

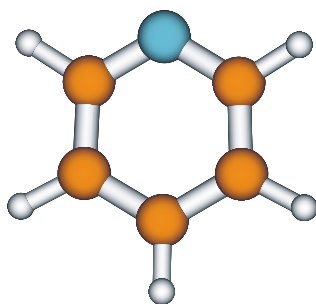
Engineering exceptionally strong oxygen superbases with 1,8-diazanaphthalene di-*N*-oxides

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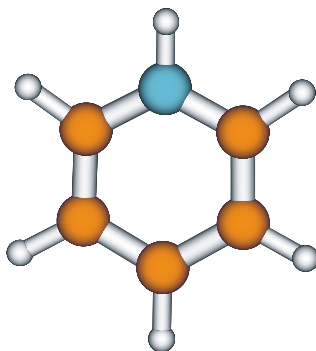
Supporting Information

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<i>Cartesian coordinates of all investigated systems (obtained by the M06-2X/6-31+G(d,p) model)</i>	S2-S107
Table S1. <i>NBO charges calculated using M06-2X/6-31+G(d,p) method.</i>	S108-S114



1a

C	-0.0143116023	0.	0.0234279507
C	-0.0234285235	0.	1.414966831
C	1.1950686216	0.	2.0875258834
C	2.3685523978	0.	1.334497657
N	2.3925278333	0.	-0.0002979968
C	1.2165048744	0.	-0.6321114115
H	-0.9603022314	0.	1.9637279508
H	1.2427128306	0.	3.1712378512
H	3.3376261175	0.	1.8279483668
H	1.2596221988	0.	-1.7188721914
H	-0.9365925692	0.	-0.5475958081

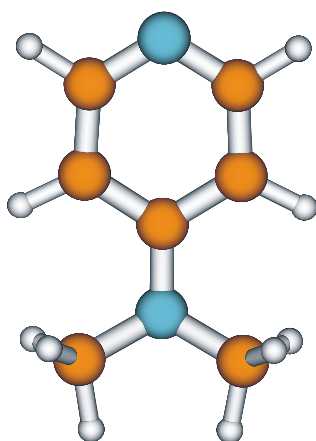


1a protonated at pyridine nitrogen

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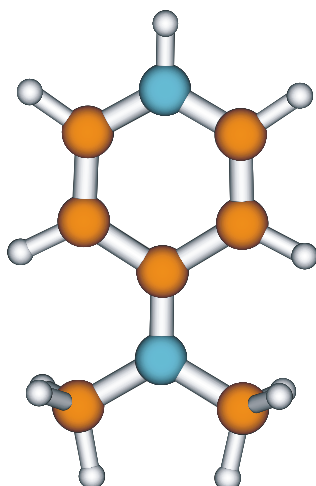
C  -0.0105947623  0.  0.0066079027
C  -0.0010575407  0.  1.4025494728
C   1.2103041619  0.  2.0958150106
C   2.3915976394  0.  1.378454065
N   2.3442946855  0.  0.0318126966
C   1.1941553263  0. -0.6703550127
H  -0.9383453055  0.  1.949859647
H   1.2446093136  0.  3.1787352716
H   3.3748978178  0.  1.8331472214
H   1.2808652214  0. -1.7502317816
H  -0.9375473434  0. -0.5542561099
H   3.2226254712  0. -0.4816833005

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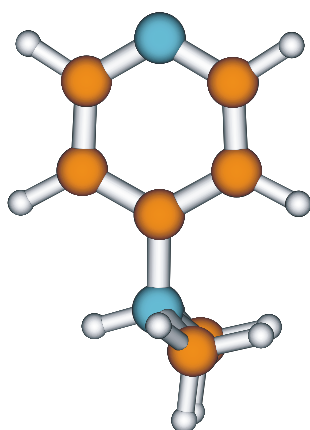
1b

N -0.0192805722 -0.0129171148 -0.0117261825
 C 0.0082443245 -0.0033111857 1.324129558
 C 1.1612301398 0.0182735412 2.0973222188
 C 2.419068202 0.0225671351 1.4586117718
 C 2.3968086547 0.027203821 0.048079032
 C 1.1749148155 0.0051386695 -0.6108315225
 N 3.5943590974 0.0178553808 2.1672387284
 C 3.5562703888 0.1949625678 3.6054262973
 C 4.8478199234 0.2040714674 1.4634227871
 H 3.3082471463 0.0480437109 -0.5357055168
 H 1.1610041695 0.0046582407 -1.6987847142
 H -0.960397344 2 -0.0106732577 1.8196237584
 H 1.0703158449 0.0318469744 3.175983295
 H 5.6684250011 0.1480056551 2.1786318315
 H 4.997222077 -0.5865003029 0.7207062703
 H 4.8967778533 1.1755514824 0.9509484688
 H 4.5720483093 0.1405986237 3.9969602015
 H 3.1219708712 1.1629141515 3.8939579458
 H 2.972381318 -0.6009430605 4.0793125408



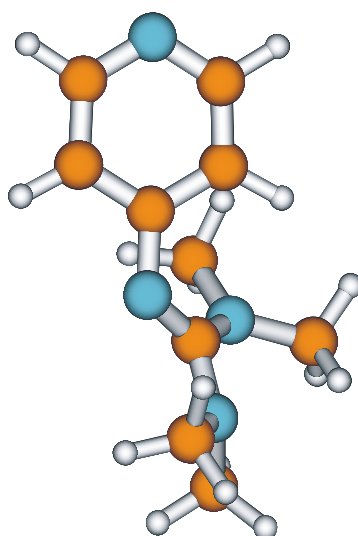
1b protonated at pyridine nitrogen

N	0.0368003154	-0.0131339269	0.0250078487
C	-0.0015673646	0.0090270256	1.379842521
C	1.146186551	0.0630908354	2.1147894578
C	2.4193573428	0.0974478661	1.4602810748
C	2.4024881286	0.0720592599	0.028643151
C	1.2162626364	0.0177203914	-0.6424194154
N	3.5595809055	0.1503045884	2.147142537
C	3.5409882584	0.1750982168	3.6113420888
C	4.8449034973	0.1844697343	1.4459903624
H	3.3159802416	0.0949749568	-0.5488537228
H	1.1610709046	-0.0030003738	-1.7239668966
H	-0.9832454531	-0.0183050188	1.8367687091
H	1.0629333634	0.0789010494	3.1924307376
H	5.6444906801	0.2258899233	2.1815133743
H	4.9794243257	-0.7161255845	0.8396322371
H	4.915141232	1.0709984907	0.8088353678
H	4.5649460535	0.2180339821	3.9742692528
H	3.007391599	1.0573341981	3.9770867027
H	3.0713604016	-0.7297973813	4.0081406842
H	-0.8299969238	-0.053562948	-0.4971693026



1b protonated at amino nitrogen

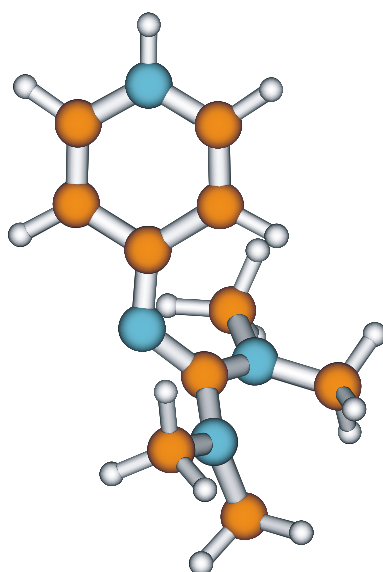
C	0.1863741678	-0.0043012981	-0.1230532842
C	0.0612603348	0.0201736618	1.2670876529
N	1.0994230508	0.0223267856	2.1033104864
C	2.3242407927	-0.0000738347	1.5847582095
C	2.5768935165	-0.0257189306	0.2094395279
C	1.4765309926	-0.0273019318	-0.6306058501
N	1.6984898962	-0.0535853355	-2.0954291333
C	1.1547025473	-1.3023050608	-2.7340581661
C	1.188785909	1.1890754447	-2.7729026333
H	-0.6998613798	-0.0046508475	-0.7490507046
H	-0.9251440819	0.0389302648	1.7216823967
H	3.1508986	0.0023106914	2.2893851801
H	3.5978555644	-0.043322418	-0.1621293268
H	1.4706537055	1.1484643969	-3.8252217825
H	0.1042341832	1.2140368274	-2.6738691481
H	1.6325577018	2.0553262066	-2.2832448949
H	1.4385888445	-1.3029431535	-3.7866155656
H	1.5734626237	-2.1647767893	-2.2164648501
H	0.0697733806	-1.2936566616	-2.6365126898
H	2.7148794648	-0.0696678624	-2.2287405592



1c

N	0.0066441281	0.0038653453	-0.0301096803
C	0.0185611586	-0.0504912251	1.3065273162
C	1.1716930143	-0.0546300975	2.0821908303
C	2.4231951372	-0.0169812483	1.4513439272
C	2.4172026524	0.0552238212	0.0472892626
C	1.2013655665	0.0614928546	-0.6267478852
N	3.5818144653	0.0423456524	2.2132268596
C	4.6528943999	-0.6010563327	1.8686510118
N	4.6979346553	-1.7663725752	1.123669744
C	3.5799515526	-2.6888617344	1.0877099998
N	5.8798630476	-0.1338688441	2.2913002764
C	5.9241353224	1.1919486414	2.8842333203
C	6.8863109809	-1.0484266925	2.8106375504
C	5.7143338559	-1.9907173416	0.1128512677
H	3.3519752254	0.1182899678	-0.5037764146
H	1.1878608654	0.1197604902	-1.7134814413
H	-0.9561885206	-0.0900993076	1.7883134977

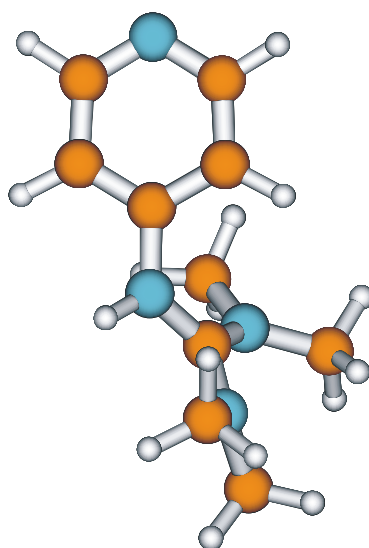
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H	2.9366131018	-2.526495241	1.9529541392
H	5.2495106412	-2.0199952863	-0.8827703198
H	6.4464511255	-1.1832160935	0.1339115402
H	6.2309405358	-2.9453900144	0.2762091591
H	6.9582096222	1.5471535917	2.857933303
H	5.2873406198	1.8699569908	2.3177911799
H	5.5723067791	1.1804137457	3.9246296219
H	6.9049083066	-1.0094935199	3.908694309
H	6.6651225057	-2.0710758132	2.5076962082
H	7.8788717003	-0.772919069	2.4384832057



1c protonated at pyridine nitrogen

N	0.1041447179	0.3216261721	0.0130474431
C	-0.0030104249	0.2358424036	1.3677808672
C	1.0942974304	-0.002833145	2.1367089262
C	2.3862876653	-0.178861719	1.5406662243
C	2.4358223494	-0.0762909782	0.1081437408
C	1.301242571	0.1738906403	-0.607288667
N	3.4300962533	-0.3464528738	2.3429475185
C	4.6166067021	-0.7947005367	1.905712547
N	4.7294876116	-1.8995169164	1.1238818536
C	3.6616067868	-2.8888977611	1.0426055472
N	5.7294885641	-0.1766445286	2.3341315137
C	5.6245265976	1.152391481	2.9345581926
C	6.9780144164	-0.8850734565	2.6150641018
C	5.8263862286	-2.0969315032	0.1802628565
H	3.3786308635	-0.1699249369	-0.4193062787
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H	-0.9957564245	0.3699383352	1.7801881622

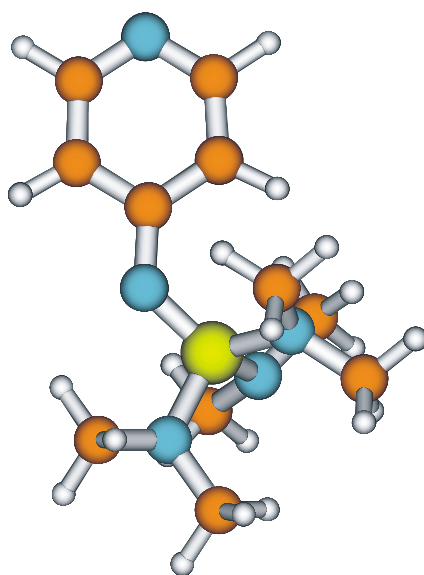
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H 3.0126483682 -2.8107097016 1.9143131946
H 5.3962378508 -2.3196940702 -0.8022129851
H 6.4228676968 -1.1887373259 0.0990557731
H 6.4704552927 -2.9328754154 0.4713178059
H 6.5740918636 1.6698764476 2.7838314244
H 4.8268853705 1.7179814526 2.4573798896
H 5.4156574576 1.0761948519 4.0068017371
H 7.2814140294 -0.6452145783 3.6378681728
H 6.8272127555 -1.9616046311 2.5471515387
H 7.7769803435 -0.5799469627 1.9330283566
H -0.7225853327 0.5063979927 -0.5402073124



