On the molecular structure and geometry of pyridylalkylamine–H^+ complexes. Application to catalytic enantioselective hydroxyalkylation of indoles

Sylvain Marque,* Vanessa Razafimahaléo, Aurelia Dinut, Guillaume Grach, Damien Prim, Xavier Moreau, and Richard Gil

[a] Université de Versailles-St-Quentin (UVSQ), Institut Lavoisier de Versailles (ILV) UMR CNRS 8180, 45 Avenue des Etats-Unis, 78 035 Versailles Cedex, France. Fax: (+33) 1 39 25 44 52; Tel: (+33) 1 39 25 44 40; E-mail: sylvain.marque@chimie.uvsq.fr

[b] Université Paris-Sud, Institut de Chimie Moléculaire et des Matériaux d'Orsay (ICMMO), Équipe de catalyse moléculaire, bâtiment 420, 91 405 Orsay Cedex, France.

Supporting Information

Contents

Analytical

Calculation part (T = 298.15 K, P = 1 atm)

Analytical

General

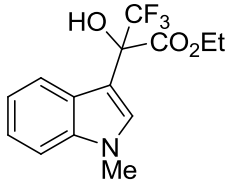
Enantiomeric excesses (ee) were determined by chiral HPLC analyses on:

CHIRALPAK IA column 250 × 4.6 (L × I.D.) 5 µm, hexane/propan-2-ol at, 254 nm, 20 °C
- for **A** hex/iPrOH v/v: 9/1, 0.5 mL.min^{-1} 18.64 min (*S*), 21.72 min (*R*);
- for **B** hex/iPrOH v/v: 85/15, 0.7 mL.min^{-1} 13.05 min (major), 15.85 min (minor);
- for **C** hex/iPrOH v/v: 85/15, 0.7 mL.min^{-1} 11.92 min (minor), 14.55 min (major);

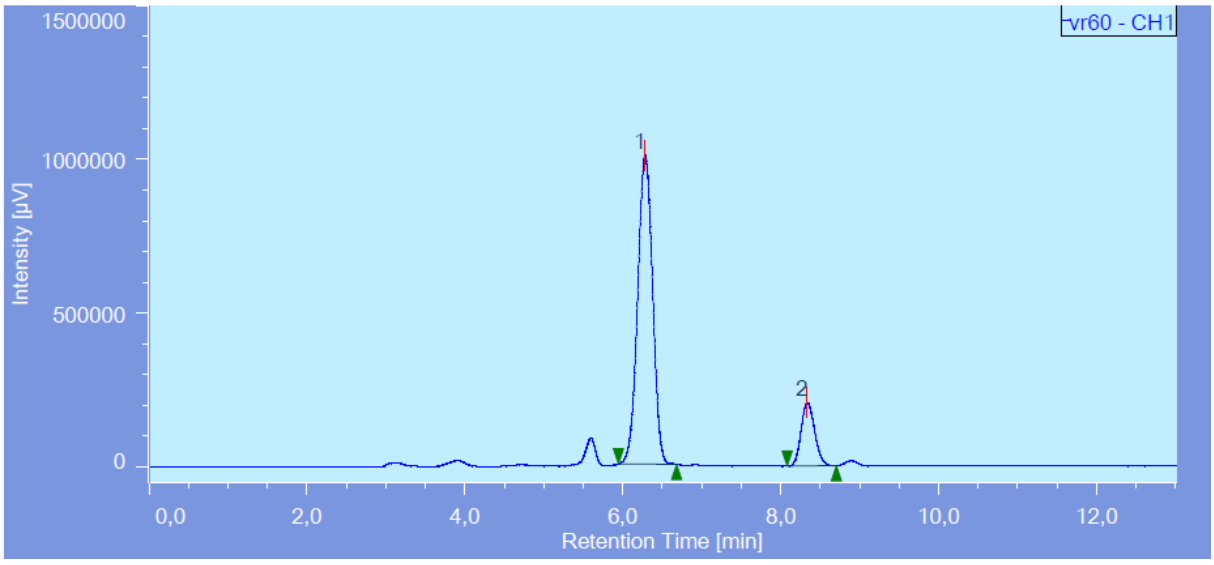
OD-H column, heptane/propan-2-ol (85/15, 1.0 mL.min^{-1}), with a UV/Vis detector at 30°C
- for **A** 6.282 min (*S*), 8.335 min (*R*);
- for **B** 7.563 min (major), 8.535 min (minor);
- for **C** 7.828 min (minor), 9.397 min (major).

A sample was prepared with 3 mL (C = 1 g.mL) of a mixture of Hept/iPrOH: 85/15 in a glass vial, then injected in the HPLC device to determine the enantiomeric excess.

HPLC Chromatogram of **A**



A

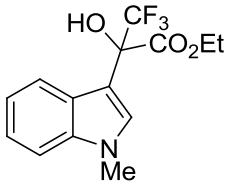


Conditions
Volume: 20,00 µL
Acquisition Sequence: OD H with Heptane/isopropanol 85/15, 1.0 mL.min^{-1}

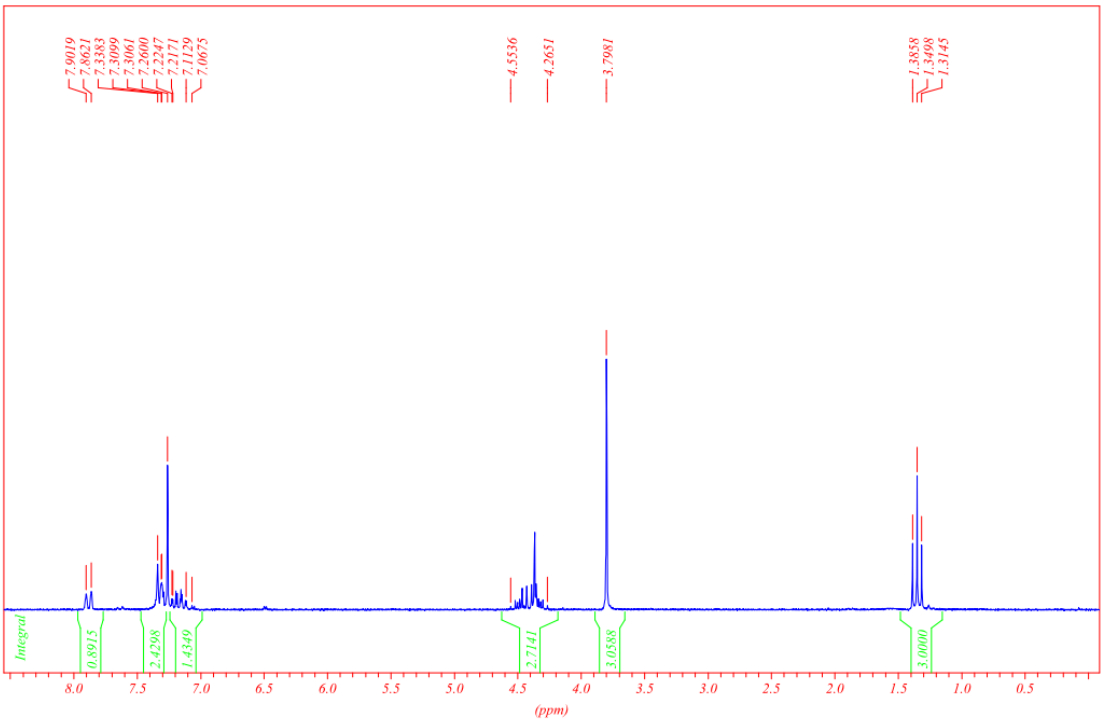
Decision

Peak	t_R (min)	Area (µV.s)	Height (µV)	Area (%)	Height (%)	Symmetry Factor
1	6.282	13187158	1002981	84.221	82.936	0.985
2	8.335	2470646	206364	15.779	17.064	1.128

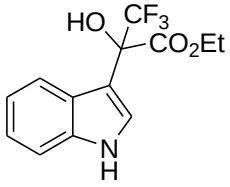
^{1}H NMR of **A**



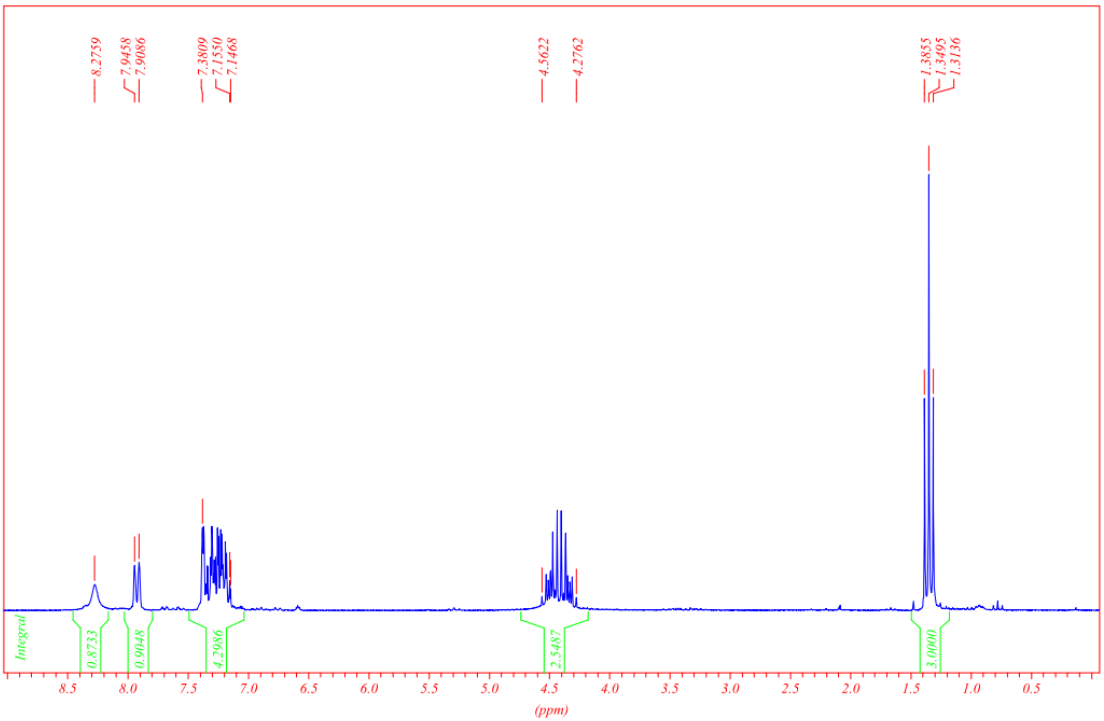
A



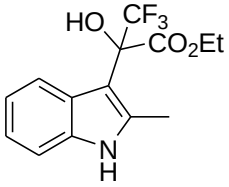
^{1}H NMR of **B**



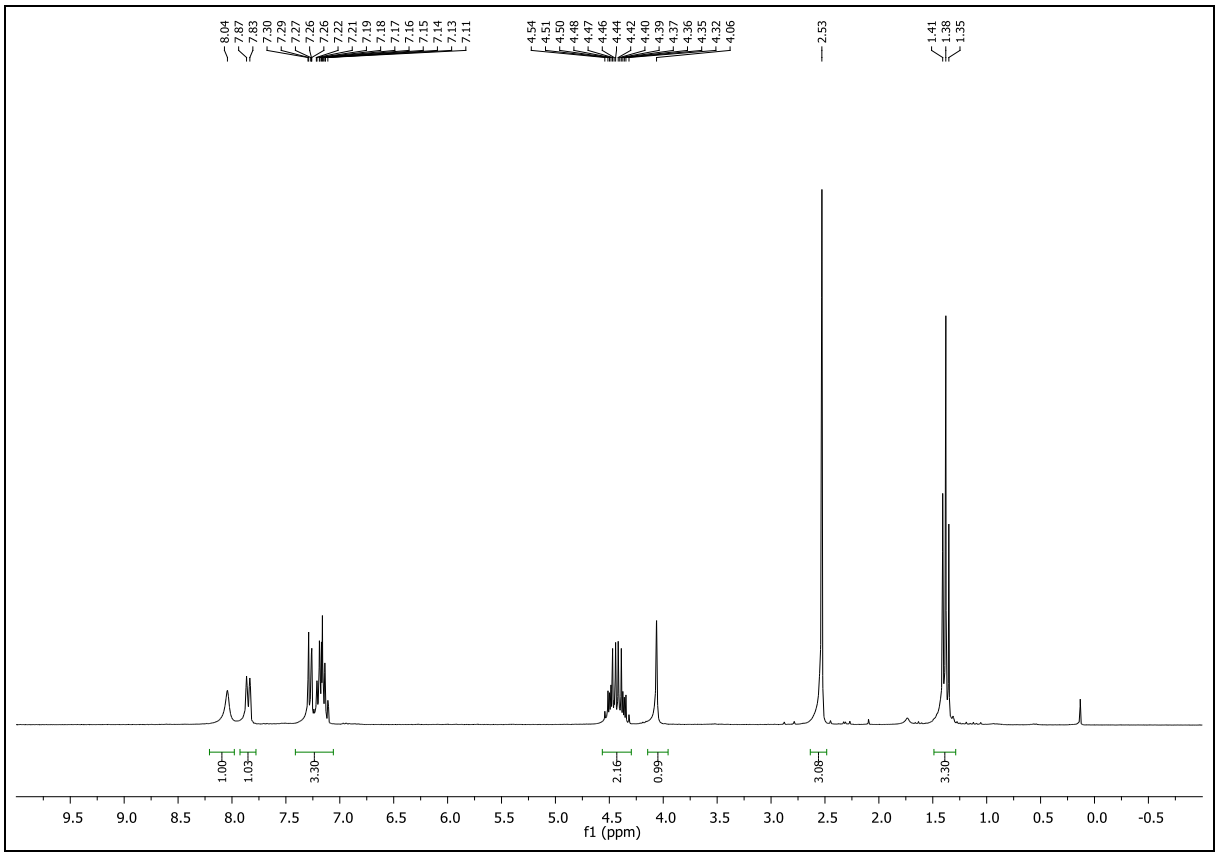
B



^{1}H NMR of **C**



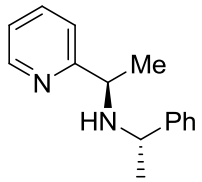
C



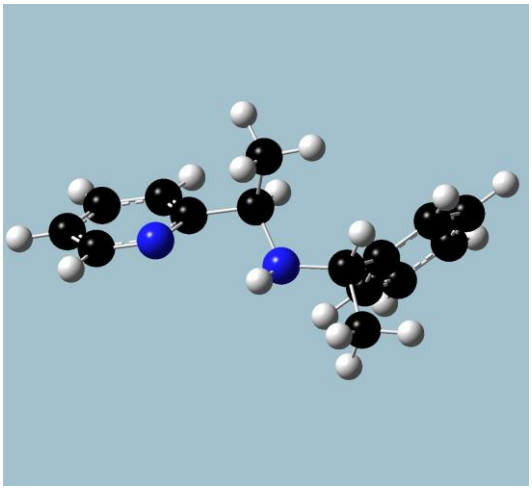
Calculation part (T = 298.15 K, P = 1 atm)

Images of the optimized geometries are given above the corresponding Cartesian coordinates

Cartesian coordinates of the (*R*,*S*)-**1** species



(*R*,*S*)-**1**

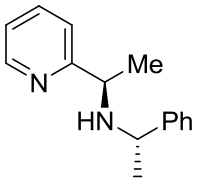


B3LYP/6-31+G(d), gas phase

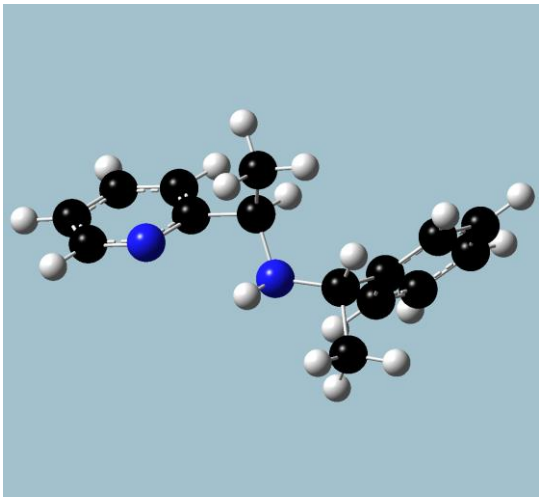
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.751064	0.338634	0.742307
2	7	0	0.123079	1.022536	-0.397666
3	1	0	0.728638	1.786079	-0.693686
4	6	0	-1.256189	1.487725	-0.229089
5	1	0	-1.383585	2.096536	0.684131
6	6	0	-1.614441	2.387436	-1.425253
7	1	0	-2.645306	2.747206	-1.341241
8	1	0	-0.950779	3.261344	-1.465464
9	1	0	-1.514961	1.833629	-2.365255
10	6	0	-2.226560	0.314078	-0.126036
11	6	0	-3.289091	0.350269	0.786136
12	6	0	-2.106592	-0.799068	-0.971556
13	6	0	-4.218387	-0.693192	0.850995
14	1	0	-3.390882	1.203460	1.455115
15	6	0	-3.030828	-1.844265	-0.908889
16	1	0	-1.274320	-0.839821	-1.669117
17	6	0	-4.091724	-1.795303	0.002144
18	1	0	-5.035347	-0.646139	1.567204
19	1	0	-2.922954	-2.700119	-1.571426
20	1	0	-4.809812	-2.610202	0.051315
21	6	0	2.128007	-0.134136	0.299881
22	6	0	2.510545	-1.478587	0.386773
23	6	0	3.794022	-1.847328	-0.017145
24	1	0	1.809147	-2.220092	0.760099
25	6	0	4.184884	0.452153	-0.555437
26	6	0	4.655519	-0.861969	-0.500847
27	1	0	4.113236	-2.885094	0.040422
28	1	0	4.822239	1.252140	-0.929181
29	1	0	5.663333	-1.099693	-0.829268
30	7	0	2.957983	0.815313	-0.164121
31	1	0	0.143020	-0.547029	0.961844
32	6	0	0.870777	1.180103	2.032681
33	1	0	1.479306	2.073096	1.849827
34	1	0	-0.113999	1.491953	2.396843
35	1	0	1.349543	0.598497	2.830347

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.753190	0.349959	0.733071
2	7	0	0.123144	1.047208	-0.401880
3	1	0	0.710792	1.840041	-0.655975
4	6	0	-1.264475	1.496698	-0.218835
5	1	0	-1.387652	2.088764	0.703917
6	6	0	-1.636916	2.413592	-1.397117
7	1	0	-2.666495	2.772263	-1.294003
8	1	0	-0.974187	3.287953	-1.430967
9	1	0	-1.549511	1.875916	-2.347941
10	6	0	-2.225227	0.314629	-0.125680
11	6	0	-3.247538	0.308204	0.833176
12	6	0	-2.141845	-0.762414	-1.021999
13	6	0	-4.171089	-0.741813	0.895362
14	1	0	-3.322526	1.132371	1.540418
15	6	0	-3.059476	-1.814594	-0.962652
16	1	0	-1.345922	-0.773899	-1.761520
17	6	0	-4.079643	-1.808155	-0.003631
18	1	0	-4.955706	-0.727532	1.648087
19	1	0	-2.978389	-2.641499	-1.664406
20	1	0	-4.792617	-2.627556	0.043337
21	6	0	2.128711	-0.129153	0.291214
22	6	0	2.503371	-1.474994	0.392629
23	6	0	3.785177	-1.857307	-0.006054
24	1	0	1.798643	-2.208028	0.775610
25	6	0	4.193395	0.433914	-0.569003
26	6	0	4.654145	-0.882902	-0.499695
27	1	0	4.096975	-2.896159	0.063762
28	1	0	4.838407	1.223586	-0.950581
29	1	0	5.660424	-1.130575	-0.824307
30	7	0	2.966380	0.810868	-0.182756
31	1	0	0.142765	-0.535131	0.945156
32	6	0	0.871892	1.180335	2.030246
33	1	0	1.474329	2.079422	1.855797
34	1	0	-0.112942	1.485048	2.399528
35	1	0	1.354924	0.592484	2.820334



(*R*,*S*)-**1**



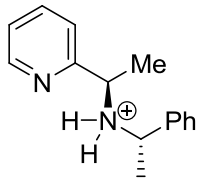
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.753416	0.348941	0.734257
2	7	0	0.122015	1.046377	-0.398815
3	1	0	0.710482	1.834796	-0.659031
4	6	0	-1.264714	1.496019	-0.215812
5	1	0	-1.389796	2.084506	0.708382
6	6	0	-1.636427	2.415876	-1.391627
7	1	0	-2.664636	2.774609	-1.287912
8	1	0	-0.973252	3.288418	-1.423288
9	1	0	-1.549224	1.879961	-2.342297
10	6	0	-2.225860	0.313977	-0.125138
11	6	0	-3.252598	0.309183	0.828806
12	6	0	-2.137441	-0.764516	-1.018995
13	6	0	-4.175674	-0.741092	0.888400
14	1	0	-3.330904	1.134152	1.533503
15	6	0	-3.054602	-1.816947	-0.961807
16	1	0	-1.337843	-0.776299	-1.753477
17	6	0	-4.079246	-1.809008	-0.007915
18	1	0	-4.963399	-0.726003	1.636631
19	1	0	-2.969828	-2.644717	-1.660796
20	1	0	-4.791387	-2.628098	0.037354
21	6	0	2.128534	-0.129294	0.291122
22	6	0	2.506687	-1.473594	0.398740
23	6	0	3.788283	-1.854476	-0.000911
24	1	0	1.804838	-2.205490	0.786795
25	6	0	4.189854	0.434650	-0.576680
26	6	0	4.653538	-0.880547	-0.501469
27	1	0	4.102765	-2.891382	0.073343
28	1	0	4.832666	1.222615	-0.963772
29	1	0	5.658885	-1.127211	-0.826910
30	7	0	2.962548	0.810433	-0.189452
31	1	0	0.145181	-0.537007	0.947326
32	6	0	0.873264	1.178881	2.031576
33	1	0	1.479195	2.074237	1.856792
34	1	0	-0.110060	1.487157	2.398532
35	1	0	1.352301	0.589761	2.821404

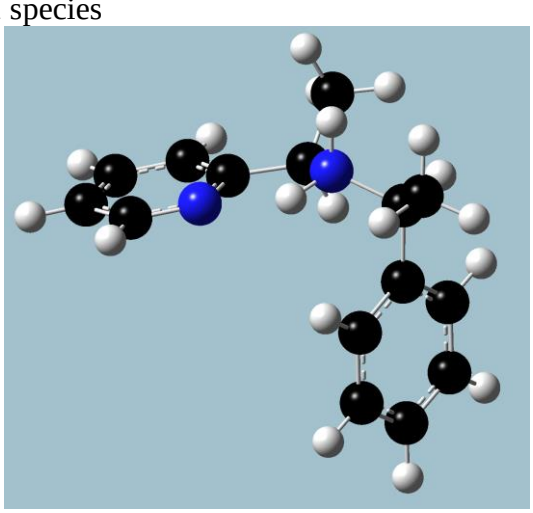
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.756723	0.444385	0.739344
2	7	0	0.117835	1.109381	-0.413918
3	1	0	0.673027	1.927073	-0.659375
4	6	0	-1.285991	1.521509	-0.232827
5	1	0	-1.420961	2.107643	0.689845
6	6	0	-1.683359	2.427216	-1.410460
7	1	0	-2.719804	2.760692	-1.302908
8	1	0	-1.040686	3.314676	-1.445217
9	1	0	-1.587224	1.892033	-2.361011
10	6	0	-2.211452	0.312452	-0.131934
11	6	0	-3.177064	0.245058	0.882193
12	6	0	-2.150134	-0.732915	-1.067775
13	6	0	-4.065476	-0.834335	0.961622
14	1	0	-3.233746	1.043465	1.618565
15	6	0	-3.032627	-1.813923	-0.991623
16	1	0	-1.402835	-0.700256	-1.855133
17	6	0	-3.995213	-1.869058	0.024289
18	1	0	-4.804864	-0.867566	1.757141
19	1	0	-2.969550	-2.614220	-1.724058
20	1	0	-4.680019	-2.710245	0.084347
21	6	0	2.108483	-0.098807	0.298132
22	6	0	2.427840	-1.455682	0.436529
23	6	0	3.686063	-1.904931	0.032723
24	1	0	1.698210	-2.144036	0.851793
25	6	0	4.186081	0.348067	-0.606430
26	6	0	4.589072	-0.984838	-0.502735
27	1	0	3.953772	-2.952924	0.130857
28	1	0	4.859815	1.095364	-1.020068
29	1	0	5.578067	-1.285281	-0.832976
30	7	0	2.980315	0.789477	-0.215438
31	1	0	0.129002	-0.413806	1.000530
32	6	0	0.915141	1.330288	1.993130
33	1	0	1.541318	2.201284	1.771375
34	1	0	-0.056414	1.681948	2.352392
35	1	0	1.387311	0.765230	2.804329

Cartesian coordinates of the ammonium-(*R*,*S*)-**1** species



(*R*,*S*)-Ammonium **1**

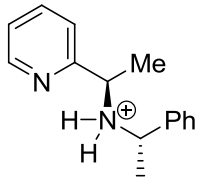


B3LYP/6-31+G(d), gas phase

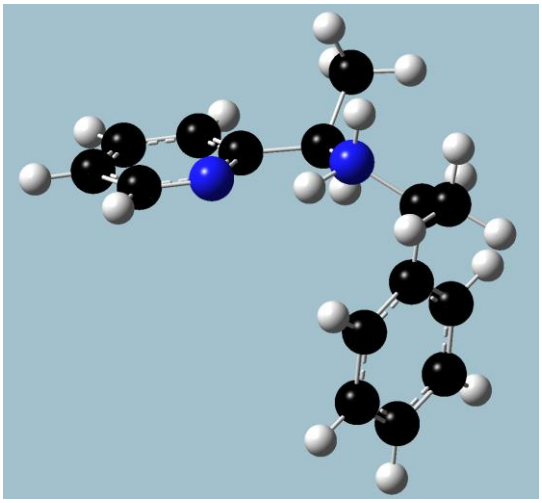
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.793479	1.060498	-0.703671
2	7	0	-0.047809	1.413160	0.568779
3	1	0	-0.426730	2.290468	0.942361
4	6	0	1.478196	1.533756	0.487556
5	1	0	1.661279	2.261113	-0.309169
6	6	0	1.975740	2.103586	1.818890
7	1	0	3.059763	2.236800	1.765587
8	1	0	1.529127	3.082395	2.033509
9	1	0	1.766028	1.428937	2.655700
10	6	0	2.092884	0.204669	0.099111
11	6	0	2.814413	0.101657	-1.098677
12	6	0	1.988120	-0.920734	0.932045
13	6	0	3.423214	-1.103508	-1.459934
14	1	0	2.916129	0.969367	-1.747607
15	6	0	2.588050	-2.126716	0.566814
16	1	0	1.446944	-0.867387	1.874702
17	6	0	3.307586	-2.219778	-0.629059
18	1	0	3.986896	-1.166817	-2.386229
19	1	0	2.501113	-2.990637	1.219453
20	1	0	3.779871	-3.157482	-0.907333
21	6	0	-1.972874	0.168017	-0.298001
22	6	0	-2.990650	-0.174019	-1.191715
23	6	0	-3.998960	-1.031639	-0.748398
24	1	0	-3.001330	0.207238	-2.207757
25	6	0	-2.905079	-1.117882	1.382036
26	6	0	-3.960023	-1.513444	0.561540
27	1	0	-4.803765	-1.318839	-1.418819
28	1	0	-2.828496	-1.462911	2.409653
29	1	0	-4.728165	-2.179560	0.940918
30	7	0	-1.932135	-0.296961	0.958440
31	1	0	-0.087746	0.463900	-1.292117
32	1	0	-0.349259	0.676329	1.248318
33	6	0	-1.172414	2.329897	-1.467190
34	1	0	-1.620371	2.072881	-2.430414
35	1	0	-1.900138	2.931521	-0.909930
36	1	0	-0.289878	2.943134	-1.679435

