Supporting Information

Electronic structural trends in divalent carbon compounds

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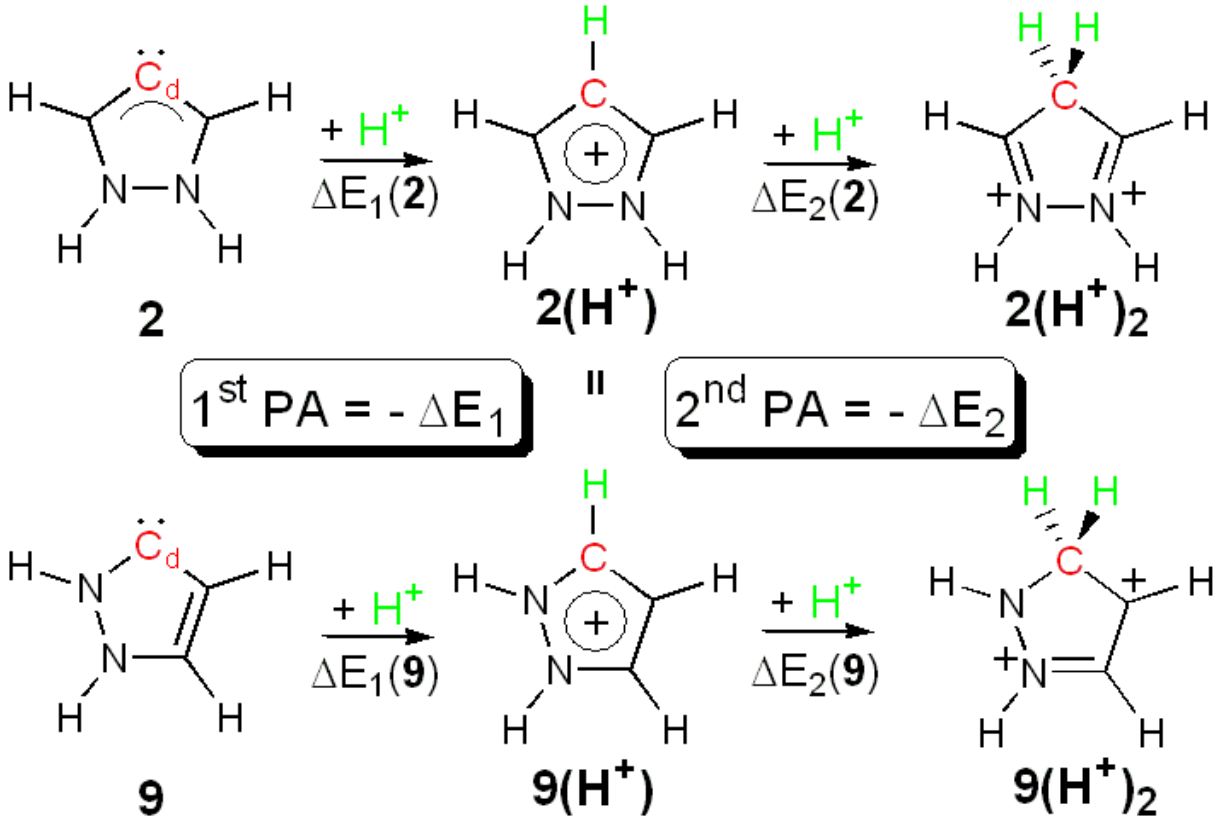

Scheme S1. Calculation of the 1st and 2nd PA illustrated for **2** and **9**.