1c protonated at imino nitrogen

C	0.0472586967	0.2081068624	-0.061886642
N	-0.0590970189	0.206213958	1.2672657381
C	1.0630933791	0.0686301732	1.9736936569
C	2.3256567796	-0.0875982697	1.4015553729
C	2.4128965637	-0.0842616399	0.0138409903
C	1.255462293	0.0751095472	-0.744592579
N	3.6893474192	-0.2088517516	-0.6053126477
C	3.9312974729	-0.7767940696	-1.8118499616
N	4.887601317	-0.2510954009	-2.5882866724
C	5.6950983116	-1.0719023091	-3.4945430299
N	3.2373084638	-1.853966726	-2.1982838389
C	2.8957486833	-2.0949137431	-3.6014637503
C	2.6432622514	-2.7904438048	-1.2415988543
C	5.3183259139	1.1419999652	-2.446548414
H	1.2836405437	0.1113858461	-1.8297685747
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H	0.9541953642	0.0734040797	3.0546456036

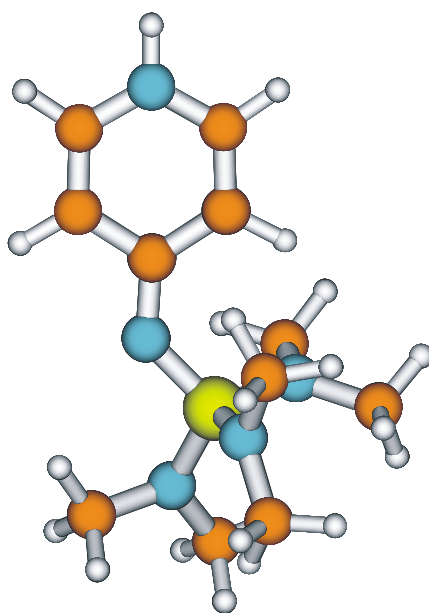
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H 3.0995463256 -2.6666699869 -0.2604824906
H 1.8212994489 -2.2917802365 -3.6570992543
H 3.1219393718 -1.2132492737 -4.2005378824
H 3.432297513 -2.9607177014 -3.9997477372
H 5.5581999691 1.5277454446 -3.4394126861
H 4.5140977169 1.7450773211 -2.024924904
H 6.2135321976 1.217387353 -1.8196555714
H 6.7471227594 -0.8288499832 -3.3257453856
H 5.5425836444 -2.1282859046 -3.2770566679
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H 4.4626776362 0.2673710404 -0.1575357115



1d

C	0.1272396314	-0.1670460287	0.495405675
N	0.2436907535	-0.7228953449	1.7093466313
C	1.4932521749	-0.9487047568	2.1219099973
C	2.6377407839	-0.6476105916	1.3904387055
C	2.5159026777	-0.0538488613	0.1162158287
C	1.1951524256	0.1752310387	-0.3196575713
N	3.5506846401	0.2881243087	-0.7243474392
P	5.0953512822	0.3341133628	-0.4419791283
N	5.8053848503	0.7571840872	-1.9013285278
C	7.2596432085	0.7464847762	-1.9855984909
N	5.7111244585	-1.087943379	0.216421292
C	7.0892627896	-1.2323473898	0.669393258
N	5.751773397	1.4830515793	0.6043900438
C	5.6081826466	2.8847429407	0.2037106576
C	5.1041952487	-2.3540132879	-0.1837310932
C	5.5273420643	1.3165762271	2.0420602471
C	5.1524061073	0.3897736922	-3.1541235256

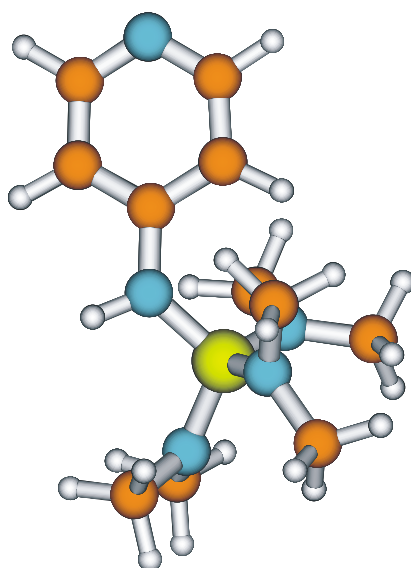
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H 3.6155891795 -0.8769813299 1.8033545356
H 4.0730751871 0.4680472706 -3.0365094352
H 5.4108982026 -0.6344670702 -3.46308588
H 5.4865435864 1.0795457543 -3.9363610178
H 7.5752031148 1.419897187 -2.7894937189
H 7.653434343 -0.257668907 -2.2067821333
H 7.6968988767 1.1013009417 -1.0496283479
H 6.3421014742 3.481448376 0.7547751988
H 5.7931932216 2.9909530331 -0.8652433565
H 7.5083781882 -0.2615570649 0.9375441236
H 6.2700695361 1.9131625702 2.5821333865
H 4.5243625301 1.6533616726 2.3388744118
H 5.6442353744 0.2715715652 2.3317303005
H 7.7226362181 -1.690045978 -0.1035416997
H 7.1127525362 -1.879838464 1.5546437687
H 5.1045903617 -3.0419672625 0.6693953598
H 5.6630647915 -2.8213144027 -1.0073556385
H 4.0724115667 -2.1965954347 -0.5004462147
H 4.6029739578 3.267833413 0.4283105396
H -0.8896263116 0.016521598 0.1540434668
H 1.0325720797 0.6261567148 -1.2929450877



1d protonated at pyridine nitrogen

C	0.0193616425	-0.0832646638	-0.0958313469
N	0.013828157	0.0189888836	1.2633592536
C	1.1750661302	0.1002050512	1.9600632193
C	2.3826813577	0.0849003027	1.326741848
C	2.4597393578	-0.0192425422	-0.1101207728
C	1.1904316518	-0.1042784869	-0.785427764
N	3.5541642937	-0.0446716449	-0.8467108862
P	5.111085819	0.0831438945	-0.4403162592
N	5.8766197138	0.7534856698	-1.7368512232
C	7.0551263785	1.6053318775	-1.6185618567
N	5.7355752929	-1.4184912026	-0.1442460329
C	7.1244760186	-1.7660908787	-0.4322753051
N	5.3620919131	1.0573524879	0.8836213017
C	4.8013652636	2.4081945398	0.8877808389
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C	6.4292239745	0.8383106157	1.8551458195

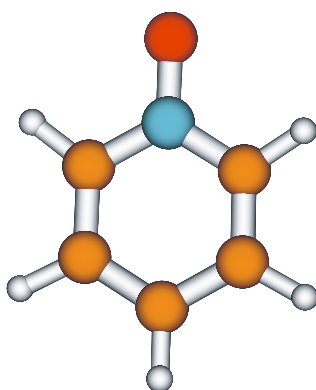
C	5.6435268114	0.2240554444	-3.0812574602
H	1.0824117547	0.1742343754	3.0372577917
H	3.2869797734	0.1500343152	1.9196815662
H	4.6940011073	-0.3103707436	-3.1103206963
H	6.4543358947	-0.451893543	-3.3826059381
H	5.598262371	1.0569992864	-3.7890433741
H	6.9270164575	2.490251267	-2.2498969109
H	7.9616324545	1.0781332021	-1.9434629418
H	7.1946706672	1.9332503682	-0.5876345953
H	5.5682906293	3.1592254875	0.6581379464
H	4.0036665918	2.4888620225	0.1454736735
H	7.5673878547	-1.0341863536	-1.1092807575
H	7.2955400655	1.484916185	1.6615475819
H	6.0535944526	1.0633297155	2.8589295205
H	6.7549098798	-0.2026543202	1.8355230112
H	7.1573533761	-2.747435493	-0.9153918165
H	7.7286800813	-1.8091912924	0.4833003907
H	5.4093200727	-2.3201539406	1.7552839549
H	5.1808919485	-3.3745887055	0.3395604383
H	3.9635192392	-2.1523531995	0.7224240937
H	4.3841788486	2.6291943541	1.8763154141
H	-0.9497345669	-0.1442709122	-0.5762359717
H	1.1854440718	-0.1844454269	-1.8653672817
H	-0.8672426607	0.0311085354	1.7593748963



1d protonated at imino nitrogen

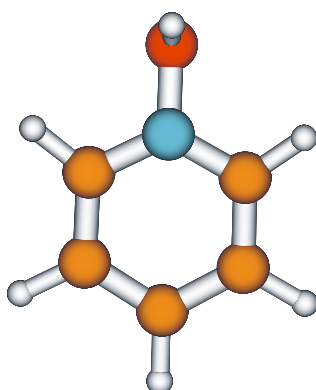
C	0.1884908827	0.4869998962	0.0094709656
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N	1.4327412376	0.1847016539	2.0472475059
C	2.4823397657	-0.1634531037	1.3051385063
C	2.4760904122	-0.2209793686	-0.0882564627
C	1.2971118576	0.1194259297	-0.7535298141
N	1.174601551	0.1060503392	-2.1657050378
P	2.345289051	0.0263600631	-3.3430161557
N	3.58982985	0.9311178571	-2.7873043584
C	4.9854901635	0.5915306353	-3.0740013184
N	1.7408604255	0.5917784593	-4.7629956831
C	0.679083997	-0.1339881582	-5.4717900597
N	2.7484523862	-1.5327828388	-3.6423022962
C	2.7142846464	-2.5639407127	-2.5991337584
C	1.8419273384	2.0107881034	-5.1194629084
C	3.4308536065	-1.9439944387	-4.8755222193
C	3.4048733744	2.2224819231	-2.1149483141
H	3.3890993465	-0.4211925512	1.8464933606

H 3.3712880813 -0.525458997 -0.6194547193
H 0.6522875918 -1.1769963828 -5.1512997058
H 0.8818347859 -0.1030695568 -6.5460661352
H -0.2996113014 0.3260985623 -5.2892969488
H 0.9781529973 2.5818911372 -4.7590922262
H 1.8845661334 2.0889816104 -6.2085515722
H 2.7576207291 2.4415904398 -4.7133444252
H 3.8565462837 3.0249656095 -2.7079606494
H 2.3442887244 2.4376102797 -1.9748379505
H 3.5010106255 -1.1084987542 -5.5734403732
H 5.4000235814 1.244995135 -3.8491626688
H 5.5713194569 0.7149096786 -2.1579490395
H 5.0704698807 -0.4465351215 -3.3979642339
H 2.8652803329 -2.7535995983 -5.3476910261
H 4.4391859319 -2.3084767004 -4.6505500792
H 3.7081250356 -2.7205030579 -2.1637394049
H 2.3772035402 -3.5001112488 -3.0520398758
H 2.0117681087 -2.2931874314 -1.8105761169
H 3.8845538435 2.1901626983 -1.1315522689
H -0.540867274 0.7761538986 2.010484364
H -0.752013545 0.7617864502 -0.4587717318
H 0.2246297303 0.2048022028 -2.5090676736



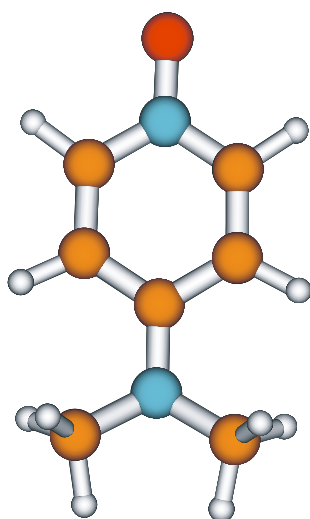
2a

C	-0.0006470209	0.	0.0212863665
C	-0.0210384992	0.	1.4139313106
C	1.2020164089	0.	2.0802768931
C	2.3869758403	0.	1.367787781
N	2.3924960988	0.	0.0041758391
C	1.2020353571	0.	-0.6608594607
H	-0.9565113151	0.	1.9603428797
H	1.2536118821	0.	3.16343027
H	3.375912127	0.	1.8056220746
H	1.3064552697	0.	-1.7373299968
H	-0.9187652445	0.	-0.5557256183
O	3.4927457392	0.	-0.6384832557



2a protonated at *N*-oxide oxygen

C	-0.0598110979	0.0324613264	0.0083423312
C	0.0048357579	-0.0499155992	1.3996566323
C	1.2442888363	-0.0450129014	2.0403293684
C	2.3969258826	0.0377251265	1.2809254197
N	2.2858686145	0.0936836096	-0.0587935528
C	1.113546067	0.1139783522	-0.7187728703
H	-0.907990576	-0.1087477369	1.9832610242
H	1.3278442898	-0.0946449669	3.1196131337
H	3.4067738631	0.0704715311	1.6730586653
H	1.1798214266	0.2027483305	-1.7969013972
H	-1.0068533691	0.0440531277	-0.5182280261
O	3.432737827	0.2700461201	-0.7881174329
H	3.7616266421	-0.6137219917	-1.0328602665