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.803069	1.084743	-0.676212
2	7	0	-0.039916	1.427490	0.587998
3	1	0	-0.405018	2.306306	0.972208
4	6	0	1.481539	1.540876	0.475706
5	1	0	1.653948	2.259954	-0.328907
6	6	0	2.013718	2.116253	1.790610
7	1	0	3.097387	2.237686	1.710327
8	1	0	1.577469	3.099579	1.998571
9	1	0	1.809234	1.453881	2.637977
10	6	0	2.087669	0.205449	0.087595
11	6	0	2.758165	0.082584	-1.137537
12	6	0	2.025010	-0.905525	0.943891
13	6	0	3.356473	-1.126909	-1.503842
14	1	0	2.819836	0.937582	-1.807089
15	6	0	2.614445	-2.116375	0.574860
16	1	0	1.522303	-0.837392	1.905836
17	6	0	3.282909	-2.229493	-0.649135
18	1	0	3.876373	-1.204817	-2.454635
19	1	0	2.556118	-2.968937	1.245741
20	1	0	3.745092	-3.171224	-0.932028
21	6	0	-1.968830	0.175299	-0.274705
22	6	0	-3.003975	-0.134239	-1.162230
23	6	0	-4.001162	-1.012485	-0.736904
24	1	0	-3.033559	0.289932	-2.160033
25	6	0	-2.867427	-1.181306	1.366736
26	6	0	-3.936553	-1.548246	0.551426
27	1	0	-4.817211	-1.273965	-1.404112
28	1	0	-2.771548	-1.568520	2.377722
29	1	0	-4.694732	-2.232832	0.917614
30	7	0	-1.904098	-0.340372	0.960672
31	1	0	-0.105505	0.501170	-1.285837
32	1	0	-0.321354	0.693677	1.272793
33	6	0	-1.203679	2.356927	-1.423151
34	1	0	-1.640020	2.099563	-2.391242
35	1	0	-1.941682	2.936407	-0.857918
36	1	0	-0.330431	2.986805	-1.620321



(*R*,*S*)-Ammonium **1**



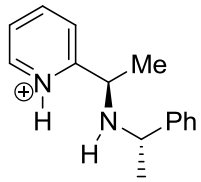
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.802954	1.105627	-0.680652
2	7	0	-0.039927	1.443616	0.583502
3	1	0	-0.397841	2.324844	0.965315
4	6	0	1.481478	1.544550	0.473739
5	1	0	1.662785	2.260817	-0.331021
6	6	0	2.017176	2.116064	1.788565
7	1	0	3.100785	2.228186	1.709434
8	1	0	1.589031	3.102097	1.994778
9	1	0	1.805921	1.456241	2.634991
10	6	0	2.077193	0.204218	0.085891
11	6	0	2.746174	0.075514	-1.139317
12	6	0	2.004141	-0.906073	0.942047
13	6	0	3.332689	-1.139461	-1.505887
14	1	0	2.815544	0.929546	-1.808129
15	6	0	2.581829	-2.122172	0.572531
16	1	0	1.502311	-0.833157	1.903151
17	6	0	3.248744	-2.241265	-0.651518
18	1	0	3.851178	-1.222293	-2.456115
19	1	0	2.515661	-2.973865	1.242498
20	1	0	3.701375	-3.186652	-0.934618
21	6	0	-1.956491	0.182011	-0.277531
22	6	0	-2.990602	-0.142923	-1.160316
23	6	0	-3.974132	-1.032779	-0.728478
24	1	0	-3.029021	0.278629	-2.158110
25	6	0	-2.830812	-1.182124	1.371688
26	6	0	-3.897522	-1.564367	0.560887
27	1	0	-4.788985	-1.306595	-1.390976
28	1	0	-2.726968	-1.565793	2.382566
29	1	0	-4.644868	-2.257295	0.931242
30	7	0	-1.880484	-0.329316	0.958842
31	1	0	-0.105237	0.531061	-1.298049
32	1	0	-0.334881	0.707187	1.262594
33	6	0	-1.220211	2.377354	-1.418177
34	1	0	-1.664506	2.120338	-2.381582
35	1	0	-1.955591	2.948537	-0.843258
36	1	0	-0.354029	3.013025	-1.621954

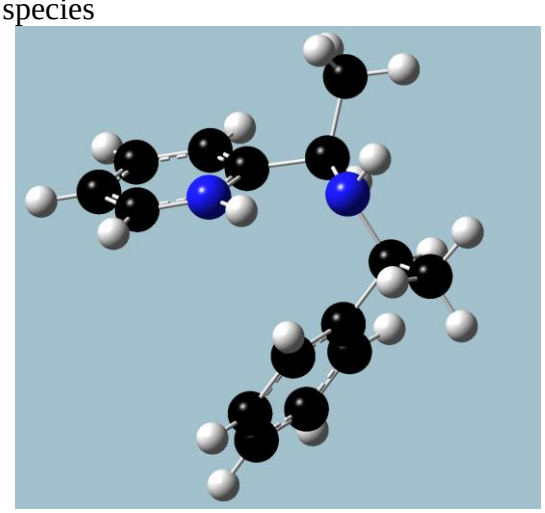
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.810203	1.107821	-0.687044
2	7	0	-0.025550	1.478379	0.552922
3	1	0	-0.362239	2.381794	0.900287
4	6	0	1.491360	1.556889	0.406279
5	1	0	1.660307	2.230811	-0.436319
6	6	0	2.067396	2.186781	1.676386
7	1	0	3.150365	2.279094	1.563809
8	1	0	1.654581	3.187237	1.839612
9	1	0	1.864966	1.572464	2.558456
10	6	0	2.074223	0.195214	0.071671
11	6	0	2.736073	0.012326	-1.150914
12	6	0	2.005964	-0.878866	0.974304
13	6	0	3.321452	-1.217748	-1.468888
14	1	0	2.798026	0.836503	-1.856605
15	6	0	2.582698	-2.110270	0.654327
16	1	0	1.504838	-0.763395	1.931399
17	6	0	3.243873	-2.282527	-0.567246
18	1	0	3.833449	-1.341546	-2.418482
19	1	0	2.519785	-2.932679	1.360677
20	1	0	3.695429	-3.239344	-0.811876
21	6	0	-1.950208	0.177549	-0.268150
22	6	0	-2.913247	-0.249749	-1.189835
23	6	0	-3.906717	-1.126448	-0.755880
24	1	0	-2.885295	0.085651	-2.220518
25	6	0	-2.910317	-1.075190	1.421723
26	6	0	-3.911396	-1.548204	0.576579
27	1	0	-4.665474	-1.476415	-1.448765
28	1	0	-2.868992	-1.376937	2.464713
29	1	0	-4.668602	-2.227854	0.952016
30	7	0	-1.948746	-0.232320	1.007985
31	1	0	-0.121553	0.538767	-1.318192
32	1	0	-0.308916	0.789629	1.276269
33	6	0	-1.263123	2.368228	-1.427032
34	1	0	-1.742331	2.094420	-2.369070
35	1	0	-1.979016	2.939428	-0.827370
36	1	0	-0.406229	3.005117	-1.664063

Cartesian coordinates of the pyridinium-(*R*,*S*)-**1** species



(*R*,*S*)-Pyridinium **1**

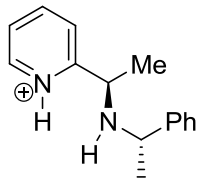


B3LYP/6-31+G(d), gas phase

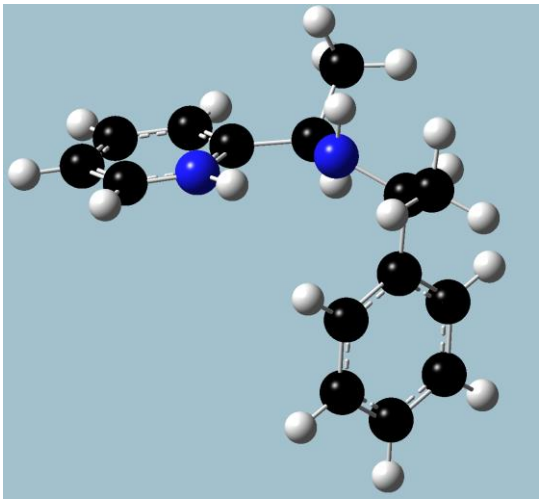
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.016092	1.618381	0.526685
2	7	0	-0.050508	1.871477	-0.450478
3	1	0	0.056096	2.806558	-0.837437
4	6	0	-1.451010	1.705354	0.043894
5	1	0	-1.526243	2.150261	1.049054
6	6	0	-2.394580	2.482137	-0.881711
7	1	0	-3.429467	2.363397	-0.548335
8	1	0	-2.158695	3.553365	-0.867730
9	1	0	-2.329295	2.131488	-1.917083
10	6	0	-1.810543	0.229068	0.170379
11	6	0	-1.950403	-0.357358	1.435025
12	6	0	-2.020813	-0.571509	-0.965226
13	6	0	-2.281528	-1.710757	1.569149
14	1	0	-1.819817	0.251862	2.327594
15	6	0	-2.354933	-1.921240	-0.836611
16	1	0	-1.953015	-0.134013	-1.959447
17	6	0	-2.482167	-2.496592	0.433050
18	1	0	-2.395292	-2.143316	2.559489
19	1	0	-2.536650	-2.520246	-1.725445
20	1	0	-2.753361	-3.543932	0.532865
21	6	0	1.705443	0.293027	0.204537
22	6	0	2.636568	-0.365944	1.006658
23	6	0	3.203793	-1.557951	0.558000
24	1	0	2.905479	0.050506	1.971938
25	6	0	1.907640	-1.413018	-1.450970
26	6	0	2.841245	-2.089977	-0.688847
27	1	0	3.927686	-2.078968	1.177829
28	1	0	1.551274	-1.750539	-2.417297
29	1	0	3.269516	-3.016154	-1.055156
30	7	0	1.386364	-0.260402	-0.979386
31	1	0	0.594253	1.516559	1.537117
32	1	0	0.657757	0.282546	-1.476168
33	6	0	2.048350	2.762857	0.543885
34	1	0	2.872805	2.553373	1.232072
35	1	0	2.472124	2.922238	-0.454513
36	1	0	1.564932	3.688616	0.872325

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.787955	1.162804	-0.619623
2	7	0	-0.035246	1.388881	0.624852
3	1	0	-0.391322	2.229408	1.081143
4	6	0	1.434439	1.530043	0.464801
5	1	0	1.657860	2.251535	-0.336810
6	6	0	2.012968	2.092297	1.770795
7	1	0	3.095811	2.220138	1.678209
8	1	0	1.574467	3.071344	2.000156
9	1	0	1.816060	1.418397	2.611721
10	6	0	2.078016	0.204215	0.078136
11	6	0	2.883952	0.121617	-1.065386
12	6	0	1.915431	-0.944610	0.868794
13	6	0	3.517077	-1.076973	-1.414206
14	1	0	3.020408	1.003003	-1.688810
15	6	0	2.542606	-2.143880	0.523437
16	1	0	1.298961	-0.900392	1.763226
17	6	0	3.346430	-2.214074	-0.620819
18	1	0	4.138456	-1.120028	-2.305034
19	1	0	2.407750	-3.023205	1.148326
20	1	0	3.834989	-3.147176	-0.888938
21	6	0	-1.952694	0.218542	-0.327773
22	6	0	-2.970400	-0.138138	-1.211326
23	6	0	-3.948262	-1.043369	-0.799326
24	1	0	-2.993353	0.282145	-2.209664
25	6	0	-2.890307	-1.210849	1.340891
26	6	0	-3.913928	-1.588003	0.491774
27	1	0	-4.740918	-1.327014	-1.484568
28	1	0	-2.774992	-1.571887	2.355495
29	1	0	-4.666202	-2.290021	0.831297
30	7	0	-1.963081	-0.335246	0.900797
31	1	0	-0.126929	0.618789	-1.306795
32	1	0	-1.170036	-0.018116	1.482593
33	6	0	-1.252731	2.457878	-1.308208
34	1	0	-1.748808	2.257869	-2.262726
35	1	0	-1.947439	3.012952	-0.667769
36	1	0	-0.384326	3.091803	-1.512358



(*R*,*S*)-Pyridinium **1**



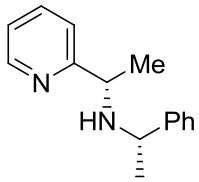
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.787340	1.171549	-0.620165
2	7	0	-0.033531	1.400319	0.622751
3	1	0	-0.385582	2.242560	1.076111
4	6	0	1.436992	1.534068	0.462801
5	1	0	1.664406	2.251384	-0.340607
6	6	0	2.018342	2.096644	1.766862
7	1	0	3.100552	2.219387	1.673522
8	1	0	1.584313	3.076926	1.993578
9	1	0	1.818794	1.425938	2.608366
10	6	0	2.072787	0.204217	0.077168
11	6	0	2.866367	0.112556	-1.074138
12	6	0	1.913009	-0.939908	0.875077
13	6	0	3.489616	-1.090734	-1.423821
14	1	0	3.000509	0.989901	-1.702374
15	6	0	2.530394	-2.143652	0.528665
16	1	0	1.306909	-0.888610	1.775277
17	6	0	3.321529	-2.223081	-0.623557
18	1	0	4.101103	-1.141162	-2.320077
19	1	0	2.398092	-3.018784	1.158514
20	1	0	3.802188	-3.159138	-0.892269
21	6	0	-1.946792	0.222527	-0.325749
22	6	0	-2.965330	-0.138287	-1.206617
23	6	0	-3.935793	-1.049708	-0.792125
24	1	0	-2.993980	0.283487	-2.203418
25	6	0	-2.868742	-1.214084	1.343712
26	6	0	-3.892942	-1.596026	0.497888
27	1	0	-4.729066	-1.337091	-1.474072
28	1	0	-2.748768	-1.576667	2.356614
29	1	0	-4.639045	-2.302708	0.838993
30	7	0	-1.948685	-0.332173	0.901680
31	1	0	-0.127782	0.627686	-1.308448
32	1	0	-1.154400	-0.007663	1.477344
33	6	0	-1.256652	2.463985	-1.309534
34	1	0	-1.756786	2.260814	-2.259949
35	1	0	-1.947938	3.018999	-0.667226
36	1	0	-0.390680	3.097322	-1.519706

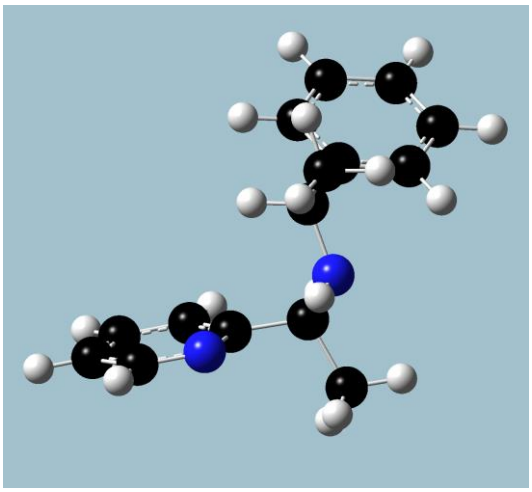
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.800728	1.172859	-0.601695
2	7	0	-0.030993	1.382968	0.634312
3	1	0	-0.381127	2.217641	1.102221
4	6	0	1.432301	1.529084	0.446883
5	1	0	1.640809	2.238054	-0.368964
6	6	0	2.035374	2.110278	1.733607
7	1	0	3.115390	2.237217	1.618787
8	1	0	1.598424	3.090622	1.955026
9	1	0	1.853773	1.447496	2.585979
10	6	0	2.078061	0.201082	0.068516
11	6	0	2.908469	0.119513	-1.057968
12	6	0	1.896574	-0.949630	0.852961
13	6	0	3.548814	-1.079180	-1.394749
14	1	0	3.056773	1.001107	-1.677136
15	6	0	2.530860	-2.149140	0.519160
16	1	0	1.258705	-0.906741	1.731184
17	6	0	3.360475	-2.218160	-0.607024
18	1	0	4.188142	-1.121767	-2.272017
19	1	0	2.380675	-3.029280	1.138296
20	1	0	3.853367	-3.150722	-0.866147
21	6	0	-1.957931	0.220206	-0.317943
22	6	0	-2.974548	-0.124468	-1.208817
23	6	0	-3.952820	-1.034861	-0.811472
24	1	0	-2.995275	0.310731	-2.200125
25	6	0	-2.894285	-1.235642	1.325221
26	6	0	-3.918451	-1.599143	0.471232
27	1	0	-4.744606	-1.308407	-1.501021
28	1	0	-2.777234	-1.614838	2.332271
29	1	0	-4.669643	-2.306394	0.800263
30	7	0	-1.967088	-0.352468	0.900745
31	1	0	-0.150584	0.644439	-1.310054
32	1	0	-1.177251	-0.052150	1.491349
33	6	0	-1.276605	2.480208	-1.258495
34	1	0	-1.781984	2.296868	-2.210348
35	1	0	-1.964329	3.016121	-0.595877
36	1	0	-0.410820	3.118466	-1.455584

Cartesian coordinates of the (*S*,*S*)-**1** species



(*S*,*S*)-**1**

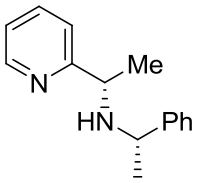


B3LYP/6-31+G(d), gas phase

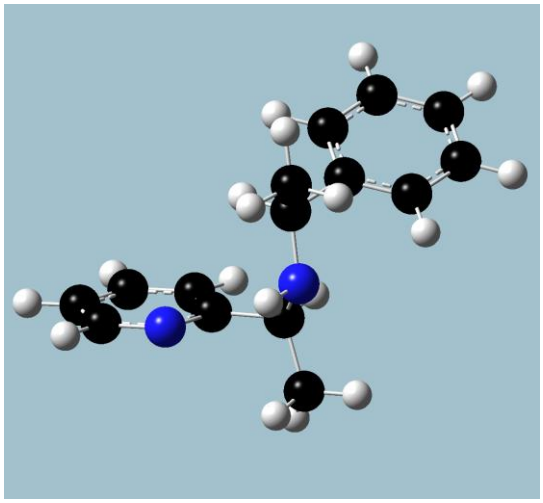
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.730058	-0.836778	-0.996106
2	1	0	-0.019919	-0.140104	-1.457430
3	7	0	-0.004807	-1.568479	0.048654
4	1	0	-0.671484	-2.174110	0.526597
5	6	0	0.680469	-0.735860	1.048143
6	1	0	0.011373	0.046972	1.449348
7	6	0	1.099035	-1.630604	2.227183
8	1	0	1.628434	-1.045601	2.986570
9	1	0	0.218113	-2.084562	2.699532
10	1	0	1.761861	-2.432704	1.883538
11	6	0	1.891487	-0.032134	0.443670
12	6	0	2.169746	1.302452	0.766617
13	6	0	2.775618	-0.714415	-0.405592
14	6	0	3.306932	1.942905	0.263348
15	1	0	1.487822	1.847908	1.417026
16	6	0	3.911358	-0.078490	-0.911966
17	1	0	2.555926	-1.744153	-0.673908
18	6	0	4.182585	1.253066	-0.578597
19	1	0	3.503977	2.979958	0.524894
20	1	0	4.585788	-0.622142	-1.569665
21	1	0	5.066044	1.747997	-0.974435
22	6	0	-1.912881	-0.023200	-0.465068
23	6	0	-2.112527	1.315003	-0.829030
24	6	0	-3.224642	1.997353	-0.334096
25	1	0	-1.401198	1.810722	-1.485039
26	6	0	-3.820594	-0.009329	0.827629
27	6	0	-4.103762	1.322575	0.513753
28	1	0	-3.398270	3.037073	-0.600928
29	1	0	-4.477285	-0.572244	1.489420
30	1	0	-4.982071	1.810598	0.926590
31	7	0	-2.757371	-0.670982	0.356304
32	6	0	-1.205940	-1.830467	-2.067242
33	1	0	-1.910485	-2.550157	-1.633665
34	1	0	-1.715434	-1.312349	-2.888187
35	1	0	-0.348901	-2.379341	-2.470834

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.733000	-0.839993	-1.006438
2	1	0	-0.024313	-0.139301	-1.462718
3	7	0	-0.002423	-1.584272	0.029756
4	1	0	-0.670725	-2.188356	0.508236
5	6	0	0.681534	-0.756260	1.038139
6	1	0	0.007693	0.019540	1.442256
7	6	0	1.101214	-1.656803	2.212208
8	1	0	1.616069	-1.071091	2.981018
9	1	0	0.222288	-2.125057	2.673570
10	1	0	1.776979	-2.448892	1.869751
11	6	0	1.889379	-0.039734	0.442003
12	6	0	2.131139	1.308145	0.741257
13	6	0	2.807777	-0.719079	-0.373637
14	6	0	3.263987	1.964439	0.246194
15	1	0	1.424638	1.851961	1.365813
16	6	0	3.939632	-0.068346	-0.871918
17	1	0	2.623686	-1.760352	-0.623339
18	6	0	4.173085	1.277222	-0.563159
19	1	0	3.431120	3.011254	0.488479
20	1	0	4.639750	-0.610718	-1.503145
21	1	0	5.052579	1.784058	-0.952469
22	6	0	-1.911512	-0.026988	-0.464289
23	6	0	-2.096248	1.318136	-0.809638
24	6	0	-3.202549	2.006172	-0.308142
25	1	0	-1.379656	1.815803	-1.457906
26	6	0	-3.825971	-0.010315	0.822980
27	6	0	-4.091831	1.329240	0.527964
28	1	0	-3.363625	3.050965	-0.560975
29	1	0	-4.492646	-0.573295	1.474106
30	1	0	-4.965401	1.820884	0.945652
31	7	0	-2.767309	-0.678581	0.344224
32	6	0	-1.212331	-1.819243	-2.089077
33	1	0	-1.904886	-2.554934	-1.662568
34	1	0	-1.734717	-1.289606	-2.894028
35	1	0	-0.356529	-2.352452	-2.516268



(*S,S*)-**1**



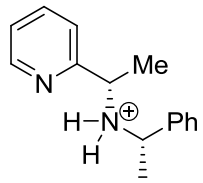
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.733231	-0.843291	-1.004312
2	1	0	-0.026197	-0.143112	-1.463073
3	7	0	-0.002608	-1.584021	0.033491
4	1	0	-0.667719	-2.189798	0.511313
5	6	0	0.681490	-0.755236	1.040241
6	1	0	0.009776	0.022199	1.443230
7	6	0	1.101160	-1.653906	2.215366
8	1	0	1.614925	-1.067686	2.982832
9	1	0	0.223018	-2.121659	2.675771
10	1	0	1.776804	-2.444895	1.873424
11	6	0	1.888799	-0.039252	0.442365
12	6	0	2.134511	1.306889	0.745661
13	6	0	2.802292	-0.717939	-0.379063
14	6	0	3.266848	1.962065	0.248631
15	1	0	1.431900	1.849416	1.374295
16	6	0	3.933392	-0.067935	-0.879416
17	1	0	2.613848	-1.757049	-0.631316
18	6	0	4.171031	1.275737	-0.566645
19	1	0	3.437426	3.006792	0.493720
20	1	0	4.629318	-0.608998	-1.514942
21	1	0	5.049395	1.781661	-0.957310
22	6	0	-1.910816	-0.027886	-0.463941
23	6	0	-2.093957	1.316424	-0.813062
24	6	0	-3.199268	2.006786	-0.313450
25	1	0	-1.377166	1.810689	-1.462309
26	6	0	-3.825138	-0.005617	0.823434
27	6	0	-4.089061	1.333213	0.524530
28	1	0	-3.359259	3.050285	-0.568893
29	1	0	-4.492869	-0.564595	1.475945
30	1	0	-4.961354	1.826621	0.940626
31	7	0	-2.767076	-0.676432	0.346289
32	6	0	-1.213598	-1.825191	-2.083716
33	1	0	-1.905302	-2.557970	-1.653616
34	1	0	-1.736244	-1.298321	-2.888635
35	1	0	-0.359243	-2.359572	-2.509264

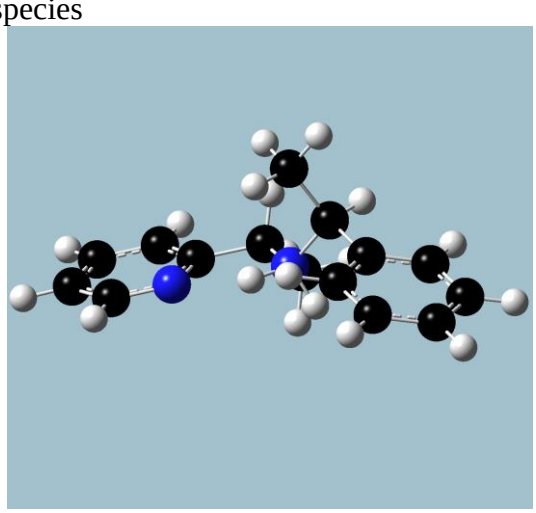
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.734849	-0.838478	-1.018594
2	1	0	-0.030728	-0.130317	-1.468436
3	7	0	0.001924	-1.597029	0.004727
4	1	0	-0.658622	-2.213679	0.475612
5	6	0	0.685135	-0.782148	1.027375
6	1	0	0.009161	-0.015255	1.440186
7	6	0	1.105629	-1.699007	2.187630
8	1	0	1.612710	-1.121999	2.966582
9	1	0	0.227184	-2.178910	2.634587
10	1	0	1.787469	-2.480647	1.835806
11	6	0	1.888651	-0.049205	0.442087
12	6	0	2.095476	1.307908	0.727191
13	6	0	2.836511	-0.718216	-0.349063
14	6	0	3.220933	1.983679	0.240548
15	1	0	1.367754	1.842517	1.333407
16	6	0	3.960523	-0.047751	-0.839736
17	1	0	2.688142	-1.767780	-0.585437
18	6	0	4.157904	1.307273	-0.546283
19	1	0	3.360336	3.036239	0.471597
20	1	0	4.682435	-0.582110	-1.451502
21	1	0	5.030655	1.828796	-0.929040
22	6	0	-1.908618	-0.028311	-0.462342
23	6	0	-2.082961	1.322569	-0.790393
24	6	0	-3.184198	2.012830	-0.281333
25	1	0	-1.362071	1.821428	-1.431216
26	6	0	-3.827546	-0.011891	0.823896
27	6	0	-4.080493	1.333038	0.545436
28	1	0	-3.336270	3.061238	-0.521026
29	1	0	-4.500318	-0.575961	1.466440
30	1	0	-4.949684	1.826164	0.968276
31	7	0	-2.772245	-0.682962	0.336562
32	6	0	-1.218690	-1.802015	-2.113251
33	1	0	-1.899750	-2.550566	-1.693046
34	1	0	-1.752078	-1.260630	-2.901152
35	1	0	-0.364525	-2.320228	-2.559671

Cartesian coordinates of the ammonium-(*S*,*S*)-**1** species



(*S*,*S*)-Ammonium **1**

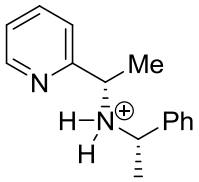


B3LYP/6-31+G(d), gas phase

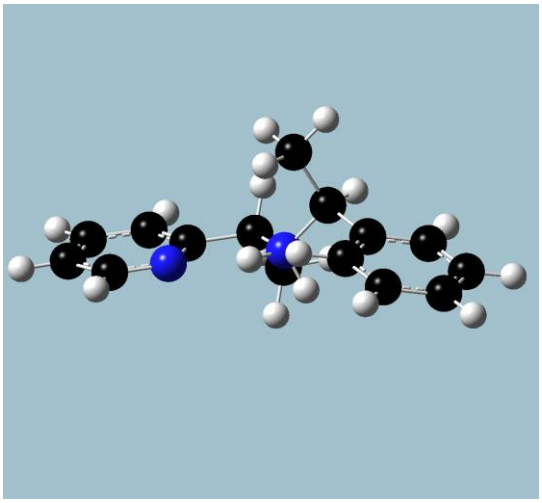
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.263365	1.401803	-0.092713
2	1	0	-1.198570	1.903688	0.877179
3	7	0	0.052278	0.671772	-0.300169
4	1	0	-0.236525	-0.290452	-0.595956
5	6	0	1.025216	0.591898	0.891263
6	1	0	1.138087	1.630731	1.218425
7	6	0	0.413205	-0.240277	2.017356
8	1	0	1.109962	-0.245479	2.860428
9	1	0	-0.535816	0.175857	2.370590
10	1	0	0.244062	-1.277771	1.715046
11	6	0	2.358111	0.093395	0.368772
12	6	0	3.439363	0.982502	0.281139
13	6	0	2.531997	-1.237634	-0.044957
14	6	0	4.675355	0.550587	-0.207007
15	1	0	3.323002	2.013488	0.609762
16	6	0	3.764575	-1.666121	-0.540531
17	1	0	1.715123	-1.952632	0.026410
18	6	0	4.837938	-0.773257	-0.621071
19	1	0	5.507617	1.246466	-0.259949
20	1	0	3.889030	-2.698047	-0.855894
21	1	0	5.798138	-1.110994	-1.000204
22	6	0	-2.375603	0.351013	-0.071270
23	6	0	-3.663071	0.656517	0.374727
24	6	0	-4.634902	-0.343705	0.317582
25	1	0	-3.902791	1.644072	0.759536
26	6	0	-2.974784	-1.816360	-0.592846
27	6	0	-4.288592	-1.602796	-0.178830
28	1	0	-5.646579	-0.143267	0.658108
29	1	0	-2.653554	-2.780036	-0.978754
30	1	0	-5.017460	-2.404546	-0.239132
31	7	0	-2.037400	-0.856960	-0.538031
32	1	0	0.562391	1.084389	-1.086808
33	6	0	-1.455081	2.446018	-1.199806
34	1	0	-1.496784	1.971803	-2.186989
35	1	0	-2.397528	2.979453	-1.047528
36	1	0	-0.648127	3.188092	-1.187718