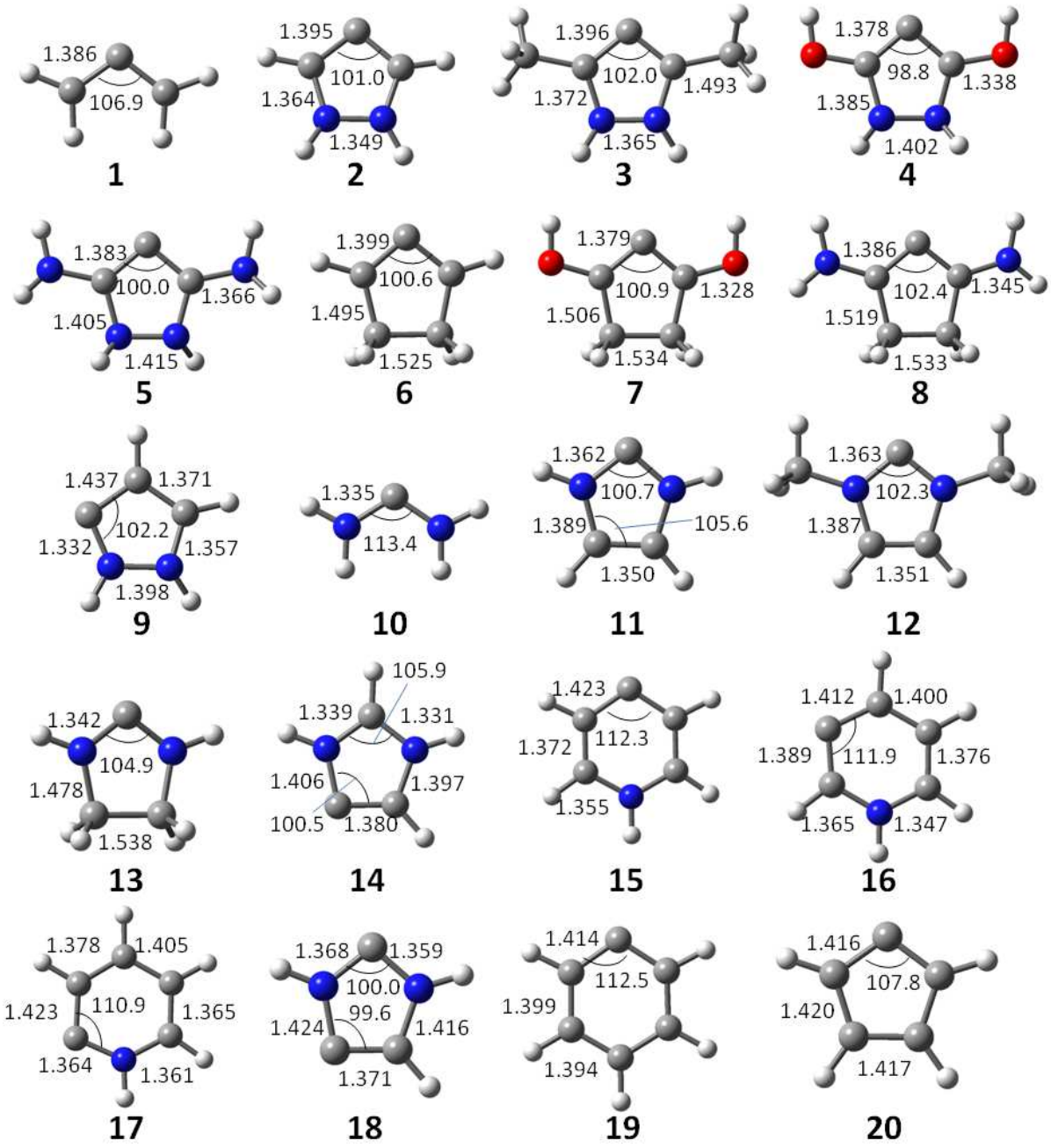

Figure S1. Optimized geometries (bond lengths [Å] and angles [°]) at the B3LYP/aug-cc-pVTZ level of **1**-**20**. All structures are minima on the PES except for **1** and **6**, which are planar ("eclipsed") transition states connecting "staggered" **1'** with itself and "staggered" **6'** with itself, respectively (see computational methods for details).