2b

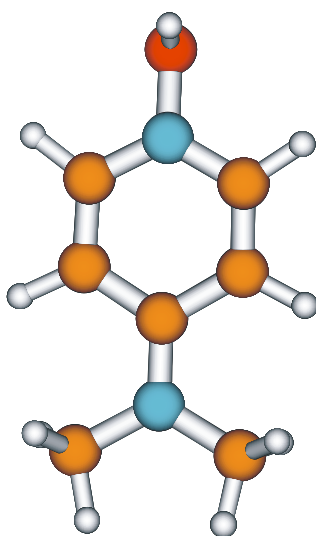
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C 0.0096293131 -0.1137623949 -0.0812725728
C -0.0297816873 0.0359066187 1.2903821816
C 1.1542547782 0.2068601648 2.0347562216
C 2.3458131957 0.2412909606 1.2836523117
C 2.3249294315 0.0864480668 -0.0878592647
N 1.1723474967 -0.094940573 -0.7803839631
O 1.1809001328 -0.2362005981 -2.0619427731
N 1.1482517686 0.3209792516 3.4094222058
H 3.3098784166 0.3881242351 1.7525897457
H 3.2101290703 0.1010404877 -0.7097935585
H -0.8683906662 -0.2516525713 -0.6982523338
H -1.0020634196 0.0155277541 1.76487091
C 2.3613963447 0.7569159018 4.0731271391
C -0.1181600046 0.5413343689 4.0801598977
H 2.1864774873 0.782070112 5.1487440459
H 3.1765578144 0.050521914 3.8884515957
H 2.6843075432 1.7568649238 3.7459263031
H 0.0557535247 0.5960511505 5.1548386204

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H -0.6103528654 1.4707565825 3.7558655846

H -0.800385396 -0.2949381131 3.8990098572



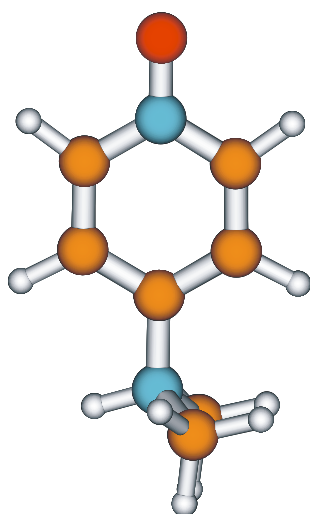
2b protonated at *N*-oxide oxygen

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C -0.1136870712 0.0381003221 -0.0492765255
C -0.1234396005 0.1947970687 1.3070949853
C 1.1044538842 0.342915938 2.0274572652
C 2.3055815229 0.3318077424 1.2490564638
C 2.2489930514 0.1713564418 -0.1056942471
N 1.0581551897 -0.0007324761 -0.7229117218
O 1.0278790021 -0.0436922082 -2.0941181475
N 1.1275130327 0.4950974259 3.3516692355
H 3.2781133698 0.4620814847 1.7028729272
H 3.1170468286 0.1749596663 -0.7540897906
H -1.0065771195 -0.0575776448 -0.6555317368
H -1.0817827268 0.2161531429 1.8069570944
C 2.4013870344 0.6600914325 4.0543529295
C -0.1219721109 0.5176562079 4.1145722862
H 2.2046545127 0.7547175243 5.1194621237
H 3.0447531819 -0.2108580276 3.8984279512
H 2.9173147332 1.5640383367 3.7165591008

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H 0.1132889809 0.6363535741 5.1694097639
H -0.7516337098 1.3571153157 3.8043245012
H -0.6701336797 -0.420417218 3.9868004303
H 1.0744000225 -0.980297025 -2.3516211128



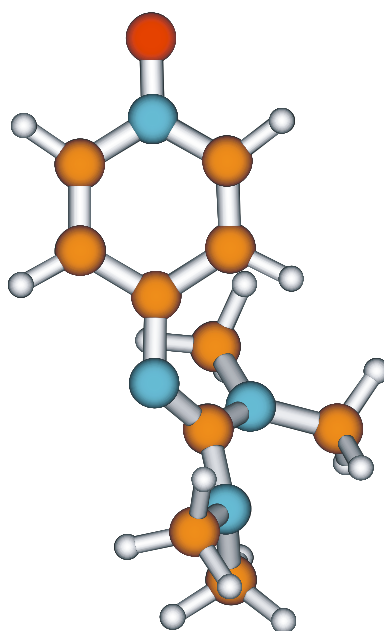
2b protonated at amino nitrogen

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C 0.3092922916 0.7277799228 -0.0612855204
C 0.3587598841 0.8370463528 1.3107120942
C 1.3113224815 0.1065949254 2.014776695
C 2.1939119915 -0.7176159859 1.3291749466
C 2.1150720311 -0.8022553828 -0.0457262607
N 1.1793609973 -0.0860607758 -0.7469676009
O 1.1156689734 -0.1696643243 -1.9937778177
N 1.3932276071 0.1987119088 3.4852042786
H 2.9538772027 -1.306280288 1.8361513632
H 2.7573513241 -1.4151483581 -0.6643037027
H -0.391750916 1.2524109618 -0.6968952662
H -0.3552131348 1.4961134023 1.7945151258
C 1.7572740797 1.5796950083 3.9606225732
C 0.1532478411 -0.3124944323 4.1685030747
H 1.8943588094 1.5496641235 5.0418805325
H 2.6741742459 1.8861218117 3.4585848151
H 0.9425349018 2.2560716533 3.7040588186
H 0.3225514134 -0.3055087964 5.2455828254

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H -0.67497153 0.348195514 3.9142390621
H -0.0458303285 -1.3218551687 3.8104954089
H 2.1601140646 -0.420411145 3.766983324



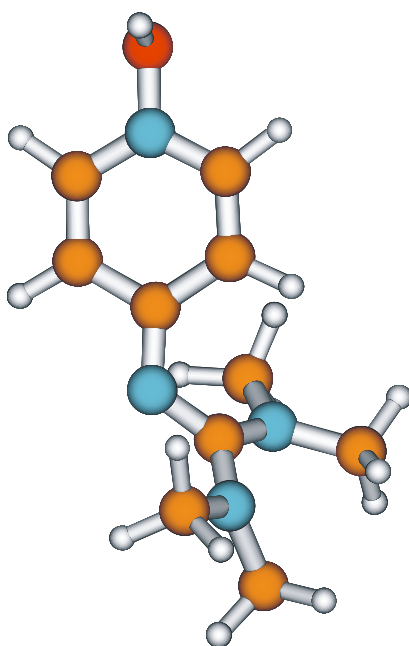
2c

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C -0.0931315694 -0.2359381204 0.2515980187
C -0.0016011894 -0.0433680655 1.6152040014
C 1.2432628216 -0.0092061418 2.260042271
C 2.3707276823 -0.1411415458 1.4312505979
C 2.2334359265 -0.3238459 0.0689237257
N 1.0128907885 -0.3829118776 -0.5266358731
O 0.907317126 -0.5641177031 -1.7962973131
N 1.303565859 0.2482590398 3.6232530146
H 3.3709991816 -0.0904413279 1.851642843
H 3.0597842758 -0.4289969233 -0.6217900694
H -1.0220098205 -0.2810006797 -0.3015237004
H -0.9073143789 0.0796795051 2.198881896
C 2.1874522872 -0.3202244838 4.383691748
N 2.5565338104 0.3023331126 5.5570827049
N 2.8032463697 -1.5370026465 4.1488594462

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C 4.2054313524 -1.7618687019 4.4459982473
C 2.1603150056 -2.5805345296 3.3748373174
C 2.6900413528 -0.4582922822 6.7916240485
C 2.1247343797 1.6759694822 5.7543529568
H 2.5590800231 -2.6465175639 2.3534621733
H 2.3246039529 -3.5407086688 3.8773630131
H 1.0877813381 -2.3930895401 3.3156411837
H 4.7561935765 -1.9591817206 3.5155273134
H 4.63113855 -0.8799253603 4.9250096739
H 4.3379507255 -2.6271210376 5.108459104
H 2.7470183883 2.1239317482 6.5341518307
H 2.237894594 2.2347130507 4.8264620798
H 1.0708319965 1.7274033844 6.0589610895
H 1.8033766446 -0.3135784747 7.4241032083
H 2.7870826136 -1.5217009073 6.5767097698
H 3.5711173785 -0.1253308705 7.3502309482



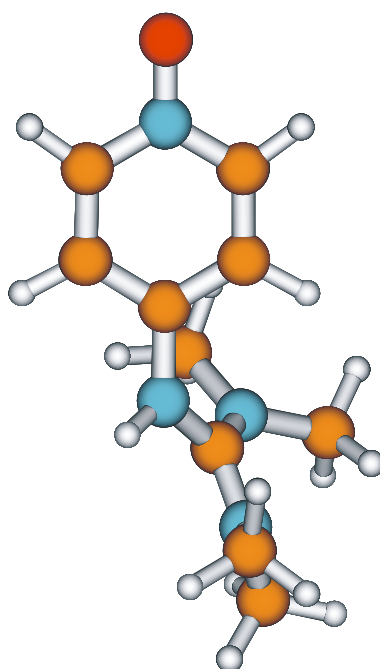
2c protonated at *N*-oxide oxygen

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C -0.0861366286 -0.0546923947 0.2243462925
C -0.0554886738 -0.0516406577 1.5865655523
C 1.1823698663 -0.1665884899 2.2994869337
C 2.3630322118 -0.2788220635 1.4901917146
C 2.2768367567 -0.2650699232 0.1268008096
N 1.0739614727 -0.1321565339 -0.4769826734
O 1.0132308344 -0.2375530546 -1.8452849821
N 1.1491279587 -0.0992303358 3.6261016978
H 3.3425611749 -0.3607318052 1.9477053992
H 3.124615307 -0.354448195 -0.5423501146
H -0.9889238597 -0.0005028577 -0.3725555997
H -0.9778077481 0.026007863 2.1492208876
C 2.1710279477 -0.4893961261 4.401157253
N 2.5054016614 0.2810906863 5.4500530347
N 2.8162596299 -1.6706645519 4.2147699566

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C 4.2088752921 -1.8849522917 4.5981725459
C 2.2057698501 -2.7680314036 3.474198397
C 2.9587749137 -0.2668333111 6.7283445698
C 2.0284857835 1.6618928136 5.5054048982
H 2.6093968981 -2.839297919 2.4565920915
H 2.4215284671 -3.7023247027 3.9993814251
H 1.1256326819 -2.6331046814 3.4268753138
H 4.7461963197 -2.278327392 3.7284500598
H 4.6684753506 -0.9419776773 4.8927292705
H 4.3013785946 -2.6079197126 5.4149602335
H 1.032601121 1.7088373767 5.9584824102
H 2.7310551824 2.2404068369 6.1086585324
H 1.9824504738 2.0830507168 4.5032428811
H 2.3115657025 0.129021838 7.5160073336
H 2.8716806143 -1.3524470881 6.7287066676
H 3.991252512 0.0211659934 6.9468100363
H 1.0413424476 0.6670145124 -2.1994221178



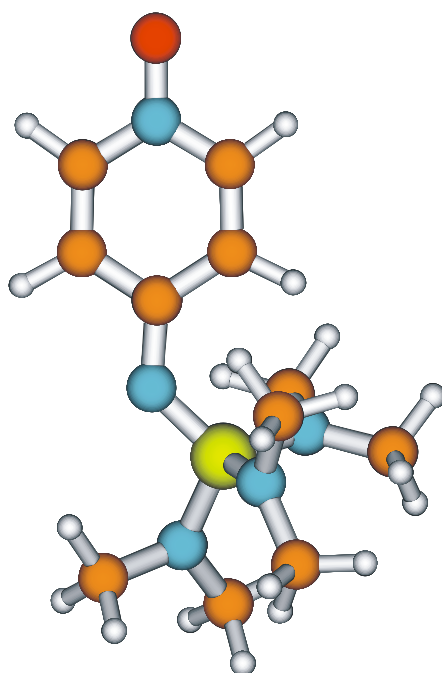
2c protonated at imino nitrogen

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C -0.0253472112 -0.4023414576 0.1525518693
C -0.0423280552 -0.3109784546 1.5294654336
C 1.1401735493 -0.0717708646 2.2253226907
C 2.322294903 0.0698147137 1.5000797954
C 2.3058448124 -0.0509537589 0.1260070827
N 1.1408765166 -0.2848301548 -0.5546826885
O 1.1438191564 -0.3863876643 -1.8105743722
N 1.129167731 0.0461272241 3.6462958395
H 3.2667228066 0.2818997591 1.9929295641
H 3.173342838 0.046835131 -0.5130892564
H -0.8963600486 -0.5786216073 -0.4646213927
H -0.987854245 -0.4321881011 2.0486887487
C 2.0838703446 -0.4474845928 4.4693468952
N 2.4027354528 0.2411583944 5.5740482509
N 2.6838750573 -1.6098987604 4.1811775449