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.262455	1.252687	0.060323
2	1	0	-1.228450	1.630856	1.085784
3	7	0	0.007151	0.443025	-0.138076
4	1	0	-0.314322	-0.549780	-0.180630
5	6	0	1.120322	0.628448	0.901107
6	1	0	1.200957	1.711181	1.030228
7	6	0	0.715016	-0.023052	2.223300
8	1	0	1.508863	0.152988	2.954534
9	1	0	-0.209068	0.402759	2.626023
10	1	0	0.581391	-1.104203	2.121364
11	6	0	2.422281	0.110355	0.315667
12	6	0	3.413950	1.025060	-0.067241
13	6	0	2.660269	-1.263142	0.145399
14	6	0	4.623973	0.579117	-0.606677
15	1	0	3.243872	2.091245	0.063737
16	6	0	3.865902	-1.708783	-0.401084
17	1	0	1.914180	-1.995732	0.442131
18	6	0	4.850745	-0.789197	-0.776831
19	1	0	5.385342	1.299790	-0.891776
20	1	0	4.037294	-2.774152	-0.527567
21	1	0	5.790121	-1.138644	-1.196399
22	6	0	-2.453528	0.299233	-0.073022
23	6	0	-3.770066	0.760715	0.026045
24	6	0	-4.805891	-0.166241	-0.086043
25	1	0	-3.984318	1.811368	0.193253
26	6	0	-3.156566	-1.881309	-0.370844
27	6	0	-4.498018	-1.513829	-0.292035
28	1	0	-5.839303	0.159444	-0.012415
29	1	0	-2.863434	-2.916379	-0.524782
30	1	0	-5.277248	-2.263133	-0.386120
31	7	0	-2.156463	-0.992291	-0.261276
32	1	0	0.394984	0.648103	-1.064539
33	6	0	-1.290079	2.434325	-0.912469
34	1	0	-1.332083	2.092492	-1.952652
35	1	0	-2.171019	3.052035	-0.721531
36	1	0	-0.407707	3.068308	-0.776763



(*S,S*)-Ammonium **1**



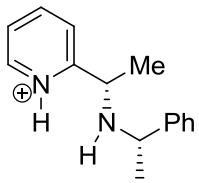
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.263520	1.260068	0.062259
2	1	0	-1.232902	1.635413	1.088638
3	7	0	0.002881	0.447941	-0.135975
4	1	0	-0.331768	-0.542671	-0.173756
5	6	0	1.116849	0.632899	0.900579
6	1	0	1.201925	1.714979	1.028674
7	6	0	0.713267	-0.015731	2.224442
8	1	0	1.506416	0.163000	2.954015
9	1	0	-0.210246	0.409649	2.626040
10	1	0	0.581440	-1.096266	2.124305
11	6	0	2.417436	0.111841	0.314635
12	6	0	3.410905	1.023818	-0.069437
13	6	0	2.651567	-1.262261	0.145117
14	6	0	4.619135	0.574320	-0.609446
15	1	0	3.243552	2.089727	0.060889
16	6	0	3.855405	-1.711202	-0.402033
17	1	0	1.903978	-1.991963	0.442408
18	6	0	4.842192	-0.794463	-0.778847
19	1	0	5.381680	1.292188	-0.895456
20	1	0	4.023975	-2.776259	-0.528148
21	1	0	5.779655	-1.146281	-1.198653
22	6	0	-2.451331	0.303107	-0.072945
23	6	0	-3.771303	0.756246	0.014219
24	6	0	-4.799243	-0.179044	-0.098207
25	1	0	-3.993517	1.805862	0.172182
26	6	0	-3.136781	-1.885316	-0.359961
27	6	0	-4.480678	-1.525788	-0.292455
28	1	0	-5.834807	0.139227	-0.033903
29	1	0	-2.836648	-2.919062	-0.504663
30	1	0	-5.253645	-2.280434	-0.386230
31	7	0	-2.144190	-0.987638	-0.250099
32	1	0	0.389436	0.650074	-1.062169
33	6	0	-1.292328	2.443353	-0.907644
34	1	0	-1.328982	2.103426	-1.947603
35	1	0	-2.175753	3.056248	-0.718840
36	1	0	-0.414064	3.079945	-0.766872

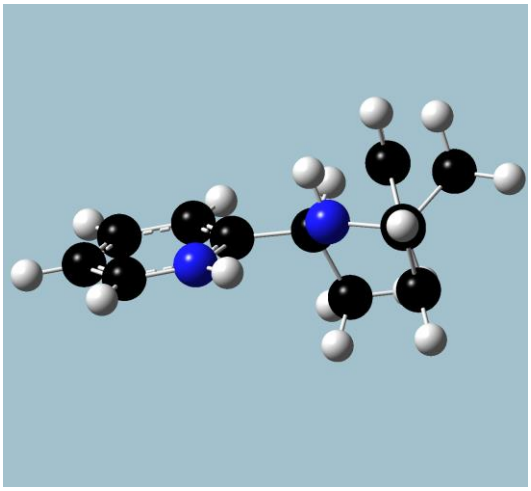
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.248620	1.231445	0.017745
2	1	0	-1.205961	1.637576	1.031318
3	7	0	0.009718	0.408889	-0.170987
4	1	0	-0.308056	-0.580470	-0.199772
5	6	0	1.111675	0.612705	0.868753
6	1	0	1.179601	1.695896	0.993111
7	6	0	0.707810	-0.040278	2.190673
8	1	0	1.486459	0.159952	2.930666
9	1	0	-0.232714	0.365875	2.573145
10	1	0	0.602752	-1.123599	2.085285
11	6	0	2.427183	0.106894	0.303033
12	6	0	3.448221	1.023022	0.012093
13	6	0	2.652576	-1.259873	0.070833
14	6	0	4.675586	0.584657	-0.495343
15	1	0	3.285623	2.082998	0.188663
16	6	0	3.875118	-1.697741	-0.444589
17	1	0	1.877811	-1.989047	0.291021
18	6	0	4.890631	-0.777047	-0.726370
19	1	0	5.458649	1.305788	-0.709910
20	1	0	4.035681	-2.757138	-0.621240
21	1	0	5.842226	-1.119854	-1.121692
22	6	0	-2.455047	0.297082	-0.079713
23	6	0	-3.758002	0.785870	0.070645
24	6	0	-4.819144	-0.114308	-0.011820
25	1	0	-3.938394	1.839379	0.254872
26	6	0	-3.221949	-1.863874	-0.370636
27	6	0	-4.550697	-1.467006	-0.240886
28	1	0	-5.840644	0.234444	0.103041
29	1	0	-2.962289	-2.904648	-0.543268
30	1	0	-5.348985	-2.197608	-0.312674
31	7	0	-2.194922	-1.000070	-0.289803
32	1	0	0.398168	0.603052	-1.098086
33	6	0	-1.269239	2.386937	-0.986025
34	1	0	-1.317026	2.011317	-2.013150
35	1	0	-2.140423	3.020347	-0.807176
36	1	0	-0.372652	3.003113	-0.868991

Cartesian coordinates of the pyridinium-(*S*,*S*)-**1** species



(*S*,*S*)-Pyridinium **1**

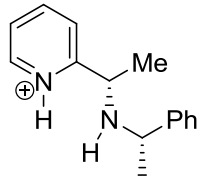


B3LYP/6-31+G(d), gas phase

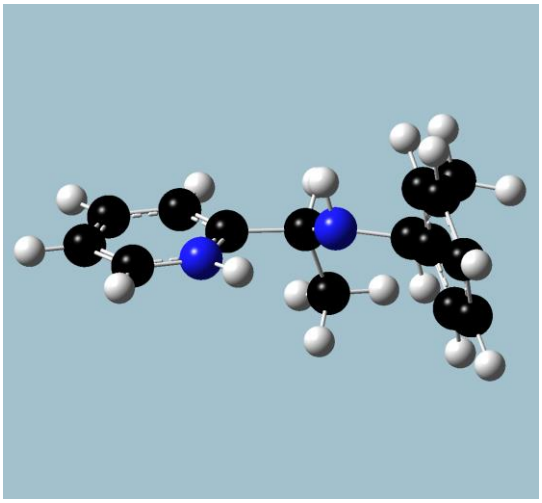
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.330599	1.307438	-0.087386
2	1	0	1.533350	2.028394	-0.894556
3	7	0	0.044268	0.608623	-0.245657
4	1	0	-0.061982	0.335747	-1.224767
5	6	0	-1.221011	1.296237	0.159292
6	1	0	-1.102534	1.562131	1.213423
7	6	0	-1.498379	2.575695	-0.646502
8	1	0	-2.434908	3.036089	-0.315416
9	1	0	-0.699764	3.315891	-0.519435
10	1	0	-1.592352	2.366814	-1.718382
11	6	0	-2.346327	0.272965	0.075117
12	6	0	-2.859813	-0.299030	1.247275
13	6	0	-2.875372	-0.135962	-1.158788
14	6	0	-3.875964	-1.256844	1.192573
15	1	0	-2.470127	0.014323	2.214046
16	6	0	-3.886438	-1.098746	-1.218193
17	1	0	-2.516465	0.304877	-2.086579
18	6	0	-4.389578	-1.661715	-0.042091
19	1	0	-4.269364	-1.680247	2.112807
20	1	0	-4.288729	-1.399135	-2.181933
21	1	0	-5.182885	-2.402599	-0.087720
22	6	0	2.418638	0.238424	-0.147311
23	6	0	3.767465	0.445451	-0.428848
24	6	0	4.650287	-0.633960	-0.380850
25	1	0	4.114857	1.441877	-0.682767
26	6	0	2.838071	-2.086355	0.209858
27	6	0	4.185326	-1.916596	-0.053458
28	1	0	5.702739	-0.481125	-0.601533
29	1	0	2.381756	-3.037961	0.458259
30	1	0	4.855376	-2.768044	-0.012841
31	7	0	2.017792	-1.015290	0.151788
32	1	0	0.992258	-1.066945	0.303248
33	6	0	1.452327	2.047230	1.261101
34	1	0	0.763450	2.894040	1.304016
35	1	0	1.236400	1.376181	2.099541
36	1	0	2.465512	2.440970	1.386958

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.312378	1.254777	-0.058325
2	1	0	1.488779	1.971879	-0.873699
3	7	0	0.038837	0.527578	-0.199492
4	1	0	-0.027384	0.179931	-1.157697
5	6	0	-1.221022	1.256479	0.107298
6	1	0	-1.141536	1.593193	1.144386
7	6	0	-1.457142	2.486559	-0.788845
8	1	0	-2.396212	2.980447	-0.515927
9	1	0	-0.650098	3.219991	-0.680788
10	1	0	-1.517826	2.207312	-1.847267
11	6	0	-2.373318	0.260571	0.047339
12	6	0	-3.012351	-0.148082	1.226485
13	6	0	-2.815763	-0.274765	-1.172834
14	6	0	-4.065658	-1.067678	1.192807
15	1	0	-2.685801	0.259140	2.181150
16	6	0	-3.863462	-1.199388	-1.211333
17	1	0	-2.349138	0.030789	-2.106712
18	6	0	-4.493239	-1.598321	-0.027707
19	1	0	-4.550750	-1.366859	2.118478
20	1	0	-4.191302	-1.602824	-2.166050
21	1	0	-5.312023	-2.312419	-0.057813
22	6	0	2.430165	0.223798	-0.120772
23	6	0	3.751298	0.483120	-0.475737
24	6	0	4.689173	-0.548260	-0.425539
25	1	0	4.035031	1.483052	-0.786296
26	6	0	2.982298	-2.058778	0.309919
27	6	0	4.305228	-1.835087	-0.024485
28	1	0	5.720513	-0.353561	-0.702298
29	1	0	2.585604	-3.018082	0.618754
30	1	0	5.016987	-2.650919	0.019475
31	7	0	2.106631	-1.033434	0.248938
32	1	0	1.107049	-1.158747	0.460767
33	6	0	1.415845	2.010249	1.282144
34	1	0	0.719238	2.851869	1.310749
35	1	0	1.199240	1.342671	2.123171
36	1	0	2.424765	2.412967	1.409018



(*S*,*S*)-Pyridinium **1**



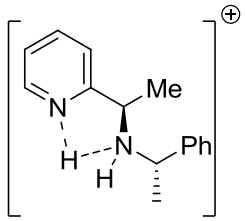
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.313564	1.256442	-0.059803
2	1	0	1.494329	1.973225	-0.873795
3	7	0	0.039040	0.531997	-0.203848
4	1	0	-0.029127	0.188723	-1.161978
5	6	0	-1.220483	1.257854	0.110142
6	1	0	-1.140316	1.589463	1.148376
7	6	0	-1.460411	2.491910	-0.779154
8	1	0	-2.396743	2.984459	-0.499363
9	1	0	-0.653150	3.223476	-0.672010
10	1	0	-1.526545	2.217035	-1.837299
11	6	0	-2.371541	0.260838	0.049027
12	6	0	-3.004167	-0.157025	1.228220
13	6	0	-2.818314	-0.266797	-1.172790
14	6	0	-4.055805	-1.078140	1.192747
15	1	0	-2.674267	0.244173	2.183363
16	6	0	-3.864267	-1.192962	-1.212840
17	1	0	-2.356709	0.045846	-2.105844
18	6	0	-4.487794	-1.601066	-0.029293
19	1	0	-4.535979	-1.384419	2.117687
20	1	0	-4.195555	-1.590245	-2.168007
21	1	0	-5.304801	-2.315875	-0.060577
22	6	0	2.429244	0.223690	-0.121720
23	6	0	3.751473	0.481954	-0.473277
24	6	0	4.686802	-0.551233	-0.423616
25	1	0	4.037097	1.481494	-0.780825
26	6	0	2.975714	-2.059963	0.304919
27	6	0	4.299442	-1.838043	-0.026257
28	1	0	5.718513	-0.358278	-0.697694
29	1	0	2.577920	-3.019237	0.610475
30	1	0	5.008911	-2.654917	0.017166
31	7	0	2.102180	-1.032993	0.244344
32	1	0	1.102316	-1.154173	0.453818
33	6	0	1.416592	2.010779	1.281143
34	1	0	0.719935	2.850911	1.310353
35	1	0	1.200982	1.342412	2.120471
36	1	0	2.424341	2.413471	1.407527

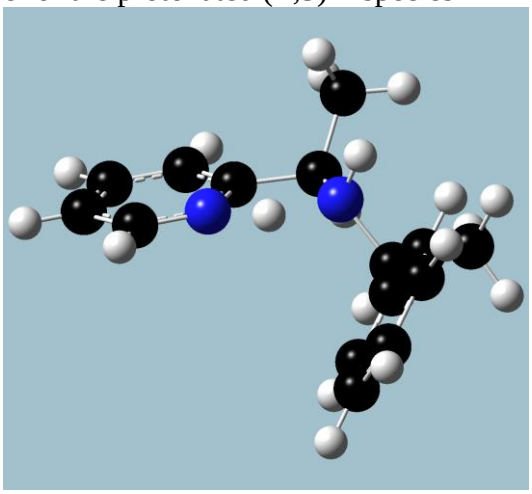
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.303662	1.230749	-0.048174
2	1	0	1.481376	1.936585	-0.872204
3	7	0	0.033421	0.496967	-0.188084
4	1	0	-0.005905	0.111494	-1.132101
5	6	0	-1.227661	1.249989	0.043518
6	1	0	-1.173116	1.654831	1.056926
7	6	0	-1.440715	2.418523	-0.937295
8	1	0	-2.382470	2.931319	-0.716403
9	1	0	-0.632569	3.153048	-0.860533
10	1	0	-1.480898	2.063415	-1.972815
11	6	0	-2.387463	0.260497	0.023534
12	6	0	-3.099186	-0.012848	1.200723
13	6	0	-2.768209	-0.400216	-1.156508
14	6	0	-4.163769	-0.921001	1.204869
15	1	0	-2.819565	0.490161	2.123216
16	6	0	-3.826885	-1.313484	-1.155742
17	1	0	-2.242259	-0.204385	-2.087562
18	6	0	-4.529713	-1.576604	0.025561
19	1	0	-4.703662	-1.114817	2.127449
20	1	0	-4.105656	-1.815262	-2.078114
21	1	0	-5.355212	-2.282462	0.024803
22	6	0	2.433724	0.215770	-0.095298
23	6	0	3.750512	0.507701	-0.443297
24	6	0	4.712952	-0.499696	-0.393345
25	1	0	4.006800	1.515776	-0.748319
26	6	0	3.039368	-2.053321	0.328065
27	6	0	4.357558	-1.797493	-0.000698
28	1	0	5.739982	-0.278788	-0.664500
29	1	0	2.663321	-3.021901	0.631357
30	1	0	5.087583	-2.596236	0.041508
31	7	0	2.139503	-1.048594	0.269972
32	1	0	1.150149	-1.209854	0.487173
33	6	0	1.394413	2.009806	1.279138
34	1	0	0.688805	2.843263	1.290048
35	1	0	1.182025	1.352210	2.128186
36	1	0	2.399267	2.422767	1.398354

Cartesian coordinates of the TS for the proton transfer of the protonated (*R*,*S*)-**1** species



(*R*,*S*)-TS-**1**



B3LYP/6-31+G(d), gas phase

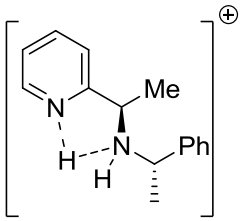
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.454646	1.455985	0.045342
2	7	0	0.099891	0.933793	-0.294940
3	1	0	-0.228624	1.321569	-1.180150
4	6	0	-0.983737	1.051971	0.747566
5	1	0	-0.545607	0.629856	1.659627
6	6	0	-1.370010	2.512693	1.008967
7	1	0	-2.135155	2.557294	1.789991
8	1	0	-0.512636	3.105654	1.347288
9	1	0	-1.783315	2.987981	0.112547
10	6	0	-2.149482	0.170038	0.330439
11	6	0	-2.428932	-1.003020	1.045071
12	6	0	-2.955052	0.499201	-0.771067
13	6	0	-3.489619	-1.832276	0.669310
14	1	0	-1.824058	-1.264787	1.911328
15	6	0	-4.009530	-0.332472	-1.153800
16	1	0	-2.779104	1.414525	-1.333182
17	6	0	-4.279390	-1.500078	-0.433713
18	1	0	-3.700159	-2.731955	1.240869
19	1	0	-4.626069	-0.063194	-2.006838
20	1	0	-5.105561	-2.141700	-0.726575
21	6	0	2.354189	0.205747	0.038244
22	6	0	3.711732	0.120690	0.332536
23	6	0	4.321902	-1.134019	0.252789
24	1	0	4.278585	1.000959	0.618593
25	6	0	2.221345	-2.104896	-0.392147
26	6	0	3.574214	-2.260507	-0.115056
27	1	0	5.379579	-1.236048	0.477671
28	1	0	1.574242	-2.927175	-0.679599
29	1	0	4.032915	-3.241119	-0.182550
30	7	0	1.660657	-0.888009	-0.305839
31	1	0	1.432414	1.863474	1.062205
32	1	0	0.551128	-0.352920	-0.455651
33	6	0	1.939668	2.537229	-0.927588
34	1	0	2.954845	2.858931	-0.675551
35	1	0	1.952572	2.164782	-1.958634
36	1	0	1.288518	3.415673	-0.877291

Imaginary frequency of -1211.9917 cm^{-1}

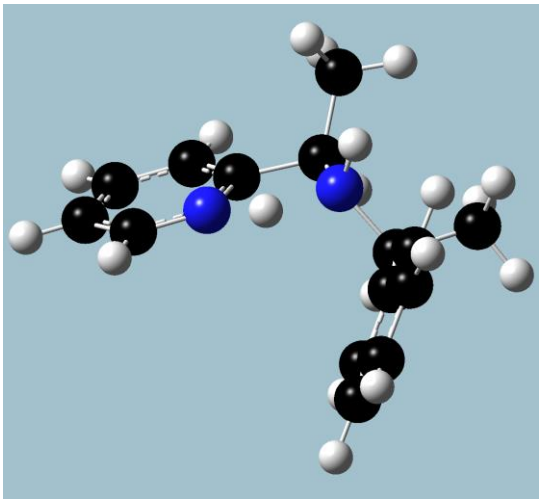
B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.454344	1.439254	0.068997
2	7	0	0.103665	0.909846	-0.286966
3	1	0	-0.200071	1.280355	-1.188445
4	6	0	-0.992462	1.059352	0.729425
5	1	0	-0.577809	0.660880	1.661233
6	6	0	-1.378773	2.527973	0.946205
7	1	0	-2.169674	2.593824	1.700061
8	1	0	-0.525715	3.115383	1.302083
9	1	0	-1.749664	2.988147	0.024001
10	6	0	-2.161039	0.174460	0.319748
11	6	0	-2.461916	-0.973109	1.067070
12	6	0	-2.949013	0.473685	-0.803125
13	6	0	-3.526234	-1.804897	0.704971
14	1	0	-1.862851	-1.216512	1.942023
15	6	0	-4.008162	-0.359795	-1.171925
16	1	0	-2.749093	1.362431	-1.397449
17	6	0	-4.300692	-1.501189	-0.417992
18	1	0	-3.747752	-2.687040	1.299816
19	1	0	-4.607679	-0.114046	-2.044405
20	1	0	-5.128023	-2.145798	-0.702382
21	6	0	2.362798	0.198416	0.044856
22	6	0	3.726078	0.129487	0.316294
23	6	0	4.346354	-1.119077	0.229867
24	1	0	4.287927	1.016486	0.589174
25	6	0	2.245128	-2.111341	-0.379215
26	6	0	3.603430	-2.253602	-0.122174
27	1	0	5.408202	-1.209778	0.437304
28	1	0	1.602733	-2.940408	-0.655469
29	1	0	4.069528	-3.229964	-0.193862
30	7	0	1.674065	-0.900692	-0.287342
31	1	0	1.423904	1.824921	1.093253
32	1	0	0.552442	-0.361435	-0.429847
33	6	0	1.933413	2.542584	-0.879212
34	1	0	2.939756	2.870813	-0.602728
35	1	0	1.963429	2.185966	-1.914807
36	1	0	1.266799	3.408485	-0.822136

Imaginary frequency of -1312.4095 cm^{-1}



(*R*,*S*)-TS-**1**



B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.454641	1.439598	0.066029
2	7	0	0.103732	0.911023	-0.290569
3	1	0	-0.202277	1.290294	-1.186466
4	6	0	-0.989765	1.056781	0.730029
5	1	0	-0.574610	0.654061	1.659269
6	6	0	-1.374936	2.524198	0.954302
7	1	0	-2.161263	2.586805	1.711490
8	1	0	-0.520990	3.109506	1.307936
9	1	0	-1.750018	2.986858	0.036293
10	6	0	-2.159569	0.173581	0.320391
11	6	0	-2.453948	-0.980505	1.059997
12	6	0	-2.954515	0.480882	-0.795217
13	6	0	-3.518874	-1.810852	0.697245
14	1	0	-1.849681	-1.229703	1.928748
15	6	0	-4.014183	-0.351328	-1.164559
16	1	0	-2.759807	1.374175	-1.382917
17	6	0	-4.300277	-1.499178	-0.418424
18	1	0	-3.735481	-2.697577	1.285554
19	1	0	-4.618889	-0.099767	-2.030769
20	1	0	-5.127588	-2.142341	-0.703021
21	6	0	2.361289	0.198695	0.042701
22	6	0	3.724246	0.129134	0.315658
23	6	0	4.343080	-1.119786	0.230816
24	1	0	4.285707	1.015593	0.588085
25	6	0	2.241841	-2.110623	-0.379861
26	6	0	3.599379	-2.253645	-0.121225
27	1	0	5.403924	-1.211634	0.439340
28	1	0	1.600632	-2.939890	-0.656136
29	1	0	4.064166	-3.229878	-0.191654
30	7	0	1.671271	-0.899348	-0.289450
31	1	0	1.426096	1.824649	1.090261
32	1	0	0.557142	-0.355534	-0.432547
33	6	0	1.935198	2.542832	-0.881163
34	1	0	2.941963	2.866982	-0.605910
35	1	0	1.962426	2.187308	-1.916131
36	1	0	1.271882	3.409661	-0.821622

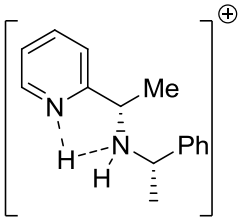
Imaginary frequency of -1214.8351 cm^{-1}

B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

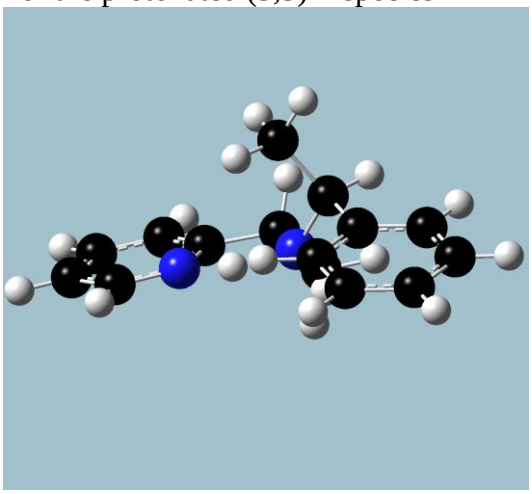
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.461607	1.446327	0.058157
2	7	0	0.110189	0.938471	-0.319521
3	1	0	-0.194816	1.352762	-1.199732
4	6	0	-0.968553	1.055433	0.714620
5	1	0	-0.536686	0.641653	1.630999
6	6	0	-1.368115	2.515174	0.965775
7	1	0	-2.128921	2.560146	1.750531
8	1	0	-0.508700	3.108651	1.291919
9	1	0	-1.780624	2.973747	0.061468
10	6	0	-2.142390	0.172953	0.313649
11	6	0	-2.448206	-0.967706	1.069981
12	6	0	-2.937515	0.472745	-0.804710
13	6	0	-3.523738	-1.792089	0.721592
14	1	0	-1.843659	-1.211144	1.940164
15	6	0	-4.007893	-0.352997	-1.159775
16	1	0	-2.729571	1.354877	-1.404939
17	6	0	-4.305487	-1.487634	-0.396581
18	1	0	-3.747889	-2.668713	1.322516
19	1	0	-4.611698	-0.107451	-2.028656
20	1	0	-5.140509	-2.125871	-0.670246
21	6	0	2.352382	0.195740	0.044761
22	6	0	3.702949	0.101589	0.370104
23	6	0	4.309496	-1.152937	0.280278
24	1	0	4.260626	0.976337	0.685164
25	6	0	2.221240	-2.102724	-0.434131
26	6	0	3.566188	-2.269002	-0.127550
27	1	0	5.360083	-1.264136	0.528504
28	1	0	1.580499	-2.917249	-0.752444
29	1	0	4.021569	-3.249511	-0.202853
30	7	0	1.663061	-0.886017	-0.337401
31	1	0	1.427002	1.832129	1.081558
32	1	0	0.563256	-0.336653	-0.495122
33	6	0	1.971184	2.542377	-0.882832
34	1	0	2.982021	2.845747	-0.597616
35	1	0	1.997357	2.185969	-1.917821
36	1	0	1.319009	3.418040	-0.824959

Imaginary frequency of -1253.4500 cm^{-1}

Cartesian coordinates of the TS for the proton transfer of the protonated (*S*,*S*)-**1** species