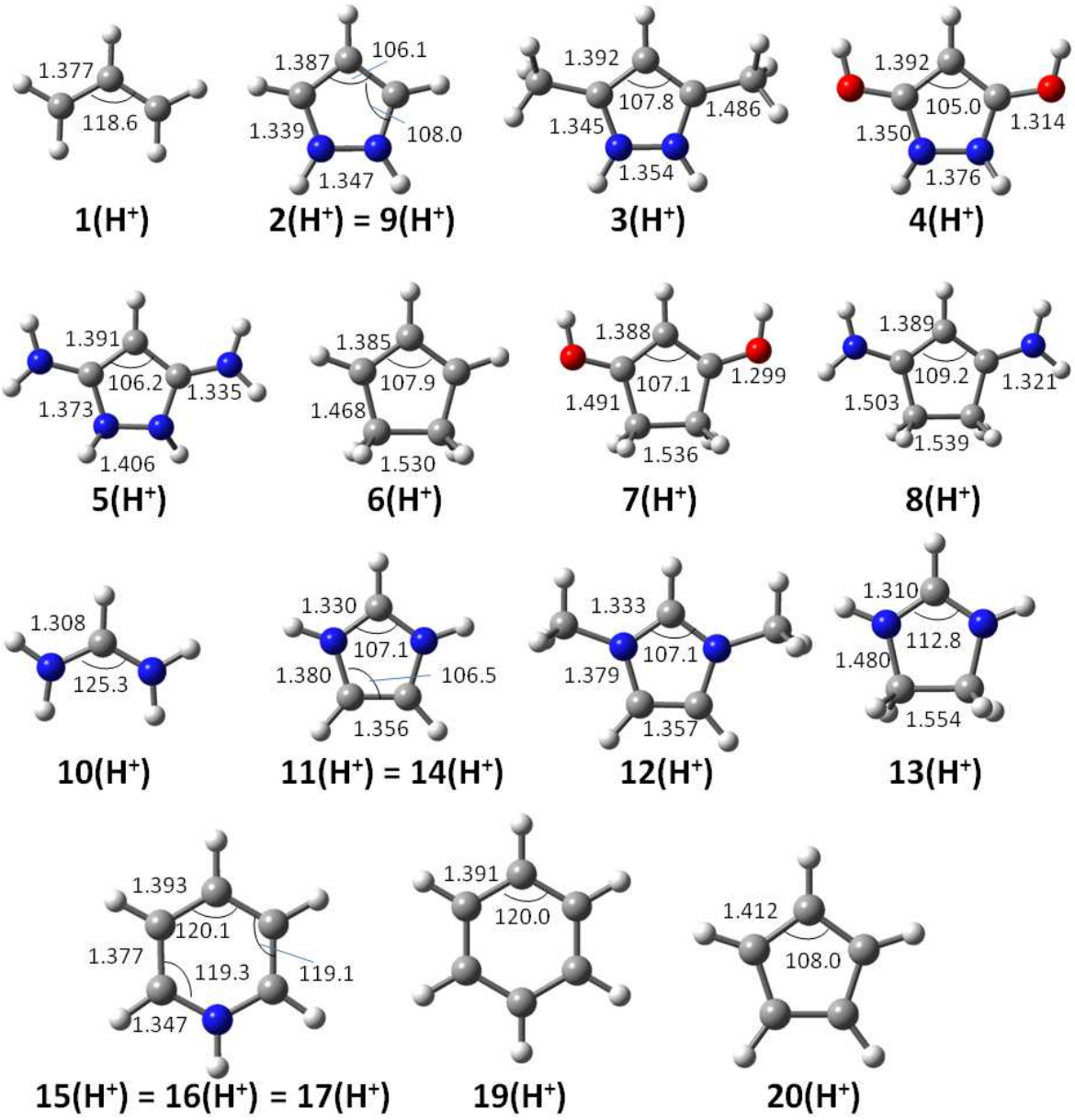

Figure S2. Optimized geometries (bond lengths [Å] and angles [°]) at the B3LYP/aug-cc-pVTZ level of **1(H$^+$)**-**20(H$^+$)**. All structures are minima on the PES.