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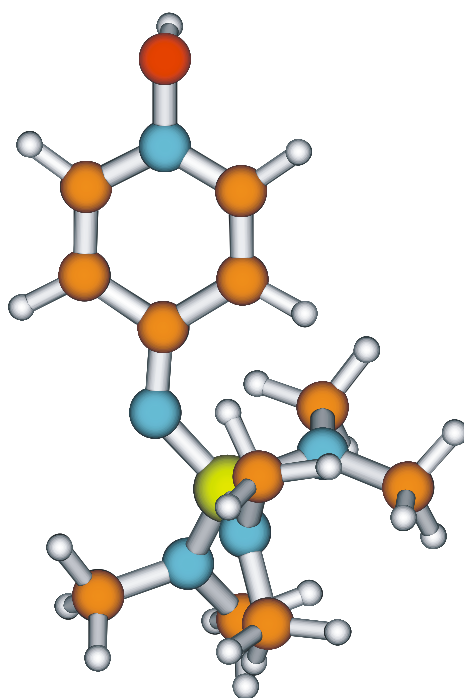
C 4.0880718216 -1.8605573596 4.5107407237
C 2.0292700116 -2.651741656 3.3867206899
C 2.8365899802 -0.4231494418 6.8062496706
C 2.159222932 1.681150164 5.6860294815
H 2.3838427267 -2.6386206956 2.350980017
H 2.2693072664 -3.6173662129 3.8376938243
H 0.9490937761 -2.5121061855 3.4029198443
H 4.5884379931 -2.2224503151 3.6081085123
H 4.5690939411 -0.9370694793 4.8319276636
H 4.1846292859 -2.6182825278 5.2935576931
H 2.9653553457 2.1180872164 6.2788710995
H 2.1665192622 2.1443425378 4.6989326466
H 1.2084587464 1.8856074123 6.1906029248
H 2.250685885 -0.0186311635 7.6353374551
H 2.6500778415 -1.4941858754 6.7383405879
H 3.8972076419 -0.2421157659 7.0022703647
H 0.4489531413 0.674540595 4.0561516867



2d

N -0.0037322112 0.4056113693 0.1090592588
 C -0.0147716822 0.1233295235 1.4335961775
 C 1.144374856 -0.1389310694 2.1416399498
 C 2.4085849575 -0.1214623944 1.512354149
 C 2.379547707 0.1761402355 0.1332064528
 C 1.1976418922 0.4273960756 -0.5285451184
 H -1.0053688779 0.1211347931 1.87000022
 O -1.1017176908 0.6443842304 -0.5324206969
 H 1.0541418167 -0.3566400242 3.2012442929
 N 3.6224714026 -0.353488314 2.1099174494
 P 3.9717334341 -0.6175386171 3.61710426
 N 3.8446267107 -2.2302492325 4.0429642473
 C 2.7115784685 -3.0148644069 3.5735003559
 C 4.6317453405 -2.8603137056 5.088207923
 N 3.053908731 0.2634956821 4.703933183
 C 2.6088189457 -0.2104675749 6.000335087

C 2.8453293758 1.6852483394 4.4632726628
N 5.5626759141 -0.1954555776 3.8759087899
C 6.5859306225 -0.6839216007 2.9626584609
C 6.0666205647 0.3783071024 5.1083950731
H 6.1230566117 -0.984143167 2.0216332531
H 7.1302484025 -1.5378888302 3.3930628833
H 7.3040213597 0.1173509424 2.7552057675
H 6.6854379043 1.2556097285 4.8840818504
H 6.6874960194 -0.3393542122 5.666327609
H 5.2427021971 0.6949051105 5.7502852072
H 3.4137038108 2.2980620391 5.1778105589
H 3.1605004523 1.9405861072 3.4490732285
H 5.4666514424 -2.2191391965 5.3765502508
H 3.1796637463 0.2464661299 6.8230988152
H 1.5508679035 0.0435727128 6.141875708
H 2.7107398178 -1.2945433455 6.0643282999
H 5.0385030593 -3.8100069986 4.7204732015
H 4.0312937605 -3.0741841668 5.9850071533
H 1.9104065889 -3.0717930972 4.3257006523
H 3.0460129655 -4.0334189293 3.3483100171
H 2.3088789273 -2.5794691546 2.6570843437
H 1.7808371121 1.9285956209 4.5646710051
H 1.1250351852 0.6589012278 -1.5832860917
H 3.3138001643 0.207321342 -0.4160299516



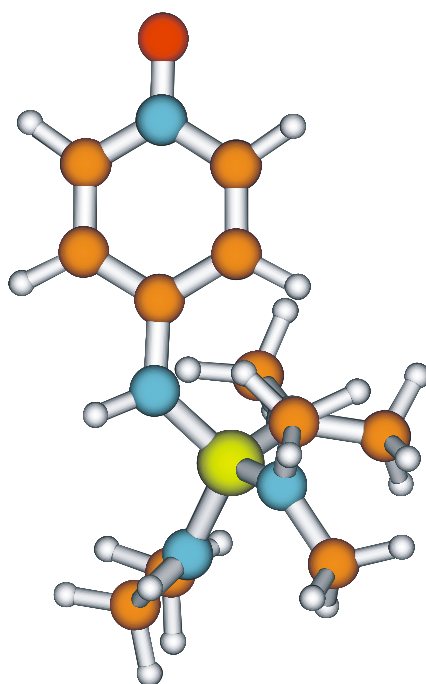
2d protonated at *N*-oxide oxygen

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N 0.1363183539 0.3258983915 0.0313774488
C 0.0381990908 0.1393676925 1.3675240226
C 1.1526714195 -0.1125888593 2.1145066916
C 2.4523877829 -0.2091834492 1.4968986718
C 2.462293148 -0.0366090643 0.0670660016
C 1.3191730595 0.2105285474 -0.6283219596
H -0.9661560305 0.1981064724 1.7707621072
O -1.0191187789 0.4632451292 -0.7000652213
H 1.0412437874 -0.251859225 3.1828421625
N 3.6026620119 -0.4481514025 2.0988974412
P 3.9555666342 -0.6571187262 3.6601414885
N 3.8497165825 -2.2607463473 4.0463508229
C 2.68913748 -3.0520309077 3.6481793257
C 4.6984082344 -2.8854378015 5.0575392728
N 2.9731548935 0.2220278564 4.6739639512
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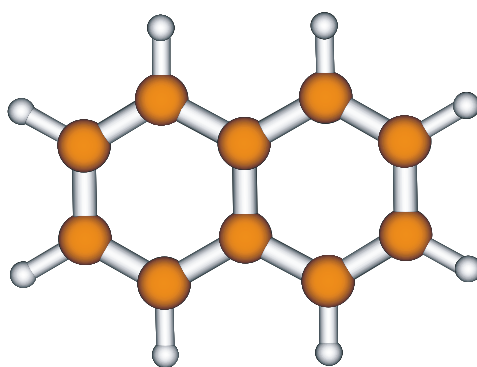
C 2.8337814291 1.6613919732 4.4564877427
N 5.5078894483 -0.1407980058 3.8599168256
C 6.5533139605 -0.5896564259 2.9389572934
C 6.0053324515 0.4377232755 5.1037137118
H 6.1070661244 -0.8998437175 1.994133964
H 7.1223178284 -1.4247110566 3.3678923566
H 7.2384207939 0.2411300592 2.7465983954
H 6.580049536 1.3416249538 4.8783201191
H 6.6612213401 -0.264283992 5.6348932037
H 5.1795423636 0.7083324 5.7631673982
H 3.4266214345 2.2329912242 5.1820789856
H 3.1688930573 1.9261009189 3.4507622437
H 5.5537275148 -2.247408706 5.284289198
H 3.1613066317 0.210487598 6.7928102652
H 1.5098946903 0.0462010719 6.1601463302
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H 5.0718258222 -3.8402688061 4.6747847582
H 4.1455536928 -3.0759594059 5.9866112626
H 1.9433723703 -3.113914365 4.4522744126
H 3.0169543456 -4.0655072065 3.399099543
H 2.2232635028 -2.6223706522 2.7594545192
H 1.7823277725 1.9499894729 4.5640637574
H 1.2653553805 0.3254117934 -1.7044023576
H 3.405872406 -0.1192148759 -0.4579339403
H -1.1745619188 1.4166873002 -0.8015588536



2d protonated at imino nitrogen

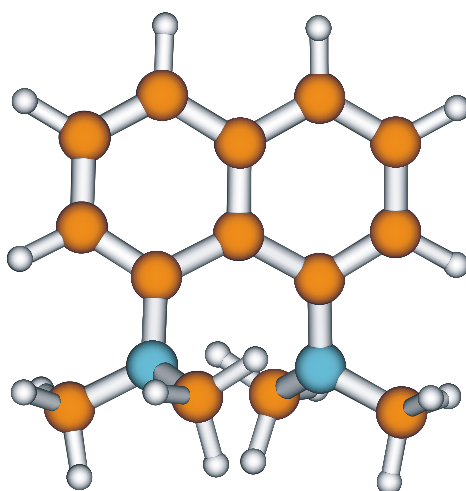
N	0.0042090079	0.6347098311	0.3442491678
C	0.0149314304	0.0071717606	1.5552222738
C	1.194624138	-0.3372109394	2.1875322018
C	2.4217403694	-0.0288733258	1.5982439628
C	2.3992930618	0.6163891463	0.3600232448
C	1.2002774062	0.9283008223	-0.2463943627
H	-0.9715486595	-0.1968973151	1.9503454115
O	-1.089230167	0.9361903371	-0.2191497146
H	1.1282420828	-0.8414774741	3.1452945743
N	3.6750482889	-0.3373100739	2.1936234341
P	4.0428339819	-0.7051742149	3.7700035228
N	3.8780865816	-2.3139184061	4.0339178112
C	2.8915239651	-3.1279366582	3.3159310893
C	4.4991152618	-2.9902253766	5.1798441924

N 3.0299519929 0.2115753382 4.6716854515
C 2.4973255077 -0.2551147026 5.9540930595
C 2.748339294 1.6210780487 4.3734240157
N 5.6272551641 -0.3875924014 4.0706517391
C 6.6881791613 -1.1722807051 3.4256541124
C 6.0570759657 0.9340087614 4.539749428
H 6.2983446383 -2.1346852698 3.0892963678
H 7.4883254642 -1.3525275472 4.1490560864
H 7.1090969371 -0.6323914096 2.5687665564
H 6.2713175882 1.6118627658 3.7049701269
H 6.9668575178 0.8081121981 5.131587589
H 5.2953328108 1.3769802827 5.1820544395
H 3.1146838619 2.2598970313 5.184180967
H 3.2271552955 1.9220827305 3.4401411576
H 5.1522689513 -2.3055672753 5.7225809965
H 3.0316954211 0.2002656915 6.7948925514
H 1.4408071798 0.0227010123 6.0160294411
H 2.5710454689 -1.3409114632 6.028227727
H 5.093080748 -3.8366413816 4.8205896576
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3a

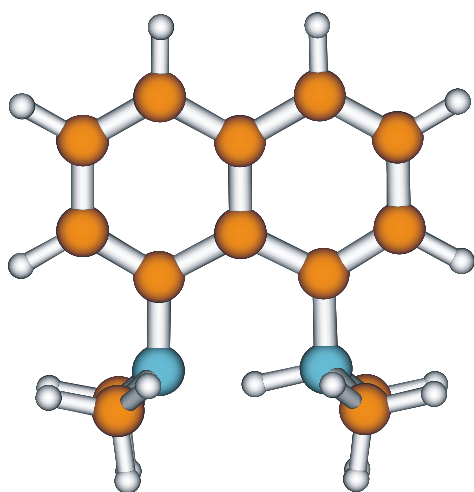
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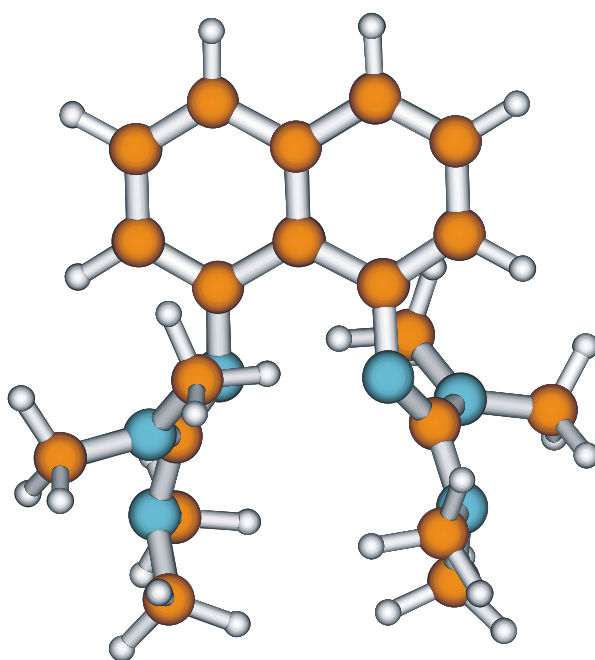
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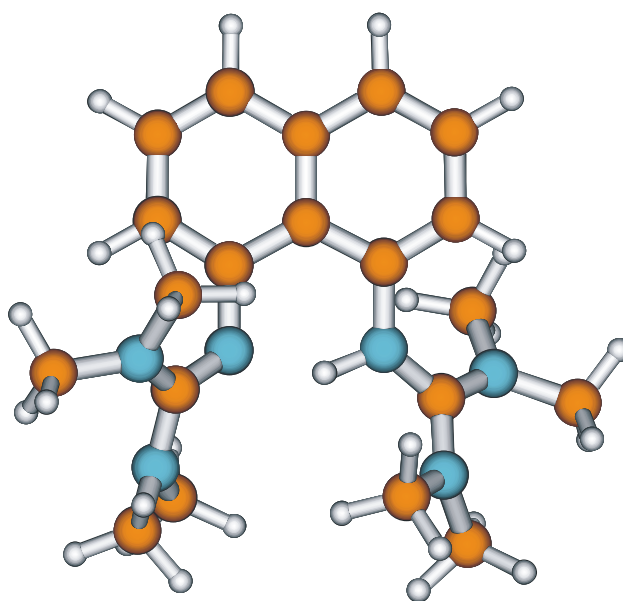
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3c protonated at imino nitrogen