(*S*,*S*)-TS-**1**



B3LYP/6-31+G(d), gas phase

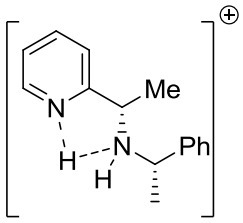
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.259008	1.419771	-0.027772
2	1	0	-1.227964	1.883413	0.964414
3	7	0	-0.032071	0.585007	-0.198022
4	1	0	-0.751394	-0.581154	-0.277316
5	6	0	1.028757	0.685874	0.874199
6	1	0	1.175637	1.753971	1.081642
7	6	0	0.559925	-0.005777	2.158758
8	1	0	1.315898	0.130010	2.937631
9	1	0	-0.380055	0.414865	2.535505
10	1	0	0.423844	-1.082191	2.011765
11	6	0	2.330425	0.131623	0.321228
12	6	0	3.428742	0.983985	0.143222
13	6	0	2.460963	-1.223199	-0.023899
14	6	0	4.635547	0.495159	-0.365488
15	1	0	3.346635	2.035181	0.412239
16	6	0	3.663025	-1.711588	-0.538948
17	1	0	1.628748	-1.909749	0.116880
18	6	0	4.753556	-0.852882	-0.709779
19	1	0	5.479785	1.167230	-0.490656
20	1	0	3.751283	-2.762520	-0.800046
21	1	0	5.690406	-1.234996	-1.105128
22	6	0	-2.419787	0.412204	-0.063199
23	6	0	-3.783191	0.663560	0.059589
24	6	0	-4.659016	-0.423098	-0.009449
25	1	0	-4.154694	1.672409	0.207804
26	6	0	-2.788227	-1.899138	-0.311310
27	6	0	-4.161493	-1.719115	-0.199344
28	1	0	-5.729023	-0.262030	0.084301
29	1	0	-2.327553	-2.870773	-0.457370
30	1	0	-4.827538	-2.573234	-0.257928
31	7	0	-1.968638	-0.837944	-0.238910
32	1	0	0.402089	0.781700	-1.101174
33	6	0	-1.383641	2.513490	-1.094622
34	1	0	-1.403414	2.083972	-2.103003
35	1	0	-2.304604	3.088160	-0.955707
36	1	0	-0.542593	3.211081	-1.024457

Imaginary frequency of -1237.2225 cm^{-1}

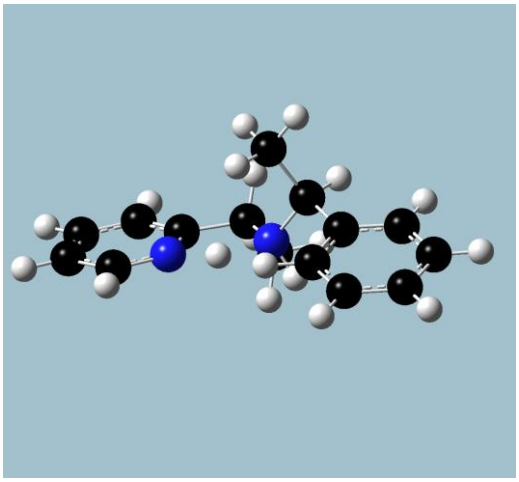
B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.276655	1.428866	-0.035207
2	1	0	-1.247564	1.895532	0.954249
3	7	0	-0.036445	0.611747	-0.215672
4	1	0	-0.720804	-0.550705	-0.286500
5	6	0	1.026879	0.735994	0.843179
6	1	0	1.187518	1.806469	1.020097
7	6	0	0.565198	0.084328	2.151785
8	1	0	1.334352	0.230752	2.916047
9	1	0	-0.361946	0.532425	2.525251
10	1	0	0.405599	-0.992051	2.033475
11	6	0	2.323630	0.149269	0.307122
12	6	0	3.432458	0.982878	0.105322
13	6	0	2.441571	-1.217220	0.005162
14	6	0	4.636725	0.465944	-0.383529
15	1	0	3.356517	2.043266	0.335495
16	6	0	3.640980	-1.734665	-0.489884
17	1	0	1.600051	-1.888388	0.158597
18	6	0	4.742803	-0.894388	-0.684360
19	1	0	5.487370	1.126312	-0.529452
20	1	0	3.716148	-2.794205	-0.719651
21	1	0	5.676585	-1.298769	-1.065762
22	6	0	-2.417331	0.400870	-0.063624
23	6	0	-3.783734	0.632572	0.063460
24	6	0	-4.641057	-0.468482	0.002330
25	1	0	-4.169068	1.635944	0.208999
26	6	0	-2.747040	-1.914555	-0.300970
27	6	0	-4.122798	-1.756722	-0.183660
28	1	0	-5.712776	-0.324579	0.099413
29	1	0	-2.270578	-2.878333	-0.444111
30	1	0	-4.774142	-2.622093	-0.235055
31	7	0	-1.945257	-0.840704	-0.236960
32	1	0	0.377191	0.812844	-1.127075
33	6	0	-1.424936	2.518594	-1.101111
34	1	0	-1.455543	2.085763	-2.106973
35	1	0	-2.349732	3.081812	-0.943669
36	1	0	-0.587429	3.221004	-1.041025

Imaginary frequency of -1336.5017 cm^{-1}



(*S,S*)-TS-**1**



B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.277552	1.429753	-0.035925
2	1	0	-1.250990	1.894935	0.954010
3	7	0	-0.036359	0.614648	-0.217802
4	1	0	-0.722682	-0.542968	-0.287810
5	6	0	1.025816	0.737770	0.842981
6	1	0	1.188718	1.807179	1.020722
7	6	0	0.562495	0.086056	2.150745
8	1	0	1.330842	0.230496	2.914455
9	1	0	-0.362900	0.535312	2.523790
10	1	0	0.401471	-0.988942	2.031119
11	6	0	2.322314	0.150142	0.307496
12	6	0	3.431498	0.982842	0.105017
13	6	0	2.438798	-1.216494	0.006116
14	6	0	4.634961	0.464557	-0.383806
15	1	0	3.356332	2.042596	0.334662
16	6	0	3.637432	-1.734973	-0.489024
17	1	0	1.597283	-1.886285	0.159918
18	6	0	4.739712	-0.895772	-0.684029
19	1	0	5.485613	1.123469	-0.530198
20	1	0	3.711741	-2.793844	-0.718322
21	1	0	5.672355	-1.300769	-1.065232
22	6	0	-2.415543	0.400183	-0.064320
23	6	0	-3.782269	0.629938	0.062968
24	6	0	-4.637229	-0.472471	0.002688
25	1	0	-4.168527	1.632244	0.207796
26	6	0	-2.740976	-1.915357	-0.300444
27	6	0	-4.116580	-1.759678	-0.182762
28	1	0	-5.708553	-0.330856	0.099909
29	1	0	-2.264617	-2.878618	-0.443277
30	1	0	-4.765821	-2.625710	-0.233504
31	7	0	-1.940564	-0.840143	-0.237060
32	1	0	0.379453	0.823584	-1.125212
33	6	0	-1.428685	2.520660	-1.099905
34	1	0	-1.456213	2.089019	-2.105273
35	1	0	-2.355167	3.078997	-0.942817
36	1	0	-0.595044	3.225688	-1.037483

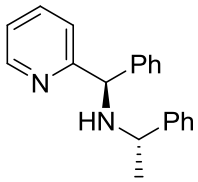
Imaginary frequency of -1239.4090 cm^{-1}

B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

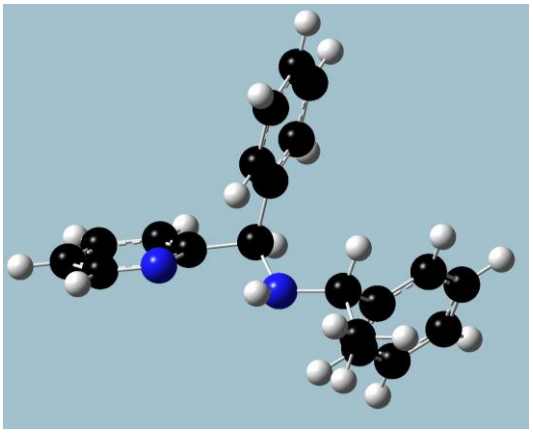
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.277236	1.423635	-0.076147
2	1	0	-1.248589	1.913371	0.901674
3	7	0	-0.041989	0.599113	-0.237705
4	1	0	-0.737695	-0.566633	-0.256548
5	6	0	1.028503	0.770265	0.800043
6	1	0	1.190211	1.845800	0.937069
7	6	0	0.588751	0.161973	2.137726
8	1	0	1.364653	0.340627	2.887009
9	1	0	-0.338427	0.616076	2.500814
10	1	0	0.436248	-0.917964	2.049844
11	6	0	2.323092	0.164033	0.281296
12	6	0	3.471207	0.960688	0.169666
13	6	0	2.402072	-1.190593	-0.081948
14	6	0	4.676687	0.418330	-0.289372
15	1	0	3.423568	2.011302	0.444659
16	6	0	3.602832	-1.732798	-0.547840
17	1	0	1.526075	-1.828290	-0.001336
18	6	0	4.744806	-0.930053	-0.651157
19	1	0	5.557033	1.049780	-0.366899
20	1	0	3.647733	-2.781577	-0.827045
21	1	0	5.678342	-1.353196	-1.010353
22	6	0	-2.420053	0.400001	-0.071842
23	6	0	-3.786723	0.638180	0.047809
24	6	0	-4.645449	-0.462842	0.026832
25	1	0	-4.167855	1.647152	0.156331
26	6	0	-2.753842	-1.922471	-0.223366
27	6	0	-4.129133	-1.758257	-0.112157
28	1	0	-5.716466	-0.314153	0.119116
29	1	0	-2.280200	-2.891820	-0.330541
30	1	0	-4.781580	-2.623400	-0.132104
31	7	0	-1.950563	-0.847829	-0.198903
32	1	0	0.360015	0.765763	-1.159894
33	6	0	-1.423225	2.487101	-1.167682
34	1	0	-1.443815	2.026317	-2.160594
35	1	0	-2.349784	3.050344	-1.028302
36	1	0	-0.585342	3.188355	-1.117816

Imaginary frequency of -1273.7346 cm^{-1}

Cartesian coordinates of the (*R*,*S*)-**2** species



(*R*,*S*)-**2**

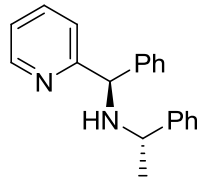


B3LYP/6-31+G(d), gas phase

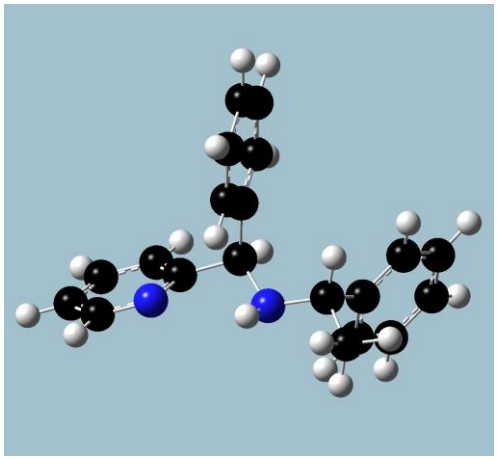
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.555078	-0.227750	-0.095917
2	7	0	0.142456	-0.661786	1.117550
3	1	0	-0.502970	-0.635627	1.903722
4	6	0	1.402865	0.015939	1.431296
5	1	0	1.295918	1.113808	1.383306
6	6	0	1.808370	-0.347855	2.870051
7	1	0	2.757618	0.129990	3.133680
8	1	0	1.046765	-0.009146	3.584817
9	1	0	1.925815	-1.432297	2.975317
10	6	0	2.500127	-0.376796	0.444966
11	6	0	3.407696	0.582212	-0.023355
12	6	0	2.654074	-1.706810	0.026445
13	6	0	4.453196	0.224748	-0.880901
14	1	0	3.292658	1.620578	0.282840
15	6	0	3.694897	-2.067877	-0.832423
16	1	0	1.942142	-2.451024	0.373533
17	6	0	4.600113	-1.103508	-1.288582
18	1	0	5.146702	0.984394	-1.234022
19	1	0	3.799550	-3.103581	-1.147811
20	1	0	5.409500	-1.384922	-1.957864
21	6	0	-1.849177	-1.025355	-0.223902
22	6	0	-2.269701	-1.529087	-1.461607
23	6	0	-3.474511	-2.226475	-1.535567
24	1	0	-1.658797	-1.376163	-2.347259
25	6	0	-3.723359	-1.865955	0.817387
26	6	0	-4.223523	-2.401727	-0.370587
27	1	0	-3.820236	-2.629566	-2.484218
28	1	0	-4.272034	-1.981060	1.750793
29	1	0	-5.166965	-2.939994	-0.377482
30	7	0	-2.568319	-1.193516	0.896644
31	6	0	-0.838617	1.281439	-0.195640
32	6	0	-1.611870	1.943139	0.770880
33	6	0	-0.314662	2.027348	-1.258894
34	6	0	-1.853325	3.314633	0.673152
35	1	0	-2.036024	1.376446	1.595825
36	6	0	-0.555681	3.401723	-1.362038
37	1	0	0.296396	1.530788	-2.010478
38	6	0	-1.326403	4.049867	-0.394764
39	1	0	-2.456786	3.810923	1.429606
40	1	0	-0.137320	3.962960	-2.194225
41	1	0	-1.515271	5.117892	-0.469776
42	1	0	0.081790	-0.488413	-0.949659

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.543068	-0.228185	-0.071052
2	7	0	0.163331	-0.644804	1.145933
3	1	0	-0.472244	-0.577822	1.938162
4	6	0	1.426022	0.046760	1.435894
5	1	0	1.306446	1.142105	1.378525
6	6	0	1.852633	-0.296507	2.873489
7	1	0	2.794107	0.203797	3.123117
8	1	0	1.091397	0.033575	3.592047
9	1	0	1.993403	-1.377351	2.988889
10	6	0	2.514577	-0.342209	0.439029
11	6	0	3.379300	0.632225	-0.078222
12	6	0	2.708171	-1.679103	0.058439
13	6	0	4.419172	0.284248	-0.947819
14	1	0	3.236662	1.674988	0.199516
15	6	0	3.743204	-2.031766	-0.811990
16	1	0	2.034793	-2.440382	0.443031
17	6	0	4.604528	-1.050936	-1.318121
18	1	0	5.077760	1.056145	-1.338827
19	1	0	3.877383	-3.072661	-1.097230
20	1	0	5.408816	-1.325149	-1.996287
21	6	0	-1.822574	-1.050638	-0.204894
22	6	0	-2.218091	-1.569570	-1.444594
23	6	0	-3.410930	-2.287762	-1.529920
24	1	0	-1.598752	-1.413168	-2.323541
25	6	0	-3.696678	-1.918014	0.818493
26	6	0	-4.172187	-2.468125	-0.373361
27	1	0	-3.737064	-2.702401	-2.480098
28	1	0	-4.256642	-2.038741	1.744073
29	1	0	-5.106349	-3.021513	-0.388945
30	7	0	-2.552604	-1.224421	0.909107
31	6	0	-0.860911	1.273421	-0.178146
32	6	0	-1.551110	1.949508	0.840119
33	6	0	-0.465499	1.995652	-1.312051
34	6	0	-1.838448	3.311829	0.724967
35	1	0	-1.871315	1.406083	1.725446
36	6	0	-0.753066	3.360065	-1.433657
37	1	0	0.077084	1.488172	-2.107496
38	6	0	-1.441100	4.022923	-0.413886
39	1	0	-2.374299	3.818992	1.523757
40	1	0	-0.435002	3.902315	-2.320828
41	1	0	-1.664653	5.083039	-0.502531
42	1	0	0.099709	-0.478344	-0.922358



(*R*,*S*)-**2**



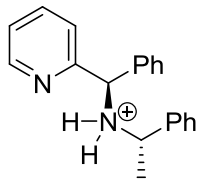
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.545435	-0.230049	-0.074972
2	7	0	0.159675	-0.649997	1.140851
3	1	0	-0.476414	-0.591234	1.931634
4	6	0	1.422946	0.037007	1.435333
5	1	0	1.308042	1.132411	1.379736
6	6	0	1.845653	-0.310810	2.872695
7	1	0	2.786392	0.186651	3.125489
8	1	0	1.083686	0.018017	3.589157
9	1	0	1.984116	-1.391305	2.984337
10	6	0	2.512401	-0.351568	0.439218
11	6	0	3.385384	0.620924	-0.067421
12	6	0	2.697633	-1.686696	0.048913
13	6	0	4.425296	0.272345	-0.936344
14	1	0	3.249044	1.661589	0.218054
15	6	0	3.732675	-2.039585	-0.821104
16	1	0	2.017572	-2.444980	0.425564
17	6	0	4.602248	-1.060973	-1.316665
18	1	0	5.090173	1.041848	-1.318986
19	1	0	3.860380	-3.078236	-1.114180
20	1	0	5.405952	-1.335176	-1.994162
21	6	0	-1.829591	-1.044622	-0.208025
22	6	0	-2.235765	-1.549365	-1.450137
23	6	0	-3.432684	-2.260119	-1.534479
24	1	0	-1.621249	-1.388107	-2.330545
25	6	0	-3.702208	-1.911427	0.818968
26	6	0	-4.187626	-2.447282	-0.375010
27	1	0	-3.766835	-2.663843	-2.485667
28	1	0	-4.257716	-2.038488	1.745689
29	1	0	-5.124108	-2.995091	-0.389947
30	7	0	-2.553393	-1.225018	0.908855
31	6	0	-0.854481	1.273440	-0.179555
32	6	0	-1.557677	1.946449	0.831791
33	6	0	-0.435700	2.000466	-1.301690
34	6	0	-1.834691	3.310982	0.721164
35	1	0	-1.895941	1.398340	1.706522
36	6	0	-0.712874	3.367315	-1.418330
37	1	0	0.116887	1.495181	-2.090443
38	6	0	-1.413829	4.027196	-0.405798
39	1	0	-2.380619	3.815752	1.513476
40	1	0	-0.377105	3.913431	-2.295509
41	1	0	-1.629292	5.088415	-0.490832
42	1	0	0.093013	-0.481842	-0.928651

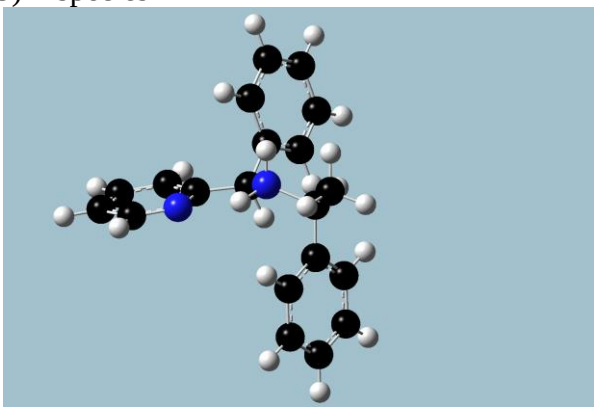
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.524170	-0.213880	-0.039126
2	7	0	0.203073	-0.577425	1.184377
3	1	0	-0.415363	-0.473329	1.985008
4	6	0	1.456875	0.156662	1.425272
5	1	0	1.308382	1.242611	1.313857
6	6	0	1.906513	-0.103707	2.872258
7	1	0	2.835890	0.432825	3.084596
8	1	0	1.143187	0.241709	3.579160
9	1	0	2.077368	-1.172556	3.039377
10	6	0	2.540400	-0.251802	0.431298
11	6	0	3.317387	0.725462	-0.206504
12	6	0	2.816694	-1.603203	0.168408
13	6	0	4.349433	0.367423	-1.082136
14	1	0	3.111955	1.776778	-0.018437
15	6	0	3.843822	-1.966169	-0.707226
16	1	0	2.218810	-2.372244	0.648820
17	6	0	4.615715	-0.981373	-1.336171
18	1	0	4.938391	1.140970	-1.567341
19	1	0	4.042378	-3.017222	-0.899138
20	1	0	5.413433	-1.263535	-2.017502
21	6	0	-1.756783	-1.105797	-0.174917
22	6	0	-2.085635	-1.690084	-1.404950
23	6	0	-3.235141	-2.475108	-1.497854
24	1	0	-1.448532	-1.531101	-2.269289
25	6	0	-3.613837	-2.040028	0.826374
26	6	0	-4.020894	-2.656654	-0.357960
27	1	0	-3.508880	-2.939448	-2.440645
28	1	0	-4.195668	-2.159671	1.737605
29	1	0	-4.922408	-3.260053	-0.379885
30	7	0	-2.511552	-1.279914	0.923572
31	6	0	-0.925091	1.266006	-0.166612
32	6	0	-1.555420	1.952326	0.883333
33	6	0	-0.679959	1.953845	-1.363702
34	6	0	-1.933034	3.290123	0.737230
35	1	0	-1.754484	1.443072	1.821950
36	6	0	-1.058536	3.292597	-1.515781
37	1	0	-0.185526	1.438954	-2.184064
38	6	0	-1.687491	3.965750	-0.464179
39	1	0	-2.418914	3.804995	1.561506
40	1	0	-0.856863	3.807550	-2.451009
41	1	0	-1.980371	5.005706	-0.576534
42	1	0	0.131484	-0.438972	-0.886014

Cartesian coordinates of the ammonium-(*R*,*S*)-**2** species



(*R*,*S*)-Ammonium **2**

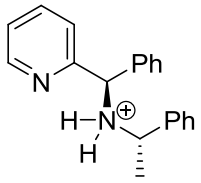


B3LYP/6-31+G(d), gas phase

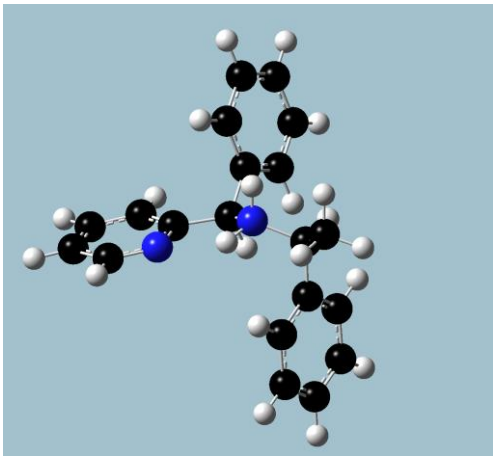
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.580871	0.045984	-0.063972
2	7	0	-0.183987	-0.132219	1.243077
3	1	0	0.489745	-0.372487	1.978292
4	6	0	-1.308508	-1.169054	1.260974
5	1	0	-0.838882	-2.092865	0.910123
6	6	0	-1.762055	-1.346224	2.713311
7	1	0	-2.539616	-2.114162	2.752144
8	1	0	-0.936660	-1.673037	3.357758
9	1	0	-2.187296	-0.423795	3.123224
10	6	0	-2.413510	-0.770778	0.303375
11	6	0	-2.750529	-1.625765	-0.755312
12	6	0	-3.138387	0.418958	0.476724
13	6	0	-3.793788	-1.300598	-1.626839
14	1	0	-2.206450	-2.558186	-0.892152
15	6	0	-4.172946	0.749340	-0.399904
16	1	0	-2.910332	1.094593	1.298924
17	6	0	-4.503322	-0.110525	-1.452330
18	1	0	-4.050261	-1.976500	-2.437587
19	1	0	-4.726533	1.672831	-0.256334
20	1	0	-5.313734	0.144947	-2.128933
21	6	0	0.989120	1.523803	-0.137404
22	6	0	1.923641	1.980667	-1.069227
23	6	0	2.180980	3.351056	-1.125606
24	1	0	2.436359	1.286596	-1.727614
25	6	0	0.599304	3.659073	0.650194
26	6	0	1.508901	4.208808	-0.251619
27	1	0	2.898942	3.742738	-1.840386
28	1	0	0.055479	4.282816	1.354576
29	1	0	1.686512	5.279386	-0.264270
30	7	0	0.341531	2.342825	0.702211
31	6	0	1.706178	-0.961871	-0.168206
32	6	0	2.826043	-0.875534	0.676092
33	6	0	1.630798	-2.004051	-1.101662
34	6	0	3.843833	-1.826775	0.595875
35	1	0	2.921005	-0.051429	1.381934
36	6	0	2.655784	-2.951080	-1.188501
37	1	0	0.775975	-2.072167	-1.771107
38	6	0	3.759481	-2.866129	-0.337193
39	1	0	4.706851	-1.750428	1.251072
40	1	0	2.590339	-3.751304	-1.920040
41	1	0	4.555898	-3.601750	-0.403337
42	1	0	-0.159036	-0.144924	-0.848275
43	1	0	-0.522448	0.829054	1.472343

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.579861	0.051047	-0.043935
2	7	0	-0.196951	-0.151437	1.249225
3	1	0	0.461686	-0.388531	1.999076
4	6	0	-1.298957	-1.211820	1.229096
5	1	0	-0.814366	-2.111330	0.840753
6	6	0	-1.741171	-1.461216	2.673000
7	1	0	-2.498298	-2.250145	2.679741
8	1	0	-0.898742	-1.794254	3.289785
9	1	0	-2.179750	-0.567298	3.127794
10	6	0	-2.416538	-0.799730	0.290102
11	6	0	-2.695189	-1.584480	-0.837896
12	6	0	-3.203570	0.335437	0.541208
13	6	0	-3.741099	-1.244016	-1.701181
14	1	0	-2.096449	-2.469769	-1.039173
15	6	0	-4.241744	0.681912	-0.325843
16	1	0	-3.019041	0.956628	1.414404
17	6	0	-4.513833	-0.107838	-1.448240
18	1	0	-3.947474	-1.864585	-2.568732
19	1	0	-4.840644	1.565057	-0.121699
20	1	0	-5.325007	0.160952	-2.119228
21	6	0	0.973025	1.531738	-0.113927
22	6	0	1.930891	1.988723	-1.022930
23	6	0	2.178649	3.360040	-1.086304
24	1	0	2.467275	1.293634	-1.660293
25	6	0	0.539823	3.670462	0.635946
26	6	0	1.472797	4.220475	-0.241799
27	1	0	2.914583	3.749882	-1.783332
28	1	0	-0.031787	4.297504	1.315016
29	1	0	1.641147	5.292365	-0.259396
30	7	0	0.291117	2.352836	0.694922
31	6	0	1.720774	-0.940287	-0.154311
32	6	0	2.827898	-0.862912	0.706464
33	6	0	1.672113	-1.954561	-1.119381
34	6	0	3.860450	-1.797251	0.610758
35	1	0	2.897866	-0.065922	1.444096
36	6	0	2.710858	-2.885349	-1.220670
37	1	0	0.824584	-2.014979	-1.797850
38	6	0	3.803213	-2.810582	-0.353095
39	1	0	4.712171	-1.729081	1.281612
40	1	0	2.663306	-3.665816	-1.974802
41	1	0	4.609903	-3.534361	-0.428958
42	1	0	-0.145470	-0.141411	-0.840293
43	1	0	-0.564157	0.792910	1.490080



(*R*,*S*)-Ammonium **2**



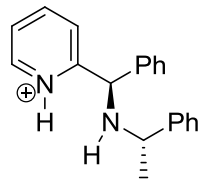
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.583025	0.046229	-0.048128
2	7	0	-0.191539	-0.170472	1.242373
3	1	0	0.469687	-0.401053	1.990069
4	6	0	-1.279695	-1.243716	1.218761
5	1	0	-0.787884	-2.135102	0.821985
6	6	0	-1.715610	-1.508414	2.661548
7	1	0	-2.464913	-2.303225	2.663950
8	1	0	-0.869500	-1.838200	3.272998
9	1	0	-2.160396	-0.622113	3.122887
10	6	0	-2.404604	-0.837946	0.285669
11	6	0	-2.668705	-1.609394	-0.854753
12	6	0	-3.210757	0.279651	0.554090
13	6	0	-3.719652	-1.273115	-1.713299
14	1	0	-2.054700	-2.480124	-1.069194
15	6	0	-4.253971	0.621779	-0.308234
16	1	0	-3.037157	0.889595	1.436524
17	6	0	-4.511749	-0.154720	-1.442967
18	1	0	-3.914846	-1.882626	-2.590215
19	1	0	-4.867831	1.490441	-0.091053
20	1	0	-5.326546	0.110396	-2.109725
21	6	0	0.939026	1.536084	-0.115476
22	6	0	1.879761	2.023007	-1.026533
23	6	0	2.091696	3.400391	-1.081273
24	1	0	2.429253	1.345977	-1.670841
25	6	0	0.455180	3.658319	0.651968
26	6	0	1.368904	4.236832	-0.227022
27	1	0	2.812929	3.813847	-1.778881
28	1	0	-0.127808	4.266352	1.337634
29	1	0	1.509924	5.311928	-0.238269
30	7	0	0.241272	2.334009	0.702642
31	6	0	1.748901	-0.916083	-0.155950
32	6	0	2.849867	-0.814273	0.710141
33	6	0	1.729195	-1.928007	-1.124326
34	6	0	3.905675	-1.721935	0.615146
35	1	0	2.896839	-0.020394	1.451781
36	6	0	2.791556	-2.831532	-1.224856
37	1	0	0.886171	-2.007237	-1.805157
38	6	0	3.878181	-2.732163	-0.352956
39	1	0	4.751893	-1.635346	1.289526
40	1	0	2.766905	-3.609672	-1.981328
41	1	0	4.702743	-3.434333	-0.428406
42	1	0	-0.132916	-0.162414	-0.848455
43	1	0	-0.567312	0.772571	1.479757