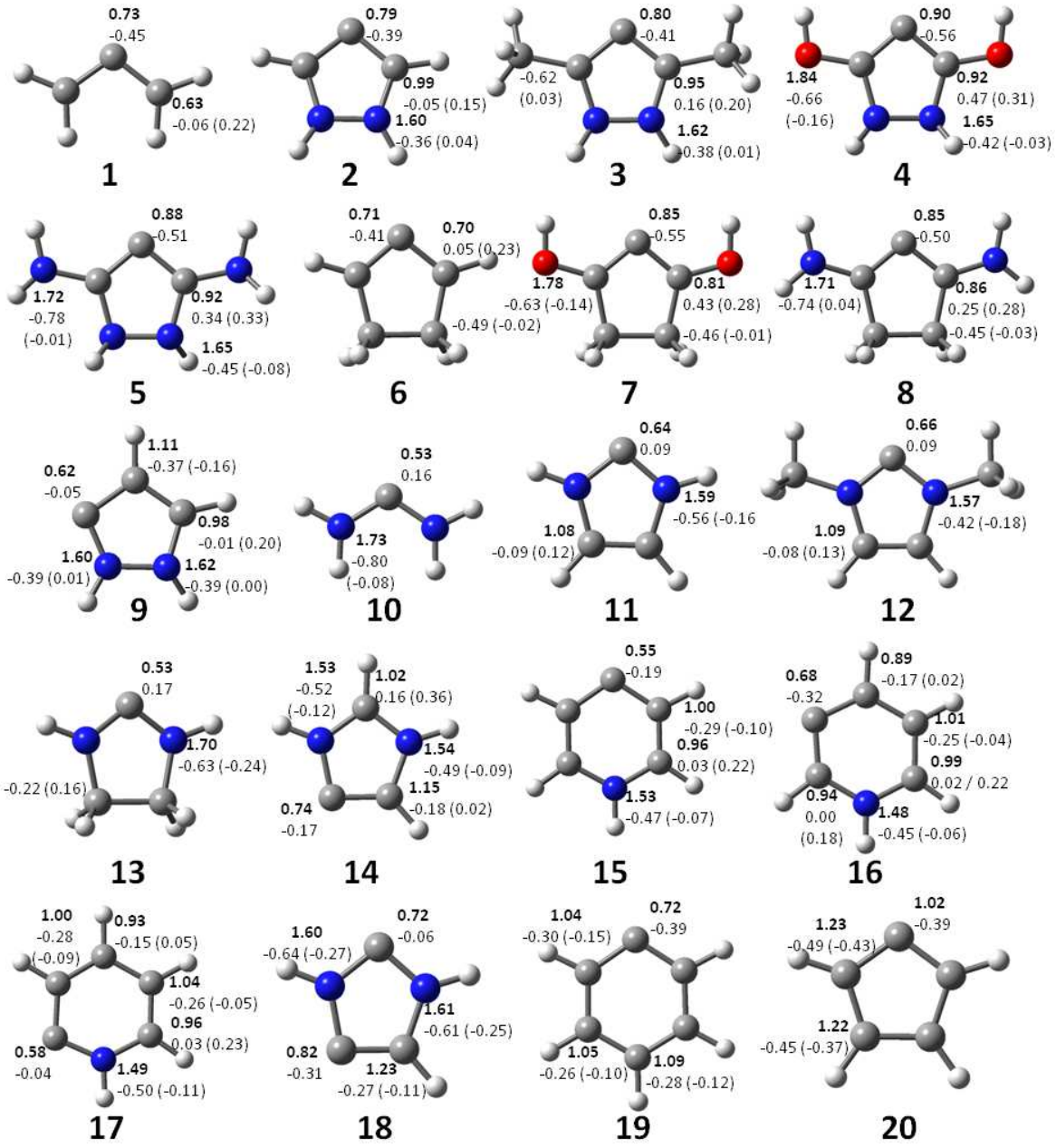

Figure S3. NPA calculated (B3LYP/aug-cc-pVTZ) π-population (bold), atomic charges, and charges with hydrogens or exocyclic substituents summed into heavy atoms (in parentheses) of **1**-**20**.