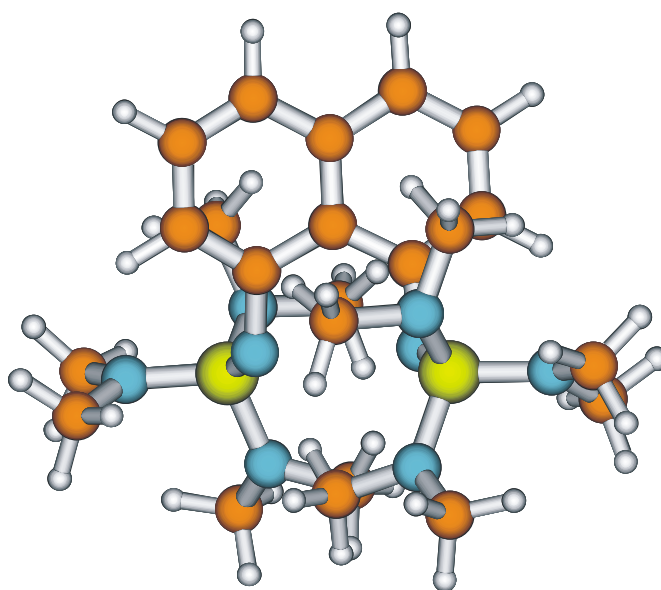
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3d

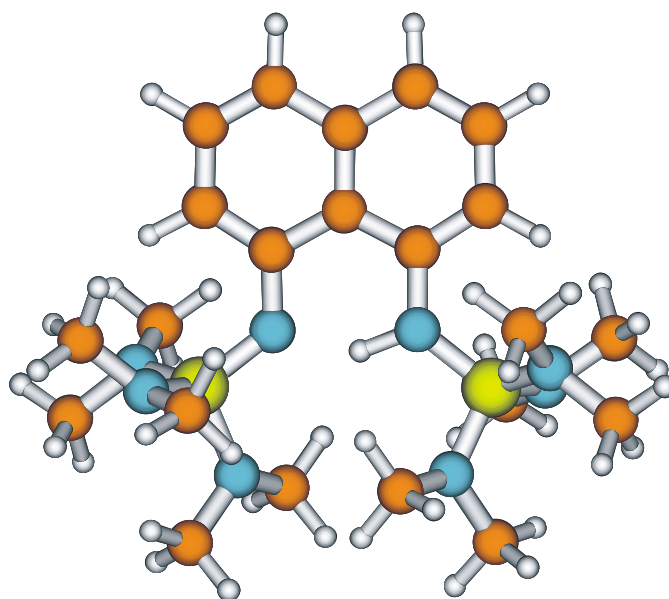
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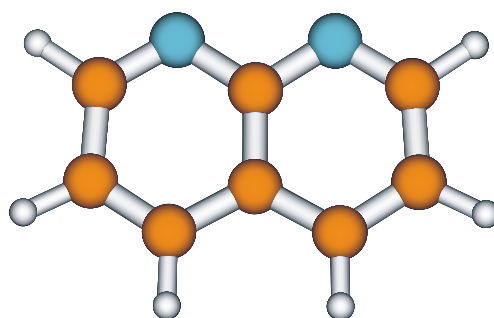


3d protonated at imino nitrogen

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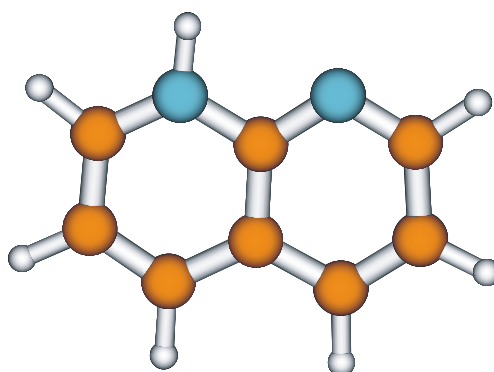
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H 1.5111178663 -1.1921778556 8.1254802914
H 0.4859061705 -2.6233766314 7.9041003476
N 5.4020828862 0.833811683 2.7268947668
N 5.1721674191 -0.3729389481 0.3912651052
N 4.5718709777 2.1947246455 0.4237361942
C 6.8527676252 0.6282973546 2.6848445107
C 5.0100386828 1.8230122005 3.7396048177
C 5.1311895186 -0.372946304 -1.0741262739

C 5.2091438848 -1.7258469008 0.9611538649
C 5.8859395847 2.6654938047 -0.0252743537
C 3.5806976451 3.2664065023 0.5637413724
H 5.3752496273 1.4904489484 4.7159541029
H 5.4411192642 2.8093892474 3.5169127908
H 3.923690516 1.9036941458 3.8020585227
H 7.1716275767 0.2040367011 3.6424075927
H 7.1232826862 -0.0639181132 1.8877125269
H 7.3890148086 1.574491259 2.5323458278
H 4.2928200325 -2.2761541422 0.7158141199
H 6.0695261978 -2.260348942 0.5483013447
H 5.3158194141 -1.6818923066 2.0469406371
H 4.3082622138 -1.0007095893 -1.4351960305
H 4.9962969273 0.6378057259 -1.4580122312
H 6.0769148766 -0.7722846282 -1.4529908545
H 6.2944169556 3.4098329962 0.6703090531
H 6.5899951556 1.8337580382 -0.1047694203
H 5.7869326412 3.1286605352 -1.0118213722
H 3.9383798411 4.0386351333 1.25589032
H 3.4151535616 3.7213093163 -0.4173224134
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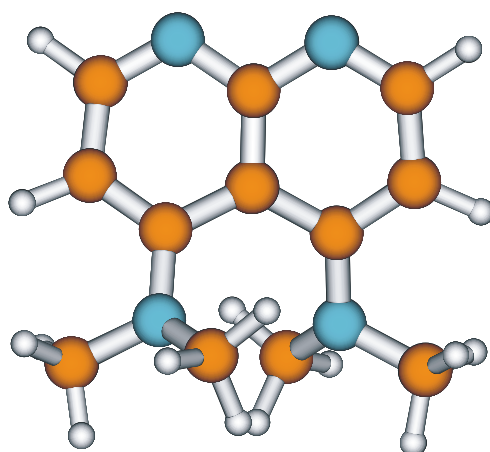
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 C 2.3535914681 0. 1.2521620479
 N 2.3516879884 0. -0.0585140586
 C 1.1467357543 0. -0.691436827
 H -0.9619990057 0. 2.0088008827
 H 1.2768431643 0. 3.1417027067
 H 3.3317063091 0. 1.7298878715
 N 1.1905752467 0. -2.0514001167
 C 0.0512224329 0. -2.7000017958
 C -1.2281844077 0. -2.0831888618
 C -1.2909114634 0. -0.715745183
 H 0.1187054738 0. -3.7864385687
 H -2.123531697 0. -2.6950664689
 H -2.2421857068 0. -0.1892848015



4a protonated at pyridine nitrogen

C -0.0927850273 0. 0.0288958858
 C -0.0301574759 0. 1.4487230013
 C 1.2002047702 0. 2.0507927043
 C 2.3697277258 0. 1.2418889853
 N 2.353071056 0. -0.0759639056
 C 1.145420778 0. -0.6512699826
 H -0.9485355089 0. 2.028066002
 H 1.3003745304 0. 3.1299483777
 H 3.3515996231 0. 1.7073544792
 N 1.1305550255 0. -2.0229902029
 C 0.0140324089 0. -2.7465407967
 C -1.2317447896 0. -2.113725386
 C -1.2827102935 0. -0.732833798
 H 0.1296141724 0. -3.8245736287
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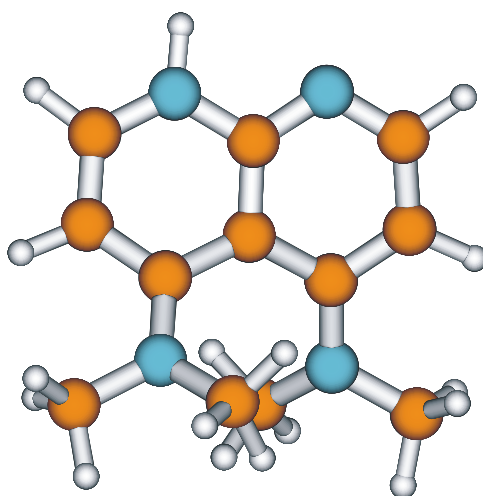
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C  2.356276942 -0.1271669647  1.4228918197
C  2.5197398452  0.2223774637  0.0917497104
C  1.3614889084  0.1163457539 -0.7614348859
H  0.9465995655 -0.7067222216  2.9482373747
H  3.1821500825 -0.0974421735  2.1222958919
C  1.3727193044  0.1477288553 -2.2034777445
C  0.1555841946  0.3348552538 -2.8394039003
C -1.0267233573  0.3465079845 -2.0733883439
N -1.0875475033  0.1160912053 -0.7846266707
H  0.0826845976  0.393496483 -3.9180018574
H -1.9788790705  0.4979077434 -2.580062504
N  2.5570501016  0.0007692446 -2.9170071878
N  3.7439814969  0.6527805475 -0.4075723158
C  3.4098358663 -1.1459782955 -2.623814404
C  2.5512809232  0.3428721924 -4.3241859947
C  3.7911098427  1.9056117368 -1.1537425366

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C 4.9223596297 0.4485775887 0.4091009145
H 3.5874219397 0.3801680949 -4.6723483551
H 2.0096723314 -0.3915725501 -4.9431120199
H 2.1036963263 1.3291232791 -4.4710166258
H 4.4651154007 -0.8524980551 -2.6528826543
H 3.2395067911 -1.9392619337 -3.3671994394
H 4.4790480474 1.8172142364 -2.0019611167
H 4.1356370414 2.7193307955 -0.4979494354
H 5.8048239309 0.6373828793 -0.2087970028
H 4.9646381217 1.1239633523 1.2796652268
H 4.9636589027 -0.5856321103 0.7602501604
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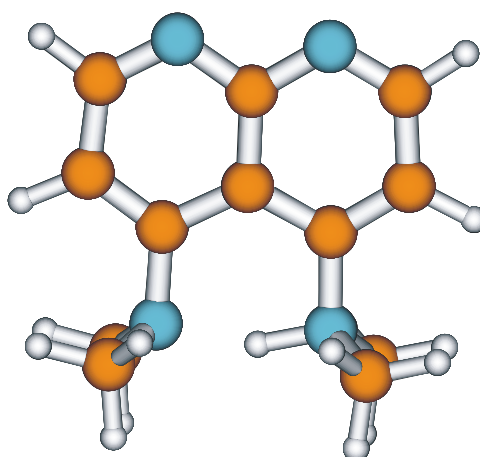
4b protonated at pyridine nitrogen

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C 2.3225424327 -0.3799454077 1.3912389917
C 2.5067525223 0.1469311943 0.1014188576
C 1.3746068641 0.0621602565 -0.7889852102
H 0.8959662903 -1.0967372475 2.8242106435
H 3.1365042186 -0.4254264707 2.1021118475
C 1.393449822 0.1764581328 -2.2314516358
C 0.1726627264 0.5557168405 -2.8651080573
C -1.0021675764 0.4585691449 -2.1690725671
N -1.0268912096 0.0441531858 -0.8921386422
H 0.1279930767 0.7968129005 -3.9169480317
H -1.9615429377 0.6539865405 -2.6339020258
N 2.4809397029 -0.1021842756 -2.9631892918
N 3.6742485307 0.7302091752 -0.2792689308
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C 2.5246412308 0.2412942016 -4.3846987989

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C 4.8596422173 0.5789702484 0.5569277665
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H 1.926206824 -0.4562647336 -4.9823772669
H 2.1717357835 1.2618046525 -4.543117507
H 3.6596787538 -1.7647230407 -3.3406974663
H 3.1957438774 -1.5795628067 -1.6399557194
H 4.2022922246 1.6436889226 -2.129560588
H 4.2558951967 2.6883250143 -0.6925995524
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H 4.8106831256 1.2109791614 1.4531286993
H 4.9844535255 -0.4643136021 0.8537055791
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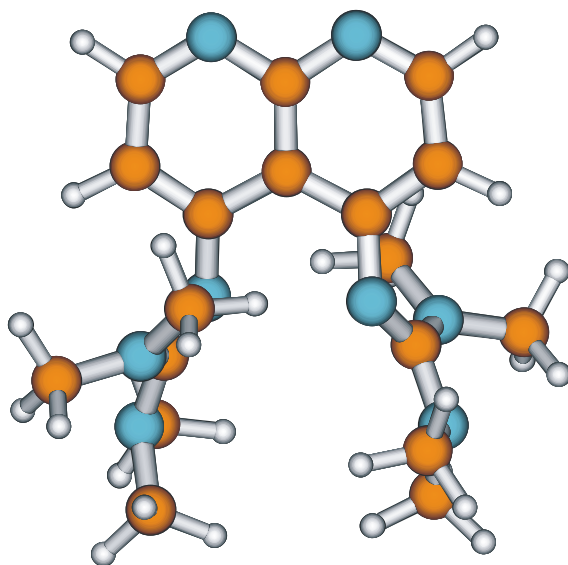
4b protonated at amino nitrogen