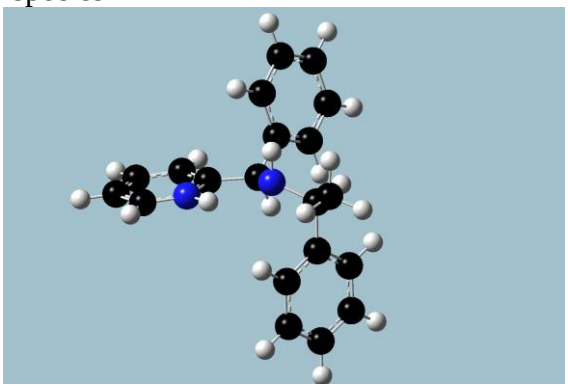
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.571640	0.044050	-0.024754
2	7	0	-0.199833	-0.145013	1.268638
3	1	0	0.457789	-0.397882	2.012571
4	6	0	-1.322638	-1.178078	1.251283
5	1	0	-0.856332	-2.093799	0.881958
6	6	0	-1.794337	-1.392798	2.691188
7	1	0	-2.571159	-2.161189	2.696281
8	1	0	-0.971641	-1.734600	3.327086
9	1	0	-2.214734	-0.477014	3.116986
10	6	0	-2.426657	-0.763357	0.295050
11	6	0	-2.718629	-1.573864	-0.811382
12	6	0	-3.193912	0.393095	0.511608
13	6	0	-3.757428	-1.239529	-1.686533
14	1	0	-2.133742	-2.472784	-0.987208
15	6	0	-4.224894	0.733339	-0.367372
16	1	0	-2.995939	1.034848	1.366219
17	6	0	-4.510728	-0.082915	-1.467735
18	1	0	-3.973057	-1.879916	-2.536616
19	1	0	-4.807584	1.632377	-0.190027
20	1	0	-5.315597	0.181179	-2.147216
21	6	0	0.989937	1.516567	-0.108472
22	6	0	1.928400	1.948481	-1.050925
23	6	0	2.209724	3.311943	-1.129337
24	1	0	2.423303	1.238012	-1.703619
25	6	0	0.637383	3.671215	0.643447
26	6	0	1.555172	4.194138	-0.265519
27	1	0	2.930995	3.679405	-1.852475
28	1	0	0.105340	4.317307	1.336193
29	1	0	1.750107	5.260696	-0.292690
30	7	0	0.355717	2.359205	0.717719
31	6	0	1.701954	-0.961016	-0.141348
32	6	0	2.818553	-0.892438	0.707886
33	6	0	1.633752	-1.977662	-1.102828
34	6	0	3.843134	-1.835092	0.602347
35	1	0	2.894689	-0.097887	1.446413
36	6	0	2.664246	-2.917293	-1.214094
37	1	0	0.777139	-2.033677	-1.768630
38	6	0	3.768041	-2.849453	-0.359789
39	1	0	4.701575	-1.773643	1.264387
40	1	0	2.601797	-3.699124	-1.964938
41	1	0	4.567888	-3.579076	-0.443538
42	1	0	-0.152901	-0.138817	-0.823019
43	1	0	-0.545397	0.800254	1.521040

Cartesian coordinates of the pyridinium-(*R*,*S*)-**2** species



(*R*,*S*)-Pyridinium **2**

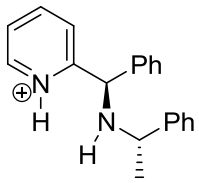


B3LYP/6-31+G(d), gas phase

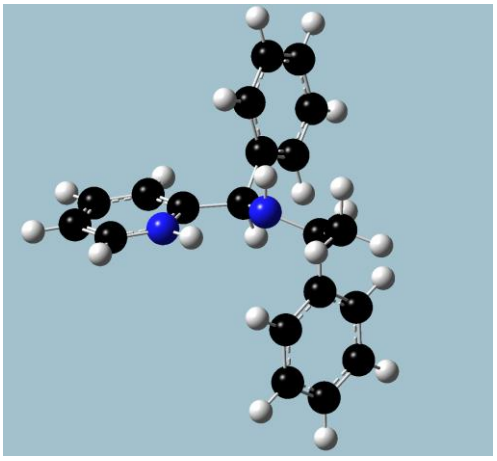
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.607851	-0.050041	-0.008490
2	7	0	-0.130913	-0.400336	1.224680
3	1	0	0.542061	-0.649469	1.949885
4	6	0	-1.096804	-1.531362	1.079318
5	1	0	-0.596444	-2.372152	0.574887
6	6	0	-1.505442	-2.002535	2.480494
7	1	0	-2.210516	-2.835381	2.404290
8	1	0	-0.632940	-2.352337	3.046530
9	1	0	-1.988084	-1.200403	3.049229
10	6	0	-2.283614	-1.113237	0.223054
11	6	0	-2.567231	-1.791984	-0.969499
12	6	0	-3.132296	-0.065320	0.615843
13	6	0	-3.667958	-1.434304	-1.756054
14	1	0	-1.932013	-2.619396	-1.280452
15	6	0	-4.230860	0.296014	-0.166003
16	1	0	-2.951744	0.454913	1.554576
17	6	0	-4.500141	-0.386972	-1.357422
18	1	0	-3.875113	-1.977489	-2.674043
19	1	0	-4.886479	1.099555	0.159573
20	1	0	-5.358757	-0.110005	-1.962688
21	6	0	0.693356	1.474412	-0.105483
22	6	0	1.447300	2.205685	-1.022783
23	6	0	1.360307	3.597189	-1.019239
24	1	0	2.092819	1.682774	-1.719955
25	6	0	-0.196189	3.496291	0.799879
26	6	0	0.530728	4.255743	-0.097871
27	1	0	1.940680	4.175860	-1.731995
28	1	0	-0.860194	3.910646	1.549902
29	1	0	0.454007	5.337065	-0.077900
30	7	0	-0.087544	2.150839	0.758482
31	6	0	1.965661	-0.721696	-0.158756
32	6	0	3.022808	-0.405642	0.710487
33	6	0	2.163601	-1.695705	-1.146105
34	6	0	4.250624	-1.059724	0.598690
35	1	0	2.894659	0.355793	1.478981
36	6	0	3.394507	-2.349668	-1.260102
37	1	0	1.355650	-1.946602	-1.830059
38	6	0	4.438130	-2.034009	-0.387737
39	1	0	5.060572	-0.807805	1.277494
40	1	0	3.534779	-3.103928	-2.029209
41	1	0	5.394251	-2.541937	-0.475284
42	1	0	-0.023140	-0.353721	-0.854543
43	1	0	-0.590881	1.501700	1.395332

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.549099	0.017665	0.019333
2	7	0	-0.224215	-0.069505	1.273486
3	1	0	0.409903	-0.288592	2.042634
4	6	0	-1.308939	-1.085300	1.271055
5	1	0	-0.909953	-2.057535	0.943250
6	6	0	-1.817104	-1.249646	2.710229
7	1	0	-2.604553	-2.008763	2.746092
8	1	0	-1.005128	-1.572339	3.373579
9	1	0	-2.226638	-0.308846	3.093827
10	6	0	-2.424208	-0.695861	0.309608
11	6	0	-2.850456	-1.598854	-0.673994
12	6	0	-3.071303	0.546586	0.405839
13	6	0	-3.900088	-1.274853	-1.541240
14	1	0	-2.358773	-2.565531	-0.762056
15	6	0	-4.116523	0.876166	-0.460146
16	1	0	-2.760150	1.259039	1.165646
17	6	0	-4.534881	-0.034588	-1.437681
18	1	0	-4.216293	-1.989612	-2.296664
19	1	0	-4.608151	1.841610	-0.370208
20	1	0	-5.349106	0.221593	-2.110442
21	6	0	1.053221	1.449580	-0.148184
22	6	0	1.971294	1.883998	-1.101142
23	6	0	2.286483	3.240346	-1.177202
24	1	0	2.428549	1.164027	-1.769868
25	6	0	0.789388	3.687983	0.637488
26	6	0	1.692964	4.156813	-0.298134
27	1	0	2.997727	3.586780	-1.920378
28	1	0	0.280640	4.313193	1.360656
29	1	0	1.928483	5.213683	-0.337629
30	7	0	0.506677	2.368529	0.672636
31	6	0	1.656337	-1.020121	-0.132908
32	6	0	2.800227	-0.982417	0.681005
33	6	0	1.520085	-2.056795	-1.065633
34	6	0	3.782904	-1.967855	0.568042
35	1	0	2.934193	-0.179305	1.403317
36	6	0	2.504682	-3.044086	-1.181010
37	1	0	0.641613	-2.094470	-1.705793
38	6	0	3.636763	-3.002226	-0.363586
39	1	0	4.663615	-1.925804	1.203204
40	1	0	2.384649	-3.842411	-1.908373
41	1	0	4.402826	-3.767767	-0.451760
42	1	0	-0.168493	-0.133122	-0.797472
43	1	0	-0.161871	1.961784	1.345157



(*R*,*S*)-Pyridinium **2**



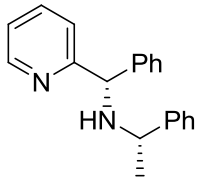
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.550353	0.016643	0.020026
2	7	0	-0.220488	-0.083108	1.274377
3	1	0	0.414757	-0.301855	2.040988
4	6	0	-1.299393	-1.105068	1.268388
5	1	0	-0.896365	-2.073000	0.934732
6	6	0	-1.804719	-1.279396	2.706919
7	1	0	-2.585987	-2.043315	2.740216
8	1	0	-0.990233	-1.598722	3.366791
9	1	0	-2.219697	-0.343745	3.094279
10	6	0	-2.416578	-0.717900	0.308377
11	6	0	-2.832131	-1.616253	-0.683865
12	6	0	-3.074719	0.517875	0.413770
13	6	0	-3.882232	-1.293959	-1.550852
14	1	0	-2.331993	-2.577068	-0.778325
15	6	0	-4.120137	0.845634	-0.452295
16	1	0	-2.772454	1.225705	1.180321
17	6	0	-4.527837	-0.060328	-1.438453
18	1	0	-4.190277	-2.004342	-2.312547
19	1	0	-4.620253	1.805114	-0.355708
20	1	0	-5.341888	0.194256	-2.110685
21	6	0	1.034231	1.454959	-0.145981
22	6	0	1.944898	1.903174	-1.099655
23	6	0	2.240289	3.263655	-1.173770
24	1	0	2.411242	1.190891	-1.769190
25	6	0	0.739144	3.687085	0.643192
26	6	0	1.634693	4.169950	-0.292572
27	1	0	2.945203	3.621408	-1.916670
28	1	0	0.223294	4.304726	1.367029
29	1	0	1.854828	5.229432	-0.330544
30	7	0	0.475284	2.363789	0.676664
31	6	0	1.670907	-1.005912	-0.134092
32	6	0	2.817049	-0.950429	0.675466
33	6	0	1.544430	-2.047130	-1.062882
34	6	0	3.811840	-1.923204	0.561767
35	1	0	2.942592	-0.144428	1.394767
36	6	0	2.541436	-3.021520	-1.178866
37	1	0	0.664705	-2.097931	-1.699015
38	6	0	3.675806	-2.962046	-0.366097
39	1	0	4.693645	-1.867949	1.192985
40	1	0	2.429498	-3.823092	-1.902711
41	1	0	4.450997	-3.717103	-0.454833
42	1	0	-0.163782	-0.141672	-0.797983
43	1	0	-0.185377	1.942938	1.347660

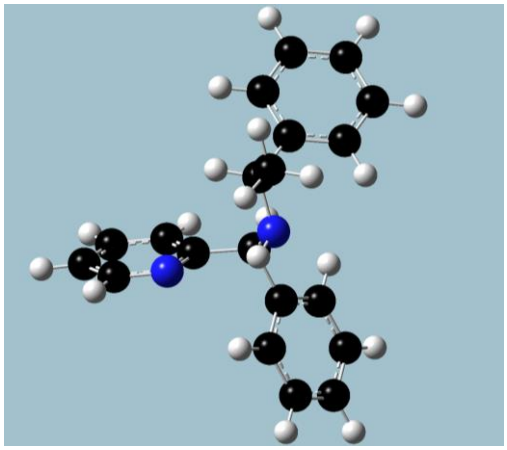
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.547409	0.021970	0.013960
2	7	0	-0.235460	-0.055071	1.259758
3	1	0	0.391566	-0.262580	2.035798
4	6	0	-1.322044	-1.063862	1.255530
5	1	0	-0.935417	-2.037796	0.919945
6	6	0	-1.831287	-1.231925	2.694422
7	1	0	-2.623387	-1.985102	2.726728
8	1	0	-1.020842	-1.561024	3.354602
9	1	0	-2.233828	-0.289142	3.079047
10	6	0	-2.441802	-0.662673	0.303119
11	6	0	-2.922320	-1.579404	-0.642426
12	6	0	-3.042498	0.604780	0.375145
13	6	0	-3.980703	-1.244636	-1.495361
14	1	0	-2.465351	-2.563612	-0.712353
15	6	0	-4.096498	0.944913	-0.477013
16	1	0	-2.684524	1.328554	1.101877
17	6	0	-4.570177	0.020216	-1.415937
18	1	0	-4.338491	-1.969181	-2.221414
19	1	0	-4.550528	1.929534	-0.407262
20	1	0	-5.389774	0.284712	-2.077789
21	6	0	1.088601	1.440607	-0.144963
22	6	0	2.027487	1.850081	-1.089442
23	6	0	2.379358	3.197111	-1.162992
24	1	0	2.471261	1.118599	-1.753584
25	6	0	0.876377	3.684078	0.635905
26	6	0	1.801380	4.129291	-0.290185
27	1	0	3.106395	3.523856	-1.899013
28	1	0	0.376275	4.321770	1.353337
29	1	0	2.064665	5.179108	-0.326914
30	7	0	0.557734	2.373370	0.668416
31	6	0	1.633408	-1.040515	-0.133046
32	6	0	2.719997	-1.089576	0.755921
33	6	0	1.537066	-2.007936	-1.141715
34	6	0	3.686987	-2.090362	0.638519
35	1	0	2.816464	-0.345545	1.543650
36	6	0	2.505956	-3.011239	-1.261473
37	1	0	0.702754	-1.978453	-1.837521
38	6	0	3.582072	-3.054894	-0.371319
39	1	0	4.522449	-2.116076	1.332014
40	1	0	2.417016	-3.755340	-2.047560
41	1	0	4.334866	-3.832359	-0.461768
42	1	0	-0.161103	-0.107624	-0.813267
43	1	0	-0.128996	1.993447	1.334334

Cartesian coordinates of the (*S*,*S*)-**2** species



(*S*,*S*)-**2**

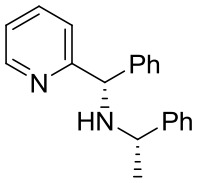


B3LYP/6-31+G(d), gas phase

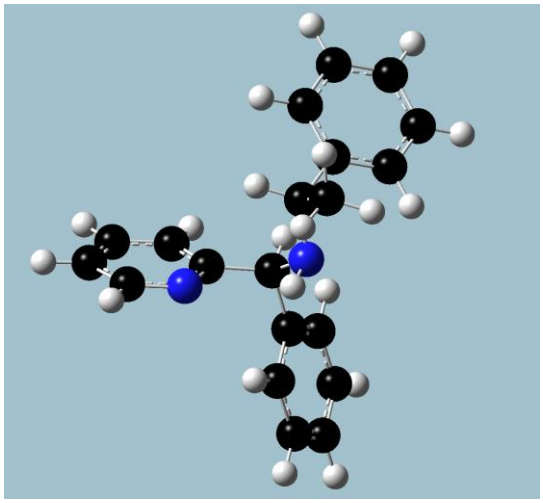
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.513175	-0.111184	-0.028703
2	1	0	0.198193	-0.308135	-0.838462
3	7	0	0.238263	-0.211857	1.228394
4	1	0	-0.381525	0.053238	1.992209
5	6	0	1.455801	0.611660	1.296318
6	1	0	1.259746	1.650041	0.974912
7	6	0	1.925068	0.665106	2.760025
8	1	0	2.845841	1.251243	2.847900
9	1	0	1.160437	1.133650	3.393137
10	1	0	2.119923	-0.344839	3.137993
11	6	0	2.550766	0.051164	0.394192
12	6	0	3.364373	0.914934	-0.350754
13	6	0	2.800013	-1.328107	0.329191
14	6	0	4.410640	0.419565	-1.135827
15	1	0	3.176130	1.986879	-0.317830
16	6	0	3.842283	-1.827196	-0.455421
17	1	0	2.160179	-2.003523	0.890493
18	6	0	4.653363	-0.955154	-1.189897
19	1	0	5.030154	1.106583	-1.707564
20	1	0	4.021921	-2.899210	-0.494938
21	1	0	5.463830	-1.344687	-1.801107
22	6	0	-1.576281	-1.209042	-0.082986
23	6	0	-2.755816	-1.126443	0.671578
24	6	0	-1.365416	-2.344586	-0.876641
25	6	0	-3.695327	-2.160115	0.638795
26	1	0	-2.941757	-0.247566	1.283257
27	6	0	-2.305910	-3.377510	-0.916196
28	1	0	-0.452562	-2.424827	-1.463242
29	6	0	-3.474875	-3.288931	-0.155935
30	1	0	-4.603245	-2.080915	1.232067
31	1	0	-2.124070	-4.249974	-1.539235
32	1	0	-4.208504	-4.090792	-0.183786
33	6	0	-1.123704	1.273718	-0.285381
34	6	0	-1.197133	1.800359	-1.582542
35	6	0	-1.782080	3.050299	-1.777375
36	1	0	-0.799508	1.234161	-2.421128
37	6	0	-2.156344	3.140292	0.585222
38	6	0	-2.277115	3.740859	-0.668944
39	1	0	-1.847272	3.479982	-2.774003
40	1	0	-2.524615	3.644182	1.477566
41	1	0	-2.739509	4.718650	-0.769028
42	7	0	-1.593773	1.940105	0.781388

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.509783	-0.115622	-0.018260
2	1	0	0.200587	-0.316552	-0.826943
3	7	0	0.238473	-0.224198	1.243842
4	1	0	-0.378688	0.069545	2.000191
5	6	0	1.465099	0.592837	1.306965
6	1	0	1.270002	1.629929	0.984488
7	6	0	1.939826	0.647372	2.768579
8	1	0	2.856461	1.240585	2.852107
9	1	0	1.175733	1.110256	3.406022
10	1	0	2.143637	-0.360765	3.146992
11	6	0	2.554823	0.031583	0.399120
12	6	0	3.318727	0.892768	-0.400710
13	6	0	2.853133	-1.340010	0.380677
14	6	0	4.361419	0.402951	-1.195671
15	1	0	3.094891	1.958066	-0.403481
16	6	0	3.891437	-1.834559	-0.413215
17	1	0	2.260085	-2.019680	0.986368
18	6	0	4.651241	-0.964405	-1.204254
19	1	0	4.940640	1.088146	-1.810008
20	1	0	4.107666	-2.900395	-0.415956
21	1	0	5.458007	-1.349936	-1.822675
22	6	0	-1.583746	-1.202146	-0.080117
23	6	0	-2.711306	-1.166239	0.755473
24	6	0	-1.442593	-2.276515	-0.969584
25	6	0	-3.666276	-2.185719	0.708597
26	1	0	-2.847258	-0.334123	1.441283
27	6	0	-2.399239	-3.295748	-1.023396
28	1	0	-0.574345	-2.320233	-1.623705
29	6	0	-3.514560	-3.254392	-0.181900
30	1	0	-4.532059	-2.142667	1.365000
31	1	0	-2.270782	-4.120134	-1.720565
32	1	0	-4.259558	-4.045100	-0.220084
33	6	0	-1.110974	1.274237	-0.273798
34	6	0	-1.168256	1.803974	-1.570173
35	6	0	-1.749411	3.056136	-1.768631
36	1	0	-0.761058	1.241081	-2.406120
37	6	0	-2.150632	3.141637	0.590744
38	6	0	-2.256180	3.744570	-0.663926
39	1	0	-1.801866	3.488325	-2.764480
40	1	0	-2.528022	3.645967	1.478575
41	1	0	-2.715778	4.723044	-0.766504
42	7	0	-1.592012	1.938253	0.790497



(*S,S*)-**2**



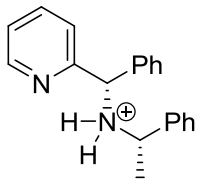
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.509351	-0.115227	-0.018839
2	1	0	0.199245	-0.315319	-0.828786
3	7	0	0.238753	-0.223428	1.242666
4	1	0	-0.377752	0.066199	1.999321
5	6	0	1.464899	0.593130	1.307737
6	1	0	1.271955	1.630010	0.985066
7	6	0	1.938267	0.646793	2.769519
8	1	0	2.853452	1.239874	2.854256
9	1	0	1.173682	1.107774	3.405603
10	1	0	2.141998	-0.360976	3.145952
11	6	0	2.554834	0.032659	0.399661
12	6	0	3.323076	0.895050	-0.394480
13	6	0	2.848172	-1.339784	0.375626
14	6	0	4.365524	0.405180	-1.189325
15	1	0	3.102716	1.960238	-0.392661
16	6	0	3.886115	-1.834103	-0.418508
17	1	0	2.251110	-2.018984	0.976574
18	6	0	4.650476	-0.962959	-1.203653
19	1	0	4.948076	1.090460	-1.798900
20	1	0	4.098530	-2.899819	-0.426006
21	1	0	5.456495	-1.348066	-1.821810
22	6	0	-1.582665	-1.202084	-0.080942
23	6	0	-2.712632	-1.163167	0.751062
24	6	0	-1.437959	-2.279751	-0.965631
25	6	0	-3.666649	-2.183282	0.705357
26	1	0	-2.850470	-0.328523	1.432205
27	6	0	-2.393898	-3.299408	-1.018144
28	1	0	-0.568446	-2.325211	-1.616547
29	6	0	-3.511561	-3.255242	-0.180246
30	1	0	-4.533848	-2.138249	1.358359
31	1	0	-2.263259	-4.125880	-1.711112
32	1	0	-4.255429	-4.045891	-0.217535
33	6	0	-1.111285	1.274028	-0.274441
34	6	0	-1.166744	1.804324	-1.570625
35	6	0	-1.748913	3.055645	-1.769235
36	1	0	-0.757252	1.242727	-2.405204
37	6	0	-2.154903	3.139692	0.589299
38	6	0	-2.258631	3.742672	-0.665235
39	1	0	-1.799977	3.488198	-2.764134
40	1	0	-2.534865	3.643879	1.475391
41	1	0	-2.718868	4.719890	-0.768058
42	7	0	-1.595058	1.936665	0.789375

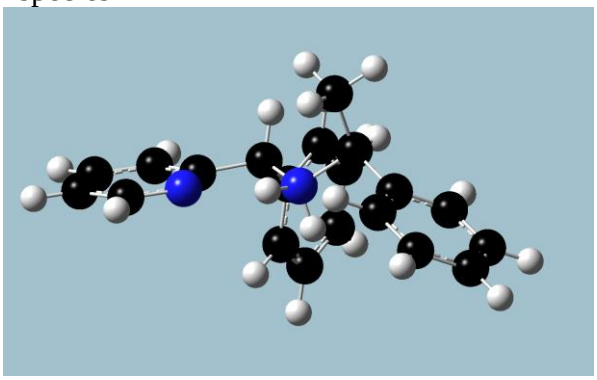
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.507240	-0.120367	0.002227
2	1	0	0.197332	-0.320885	-0.810184
3	7	0	0.243163	-0.247579	1.262530
4	1	0	-0.366125	0.034842	2.028035
5	6	0	1.476153	0.564319	1.332190
6	1	0	1.282925	1.603643	1.021516
7	6	0	1.956969	0.600005	2.791573
8	1	0	2.870690	1.195471	2.876969
9	1	0	1.193390	1.050990	3.435721
10	1	0	2.166437	-0.411133	3.156316
11	6	0	2.556955	0.013318	0.407538
12	6	0	3.256662	0.874068	-0.449730
13	6	0	2.909134	-1.346128	0.424154
14	6	0	4.287072	0.396081	-1.268401
15	1	0	2.991842	1.928492	-0.478627
16	6	0	3.935009	-1.829035	-0.392947
17	1	0	2.373172	-2.029053	1.076820
18	6	0	4.629439	-0.959017	-1.242794
19	1	0	4.815170	1.080364	-1.926808
20	1	0	4.193095	-2.884327	-0.367081
21	1	0	5.426114	-1.335234	-1.878326
22	6	0	-1.592441	-1.194752	-0.073314
23	6	0	-2.691588	-1.191977	0.800916
24	6	0	-1.492513	-2.222211	-1.022417
25	6	0	-3.660025	-2.197677	0.731604
26	1	0	-2.795567	-0.399022	1.535718
27	6	0	-2.462753	-3.227738	-1.097734
28	1	0	-0.647631	-2.238526	-1.706225
29	6	0	-3.549937	-3.219331	-0.218894
30	1	0	-4.502461	-2.180893	1.417513
31	1	0	-2.366732	-4.015183	-1.840085
32	1	0	-4.304629	-3.998662	-0.273613
33	6	0	-1.095705	1.275706	-0.250572
34	6	0	-1.141362	1.801516	-1.549296
35	6	0	-1.713465	3.056205	-1.756582
36	1	0	-0.731625	1.232713	-2.378671
37	6	0	-2.128543	3.156455	0.599936
38	6	0	-2.222846	3.753040	-0.658087
39	1	0	-1.756724	3.484097	-2.753870
40	1	0	-2.507250	3.668727	1.481698
41	1	0	-2.675322	4.733155	-0.767419
42	7	0	-1.578869	1.948370	0.808097

