13542600	-2.48214600	-0.41950500
H	-0.18990900	-3.32260400	0.16039400
H	-0.29293000	-2.76817200	-1.38630200
C	-2.95857900	0.41951000	0.83269400
H	-3.68367000	1.15336600	1.16419300

H	-1.11859200	1.79185800	-0.46226000
O	-0.23723800	1.93696500	-0.82464100
H	1.08670300	1.41846500	0.17503200
O	1.77627400	0.97549100	0.71421600
H	2.11090100	-0.50783100	0.23995100
O	2.17717800	-1.46102600	-0.06056300
H	0.90173800	-2.06671600	-0.32866700
C	-0.24727000	3.07748400	-1.70220700
H	0.76396900	3.18038000	-2.09404200
H	-0.93559800	2.92191900	-2.53730100
H	-0.51731300	3.99136900	-1.16552900
C	2.66789800	1.93605500	1.29717200
H	3.36659400	1.39116400	1.93190100
H	3.23016900	2.47605600	0.52912800
H	2.11638600	2.65017500	1.91486800
C	3.37579500	-1.68090300	-0.82578300
H	3.38352800	-2.72347700	-1.14502100
H	3.40573100	-1.03101200	-1.70455300
H	4.25382600	-1.49985100	-0.20269100

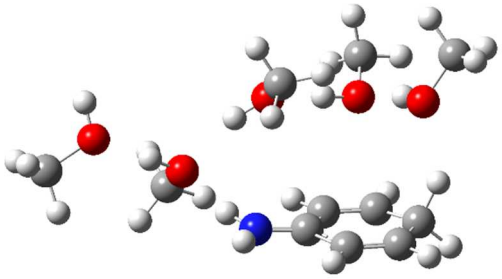
Solvent-bridged protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_4$



C	3.04840400	-0.23352900	-1.08798400
C	2.85435500	-0.27777400	1.31533100
C	1.93921800	-1.32409400	1.22489800
C	1.58741100	-1.84073900	-0.02610600
C	2.13559900	-1.28074100	-1.18434900
H	3.48634300	0.17599400	-1.99080700
H	3.13905200	0.09913600	2.29076500
H	1.51659300	-1.75416000	2.12704400
H	1.86902000	-1.67881300	-2.15800700
N	0.63730000	-2.90193500	-0.11725700
H	0.74246200	-3.43376200	-0.97598200
H	0.71821000	-3.54837500	0.66217500
C	3.41619800	0.27312700	0.16059500

H	4.15049600	1.06651700	0.23500100
H	1.53587000	1.57703500	0.19480100
O	0.90969500	2.29009000	0.00278500
H	-0.66357300	2.21334100	0.28222900
O	-2.89631700	0.30297400	-0.39722400
H	-2.47450100	-0.62908600	-0.23334200
O	-1.99274500	-1.98354200	-0.02591200
H	-1.04659200	-2.27899700	-0.08143100
O	-1.64766700	2.19159400	0.44137900
H	-2.30433500	1.13811900	0.00317000
C	1.52102200	3.25514400	-0.87097200
H	0.76856100	4.01428200	-1.08158400
H	2.37857400	3.72801000	-0.38594500
H	1.83479800	2.78999600	-1.80930500
C	-1.99593300	2.78278700	1.71130800
H	-3.07928700	2.72867400	1.80989400
H	-1.52303500	2.24228500	2.53441300
H	-1.68446100	3.82792900	1.72326100
C	-3.31651900	0.49354400	-1.77550000
H	-4.00506200	-0.30978300	-2.03037800
H	-3.82763100	1.45243600	-1.83019800
H	-2.45256600	0.48294100	-2.44176400
C	-2.77962800	-2.93179600	0.71640000
H	-2.39962200	-3.04362300	1.73562500
H	-3.79936700	-2.55001900	0.75914900
H	-2.78552800	-3.90103100	0.21205300

Solvent-bridged protonated $(C_6H_5NH_2 + H)^+ \bullet (CH_3OH)_5$



C	1.95306000	1.04264700	1.34919900
C	2.28784800	3.01127700	-0.14047500
C	0.96009700	3.05958900	-0.37260200
C	0.09061600	2.06705000	0.20788900
C	0.62773200	1.08279300	1.10543800
H	2.35258000	0.26394300	1.98721300
H	2.94208500	3.74659300	-0.59625500
H	0.52859900	3.82386100	-1.00989300
H	-0.04314900	0.35791900	1.54515600

N	-1.19873000	2.05204200	-0.08743900
H	-1.81889700	1.29719300	0.23806200
H	-1.58413100	2.73685000	-0.72250800
C	2.90580000	1.95340000	0.68418900
H	3.64616000	2.36096200	1.38400900
H	3.49864600	1.29563600	0.00760200
O	3.37898300	-0.54482600	-0.95246300
H	2.96288400	-1.14276000	-0.29865700
O	-2.73159700	-0.25026800	0.55489900
H	-3.52281000	-0.37386100	-0.01940000
O	-4.90791200	-0.57563300	-0.99823800
H	-5.02073900	-1.34783200	-1.56209800
O	1.93067700	-2.00146500	0.89537100
H	1.03398400	-1.90776200	0.51467600
O	-0.39983200	-1.50558000	-0.42886000
H	-1.28183100	-1.20941200	-0.14597200
C	4.28472100	-1.29173800	-1.76448000
H	3.77323800	-2.09858100	-2.30310400
H	4.71239700	-0.60681300	-2.49781500
H	5.10103300	-1.72323500	-1.17374200
C	2.16980100	-3.37291100	1.23148100
H	2.08461400	-4.02326800	0.35434500
H	3.18503400	-3.44127500	1.62335600
H	1.47372100	-3.71862400	2.00239800
C	-0.13884600	-1.07345300	-1.76955500
H	-0.48279600	-0.04586100	-1.93029900
H	0.94136300	-1.09834500	-1.91771200
H	-0.62265800	-1.73145400	-2.49807500
C	-3.06585600	-0.66326900	1.89397900
H	-3.40095600	-1.70342700	1.90723500
H	-2.16445700	-0.57667000	2.50150700
H	-3.84315500	-0.02238500	2.31882100
C	-6.19175100	0.01710300	-0.71746200
H	-6.83882600	-0.67834400	-0.17644000
H	-6.00227100	0.88895700	-0.09209200
H	-6.68043700	0.34095000	-1.63952300