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C 2.1293711271 0.7916966984 1.4036573086
C 2.3697387032 0.5216489923 0.0874216714
C 1.3212265256 0.0900501398 -0.7694401079
H 0.5831489601 0.8349470652 2.9258108754
H 2.9101210538 1.1226761352 2.0812961653
C 1.4451459926 -0.2224335585 -2.1567165757
C 0.3311745943 -0.6256018215 -2.8411947935
C -0.9047795759 -0.7181539679 -2.147229543
N -1.0579193655 -0.4408315611 -0.8777851608
H 0.3738938157 -0.8743438671 -3.8970321057
H -1.7943630236 -1.0377606508 -2.6845615831
N 2.7476466771 -0.1010309164 -2.78889084
N 3.7177002386 0.6684565459 -0.4841175888
C 3.2421188405 -1.400458797 -3.2899053699
C 2.7504955214 0.9198842122 -3.8573344174
C 4.2004897219 2.0787234314 -0.4553328818

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C 4.7006315974 -0.2767183705 0.1186263379
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H 2.3705995744 1.8645955739 -3.4621941923
H 2.6322407447 -1.7700302791 -4.122620381
H 3.2178267954 -2.1369702994 -2.4837604501
H 5.1400398503 2.1342008585 -1.0071860306
H 4.358297522 2.393278843 0.577636989
H 5.6360522515 -0.2048057887 -0.4383373989
H 4.8707445558 -0.0143909959 1.1641429193
H 4.2985409343 -1.2883501479 0.0543188489
H 4.2706613295 -1.2755316452 -3.636454324
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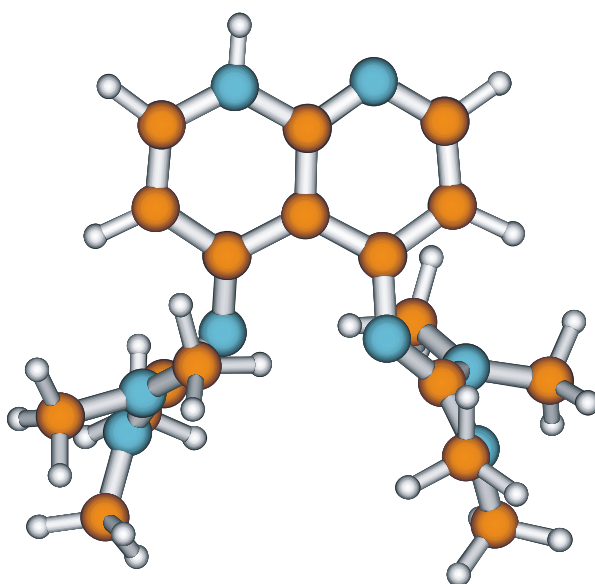


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C	2.2274669413	0.8234313697	1.6289500905
C	2.0787926629	1.3344917758	0.3505388877
C	0.8681754956	1.1267529002	-0.3382926901
C	1.1928292286	-0.6184936651	3.4224716344
C	0.0289388252	-1.2198566385	3.8711347905
C	-1.125130774	-1.1744830759	3.0653075728
N	-1.1908234394	-0.6268866497	1.8732516954
N	2.3930558559	-0.7935265833	4.0961880626
C	2.5600702815	-0.4250906924	5.3189639115
N	1.8518581804	0.5700289872	5.9709981776
N	3.3260850406	1.156399191	2.4082098815
C	4.5337642608	0.8829253641	2.0538247276
N	4.9175944669	-0.1341728485	1.1964191856
N	3.5559645867	-1.0269479949	6.0761448888

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H -2.0395606043 -1.644238632 3.4261517802
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C 4.2357363863 -2.1558877223 5.4648052783
C 1.3586445171 0.3757115506 7.3221499053
C 1.2203062625 1.6426964697 5.2230751879
H 4.8033073091 -2.6794546966 6.2388658194
H 3.5043874546 -2.8337521813 5.0251771234
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H 6.6533849037 -0.7078975556 0.1485774647

H 3.4016866808 -1.2137168272 0.1592487328
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4c protonated at pyridine nitrogen

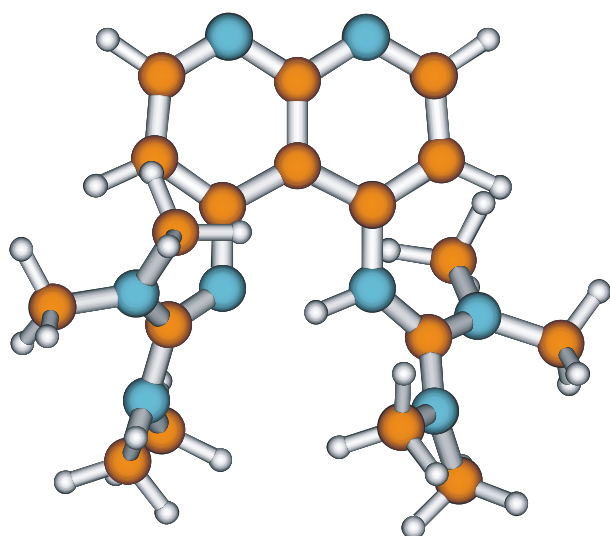
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C 2.2789863164 0.8685626897 0.1802044872
C 1.0834710191 0.744738496 -0.471497798
C 1.1893206978 -0.4587188194 3.5654432078
C -0.0718308751 -0.8050130571 4.0854926134
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N 1.8840900923 0.4996122537 6.1914195416
N 3.4328808189 0.9589127048 2.3037538131
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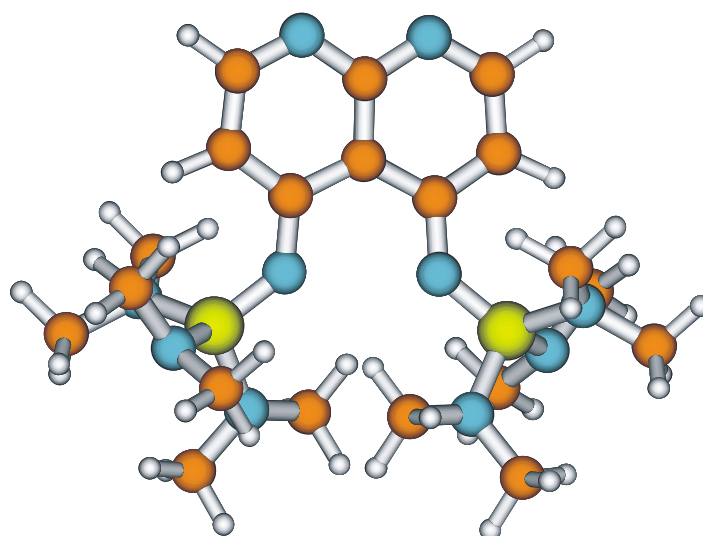


4c protonated at imino nitrogen

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C	1.0303734239	1.0005784873	-0.3508739649
C	1.2217999477	-0.3709988353	3.5880470792
C	0.0308205947	-0.9030623838	4.0497467677
C	-1.0920445517	-0.9391490979	3.1978740099
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N	1.3614739883	0.6961014858	6.2939151743
N	3.6527488142	0.3999037896	2.2128774788
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N	3.3279526941	-0.532403554	6.4372200035

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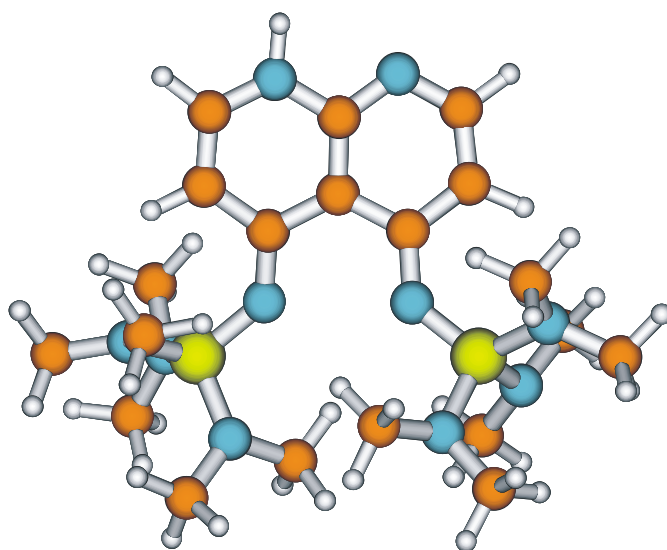


4d

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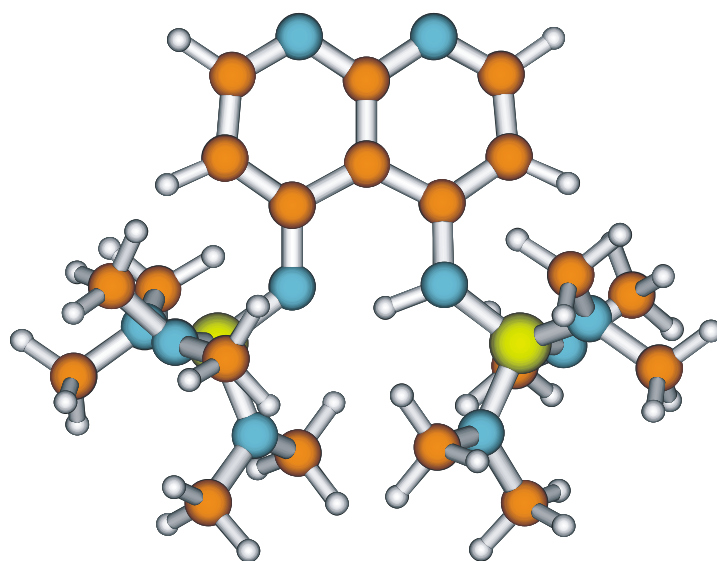


4d protonated at pyridine nitrogen

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4d protonated at imino nitrogen

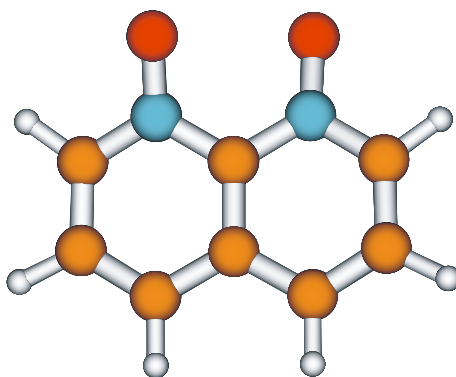
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H -0.8296216672 -0.793138359  4.7500085542
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C 4.3424786332 -1.2260383983 5.1031515482
C -0.1828761529 0.8416746013 6.8976507848
C 1.7052880916 2.2059283991 6.1891627131
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C 0.9712586767 -2.9418612046 5.288413146
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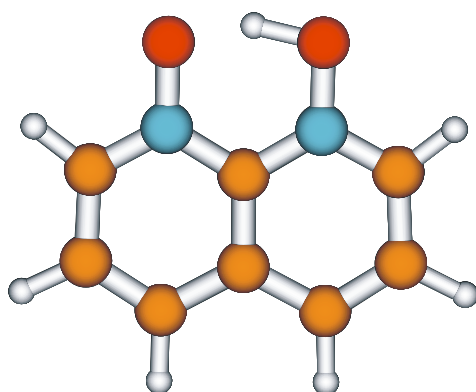


5a

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N  2.4409156705  0.3746226947  1.4690570754
C  2.4300795925  0.3255748092  0.1154530673
C  1.2583252164  0.1759455561  -0.6261066704
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C  -1.1729034026  -0.0417700388  3.5019656804
C  -1.2068586363  -0.0343183585  2.1315949612
O  2.3016580844  -0.0754173683  4.2063650519
O  3.5149272099  0.6452610646  2.0679126329
H  -0.8838616839  -0.0060918471  -0.5463251672
H  1.3375656882  0.1692560837  -1.7073604756
H  3.4115256828  0.4736104381  -0.312860854
H  0.1534972594  -0.0742987864  5.2519970483
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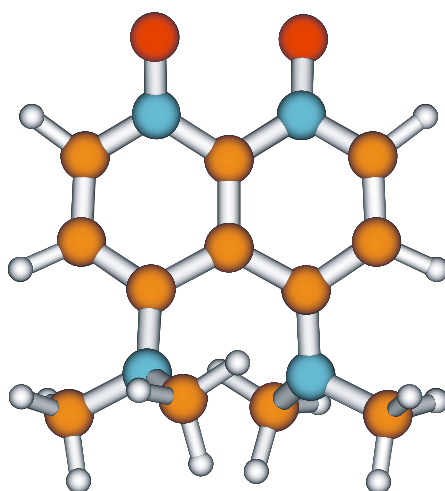