Cartesian coordinates of the ammonium-(*S*,*S*)-**2** species



(*S*,*S*)-Ammonium **2**

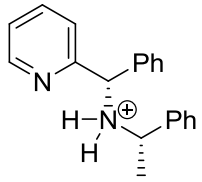


B3LYP/6-31+G(d), gas phase

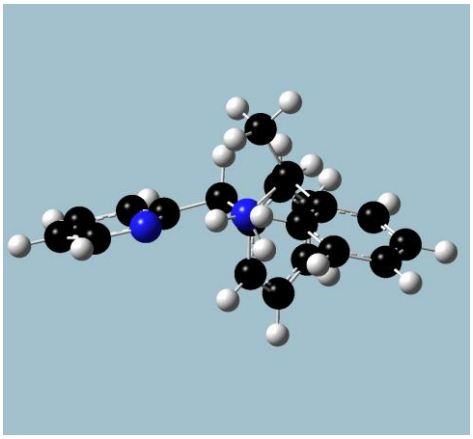
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.053611	-0.004702	0.639926
2	1	0	-1.030996	-0.045130	1.732996
3	7	0	0.339918	-0.434828	0.188376
4	1	0	0.233425	-1.446638	-0.052789
5	6	0	1.506797	-0.203707	1.158647
6	1	0	1.360167	0.815939	1.527769
7	6	0	1.424092	-1.198415	2.317412
8	1	0	2.243167	-0.993288	3.012506
9	1	0	0.486072	-1.112193	2.875602
10	1	0	1.527473	-2.233264	1.976262
11	6	0	2.797310	-0.256379	0.362974
12	6	0	3.516171	0.926486	0.137640
13	6	0	3.284480	-1.463117	-0.165476
14	6	0	4.704397	0.905614	-0.597281
15	1	0	3.154174	1.867350	0.547136
16	6	0	4.467171	-1.482003	-0.906993
17	1	0	2.755429	-2.398119	0.006174
18	6	0	5.179598	-0.298168	-1.122451
19	1	0	5.256692	1.827350	-0.755997
20	1	0	4.836086	-2.421348	-1.308807
21	1	0	6.103394	-0.316267	-1.693533
22	6	0	-1.343371	1.416733	0.204533
23	6	0	-1.564847	1.720648	-1.149089
24	6	0	-1.371502	2.447859	1.153035
25	6	0	-1.797053	3.038312	-1.545037
26	1	0	-1.578724	0.928256	-1.895699
27	6	0	-1.612816	3.766628	0.756409
28	1	0	-1.216669	2.222685	2.206383
29	6	0	-1.821524	4.062879	-0.592238
30	1	0	-1.970163	3.264061	-2.593330
31	1	0	-1.639424	4.557434	1.500506
32	1	0	-2.009938	5.086971	-0.901343
33	6	0	-2.034392	-1.076582	0.142189
34	6	0	-3.416262	-0.877939	0.177121
35	6	0	-4.242286	-1.929189	-0.222944
36	1	0	-3.833394	0.069829	0.502639
37	6	0	-2.274936	-3.230685	-0.654603
38	6	0	-3.664995	-3.128244	-0.647807
39	1	0	-5.321957	-1.811713	-0.206063
40	1	0	-1.776693	-4.139669	-0.980628
41	1	0	-4.276036	-3.965329	-0.969878
42	7	0	-1.476732	-2.225295	-0.262176
43	1	0	0.561083	0.047763	-0.689085

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.050070	-0.017296	0.631716
2	1	0	-1.030143	-0.064056	1.723713
3	7	0	0.328771	-0.482679	0.176444
4	1	0	0.210209	-1.496797	-0.035515
5	6	0	1.498186	-0.231495	1.135687
6	1	0	1.352805	0.792865	1.488496
7	6	0	1.426895	-1.202288	2.314800
8	1	0	2.243870	-0.969612	3.003586
9	1	0	0.488077	-1.108648	2.869243
10	1	0	1.539457	-2.242959	1.995698
11	6	0	2.793772	-0.293689	0.346144
12	6	0	3.521508	0.885081	0.128483
13	6	0	3.284000	-1.503037	-0.172627
14	6	0	4.720641	0.858450	-0.589365
15	1	0	3.153167	1.827620	0.526712
16	6	0	4.477707	-1.528577	-0.897478
17	1	0	2.745670	-2.433526	-0.011047
18	6	0	5.199466	-0.348539	-1.105716
19	1	0	5.276844	1.778856	-0.743898
20	1	0	4.845818	-2.470687	-1.294128
21	1	0	6.130641	-0.371522	-1.665134
22	6	0	-1.303301	1.414272	0.202577
23	6	0	-1.504815	1.733189	-1.150255
24	6	0	-1.321025	2.437713	1.159242
25	6	0	-1.710240	3.058188	-1.537659
26	1	0	-1.515260	0.949314	-1.904801
27	6	0	-1.534722	3.764180	0.771195
28	1	0	-1.174345	2.200788	2.210365
29	6	0	-1.726640	4.075989	-0.576964
30	1	0	-1.865681	3.294405	-2.586504
31	1	0	-1.550553	4.549087	1.522007
32	1	0	-1.892355	5.106205	-0.879522
33	6	0	-2.067614	-1.053819	0.137031
34	6	0	-3.441004	-0.798764	0.167270
35	6	0	-4.309168	-1.816597	-0.228127
36	1	0	-3.819812	0.165941	0.488612
37	6	0	-2.396261	-3.201019	-0.642811
38	6	0	-3.781015	-3.041809	-0.643119
39	1	0	-5.382751	-1.653472	-0.214988
40	1	0	-1.936171	-4.133204	-0.959565
41	1	0	-4.424662	-3.855201	-0.962014
42	7	0	-1.557133	-2.227718	-0.255294
43	1	0	0.545914	-0.033421	-0.719499



(*S,S*)-Ammonium **2**



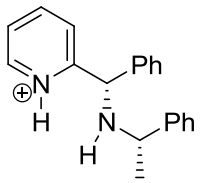
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.048685	-0.014871	0.632712
2	1	0	-1.030361	-0.059828	1.724496
3	7	0	0.331760	-0.469470	0.176195
4	1	0	0.209507	-1.483679	-0.040014
5	6	0	1.498828	-0.218647	1.136622
6	1	0	1.353571	0.804347	1.492390
7	6	0	1.429257	-1.192506	2.312905
8	1	0	2.243894	-0.959481	3.002469
9	1	0	0.490451	-1.102796	2.865880
10	1	0	1.545034	-2.230732	1.990512
11	6	0	2.795300	-0.276083	0.348065
12	6	0	3.520682	0.904489	0.133438
13	6	0	3.287909	-1.483365	-0.172949
14	6	0	4.720036	0.881473	-0.583791
15	1	0	3.150567	1.844713	0.533349
16	6	0	4.481752	-1.505002	-0.897245
17	1	0	2.751513	-2.414472	-0.013709
18	6	0	5.201251	-0.323308	-1.102436
19	1	0	5.274327	1.802472	-0.736033
20	1	0	4.851671	-2.444767	-1.295591
21	1	0	6.132039	-0.343267	-1.661068
22	6	0	-1.319398	1.412619	0.201486
23	6	0	-1.518826	1.727229	-1.152568
24	6	0	-1.356043	2.436192	1.157196
25	6	0	-1.740776	3.048673	-1.542085
26	1	0	-1.513800	0.943129	-1.905818
27	6	0	-1.586728	3.758912	0.766739
28	1	0	-1.210771	2.202206	2.208345
29	6	0	-1.776485	4.066663	-0.582417
30	1	0	-1.894019	3.281928	-2.591088
31	1	0	-1.617315	4.543800	1.515950
32	1	0	-1.955174	5.093421	-0.886492
33	6	0	-2.053473	-1.063841	0.139520
34	6	0	-3.430363	-0.830099	0.170166
35	6	0	-4.281779	-1.860995	-0.226668
36	1	0	-3.823372	0.127775	0.492301
37	6	0	-2.347759	-3.215395	-0.643796
38	6	0	-3.734436	-3.077069	-0.643427
39	1	0	-5.357112	-1.715291	-0.213551
40	1	0	-1.874416	-4.139633	-0.962215
41	1	0	-4.364964	-3.899245	-0.963276
42	7	0	-1.524553	-2.228758	-0.254801
43	1	0	0.546695	-0.013434	-0.715414

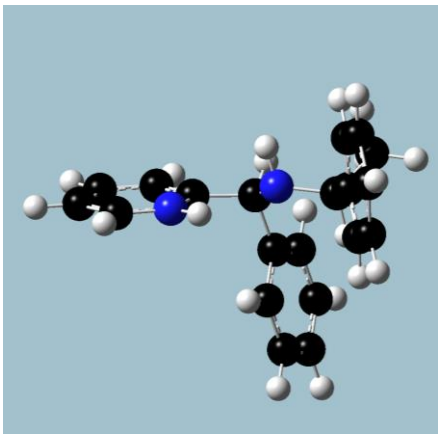
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.026711	-0.022593	0.616544
2	1	0	-1.002007	-0.064008	1.707733
3	7	0	0.350522	-0.467201	0.151826
4	1	0	0.243451	-1.470343	-0.098640
5	6	0	1.506807	-0.250842	1.129798
6	1	0	1.360071	0.759118	1.518089
7	6	0	1.427932	-1.265369	2.271501
8	1	0	2.238508	-1.059326	2.974865
9	1	0	0.483540	-1.190293	2.817389
10	1	0	1.539447	-2.290556	1.907938
11	6	0	2.811370	-0.284250	0.351596
12	6	0	3.540740	0.901855	0.183948
13	6	0	3.307429	-1.473071	-0.208035
14	6	0	4.746770	0.902611	-0.524051
15	1	0	3.166806	1.827868	0.612767
16	6	0	4.508485	-1.471646	-0.922076
17	1	0	2.762401	-2.405333	-0.090193
18	6	0	5.232073	-0.284403	-1.080240
19	1	0	5.302771	1.828097	-0.640637
20	1	0	4.879904	-2.397549	-1.351093
21	1	0	6.167444	-0.286079	-1.631954
22	6	0	-1.312766	1.405066	0.189595
23	6	0	-1.536654	1.723075	-1.159927
24	6	0	-1.348497	2.424906	1.149682
25	6	0	-1.782863	3.043579	-1.540720
26	1	0	-1.528100	0.940601	-1.914451
27	6	0	-1.602118	3.746927	0.768681
28	1	0	-1.183094	2.186348	2.196829
29	6	0	-1.817440	4.058205	-0.576542
30	1	0	-1.955122	3.279006	-2.586617
31	1	0	-1.630812	4.528401	1.521951
32	1	0	-2.014652	5.083866	-0.873687
33	6	0	-2.043205	-1.064895	0.136114
34	6	0	-3.418041	-0.829036	0.236029
35	6	0	-4.293562	-1.842349	-0.151693
36	1	0	-3.790348	0.119655	0.606869
37	6	0	-2.388303	-3.191452	-0.694841
38	6	0	-3.772665	-3.048410	-0.629058
39	1	0	-5.366409	-1.692056	-0.083796
40	1	0	-1.936350	-4.109466	-1.059940
41	1	0	-4.421102	-3.858792	-0.943772
42	7	0	-1.539620	-2.220480	-0.315513
43	1	0	0.574658	0.017175	-0.721668

Cartesian coordinates of the pyridinium-(*S*,*S*)-**2** species



(*S*,*S*)-Pyridinium **2**

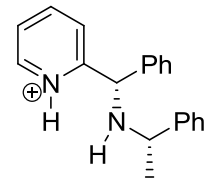


B3LYP/6-31+G(d), gas phase

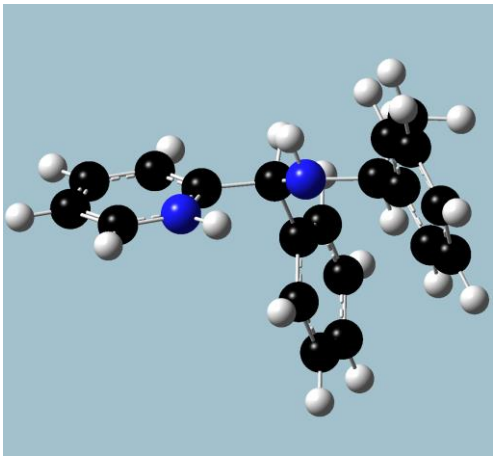
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.977285	0.054484	-0.931283
2	1	0	-1.185112	-0.077525	-2.003174
3	7	0	0.444369	0.331989	-0.650305
4	1	0	0.775694	1.018968	-1.331362
5	6	0	1.417172	-0.805435	-0.671111
6	1	0	1.054621	-1.528220	0.064113
7	6	0	1.502355	-1.502587	-2.038175
8	1	0	2.252997	-2.299023	-2.008902
9	1	0	0.544642	-1.958604	-2.311894
10	1	0	1.789218	-0.805429	-2.834603
11	6	0	2.756335	-0.272351	-0.179994
12	6	0	3.205691	-0.589689	1.109187
13	6	0	3.558231	0.550924	-0.985839
14	6	0	4.424133	-0.098156	1.585628
15	1	0	2.603428	-1.237489	1.743245
16	6	0	4.773361	1.051020	-0.510512
17	1	0	3.251432	0.796091	-2.000843
18	6	0	5.209790	0.727181	0.777199
19	1	0	4.761142	-0.364869	2.583771
20	1	0	5.384078	1.682430	-1.150325
21	1	0	6.159510	1.107273	1.143233
22	6	0	-1.529972	-1.171124	-0.200817
23	6	0	-1.447945	-1.284475	1.195817
24	6	0	-2.162096	-2.184752	-0.931871
25	6	0	-1.976682	-2.400731	1.845260
26	1	0	-0.956298	-0.511452	1.781965
27	6	0	-2.695659	-3.301137	-0.281089
28	1	0	-2.230086	-2.111691	-2.015313
29	6	0	-2.603417	-3.410970	1.107866
30	1	0	-1.900389	-2.482235	2.925926
31	1	0	-3.176907	-4.083578	-0.860909
32	1	0	-3.015803	-4.278618	1.614753
33	6	0	-1.764657	1.281903	-0.472611
34	6	0	-3.066515	1.609661	-0.849045
35	6	0	-3.672162	2.738626	-0.301231
36	1	0	-3.592237	0.976142	-1.555855
37	6	0	-1.689731	3.185565	0.969287
38	6	0	-2.980632	3.537378	0.624335
39	1	0	-4.684959	3.002775	-0.591251
40	1	0	-1.072087	3.741836	1.665277
41	1	0	-3.436183	4.418268	1.062550
42	7	0	-1.136131	2.086467	0.409260
43	1	0	-0.166267	1.773762	0.600908

B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.973708	-0.071055	0.894696
2	1	0	-1.161295	0.045150	1.971219
3	7	0	0.432020	-0.394475	0.586954
4	1	0	0.715595	-1.170899	1.188010
5	6	0	1.439061	0.691725	0.749186
6	1	0	1.117182	1.505884	0.094462
7	6	0	1.532001	1.238865	2.184435
8	1	0	2.313416	2.004089	2.247126
9	1	0	0.587916	1.701939	2.490524
10	1	0	1.771852	0.449874	2.906952
11	6	0	2.772707	0.178545	0.218493
12	6	0	3.238744	0.606650	-1.033166
13	6	0	3.554918	-0.731999	0.946730
14	6	0	4.452152	0.139717	-1.547949
15	1	0	2.648524	1.316267	-1.609166
16	6	0	4.765977	-1.206519	0.433593
17	1	0	3.230415	-1.074060	1.926746
18	6	0	5.219282	-0.771416	-0.815862
19	1	0	4.797612	0.489393	-2.517547
20	1	0	5.357741	-1.910216	1.013518
21	1	0	6.163652	-1.135178	-1.212248
22	6	0	-1.462912	1.201578	0.196927
23	6	0	-1.336892	1.362752	-1.191514
24	6	0	-2.074924	2.212922	0.947719
25	6	0	-1.806861	2.520731	-1.813755
26	1	0	-0.859818	0.591048	-1.789982
27	6	0	-2.549558	3.371904	0.324758
28	1	0	-2.178028	2.100723	2.024509
29	6	0	-2.416262	3.528196	-1.057000
30	1	0	-1.698512	2.635864	-2.888820
31	1	0	-3.018389	4.149968	0.920942
32	1	0	-2.783131	4.428253	-1.542698
33	6	0	-1.825781	-1.247668	0.427599
34	6	0	-3.106822	-1.544145	0.885597
35	6	0	-3.799139	-2.620320	0.331858
36	1	0	-3.551486	-0.933064	1.663480
37	6	0	-1.934293	-3.080991	-1.098494
38	6	0	-3.211626	-3.397728	-0.676229
39	1	0	-4.797529	-2.857745	0.685418
40	1	0	-1.390655	-3.624884	-1.860996
41	1	0	-3.732747	-4.237515	-1.120209
42	7	0	-1.296672	-2.032047	-0.534752
43	1	0	-0.336134	-1.779700	-0.802383



(*S,S*)-Pyridinium **2**



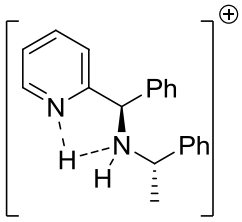
B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.974487	-0.072139	0.896695
2	1	0	-1.166100	0.044208	1.971948
3	7	0	0.431601	-0.394698	0.591535
4	1	0	0.716131	-1.168905	1.192605
5	6	0	1.437992	0.692395	0.748777
6	1	0	1.116311	1.504566	0.092151
7	6	0	1.532967	1.243803	2.182041
8	1	0	2.309641	2.012553	2.239411
9	1	0	0.588542	1.702180	2.490038
10	1	0	1.779818	0.458378	2.904462
11	6	0	2.770979	0.178649	0.217595
12	6	0	3.236973	0.606235	-1.034077
13	6	0	3.552309	-0.732327	0.946054
14	6	0	4.449866	0.138240	-1.548572
15	1	0	2.647715	1.315873	-1.609481
16	6	0	4.762633	-1.207909	0.432851
17	1	0	3.227798	-1.073618	1.925468
18	6	0	5.216066	-0.773346	-0.816520
19	1	0	4.795452	0.487101	-2.517495
20	1	0	5.353514	-1.911553	1.012204
21	1	0	6.159347	-1.137714	-1.212666
22	6	0	-1.462832	1.200626	0.198495
23	6	0	-1.335713	1.361553	-1.189804
24	6	0	-2.074473	2.212135	0.949070
25	6	0	-1.804386	2.519835	-1.811990
26	1	0	-0.859269	0.590154	-1.787742
27	6	0	-2.547718	3.371305	0.325847
28	1	0	-2.178263	2.099752	2.024959
29	6	0	-2.413333	3.527539	-1.055575
30	1	0	-1.695467	2.635053	-2.886163
31	1	0	-3.016077	4.149192	0.921151
32	1	0	-2.778916	4.427265	-1.541052
33	6	0	-1.825521	-1.247967	0.427572
34	6	0	-3.107040	-1.544253	0.884263
35	6	0	-3.798392	-2.619756	0.328960
36	1	0	-3.551834	-0.934048	1.661735
37	6	0	-1.932042	-3.079412	-1.099386
38	6	0	-3.209668	-3.396187	-0.678964
39	1	0	-4.796594	-2.857531	0.680865
40	1	0	-1.388928	-3.623381	-1.861428
41	1	0	-3.729833	-4.235068	-1.124002
42	7	0	-1.294888	-2.031250	-0.534052
43	1	0	-0.335051	-1.776935	-0.799347

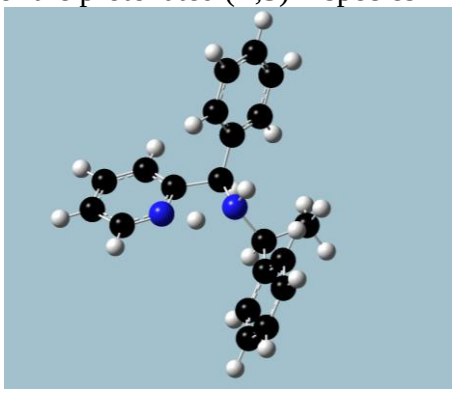
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.978255	-0.081906	0.852135
2	1	0	-1.169006	0.018213	1.928934
3	7	0	0.415935	-0.447935	0.545965
4	1	0	0.643686	-1.281356	1.089190
5	6	0	1.455500	0.577125	0.836614
6	1	0	1.167171	1.475291	0.284513
7	6	0	1.562873	0.941733	2.328195
8	1	0	2.348183	1.689635	2.478126
9	1	0	0.623216	1.363508	2.698183
10	1	0	1.806980	0.063694	2.936095
11	6	0	2.779865	0.095701	0.255362
12	6	0	3.331814	0.740617	-0.861218
13	6	0	3.472262	-0.994957	0.807218
14	6	0	4.542297	0.310726	-1.416215
15	1	0	2.811069	1.588876	-1.298762
16	6	0	4.678722	-1.432295	0.252025
17	1	0	3.076224	-1.510880	1.678006
18	6	0	5.218981	-0.780016	-0.861894
19	1	0	4.953702	0.827458	-2.278767
20	1	0	5.198548	-2.278643	0.692257
21	1	0	6.158450	-1.116850	-1.290520
22	6	0	-1.409564	1.229661	0.188796
23	6	0	-1.261143	1.433360	-1.192009
24	6	0	-1.989232	2.238505	0.968492
25	6	0	-1.680112	2.630008	-1.778029
26	1	0	-0.810436	0.663552	-1.811483
27	6	0	-2.412679	3.436192	0.381787
28	1	0	-2.105560	2.091031	2.038830
29	6	0	-2.258969	3.634455	-0.992976
30	1	0	-1.556545	2.777621	-2.846912
31	1	0	-2.857348	4.210864	0.999495
32	1	0	-2.585841	4.563407	-1.450741
33	6	0	-1.879583	-1.210205	0.366319
34	6	0	-3.167797	-1.448347	0.839403
35	6	0	-3.918364	-2.487939	0.293403
36	1	0	-3.567023	-0.818795	1.625909
37	6	0	-2.096191	-3.028492	-1.162567
38	6	0	-3.380609	-3.288837	-0.723713
39	1	0	-4.921190	-2.679159	0.660449
40	1	0	-1.589168	-3.593678	-1.933900
41	1	0	-3.944651	-4.102529	-1.162433
42	7	0	-1.401296	-2.013278	-0.605750
43	1	0	-0.441835	-1.813296	-0.904732

Cartesian coordinates of the TS for the proton transfer of the protonated (*R*,*S*)-**2** species



(*R*,*S*)-TS-**2**



B3LYP/6-31+G(d), gas phase

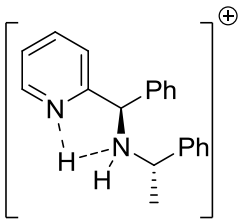
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.026559	0.011712	-0.672514
2	7	0	-0.329249	-0.294881	-0.111891
3	1	0	-0.249082	-0.965632	0.653300
4	6	0	-1.401699	-0.737415	-1.073667
5	1	0	-1.381377	0.003728	-1.881458
6	6	0	-1.114549	-2.124697	-1.660249
7	1	0	-1.900662	-2.392358	-2.373067
8	1	0	-0.155740	-2.150953	-2.189133
9	1	0	-1.093412	-2.894888	-0.881686
10	6	0	-2.747105	-0.634819	-0.372582
11	6	0	-3.673474	0.337642	-0.773495
12	6	0	-3.085069	-1.496060	0.683302
13	6	0	-4.912044	0.450131	-0.135134
14	1	0	-3.434381	1.003641	-1.600546
15	6	0	-4.318000	-1.379659	1.328462
16	1	0	-2.396079	-2.275587	1.003028
17	6	0	-5.234731	-0.406079	0.919971
18	1	0	-5.623470	1.201854	-0.465749
19	1	0	-4.566481	-2.055195	2.142269
20	1	0	-6.197237	-0.321954	1.416545
21	6	0	1.225767	1.509316	-0.360439
22	6	0	2.322644	2.307408	-0.671146
23	6	0	2.278850	3.651695	-0.295581
24	1	0	3.184642	1.889912	-1.181471
25	6	0	0.101623	3.306947	0.661714
26	6	0	1.160055	4.160871	0.379376
27	1	0	3.116271	4.304633	-0.523818
28	1	0	-0.797059	3.622806	1.181289
29	1	0	1.112738	5.201678	0.681217
30	7	0	0.167707	2.019748	0.282136
31	6	0	2.137892	-0.865721	-0.123638
32	6	0	2.844119	-1.720316	-0.979766
33	6	0	2.463997	-0.840190	1.242163
34	6	0	3.857146	-2.543499	-0.479989
35	1	0	2.604903	-1.746752	-2.040774
36	6	0	3.470225	-1.668413	1.742109
37	1	0	1.941683	-0.168810	1.922007
38	6	0	4.168937	-2.521051	0.881237
39	1	0	4.398324	-3.201255	-1.154050
40	1	0	3.713717	-1.642635	2.800451
41	1	0	4.954770	-3.161783	1.270683
42	1	0	0.986564	-0.105874	-1.760425
43	1	0	-0.514696	0.994525	0.348870

Imaginary frequency of -1198.8841 cm^{-1}

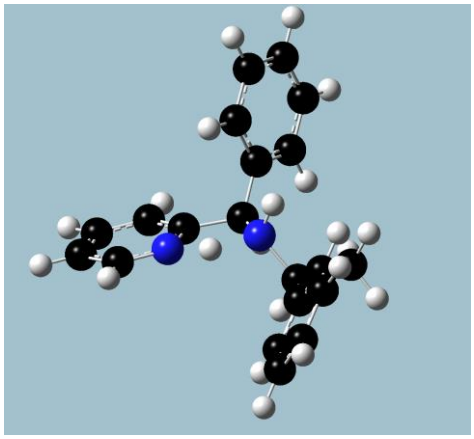
B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.027813	0.012105	-0.670697
2	7	0	-0.325403	-0.302112	-0.103064
3	1	0	-0.244710	-0.970485	0.664176
4	6	0	-1.394470	-0.737156	-1.066490
5	1	0	-1.373978	0.005610	-1.871105
6	6	0	-1.111661	-2.122850	-1.659058
7	1	0	-1.898547	-2.383399	-2.374021
8	1	0	-0.154060	-2.142068	-2.189196
9	1	0	-1.088167	-2.895456	-0.883339
10	6	0	-2.742785	-0.639168	-0.367438
11	6	0	-3.667872	0.335890	-0.765833
12	6	0	-3.084734	-1.505018	0.683648
13	6	0	-4.909226	0.446059	-0.131080
14	1	0	-3.419372	1.011792	-1.581263
15	6	0	-4.320791	-1.391798	1.325155
16	1	0	-2.392734	-2.279182	1.007647
17	6	0	-5.237305	-0.416160	0.918598
18	1	0	-5.616219	1.204477	-0.456732
19	1	0	-4.569241	-2.068817	2.138104
20	1	0	-6.200430	-0.331898	1.414745
21	6	0	1.217622	1.510442	-0.361184
22	6	0	2.302068	2.315668	-0.693692
23	6	0	2.251286	3.660442	-0.321157
24	1	0	3.156861	1.907424	-1.222246
25	6	0	0.093312	3.295902	0.671909
26	6	0	1.139173	4.159596	0.370582
27	1	0	3.077599	4.320482	-0.566643
28	1	0	-0.799375	3.605562	1.204195
29	1	0	1.085675	5.200355	0.670027
30	7	0	0.164703	2.009258	0.295805
31	6	0	2.143106	-0.861046	-0.120943
32	6	0	2.820257	-1.746555	-0.969634
33	6	0	2.504129	-0.800997	1.234766
34	6	0	3.837883	-2.566421	-0.472765
35	1	0	2.554949	-1.797598	-2.022844
36	6	0	3.515713	-1.625175	1.732374
37	1	0	2.003878	-0.108216	1.908319
38	6	0	4.185338	-2.509324	0.879513
39	1	0	4.355527	-3.247392	-1.142631
40	1	0	3.785217	-1.571154	2.783489
41	1	0	4.975398	-3.146452	1.267196
42	1	0	0.985241	-0.107613	-1.757177
43	1	0	-0.511736	0.957396	0.360680

Imaginary frequency of -1321.4278 cm^{-1}



(*R*,*S*)-TS-**2**



B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.027826	0.012695	-0.669361
2	7	0	-0.325167	-0.301929	-0.101120
3	1	0	-0.242735	-0.974775	0.660734
4	6	0	-1.393842	-0.735976	-1.066334
5	1	0	-1.375166	0.007706	-1.869537
6	6	0	-1.110453	-2.120168	-1.661313
7	1	0	-1.895649	-2.378337	-2.377168
8	1	0	-0.153142	-2.138467	-2.189626
9	1	0	-1.088636	-2.893468	-0.887633
10	6	0	-2.742411	-0.639264	-0.367728
11	6	0	-3.664603	0.340672	-0.760349
12	6	0	-3.086724	-1.510905	0.677628
13	6	0	-4.905653	0.449866	-0.125323
14	1	0	-3.414207	1.020256	-1.571053
15	6	0	-4.322472	-1.398385	1.319362
16	1	0	-2.397303	-2.288281	0.996630
17	6	0	-5.236135	-0.417980	0.918654
18	1	0	-5.610250	1.211418	-0.446082
19	1	0	-4.572937	-2.079233	2.127398
20	1	0	-6.198471	-0.334413	1.414660
21	6	0	1.216748	1.510004	-0.360102
22	6	0	2.301786	2.314917	-0.691574
23	6	0	2.250016	3.659485	-0.319982
24	1	0	3.156673	1.906236	-1.218048
25	6	0	0.090640	3.295364	0.669734
26	6	0	1.136698	4.158636	0.369518
27	1	0	3.075925	4.319368	-0.564235
28	1	0	-0.801830	3.606623	1.200352
29	1	0	1.082438	5.198800	0.668156
30	7	0	0.162336	2.008200	0.294614
31	6	0	2.143705	-0.860014	-0.120160
32	6	0	2.819913	-1.745728	-0.969162
33	6	0	2.505246	-0.799854	1.235333
34	6	0	3.837415	-2.565642	-0.472717
35	1	0	2.554162	-1.796594	-2.021452
36	6	0	3.516628	-1.624318	1.732256
37	1	0	2.005874	-0.107658	1.908797
38	6	0	4.185445	-2.508510	0.879172
39	1	0	4.354310	-3.246335	-1.142137
40	1	0	3.786550	-1.570625	2.782451
41	1	0	4.974894	-3.145415	1.266219
42	1	0	0.987103	-0.106243	-1.755681
43	1	0	-0.506430	0.956164	0.357488

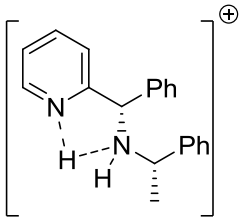
Imaginary frequency of -1228.0484 cm^{-1}

B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

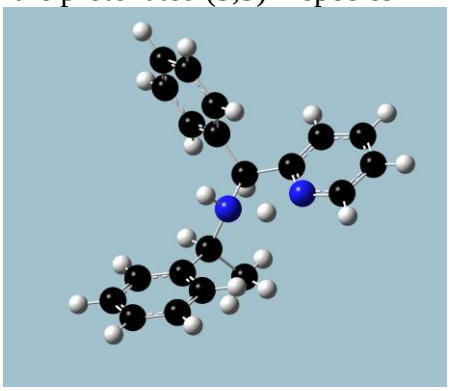
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.021065	0.016235	-0.657893
2	7	0	-0.334206	-0.275668	-0.091535
3	1	0	-0.264194	-0.946741	0.673245
4	6	0	-1.398327	-0.694033	-1.063132
5	1	0	-1.379055	0.061621	-1.854131
6	6	0	-1.115757	-2.069770	-1.679314
7	1	0	-1.899834	-2.316751	-2.401175
8	1	0	-0.156158	-2.076495	-2.204204
9	1	0	-1.094547	-2.851649	-0.913889
10	6	0	-2.751467	-0.609661	-0.370146
11	6	0	-3.670431	0.379287	-0.749795
12	6	0	-3.107043	-1.503364	0.653513
13	6	0	-4.918320	0.476001	-0.124530
14	1	0	-3.410692	1.076305	-1.542599
15	6	0	-4.349960	-1.404347	1.285241
16	1	0	-2.417229	-2.284176	0.962283
17	6	0	-5.260251	-0.414760	0.897121
18	1	0	-5.619069	1.245565	-0.435232
19	1	0	-4.608727	-2.102289	2.076275
20	1	0	-6.227614	-0.341499	1.385348
21	6	0	1.242936	1.506833	-0.343786
22	6	0	2.343175	2.292271	-0.674344
23	6	0	2.316811	3.637059	-0.300488
24	1	0	3.188390	1.867093	-1.203686
25	6	0	0.149405	3.312534	0.686848
26	6	0	1.211977	4.156648	0.388752
27	1	0	3.154858	4.282036	-0.544058
28	1	0	-0.738164	3.639986	1.216118
29	1	0	1.176599	5.197617	0.688181
30	7	0	0.198601	2.024672	0.311005
31	6	0	2.121780	-0.880732	-0.116174
32	6	0	2.826377	-1.723923	-0.985450
33	6	0	2.445740	-0.881815	1.250369
34	6	0	3.836575	-2.560380	-0.499199
35	1	0	2.584600	-1.728663	-2.044668
36	6	0	3.449819	-1.722119	1.737268
37	1	0	1.916654	-0.226898	1.938409
38	6	0	4.148864	-2.562683	0.863251
39	1	0	4.375208	-3.208128	-1.184452
40	1	0	3.689953	-1.715946	2.796317
41	1	0	4.932134	-3.212200	1.242417
42	1	0	0.980558	-0.094234	-1.744646
43	1	0	-0.492253	0.996731	0.369193

Imaginary frequency of -1248.8151 cm^{-1}

Cartesian coordinates of the TS for the proton transfer of the protonated (*S,S*)-**2** species



(*S,S*)-TS-**2**



B3LYP/6-31+G(d), gas phase

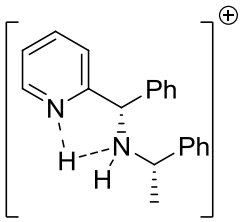
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.020409	0.065488	0.673039
2	1	0	-0.973327	0.082208	1.766693
3	7	0	0.359319	-0.224294	0.153765
4	1	0	-0.012737	-1.461922	-0.337344
5	6	0	1.495084	-0.157600	1.146837
6	1	0	1.364780	0.766938	1.724105
7	6	0	1.441869	-1.351741	2.105956
8	1	0	2.238789	-1.253551	2.848933
9	1	0	0.490689	-1.404670	2.648882
10	1	0	1.592339	-2.300241	1.580134
11	6	0	2.802325	-0.049777	0.380055
12	6	0	3.567016	1.121139	0.471878
13	6	0	3.264654	-1.098935	-0.430341
14	6	0	4.772479	1.242425	-0.225347
15	1	0	3.224379	1.942390	1.098102
16	6	0	4.464660	-0.977031	-1.133120
17	1	0	2.696212	-2.023048	-0.510721
18	6	0	5.222073	0.194151	-1.030771
19	1	0	5.356838	2.154011	-0.137631
20	1	0	4.812395	-1.797720	-1.754472
21	1	0	6.158607	0.285789	-1.573506
22	6	0	-1.585364	1.388052	0.188806
23	6	0	-1.921336	1.576762	-1.161870
24	6	0	-1.745527	2.449771	1.089127
25	6	0	-2.396181	2.812464	-1.603793
26	1	0	-1.820199	0.760178	-1.874961
27	6	0	-2.226921	3.685210	0.646708
28	1	0	-1.496178	2.314306	2.139466
29	6	0	-2.549888	3.868605	-0.699594
30	1	0	-2.652492	2.948857	-2.650553
31	1	0	-2.348709	4.500631	1.353900
32	1	0	-2.923570	4.828581	-1.043959
33	6	0	-1.848371	-1.160817	0.252555
34	6	0	-3.204979	-1.388543	0.463160
35	6	0	-3.742880	-2.595066	0.010411
36	1	0	-3.820233	-0.644244	0.958310
37	6	0	-1.582405	-3.236494	-0.823785
38	6	0	-2.927514	-3.531046	-0.641681
39	1	0	-4.797341	-2.807706	0.160653
40	1	0	-0.889623	-3.907353	-1.321258
41	1	0	-3.330633	-4.470955	-1.003194
42	7	0	-1.088959	-2.071204	-0.371635
43	1	0	0.567183	0.413915	-0.615865

Imaginary frequency of -1226.9355 cm^{-1}

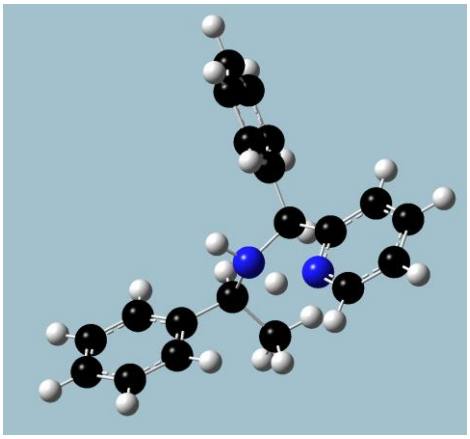
B3LYP/6-31+G(d), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.024581	0.064332	0.667376
2	1	0	-0.977125	0.087826	1.759818
3	7	0	0.359498	-0.213155	0.148649
4	1	0	0.020346	-1.436374	-0.315488
5	6	0	1.492668	-0.115046	1.135970
6	1	0	1.358956	0.817626	1.697084
7	6	0	1.457347	-1.293040	2.116501
8	1	0	2.257885	-1.171273	2.852347
9	1	0	0.509691	-1.340569	2.663909
10	1	0	1.609609	-2.248612	1.604411
11	6	0	2.801207	-0.018462	0.367738
12	6	0	3.595176	1.130626	0.485211
13	6	0	3.239247	-1.061970	-0.463448
14	6	0	4.806492	1.235879	-0.206126
15	1	0	3.267260	1.948138	1.123443
16	6	0	4.444763	-0.955928	-1.161079
17	1	0	2.643444	-1.965460	-0.568780
18	6	0	5.232999	0.193027	-1.032590
19	1	0	5.411690	2.132200	-0.099940
20	1	0	4.770205	-1.771473	-1.801435
21	1	0	6.172458	0.272940	-1.572880
22	6	0	-1.603138	1.380106	0.178212
23	6	0	-1.972938	1.557529	-1.165053
24	6	0	-1.750711	2.448005	1.074029
25	6	0	-2.467197	2.787649	-1.603802
26	1	0	-1.883522	0.738507	-1.875594
27	6	0	-2.250407	3.677839	0.635272
28	1	0	-1.477415	2.319370	2.118558
29	6	0	-2.607095	3.850445	-0.704650
30	1	0	-2.749655	2.913011	-2.645390
31	1	0	-2.361073	4.496627	1.340808
32	1	0	-2.996253	4.805393	-1.046920
33	6	0	-1.835015	-1.175213	0.253553
34	6	0	-3.189568	-1.412570	0.461591
35	6	0	-3.710892	-2.630785	0.020870
36	1	0	-3.814586	-0.670854	0.947491
37	6	0	-1.536620	-3.258354	-0.789204
38	6	0	-2.880419	-3.565272	-0.612394
39	1	0	-4.763433	-2.853085	0.167211
40	1	0	-0.833088	-3.928482	-1.270989
41	1	0	-3.270062	-4.514215	-0.963802
42	7	0	-1.059242	-2.082510	-0.351838
43	1	0	0.554972	0.405636	-0.639413

Imaginary frequency of -1329.9769 cm^{-1}



(*S*,*S*)-TS-**2**



B3LYP/6-31+G(d,p), CH_2Cl_2 (PCM-UFF)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.026338	0.061322	0.666644
2	1	0	-0.984025	0.081960	1.759081
3	7	0	0.359064	-0.215564	0.151228
4	1	0	0.019056	-1.438122	-0.303287
5	6	0	1.491426	-0.107473	1.139165
6	1	0	1.357954	0.829748	1.691529
7	6	0	1.456829	-1.276448	2.129952
8	1	0	2.257980	-1.149101	2.862381
9	1	0	0.511204	-1.317457	2.679065
10	1	0	1.606802	-2.235587	1.626061
11	6	0	2.799520	-0.015381	0.369594
12	6	0	3.583653	1.142405	0.464053
13	6	0	3.244912	-1.070648	-0.442447
14	6	0	4.792801	1.244622	-0.231106
15	1	0	3.249879	1.968297	1.086942
16	6	0	4.448238	-0.967528	-1.143791
17	1	0	2.657177	-1.980309	-0.529885
18	6	0	5.226724	0.190126	-1.038300
19	1	0	5.390294	2.147067	-0.143005
20	1	0	4.779536	-1.791538	-1.768747
21	1	0	6.163976	0.267689	-1.581124
22	6	0	-1.603948	1.377916	0.179070
23	6	0	-1.972666	1.556881	-1.164229
24	6	0	-1.750251	2.445090	1.075744
25	6	0	-2.464763	2.787940	-1.602013
26	1	0	-1.884042	0.739069	-1.875027
27	6	0	-2.247770	3.675816	0.637647
28	1	0	-1.478035	2.315010	2.119555
29	6	0	-2.603435	3.849969	-0.702110
30	1	0	-2.746292	2.914731	-2.642845
31	1	0	-2.357615	4.493724	1.343093
32	1	0	-2.990628	4.805106	-1.043534
33	6	0	-1.834297	-1.177240	0.249231
34	6	0	-3.190937	-1.411827	0.446544
35	6	0	-3.709370	-2.631217	0.006918
36	1	0	-3.818460	-0.667273	0.923037
37	6	0	-1.529081	-3.264605	-0.781614
38	6	0	-2.874314	-3.569231	-0.614638
39	1	0	-4.762676	-2.851903	0.144872
40	1	0	-0.823831	-3.938255	-1.254681
41	1	0	-3.261437	-4.518781	-0.964853
42	7	0	-1.053656	-2.087322	-0.345326
43	1	0	0.553727	0.403186	-0.635819

Imaginary frequency of -1237.2372 cm^{-1}

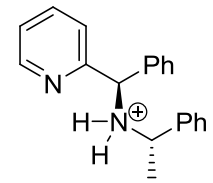
B3LYP/6-31+G(d,p), CH_2Cl_2 (CPCM-Bondi)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.027591	0.061313	0.662916
2	1	0	-0.987726	0.087254	1.754829
3	7	0	0.353250	-0.217463	0.147302
4	1	0	0.015051	-1.455363	-0.292797
5	6	0	1.482333	-0.077399	1.127070
6	1	0	1.346237	0.871827	1.657357
7	6	0	1.461533	-1.224521	2.144954
8	1	0	2.262018	-1.072668	2.874118
9	1	0	0.514539	-1.263047	2.692041
10	1	0	1.619973	-2.189956	1.655441
11	6	0	2.793157	-0.001770	0.360170
12	6	0	3.620499	1.121027	0.501569
13	6	0	3.206026	-1.044491	-0.485615
14	6	0	4.839568	1.201632	-0.180605
15	1	0	3.311254	1.936427	1.150502
16	6	0	4.419240	-0.962737	-1.174152
17	1	0	2.581825	-1.925187	-0.609064
18	6	0	5.241083	0.160099	-1.021932
19	1	0	5.469638	2.077631	-0.056646
20	1	0	4.724275	-1.776017	-1.826401
21	1	0	6.185264	0.221273	-1.555142
22	6	0	-1.603462	1.376888	0.171019
23	6	0	-1.917777	1.569380	-1.184224
24	6	0	-1.802556	2.429202	1.074855
25	6	0	-2.412375	2.798443	-1.626315
26	1	0	-1.778427	0.761205	-1.897856
27	6	0	-2.302460	3.658751	0.632919
28	1	0	-1.567758	2.287330	2.126241
29	6	0	-2.606590	3.846117	-0.718375
30	1	0	-2.651359	2.936097	-2.676649
31	1	0	-2.453177	4.465678	1.343853
32	1	0	-2.994840	4.800000	-1.062778
33	6	0	-1.837017	-1.177815	0.251373
34	6	0	-3.194206	-1.412736	0.448258
35	6	0	-3.711824	-2.634854	0.014795
36	1	0	-3.822115	-0.666368	0.921437
37	6	0	-1.529467	-3.272695	-0.765314
38	6	0	-2.875399	-3.576634	-0.600249
39	1	0	-4.765305	-2.855291	0.153280
40	1	0	-0.822301	-3.949256	-1.231620
41	1	0	-3.261490	-4.528676	-0.945438
42	7	0	-1.056091	-2.092338	-0.335498
43	1	0	0.538013	0.382521	-0.656046

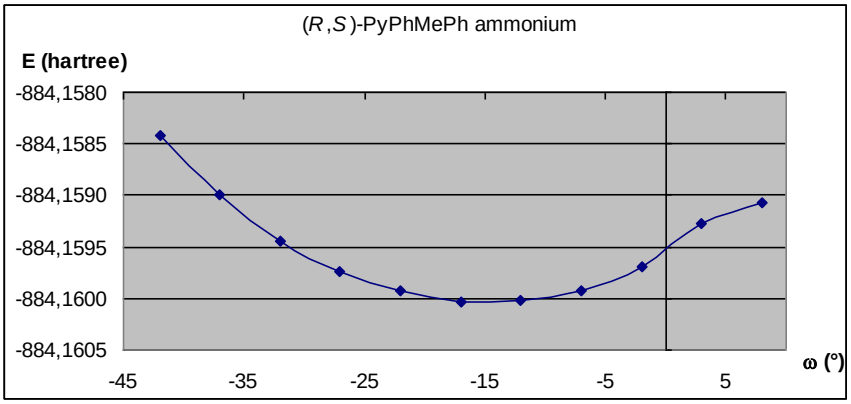
Imaginary frequency of -1282.3279 cm^{-1}

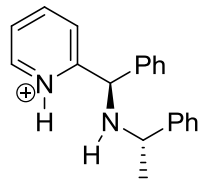
Relaxed scans of protonated (*R*,*S*) and (*S*,*S*)-**2** species

Level of theory : B3LYP/6-31+G(d) in CH_2Cl_2 solution, with PCM–UFF model

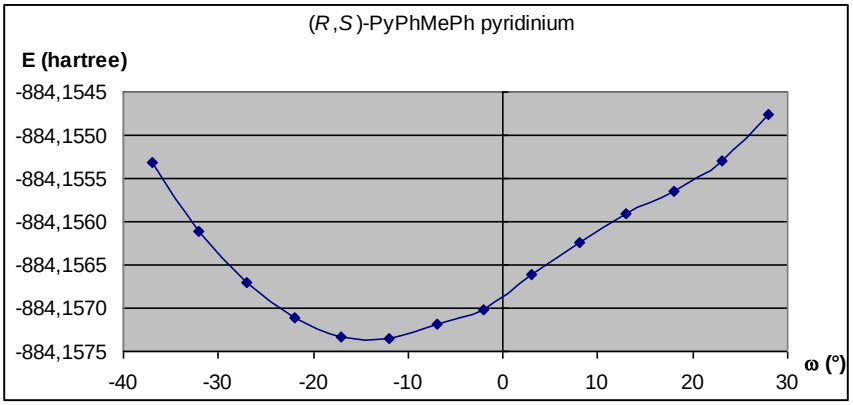


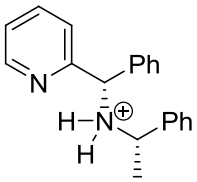
(*R*,*S*)-Ammonium **2**



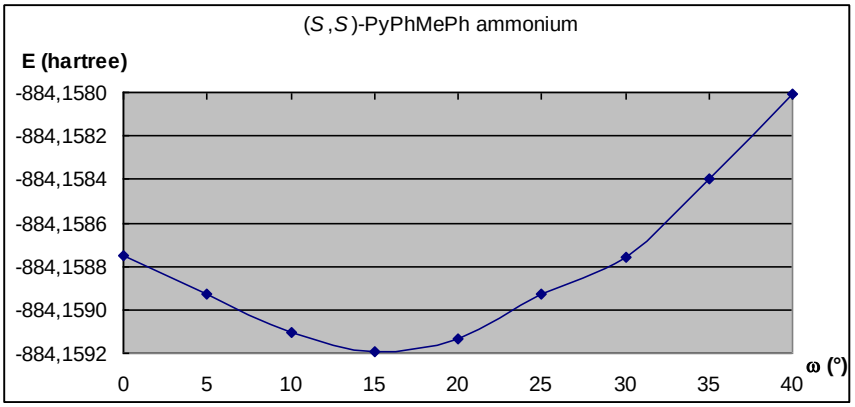


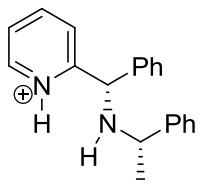
(*R*,*S*)-Pyridinium **2**



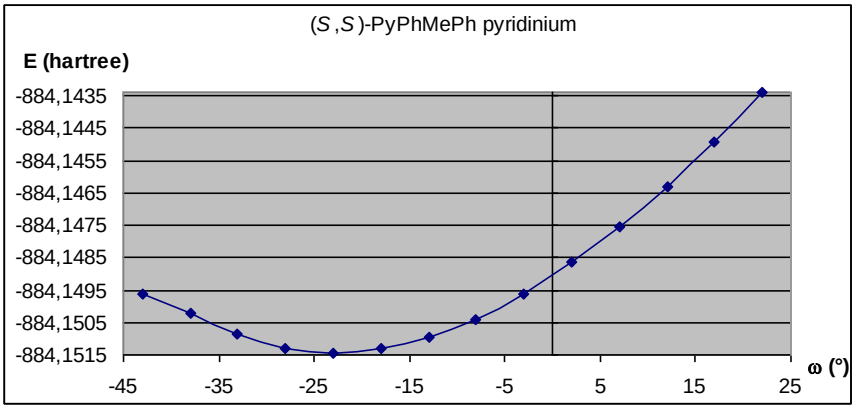


(*S*,*S*)-Ammonium **2**





(*S*,*S*)-Pyridinium **2**



$E = E_{electronic} + ZPE + E_{translation} + E_{vibration} + E_{rotation}$
$H = E + RT$
$G = H - TS$

Tables of results in energies in hartrees

Species	B3LYP/6-31+G(d) gas phase; T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G / H^+$	$\Delta G^{\ddagger} / H^+$
(*R*,*S*)-**1**	-691.962827562	-691.662621	-691.647136	-691.646192	-691.707234		
Ammonium (*R*,*S*)-**1**	-692.357340532	-692.042108	-692.026622	-692.025678	-692.086692	-0.369458	
Pyridinium (*R*,*S*)-**1**	-692.353475974	-692.039019	-692.023615	-692.022671	-692.083254	-0.366020	
(*S*,*S*)-**1**	-691.965618080	-691.665302	-691.649803	-691.648859	-691.710054		
Ammonium (*S*,*S*)-**1**	-692.357474480	-692.042077	-692.026598	-692.025654	-692.086785	-0.366731	
Pyridinium (*S*,*S*)-**1**	-692.346060150	-692.031484	-692.016134	-692.015190	-692.075463	-0.355409	
TS (*R*,*S*)-**1**	-692.344691252	-692.034463	-692.019304	-692.018360	-692.078413	-0.361179	0.0048
TS (*S*,*S*)-**1**	-692.344266485	-692.033904	-692.018771	-692.017827	-692.078000	-0.357946	-0.0025
H^+	0.000000000	0.000000	0.001416	0.002360	-0.010000		

Species	B3LYP/6-31+G(d) CH_2Cl_2 solution (PCM-UFF); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G / H^+$	$\Delta G^{\ddagger} / H^+$
(*R*,*S*)-**1**	-691.969216036	-691.669153	-691.653638	-691.652693	-691.713912		
Ammonium (*R*,*S*)-**1**	-692.418242759	-692.102405	-692.087040	-692.086096	-692.146760	-0.274824	
Pyridinium (*R*,*S*)-**1**	-692.415283167	-692.100710	-692.085350	-692.084406	-692.144484	-0.272548	
(*S*,*S*)-**1**	-691.971598617	-691.671519	-691.655984	-691.655040	-691.716485		
Ammonium (*S*,*S*)-**1**	-692.417616851	-692.101646	-692.086343	-692.085399	-692.145563	-0.271054	
Pyridinium (*S*,*S*)-**1**	-692.409940179	-692.095179	-692.079771	-692.078827	-692.139110	-0.264601	
TS (*R*,*S*)-**1**	-692.404733204	-692.094321	-692.079220	-692.078276	-692.137943	-0.266007	0.0065
TS (*S*,*S*)-**1**	-692.404425797	-692.093533	-692.078587	-692.077643	-692.136610	-0.262101	0.0025
H^+	-0.148024583	-0.148025	-0.146608	-0.145664	-0.158024		

Species	B3LYP/6-31+G(d,p) CH_2Cl_2 solution (PCM-UFF); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G / H^+$	$\Delta G^{\ddagger} / H^+$
(*R*,*S*)-**1**	-691.997055421	-691.697749	-691.682209	-691.681265	-691.742493		
Ammonium (*R*,*S*)-**1**	-692.448434464	-692.133560	-692.118169	-692.117225	-692.177859	-0.277342	
Pyridinium (*R*,*S*)-**1**	-692.446454069	-692.132709	-692.117318	-692.116373	-692.176525	-0.276008	
(*S*,*S*)-**1**	-691.999376542	-691.700056	-691.684491	-691.683547	-691.745053		
Ammonium (*S*,*S*)-**1**	-692.447785517	-692.132819	-692.117486	-692.116542	-692.176797	-0.273720	
Pyridinium (*S*,*S*)-**1**	-692.440980542	-692.127068	-692.111613	-692.110669	-692.171119	-0.268042	
TS (*R*,*S*)-**1**	-692.437481927	-692.127810	-692.112681	-692.111737	-692.171518	-0.271001	0.0050
TS (*S*,*S*)-**1**	-692.437141746	-692.126988	-692.112024	-692.111080	-692.170049	-0.266972	0.0011
H^+	-0.148024583	-0.148025	-0.146608	-0.145664	-0.158024		

Species	B3LYP/6-31+G(d,p) CH_2Cl_2 solution (CPCM-Bondi); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G / H^+$	$\Delta G^{\ddagger} / H^+$
(*R*,*S*)-**1**	-692.003489131	-691.704353	-691.688809	-691.687865	-691.749330		
Ammonium (*R*,*S*)-**1**	-692.463240281	-692.148834	-692.133276	-692.132332	-692.193729	-0.256400	
Pyridinium (*R*,*S*)-**1**	-692.458470763	-692.145487	-692.129919	-692.128975	-692.190025	-0.252696	
(*S*,*S*)-**1**	-692.005773456	-691.706682	-691.691107	-691.690163	-691.751724		
Ammonium (*S*,*S*)-**1**	-692.462628287	-692.148011	-692.132487	-692.131543	-692.193068	-0.253345	
Pyridinium (*S*,*S*)-**1**	-692.453839241	-692.140170	-692.124684	-692.123740	-692.184405	-0.244682	
TS (*R*,*S*)-**1**	-692.449435890	-692.140096	-692.124949	-692.124005	-692.183991	-0.246662	0.0060
TS (*S*,*S*)-**1**	-692.448942216	-692.139369	-692.124298	-692.123353	-692.183040	-0.243317	0.0014
H^+	-0.177999562	-0.178000	-0.176583	-0.175639	-0.187999		

Species	B3LYP/6-31+G(d) gas phase; T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G / H^+$	$\Delta G^{\ddagger} / H^+$
(*R*,*S*)-**2**	-883.705545687	-883.352520	-883.333825	-883.332880	-883.402264		
Ammonium (*R*,*S*)-**2**	-884.102923858	-883.734949	-883.716236	-883.715292	-883.785103	-0.372839	
Pyridinium (*R*,*S*)-**2**	-884.097096131	-883.730042	-883.711398	-883.710454	-883.779608	-0.367344	
(*S*,*S*)-**2**	-883.705047081	-883.352040	-883.333296	-883.332352	-883.402191		
Ammonium (*S*,*S*)-**2**	-884.102496250	-883.734442	-883.715725	-883.714781	-883.784361	-0.372170	
Pyridinium (*S*,*S*)-**2**	-884.089225745	-883.722113	-883.703452	-883.702508	-883.771353	-0.359162	
TS (*R*,*S*)-**2**	-884.088276350	-883.725282	-883.706888	-883.705944	-883.774866	-0.362602	0.0047
TS (*S*,*S*)-**2**	-884.088145638	-883.725154	-883.706738	-883.705794	-883.775025	-0.362834	-0.0037
H^+	0.000000000	0.000000	0.001416	0.002360	-0.010000		

Species	B3LYP/6-31+G(d) CH_2Cl_2 solution (PCM-UFF); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G / H^+$	$\Delta G^{\ddagger} / H^+$
(*R*,*S*)-**2**	-883.713058804	-883.360182	-883.341450	-883.340506	-883.410314		
Ammonium (*R*,*S*)-**2**	-884.160035947	-883.791640	-883.773074	-883.772130	-883.840443	-0.272105	
Pyridinium (*R*,*S*)-**2**	-884.157354065	-883.789939	-883.771407	-883.770463	-883.838781	-0.270443	
(*S*,*S*)-**2**	-883.712745305	-883.359874	-883.341086	-883.340141	-883.410454		
Ammonium (*S*,*S*)-**2**	-884.159196824	-883.790568	-883.772015	-883.771071	-883.839264	-0.270786	
Pyridinium (*S*,*S*)-**2**	-884.151442152	-883.783915	-883.765292	-883.764348	-883.832789	-0.264311	
TS (*R*,*S*)-**2**	-884.145489080	-883.782425	-883.764027	-883.763082	-883.832061	-0.263723	0.0067
TS (*S*,*S*)-**2**	-884.145552257	-883.782602	-883.764203	-883.763259	-883.832042	-0.263564	0.0007
H^+	-0.148024583	-0.148025	-0.146608	-0.145664	-0.158024		

Species	B3LYP/6-31+G(d,p) CH_2Cl_2 solution (PCM-UFF); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G / H^+$	$\Delta G^{\ddagger} / H^+$
(*R*,*S*)-**2**	-883.744782965	-883.392668	-883.373889	-883.372944	-883.443164		
Ammonium (*R*,*S*)-**2**	-884.193983893	-883.826321	-883.807784	-883.806840	-883.875040	-0.273852	
Pyridinium (*R*,*S*)-**2**	-884.192285081	-883.825652	-883.807088	-883.806144	-883.874527	-0.273339	
(*S*,*S*)-**2**	-883.744386233	-883.392242	-883.373421	-883.372477	-883.442904		
Ammonium (*S*,*S*)-**2**	-884.193106377	-883.825499	-883.806880	-883.805936	-883.874542	-0.273614	
Pyridinium (*S*,*S*)-**2**	-884.186300410	-883.819562	-883.800901	-883.799957	-883.868512	-0.267584	
TS (*R*,*S*)-**2**	-884.181995282	-883.819664	-883.801230	-883.800286	-883.869604	-0.268416	0.0049
TS (*S*,*S*)-**2**	-884.182012086	-883.819796	-883.801365	-883.800421	-883.869272	-0.268344	-0.0008
H^+	-0.148024583	-0.148025	-0.146608	-0.145664	-0.158024		

Species	B3LYP/6-31+G(d,p) CH_2Cl_2 solution (CPCM-Bondi); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G / H^+$	$\Delta G^{\ddagger} / H^+$
(*R*,*S*)-**2**	-883.752209939	-883.400246	-883.381441	-883.380497	-883.450767		
Ammonium (*R*,*S*)-**2**	-884.209783900	-883.842658	-883.823903	-883.822959	-883.893354	-0.254588	
Pyridinium (*R*,*S*)-**2**	-884.205753756	-883.839882	-883.821128	-883.820183	-883.889635	-0.250869	
(*S*,*S*)-**2**	-883.751974156	-883.400004	-883.381203	-883.380259	-883.450286		
Ammonium (*S*,*S*)-**2**	-884.209028494	-883.841707	-883.822977	-883.822033	-883.891529	-0.253244	
Pyridinium (*S*,*S*)-**2**	-884.200973257	-883.834346	-883.815643	-883.814699	-883.883604	-0.245319	
TS (*R*,*S*)-**2**	-884.195632935	-883.833330	-883.814987	-883.814043	-883.882790	-0.244024	0.0068
TS (*S*,*S*)-**2**	-884.195276291	-883.833206	-883.814833	-883.813889	-883.882300	-0.244015	0.0013
H^+	-0.177999562	-0.178000	-0.176583	-0.175639	-0.187999		

Tables of results in energies in $kJ.mol^{-1}$

Conversion factor from hartree to $kJ.mol^{-1}$: 2625.499640

according to 1 hartree = ($4.35974434.10^{-18}$ J * $6.02214129.10^{23}$ mol^{-1}) $/10^{3}$

with the fundamental constant values taken from the *National Institute of Standards and Technology* (NIST – USA).