5a protonated at *N*-oxide oxygen

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C 2.396327751 -0.0057588228 1.289496806
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C 1.1538920588 -0.0061714744 -0.700698398
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C -1.2687023703 0.0025278926 -0.7360571428
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H -2.1237260117 0.0008439589 -2.709085477
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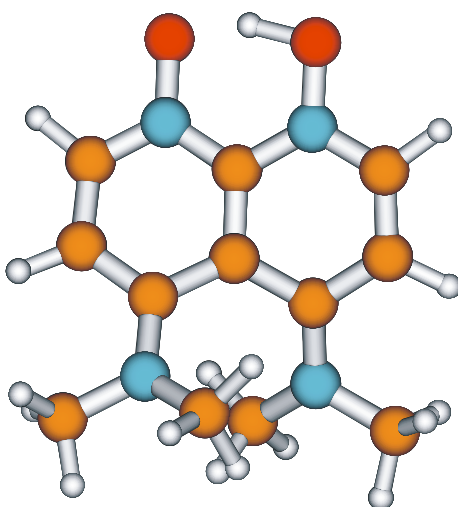
5b

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C 2.5044175417 0.2379542373 0.0895897088
C 1.337308805 0.1089023913 -0.7482905478
H 0.904647002 -0.2910801287 3.0602693057
H 3.185790335 -0.0025652179 2.1169097881
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C 0.1594587936 0.2206562017 -2.847625373
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H -2.0107963235 0.0544666136 -2.6561138824
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H 4.4039208946 -0.994653603 -2.9000631134
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H 3.98163274 2.7117982936 -0.2778515439
H 5.8045702474 0.5046034053 -0.2496553533
H 4.9951749266 0.9913563723 1.2529863962
H 4.9136643489 -0.7044858858 0.6921084449
H 3.2509401364 -1.53605653 -1.6726101333
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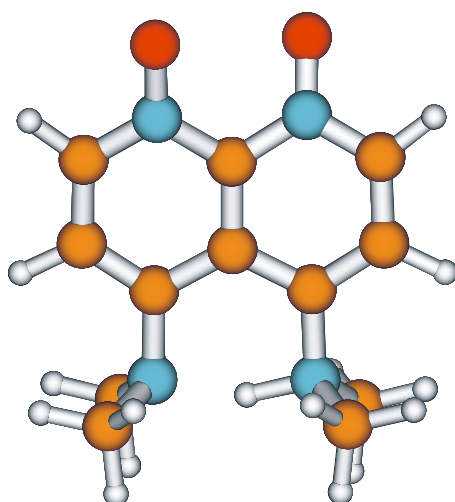


5b protonated at *N*-oxide oxygen

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C 2.4804468201 0.1788062515 0.1078912869
C 1.3395985504 0.0789682166 -0.773905047
H 0.862156068 -1.02571114 2.8780383927
H 3.1401838347 -0.3885989196 2.1062471154
C 1.3716327956 0.1560331865 -2.2202616251
C 0.1592182537 0.4915729827 -2.8627977141
C -1.0260213073 0.4531386084 -2.1641406469
N -1.0754267347 0.0998473697 -0.8762923098
H 0.1095903183 0.67446844 -3.9265312778
H -1.9972086391 0.6385570554 -2.6082857497
N 2.4893594759 -0.1008149092 -2.9273277737
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H 1.9757076055 -0.4740482007 -4.9556740076
H 2.1668784766 1.2500658964 -4.5131243879
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H 4.9650514547 -0.4556904311 0.8205373608
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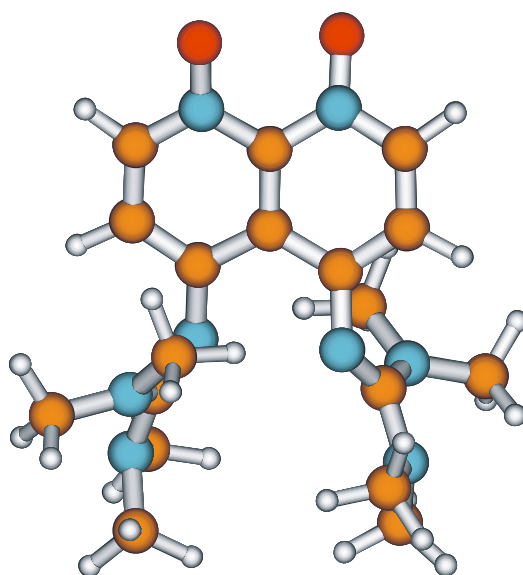
5b protonated at amino nitrogen

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5c

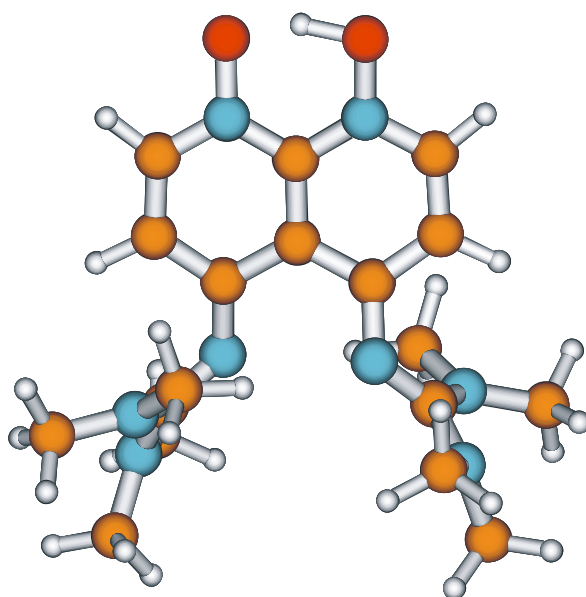
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5c protonated at *N*-oxide oxygen

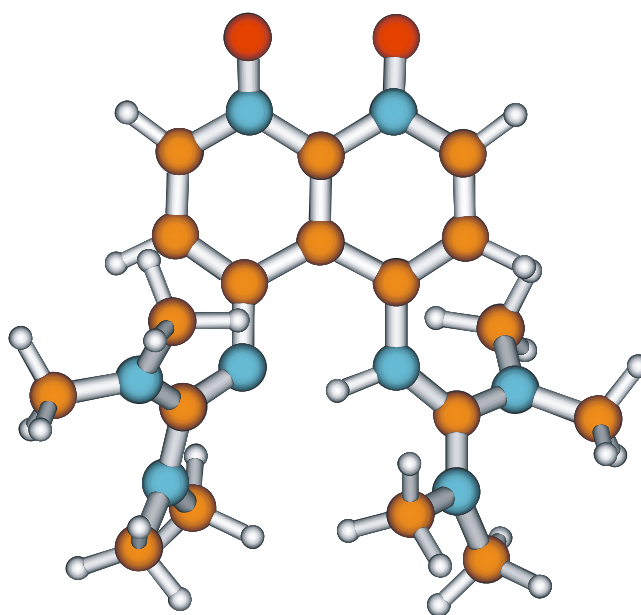
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5c protonated at imino nitrogen

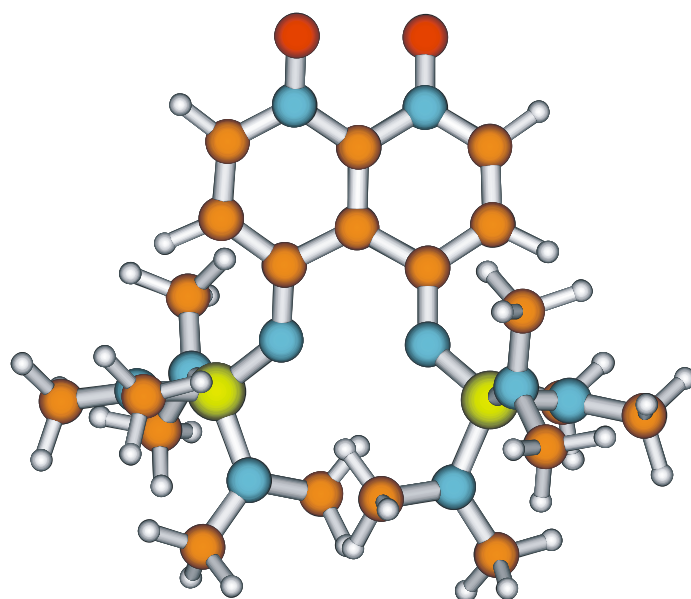
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5d

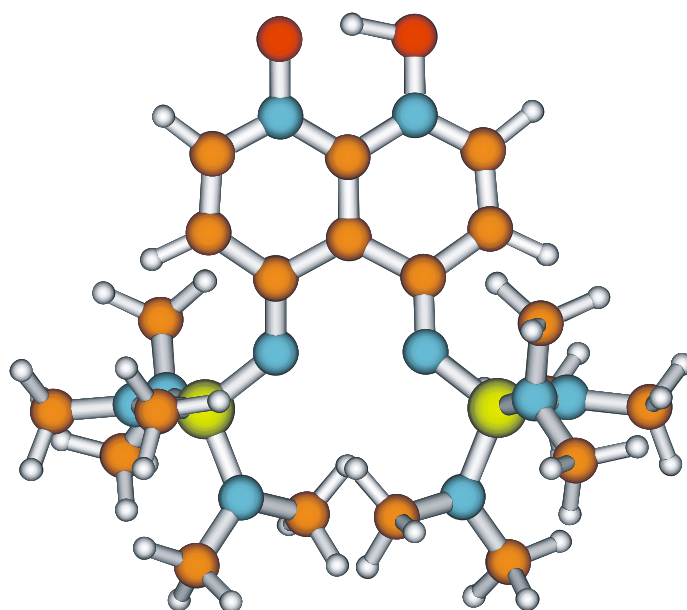
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5d protonated at *N*-oxide oxygen

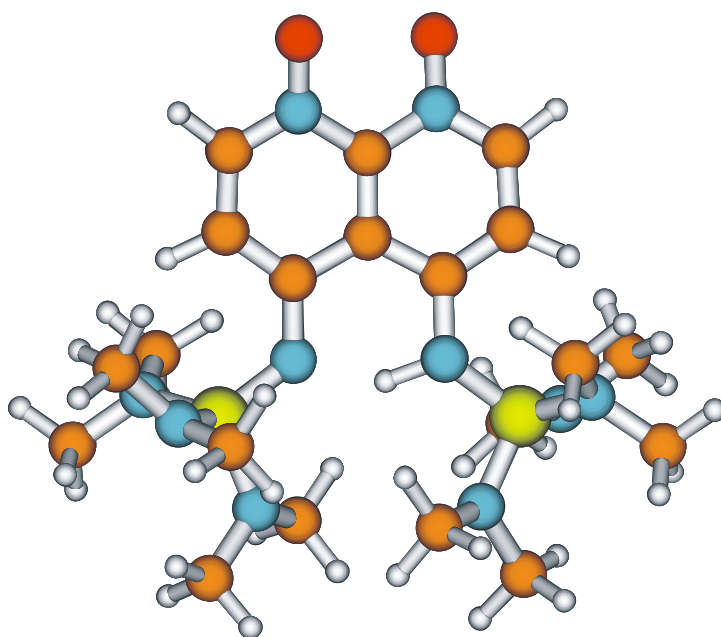
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5d protonated at imino nitrogen

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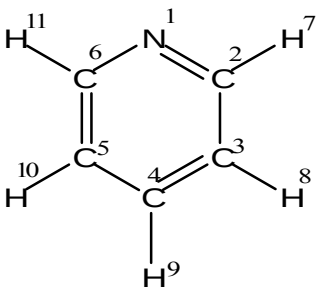
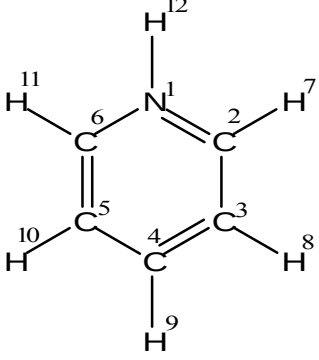
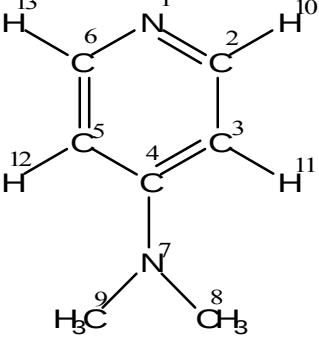
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H -0.7919236144 -0.9040445874 4.7136517566