Species	B3LYP/6-31+G(d) gas phase; T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G /H^+$	$\Delta G^{\dagger} /H^+$
(*R*,*S*)-**1**	-1816748.15	-1815959.96	-1815919.31	-1815916.83	-1816077.09		
Ammonium (*R*,*S*)-**1**	-1817783.95	-1816956.31	-1816915.65	-1816913.17	-1817073.36	**-970.01**	
Pyridinium (*R*,*S*)-**1**	-1817773.80	-1816948.20	-1816907.75	-1816905.27	-1817064.33	**-960.99**	
(*S*,*S*)-**1**	-1816755.48	-1815967.00	-1815926.31	-1815923.83	-1816084.50		
Ammonium (*S*,*S*)-**1**	-1817784.30	-1816956.22	-1816915.58	-1816913.11	-1817073.61	**-962.85**	
Pyridinium (*S*,*S*)-**1**	-1817754.33	-1816928.41	-1816888.11	-1816885.63	-1817043.88	**-933.13**	
TS (*R*,*S*)-**1**	-1817750.74	-1816936.23	-1816896.43	-1816893.96	-1817051.62	**-948.28**	**12.71**
TS (*S*,*S*)-**1**	0.00	0.00	3.72	6.20	-26.25	**-939.79**	**-6.66**
H^+	0.00	0.00	3.72	6.20	-26.25		

Species	B3LYP/6-31+G(d) CH_2Cl_2 solution (PCM-UFF); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G /H^+$	$\Delta G^{\dagger} /H^+$
(*R*,*S*)-**1**	-1816764.93	-1815977.11	-1815936.38	-1815933.90	-1816094.63		
Ammonium (*R*,*S*)-**1**	-1817943.85	-1817114.62	-1817074.27	-1817071.80	-1817231.07	**-721.55**	
Pyridinium (*R*,*S*)-**1**	-1817936.08	-1817110.17	-1817069.84	-1817067.36	-1817225.09	**-715.57**	
(*S*,*S*)-**1**	-1816771.18	-1815983.32	-1815942.54	-1815940.06	-1816101.38		
Ammonium (*S*,*S*)-**1**	-1817942.20	-1817112.62	-1817072.44	-1817069.97	-1817227.93	**-711.65**	
Pyridinium (*S*,*S*)-**1**	-1817922.05	-1817095.64	-1817055.19	-1817052.71	-1817210.98	**-694.71**	
TS (*R*,*S*)-**1**	-1817908.38	-1817093.39	-1817053.74	-1817051.26	-1817207.92	**-698.40**	**17.17**
TS (*S*,*S*)-**1**	-1817907.57	-1817091.32	-1817052.08	-1817049.60	-1817204.42	**-688.15**	**6.56**
H^+	-388.64	-388.64	-384.92	-382.44	-414.89		

Species	B3LYP/6-31+G(d,p) CH_2Cl_2 solution (PCM-UFF); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G /H^+$	$\Delta G^{\dagger} /H^+$
(*R*,*S*)-**1**	-1816838.02	-1816052.19	-1816011.39	-1816008.91	-1816169.67		
Ammonium (*R*,*S*)-**1**	-1818023.12	-1817196.41	-1817156.00	-1817153.53	-1817312.72	**-728.16**	
Pyridinium (*R*,*S*)-**1**	-1818017.92	-1817194.18	-1817153.77	-1817151.29	-1817309.22	**-724.66**	
(*S*,*S*)-**1**	-1816844.11	-1816058.25	-1816017.38	-1816014.90	-1816176.39		
Ammonium (*S*,*S*)-**1**	-1818021.41	-1817194.47	-1817154.21	-1817151.73	-1817309.93	**-718.65**	
Pyridinium (*S*,*S*)-**1**	-1818003.55	-1817179.37	-1817138.79	-1817136.31	-1817295.02	**-703.74**	
TS (*R*,*S*)-**1**	-1817994.36	-1817181.32	-1817141.60	-1817139.12	-1817296.07	**-711.51**	**13.15**
TS (*S*,*S*)-**1**	-1817993.47	-1817179.16	-1817139.87	-1817137.39	-1817292.21	**-700.93**	**2.81**
H^+	-388.64	-388.64	-384.92	-382.44	-414.89		

Species	B3LYP/6-31+G(d,p) CH_2Cl_2 solution (CPCM-Bondi); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	$\Delta G /H^+$	$\Delta G^{\dagger} /H^+$
(*R*,*S*)-**1**	-1816854.91	-1816069.53	-1816028.72	-1816026.24	-1816187.62		
Ammonium (*R*,*S*)-**1**	-1818061.99	-1817236.51	-1817195.67	-1817193.19	-1817354.39	**-673.18**	
Pyridinium (*R*,*S*)-**1**	-1818049.47	-1817227.73	-1817186.85	-1817184.37	-1817344.66	**-663.45**	
(*S*,*S*)-**1**	-1816860.91	-1816075.64	-1816034.75	-1816032.27	-1816193.90		
Ammonium (*S*,*S*)-**1**	-1818060.38	-1817234.35	-1817193.60	-1817191.12	-1817352.65	**-665.16**	
Pyridinium (*S*,*S*)-**1**	-1818037.31	-1817213.77	-1817173.11	-1817170.63	-1817329.91	**-642.41**	
TS (*R*,*S*)-**1**	-1818025.74	-1817213.57	-1817173.80	-1817171.33	-1817328.82	**-647.61**	**15.84**
TS (*S*,*S*)-**1**	-1818024.45	-1817211.66	-1817172.10	-1817169.61	-1817326.32	**-638.83**	**3.58**
H^+	-467.34	-467.34	-463.62	-461.14	-493.59		

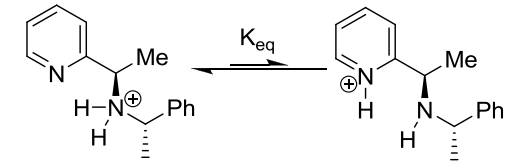
Species	B3LYP/6-31+G(d) gas phase; T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	ΔG /H^+	$\Delta G^{\dagger}$ /H^+
(*R*,*S*)-**2**	-2320168.59	-2319241.72	-2319192.64	-2319190.16	-2319372.33		
Ammonium (*R*,*S*)-**2**	-2321211.91	-2320245.79	-2320196.66	-2320194.18	-2320377.47	**-978.89**	
Pyridinium (*R*,*S*)-**2**	-2321196.61	-2320232.91	-2320183.96	-2320181.48	-2320363.04	**-964.46**	
(*S*,*S*)-**2**	-2320167.28	-2319240.46	-2319191.25	-2319188.77	-2319372.13		
Ammonium (*S*,*S*)-**2**	-2321210.79	-2320244.46	-2320195.32	-2320192.84	-2320375.52	**-977.13**	
Pyridinium (*S*,*S*)-**2**	-2321175.94	-2320212.09	-2320163.10	-2320160.62	-2320341.37	**-942.98**	
TS (*R*,*S*)-**2**	-2321173.45	-2320220.41	-2320172.12	-2320169.64	-2320350.59	**-952.01**	**12.45**
TS (*S*,*S*)-**2**	-2321173.11	-2320220.07	-2320171.72	-2320169.24	-2320351.01	**-952.62**	**-9.64**
H^+	0.00	0.00	3.72	6.20	-26.25		

Species	B3LYP/6-31+G(d) CH_2Cl_2 solution (PCM-UFF); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	ΔG /H^+	$\Delta G^{\dagger}$ /H^+
(*R*,*S*)-**2**	-2320188.32	-2319261.84	-2319212.66	-2319210.18	-2319393.46		
Ammonium (*R*,*S*)-**2**	-2321361.86	-2320394.63	-2320345.89	-2320343.41	-2320522.77	**-714.41**	
Pyridinium (*R*,*S*)-**2**	-2321354.82	-2320390.17	-2320341.51	-2320339.03	-2320518.40	**-710.05**	
(*S*,*S*)-**2**	-2320187.49	-2319261.03	-2319211.70	-2319209.22	-2319393.83		
Ammonium (*S*,*S*)-**2**	-2321359.65	-2320391.82	-2320343.11	-2320340.63	-2320519.67	**-710.95**	
Pyridinium (*S*,*S*)-**2**	-2321339.29	-2320374.35	-2320325.46	-2320322.98	-2320502.67	**-693.95**	
TS (*R*,*S*)-**2**	-2321323.66	-2320370.44	-2320322.14	-2320319.65	-2320500.76	**-692.40**	**17.64**
TS (*S*,*S*)-**2**	-2321323.83	-2320370.90	-2320322.60	-2320320.12	-2320500.71	**-691.99**	**1.96**
H^+	-388.64	-388.64	-384.92	-382.44	-414.89		

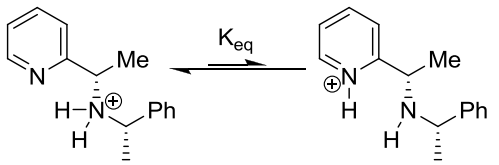
Species	B3LYP/6-31+G(d) CH_2Cl_2 solution (PCM-UFF); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	ΔG /H^+	$\Delta G^{\dagger}$ /H^+
(*R*,*S*)-**2**	-2320271.61	-2319347.13	-2319297.83	-2319295.35	-2319479.71		
Ammonium (*R*,*S*)-**2**	-2321450.99	-2320485.69	-2320437.02	-2320434.54	-2320613.60	**-719.00**	
Pyridinium (*R*,*S*)-**2**	-2321446.53	-2320483.93	-2320435.19	-2320432.71	-2320612.25	**-717.65**	
(*S*,*S*)-**2**	-2320270.57	-2319346.01	-2319296.60	-2319294.12	-2319479.03		
Ammonium (*S*,*S*)-**2**	-2321448.68	-2320483.53	-2320434.65	-2320432.17	-2320612.29	**-718.37**	
Pyridinium (*S*,*S*)-**2**	-2321430.81	-2320467.94	-2320418.95	-2320416.47	-2320596.46	**-702.54**	
TS (*R*,*S*)-**2**	-2321419.51	-2320468.21	-2320419.81	-2320417.33	-2320599.33	**-704.73**	**12.93**
TS (*S*,*S*)-**2**	-2321419.55	-2320468.56	-2320420.17	-2320417.69	-2320598.46	**-704.54**	**-2.00**
H^+	-388.64	-388.64	-384.92	-382.44	-414.89		

Species	B3LYP/6-31+G(d) CH_2Cl_2 solution (CPCM-Bondi); T = 298.15 K; P = 1 atm						
	E_{elec}	E_{elec} + ZPE	E	H	G	ΔG /H^+	$\Delta G^{\dagger}$ /H^+
(*R*,*S*)-**2**	-2320291.11	-2319367.03	-2319317.66	-2319315.18	-2319499.67		
Ammonium (*R*,*S*)-**2**	-2321492.47	-2320528.58	-2320479.34	-2320476.86	-2320661.68	**-668.42**	
Pyridinium (*R*,*S*)-**2**	-2321481.89	-2320521.29	-2320472.05	-2320469.57	-2320651.92	**-658.66**	
(*S*,*S*)-**2**	-2320290.49	-2319366.39	-2319317.03	-2319314.55	-2319498.41		
Ammonium (*S*,*S*)-**2**	-2321490.49	-2320526.08	-2320476.91	-2320474.43	-2320656.89	**-664.89**	
Pyridinium (*S*,*S*)-**2**	-2321469.34	-2320506.76	-2320457.65	-2320455.17	-2320636.08	**-644.08**	
TS (*R*,*S*)-**2**	-2321455.32	-2320504.09	-2320455.93	-2320453.45	-2320633.95	**-640.68**	**17.97**
TS (*S*,*S*)-**2**	-2321454.38	-2320503.76	-2320455.53	-2320453.05	-2320632.66	**-640.66**	**3.42**
H^+	-467.34	-467.34	-463.62	-461.14	-493.59		

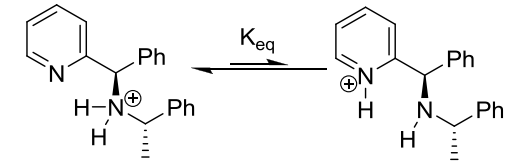
Thermodynamic equilibrium constants



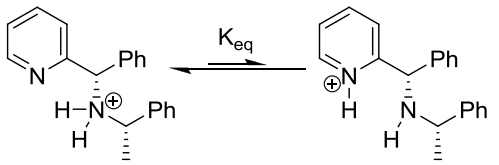
(*R*,*S*)-Ammonium **1** (*R*,*S*)-Pyridinium **1**



(*S*,*S*)-Ammonium **1** (*S*,*S*)-Pyridinium **1**



(*R*,*S*)-Ammonium **2** (*R*,*S*)-Pyridinium **2**



(*S*,*S*)-Ammonium **2** (*S*,*S*)-Pyridinium **2**

K_{eq} of the reaction of the proton transfer from the ammonium to the pyridinium forms could be calculated starting from the formula $\Delta G = - R T Ln(K_{eq})$ led to $K_{eq} = \exp[-\Delta G / (RT)]$.

With the fundamental constant values taken from the *National Institute of Standards and Technology* (NIST – USA)

Gaz constant R = 8.3144621 $J.mol^{-1}.K^{-1}$

1 hartree = $4.35974434.10^{-18}$ J

Avogadro number $N_A = 6.02214129.10^{23}$ mol^{-1},

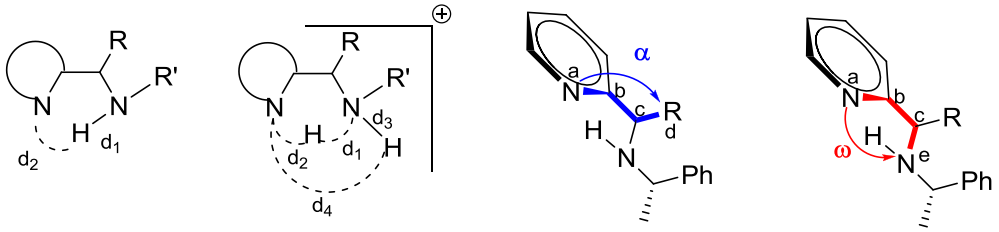
the temperature of T = 298.15 K,

and the previous results of the G value of protonated forms,

K_{eq} values are ($kJ.mol^{-1}$):

Equilibrium of protonated forms	B3LYP/6-31+G(d)		B3LYP/6-31+G(d,p)	
	Gas phase	CH_2Cl_2 (PCM-UFF)	CH_2Cl_2 (PCM-UFF)	CH_2Cl_2 (CPCM-Bondi)
(*R*,*S*)-**1**	38.139	11.14	4.11	50.55
(*S*,*S*)-**1**	Not defined	929.33	408.97	9653.84
(*R*,*S*)-**2**	336.917	5.8139	1.72	51.36
(*S*,*S*)-**2**	962187	951.24	593.75	4418.18

Define of geometric parameters



Tables of results for the geometric parameters

Distance in Å. angle in °	B3LYP/6-31+G(d) gas phase; T = 298.15 K; P = 1 atm					
Species	d_1	d_2	d_3	d_4	α	ω
(*R*,*S*)-**1**	1.01849	2.48853			-69.56543	56.89811
Ammonium (*R*,*S*)-**1**	1.04669	1.88064	1.02607	2.99354	-135.34601	-12.35298
Pyridinium (*R*,*S*)-**1**	2.01950	1.03559	1.01758	3.34604	-112.56096	10.46497
(*S*,*S*)-**1**	1.01965	2.57669			73.93142	-48.84058
Ammonium (*S*,*S*)-**1**	1.04727	1.88877	1.02434	3.29073	105.86980	-15.17614
Pyridinium (*S*,*S*)-**1**	2.00188	1.03794	1.02196	2.83649	99.40882	-22.45142
TS (*R*,*S*)-**1**	1.37298	1.24089	1.02073	3.03579	-120.53889	2.19647
TS (*S*,*S*)-**1**	1.37246	1.24463	1.02121	2.99785	126.45676	-0.45407

Distance in Å. angle in °	B3LYP/6-31+G(d) CH_2Cl_2 (PCM-UFF); T = 298.15 K; P = 1 atm					
Species	d_1	d_2	d_3	d_4	α	ω
(*R*,*S*)-**1**	1.01906	2.52405			-70.51954	56.10800
Ammonium (*R*,*S*)-**1**	1.04242	1.91618	1.02627	3.04176	-137.28375	-13.77467
Pyridinium (*R*,*S*)-**1**	2.00078	1.03343	1.02053	3.01337	-134.82025	-8.05104
(*S*,*S*)-**1**	1.02004	2.58882			73.49464	-49.59713
Ammonium (*S*,*S*)-**1**	1.04442	1.89626	1.02509	3.13783	125.76684	2.98475
Pyridinium (*S*,*S*)-**1**	2.10255	1.02944	1.02147	2.82929	96.29041	-25.53704
TS (*R*,*S*)-**1**	1.35572	1.25265	1.02088	3.01353	-122.23773	0.61527
TS (*S*,*S*)-**1**	1.35080	1.25930	1.02088	2.98669	122.58972	-0.13596

Distance in Å. angle in °	B3LYP/6-31+G(d,p) CH_2Cl_2 (PCM-UFF); T = 298.15 K; P = 1 atm					
Species	d_1	d_2	d_3	d_4	α	ω
(*R*,*S*)-**1**	1.01765	2.51826			-70.84381	55.76633
Ammonium (*R*,*S*)-**1**	1.04427	1.88560	1.02491	3.04020	-136.79916	-13.20326
Pyridinium (*R*,*S*)-**1**	1.99226	1.03324	1.01924	3.01711	-135.04387	-8.18366
(*S*,*S*)-**1**	1.01865	2.59332			73.46326	-49.66621
Ammonium (*S*,*S*)-**1**	1.04629	1.86781	1.02378	3.12423	126.36969	3.52086
Pyridinium (*S*,*S*)-**1**	2.09911	1.02873	1.02005	2.83069	96.39986	-25.46248
TS (*R*,*S*)-**1**	1.35274	1.24800	1.01986	3.01817	-122.28236	0.60913
TS (*S*,*S*)-**1**	1.34760	1.25464	1.01978	2.98986	122.71647	-0.05352

Distance in Å. angle in °	B3LYP/6-31+G(d,p) CH_2Cl_2 (CPCM-Bondi); T = 298.15 K; P = 1 atm					
Species	d_1	d_2	d_3	d_4	α	ω
(*R*,*S*)-**1**	1.01838	2.61051			-69.54135	57.22133
Ammonium (*R*,*S*)-**1**	1.03822	1.95074	1.02478	3.05977	-130.42015	-7.04001
Pyridinium (*R*,*S*)-**1**	2.02682	1.03094	1.01893	3.02677	-134.22463	-7.52116
(*S*,*S*)-**1**	1.01898	2.61339			73.23186	-50.09890
Ammonium (*S*,*S*)-**1**	1.03954	1.93505	1.02377	3.15396	123.26196	0.52137
Pyridinium (*S*,*S*)-**1**	2.14856	1.02567	1.02044	2.81325	97.32065	-24.97899
TS (*R*,*S*)-**1**	1.36457	1.23945	1.01953	3.03438	-120.36977	2.36528
TS (*S*,*S*)-**1**	1.35769	1.24637	1.01971	2.97758	123.32255	0.46831

Distance in Å. angle in °	B3LYP/6-31+G(d) gas phase; T = 298.15 K; P = 1 atm					
Species	d_1	d_2	d_3	d_4	α	ω
(*R*,*S*)-**2**	1.01751	2.36455			-84.53000	43.23568
Ammonium (*R*,*S*)-**2**	1.04459	1.90554	1.02576	3.00388	-139.88372	-15.95430
Pyridinium (*R*,*S*)-**2**	1.96429	1.03938	1.02024	3.10766	-139.85077	-11.41046
(*S*,*S*)-**2**	1.01874	2.54871			88.29038	-36.62220
Ammonium (*S*,*S*)-**2**	1.04559	1.89071	1.02555	3.08249	138.63885	14.55037
Pyridinium (*S*,*S*)-**2**	2.00428	1.03689	1.02252	2.79721	103.34887	-19.87789
TS (*R*,*S*)-**2**	1.38176	1.23337	1.02071	3.03710	-124.22927	0.05999
TS (*S*,*S*)-**2**	1.38251	1.23720	1.02120	2.99638	126.52782	2.14765

Distance in Å. angle in °	B3LYP/6-31+G(d) CH_2Cl_2 (PCM-UFF); T = 298.15 K; P = 1 atm					
Species	d_1	d_2	d_3	d_4	α	ω
(*R*,*S*)-**2**	1.01787	2.40934			-84.16588	43.80450
Ammonium (*R*,*S*)-**2**	1.04146	1.94862	1.02581	3.04056	-142.04270	-17.37638
Pyridinium (*R*,*S*)-**2**	2.03351	1.03183	1.02063	2.99108	-141.58087	-12.56760
(*S*,*S*)-**2**	1.01943	2.53527			87.72763	-37.19588
Ammonium (*S*,*S*)-**2**	1.04279	1.92511	1.02552	3.07461	139.83605	15.52783
Pyridinium (*S*,*S*)-**2**	2.10693	1.02856	1.02202	2.78544	99.43917	-23.28441
TS (*R*,*S*)-**2**	1.35504	1.25227	1.02073	3.03021	-123.36163	0.66180
TS (*S*,*S*)-**2**	1.35156	1.25870	1.02086	2.97981	127.18821	2.78726

Distance in Å. angle in °	B3LYP/6-31+G(d,p) CH_2Cl_2 (PCM-UFF); T = 298.15 K; P = 1 atm					
Species	d_1	d_2	d_3	d_4	α	ω
(*R*,*S*)-**2**	1.01656	2.40033			-84.69754	43.18142
Ammonium (*R*,*S*)-**2**	1.04254	1.92245	1.02442	3.03154	-141.42333	-16.73770
Pyridinium (*R*,*S*)-**2**	2.02767	1.03142	1.01935	2.99511	-141.57009	-12.56540
(*S*,*S*)-**2**	1.01808	2.53859			87.61244	-37.32497
Ammonium (*S*,*S*)-**2**	1.04418	1.89954	1.02427	3.06755	139.60520	15.27407
Pyridinium (*S*,*S*)-**2**	2.10544	1.02779	1.02061	2.78733	99.43041	-23.28986
TS (*R*,*S*)-**2**	1.35129	1.24819	1.01977	3.03253	-123.49842	0.52794
TS (*S*,*S*)-**2**	1.34790	1.25457	1.01990	2.97837	127.73562	3.28368

Distance in Å. angle in °	B3LYP/6-31+G(d,p) CH_2Cl_2 (CPCM-Bondi); T = 298.15 K; P = 1 atm					
Species	d_1	d_2	d_3	d_4	α	ω
(*R*,*S*)-**2**	1.01701	2.48420			-82.37266	45.90215
Ammonium (*R*,*S*)-**2**	1.03762	1.97171	1.02462	3.04772	-140.72830	-15.81479
Pyridinium (*R*,*S*)-**2**	2.05264	1.02926	1.01905	2.97415	-141.81340	-12.92614
(*S*,*S*)-**2**	1.01833	2.57305			87.88137	-37.51853
Ammonium (*S*,*S*)-**2**	1.03947	1.94656	1.02364	3.10519	137.62622	12.89754
Pyridinium (*S*,*S*)-**2**	2.16899	1.02467	1.02057	2.75508	100.01718	-23.14155
TS (*R*,*S*)-**2**	1.36244	1.23989	1.01987	3.02898	-123.83155	0.35909
TS (*S*,*S*)-**2**	1.35664	1.24696	1.01955	2.96122	127.96572	3.57947

Example of Gaussian 09 input file

```
%mem=1GB
%nproc=1
#p B3LYP/6-31+G(d,p) opt=(CalcFC, tight, TS, Noeigentest) SCRF=(CPCM, read, solvent=dichloromethane)
gfprint pop=full freq

TS (R,S)-Py,Me,Me,Ph with H+ B3LYP/6-31+G(d,p) in CH2Cl2 CPCM-Bondi opt

1 1
```

6	1.461675	1.446406	0.058044
7	0.110182	0.938650	-0.319529
1	-0.194904	1.353106	-1.199631
6	-0.968475	1.055446	0.714736
1	-0.536518	0.641589	1.631035
6	-1.368106	2.515135	0.966078
1	-2.128518	2.560004	1.751222
1	-0.508609	3.108744	1.291770
1	-1.781146	2.973630	0.061978
6	-2.142296	0.172967	0.313706
6	-2.448163	-0.967730	1.069956
6	-2.937338	0.472813	-0.804700
6	-3.523652	-1.792110	0.721423
1	-1.843683	-1.211217	1.940171
6	-4.007673	-0.352921	-1.159906
1	-2.729357	1.354990	-1.404847
6	-4.305309	-1.487609	-0.396803
1	-3.747842	-2.668775	1.322274
1	-4.611405	-0.107338	-2.028826
1	-5.140290	-2.125851	-0.670582
6	2.352345	0.195751	0.044685
6	3.702930	0.101522	0.369932
6	4.309338	-1.153082	0.280266
1	4.260709	0.976278	0.684791
6	2.220928	-2.102772	-0.433834
6	3.565877	-2.269140	-0.127309
1	5.359933	-1.264352	0.528425
1	1.580087	-2.917279	-0.751989
1	4.021149	-3.249711	-0.202474
7	1.662887	-0.885987	-0.337277
1	1.427208	1.832311	1.081409
1	0.563155	-0.336502	-0.495112
6	1.971247	2.542348	-0.883070
1	2.982151	2.845623	-0.597995
1	1.997253	2.185892	-1.918045
1	1.319166	3.418080	-0.825150

```
Radii=Bondi
```