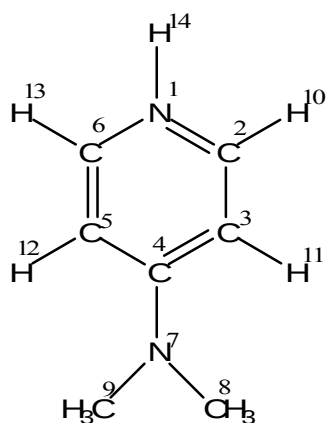
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N 1.1499138491 -1.7436375985 6.130006708
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C 4.3566584281 -1.2332016617 5.1213668019
C -0.1918384975 0.8700629896 6.8319894168
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C 1.2360346099 -2.0257716674 7.5644943844
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H 5.3812637456 -0.8466485918 5.0762626747
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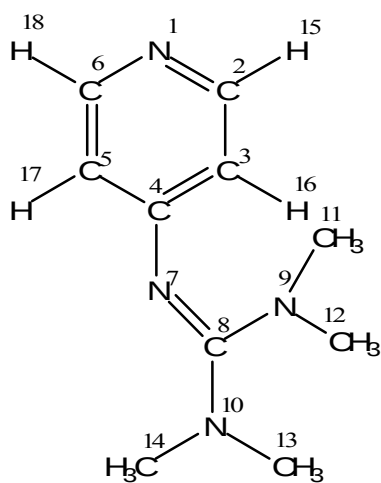
Table S1. NBO charges calculated using M06-2X/6-31+G(d,p) method.

system	atom	charge
 1a	N1	-0.46
	C2	0.00
	C3	-0.29
	C4	-0.22
	C5	-0.29
	C6	0.00
	H7	0.24
	H8	0.26
	H9	0.26
	H10	0.26
	H11	0.24
 1a protonated at pyridine nitrogen	N1	-0.49
	C2	0.06
	C3	-0.26
	C4	-0.13
	C5	-0.26
	C6	0.06
	H7	0.30
	H8	0.31
	H9	0.30
	H10	0.31
	H11	0.30
	H12	0.50
 1b	N1	-0.50
	C2	0.02
	C3	-0.35
	C4	0.22
	C5	-0.35
	C6	0.02
	N7	-0.51
	C8	-0.48
	C9	-0.48
	H10	0.24
	H11	0.25
	H12	0.25
	H13	0.24



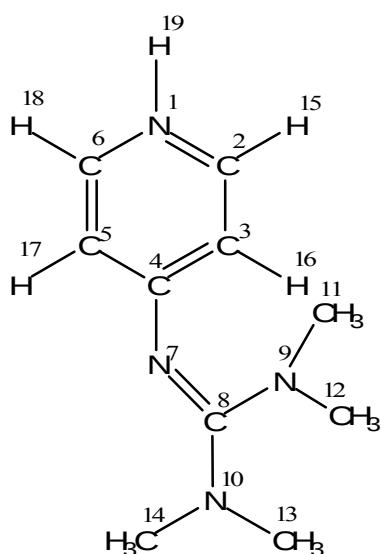
1b protonated at pyridine nitrogen

N1	-0.55
C2	0.06
C3	-0.33
C4	0.29
C5	-0.33
C6	0.06
N7	-0.42
C8	-0.50
C9	-0.50
H10	0.29
H11	0.29
H12	0.29
H13	0.29
H14	0.49



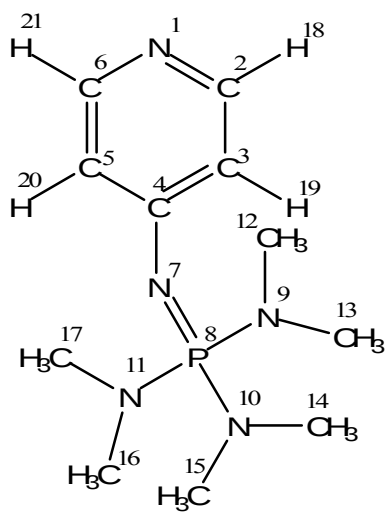
1c

N1	-0.49
C2	0.01
C3	-0.34
C4	0.18
C5	-0.31
C6	0.01
N7	-0.60
C8	0.68
N9	-0.55
N10	-0.53
C11	-0.48
C12	-0.49
C13	-0.49
C14	-0.48
H15	0.23
H16	0.25
H17	0.26
H18	0.23



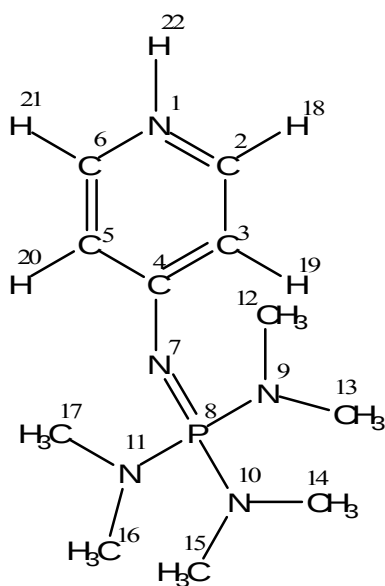
1c protonated at pyridine nitrogen

N1	-0.56
C2	0.04
C3	-0.34
C4	0.26
C5	-0.30
C6	0.03
N7	-0.60
C8	0.72
N9	-0.51
N10	-0.47
C11	-0.49
C12	-0.50
C13	-0.50
C14	-0.49
H15	0.28
H16	0.27
H17	0.29
H18	0.28
H19	0.48



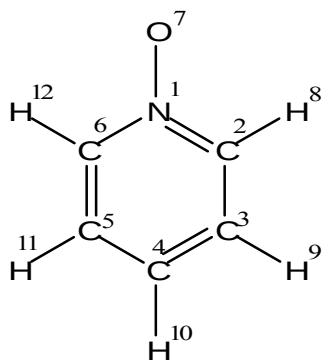
1d

N1	-0.50
C2	0.01
C3	-0.37
C4	0.20
C5	-0.31
C6	0.01
N7	-1.12
P8	2.44
N9	-0.91
N10	-0.93
N11	-0.91
C12	-0.49
C13	-0.49
C14	-0.49
C15	-0.49
C16	-0.49
C17	-0.48
H18	0.23
H19	0.24
H20	0.25
H21	0.23



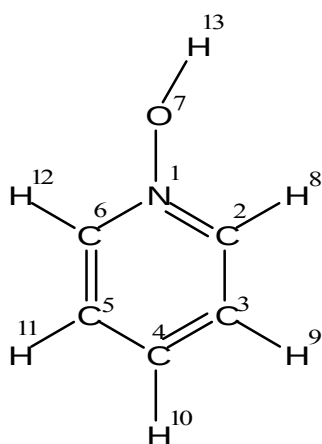
1d protonated at pyridine nitrogen

N1	-0.56
C2	0.04
C3	-0.35
C4	0.28
C5	-0.30
C6	0.03
N7	-1.01
P8	2.48
N9	-0.93
N10	-0.92
N11	-0.91
C12	-0.48
C13	-0.49
C14	-0.48
C15	-0.49
C16	-0.48
C17	-0.49
H18	0.27
H19	0.28
H20	0.29
H21	0.28
H22	0.48



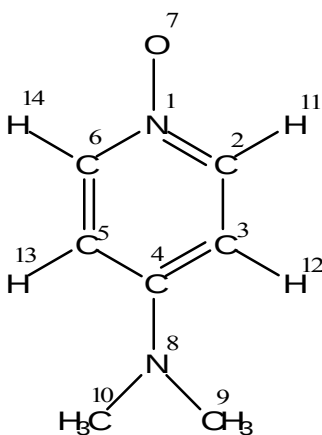
2a

N1	0.08
C2	-0.04
C3	-0.26
C4	-0.26
C5	-0.26
C6	-0.04
O7	-0.56
H8	0.27
H9	0.27
H10	0.26
H11	0.27
H12	0.27



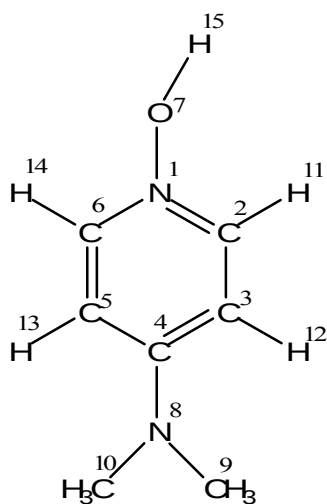
2a protonated at N-oxide oxygen

N1	-0.02
C2	0.06
C3	-0.25
C4	-0.13
C5	-0.25
C6	0.06
O7	-0.54
H8	0.31
H9	0.31
H10	0.30
H11	0.31
H12	0.31
H13	0.55



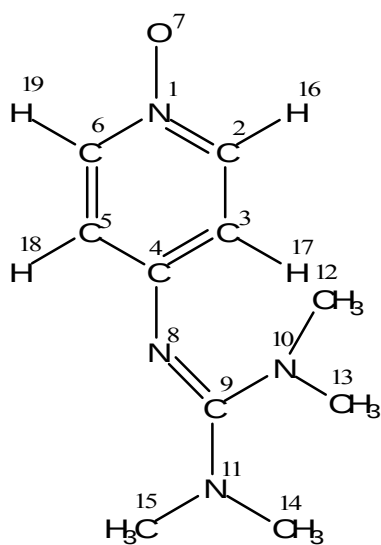
2b

N1	0.04
C2	-0.01
C3	-0.32
C4	0.19
C5	-0.32
C6	-0.01
O7	-0.61
N8	-0.51
C9	-0.49
C10	-0.49
H11	0.27
H12	0.26
H13	0.26
H14	0.27



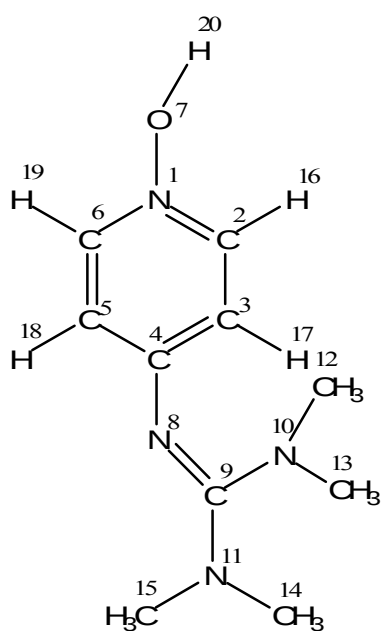
2b protonated at *N*-oxide oxygen

N1	-0.08
C2	0.05
C3	-0.32
C4	0.28
C5	-0.32
C6	0.05
O7	-0.55
N8	-0.42
C9	-0.50
C10	-0.50
H11	0.30
H12	0.29
H13	0.29
H14	0.30
H15	0.54



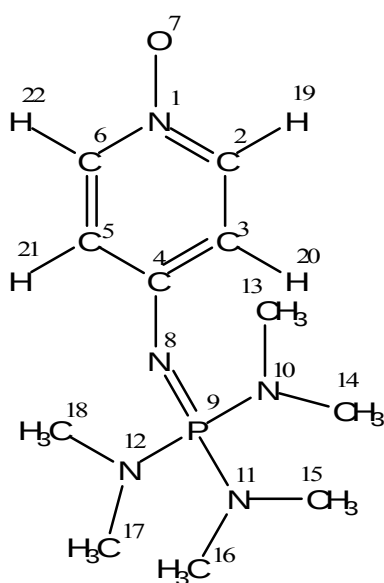
2c

N1	0.05
C2	-0.02
C3	-0.30
C4	0.14
C5	-0.28
C6	-0.02
O7	-0.60
N8	-0.60
C9	0.68
N10	-0.56
N11	-0.53
C12	-0.48
C13	-0.49
C14	-0.49
C15	-0.48
H16	0.27
H17	0.26
H18	0.27
H19	0.27



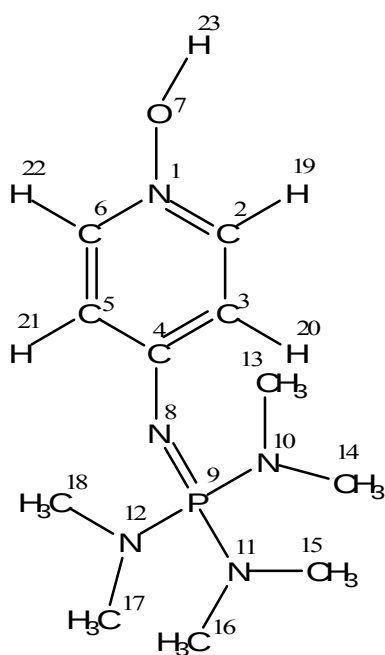
2c protonated at *N*-oxide oxygen

N1	-0.08
C2	0.04
C3	-0.34
C4	0.26
C5	-0.29
C6	0.03
O7	-0.55
N8	-0.60
C9	0.72
N10	-0.51
N11	-0.48
C12	-0.49
C13	-0.50
C14	-0.50
C15	-0.49
H16	0.29
H17	0.28
H18	0.30
H19	0.29
H20	0.53



2d

N1	0.04
C2	-0.02
C3	-0.34
C4	0.17
C5	-0.29
C6	-0.02
O7	-0.63
N8	-1.11
P9	2.46
N10	-0.93
N11	-0.92
N12	-0.91
C13	-0.49
C14	-0.47
C15	-0.48
C16	-0.47
C17	-0.47
C18	-0.48
H19	0.26
H20	0.25
H21	0.27
H22	0.27



2d protonated at *N*-oxide oxygen

N1	-0.09
C2	0.04
C3	-0.35
C4	0.27
C5	-0.29
C6	0.02
O7	-0.55
N8	-1.01
P9	2.48
N10	-0.93
N11	-0.92
N12	-0.91
C13	-0.49
C14	-0.48
C15	-0.48
C16	-0.48
C17	-0.48
C18	-0.49
H19	0.29
H20	0.28
H21	0.29
H22	0.29