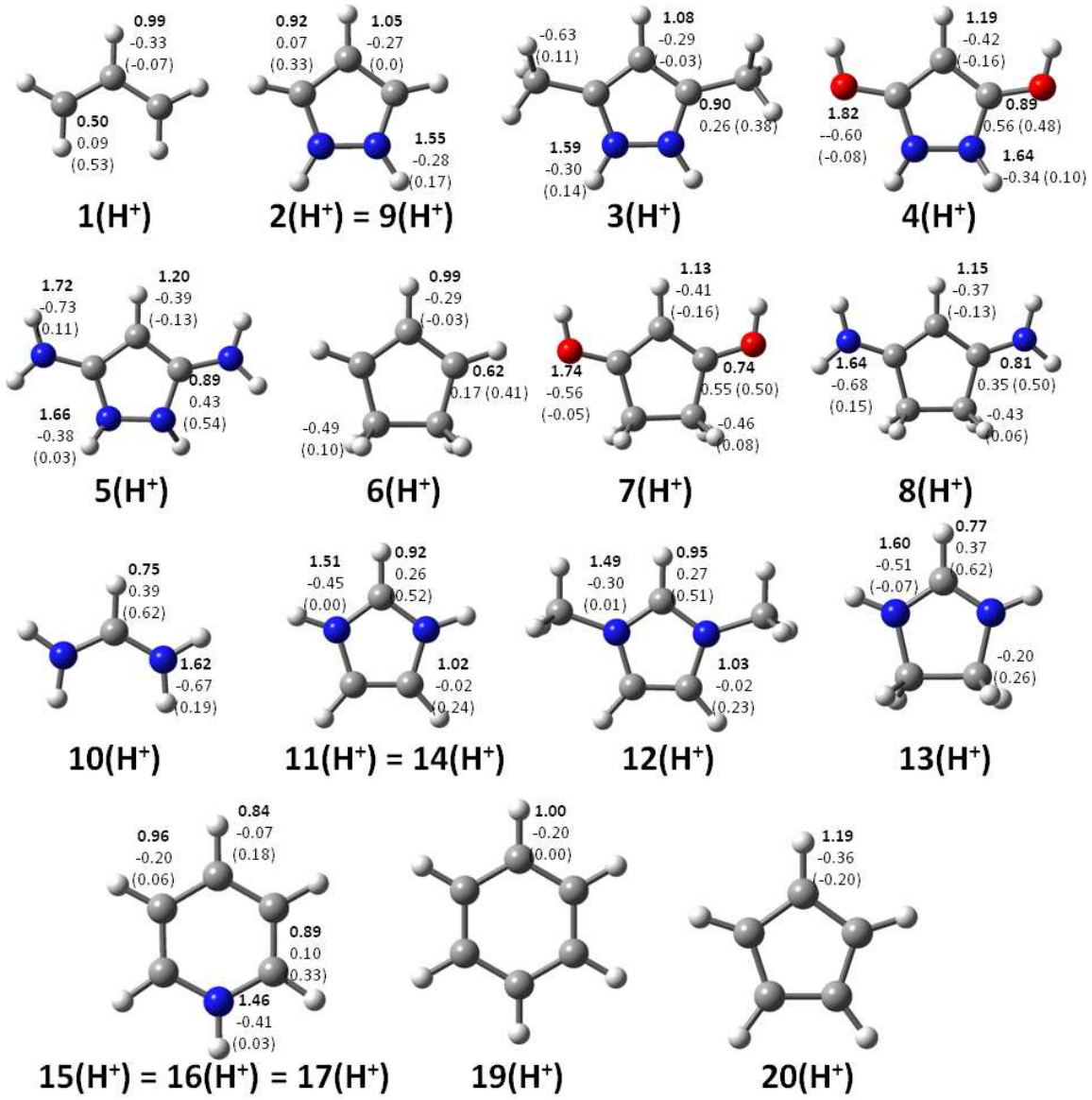

Figure S4. NPA calculated (B3LYP/aug-cc-pVTZ) π-population (bold), atomic charges, and charges with hydrogens or exocyclic substituents summed into heavy atoms (in parentheses) of **1(H$^+$)**-**20(H$^+$)**.

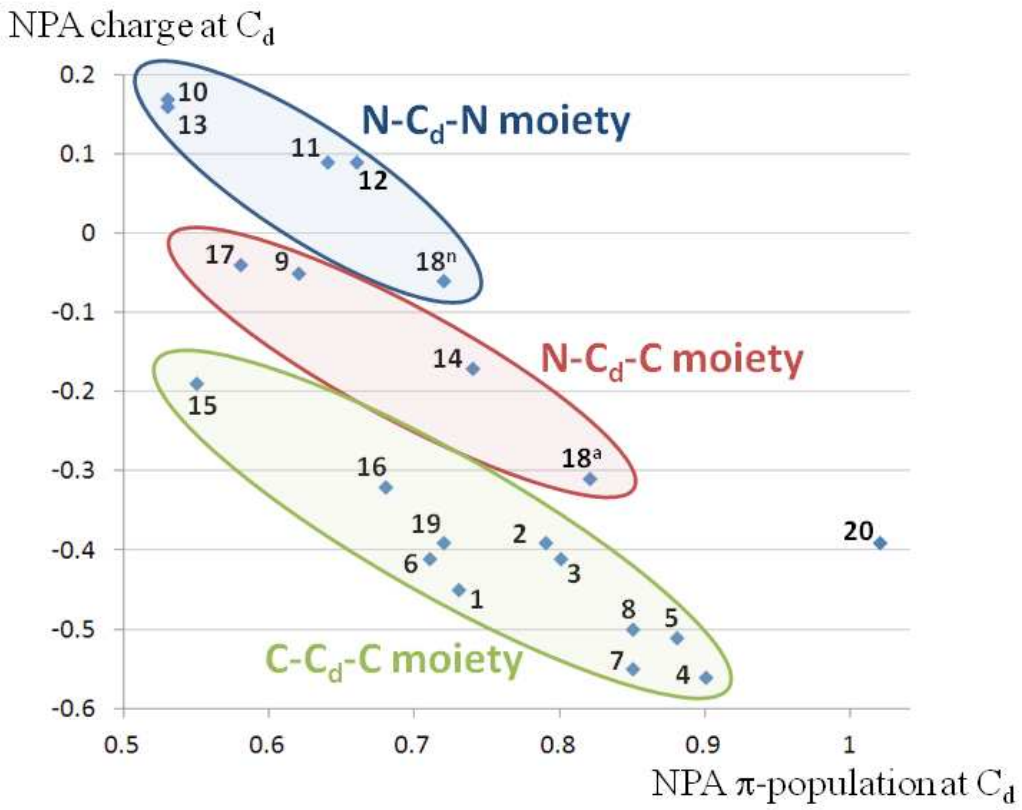

Figure S5. Plot of calculated B3LYP/aug-cc-pVTZ NPA π-population at C_d versus the NPA charge at C_d for **1**-**20**.

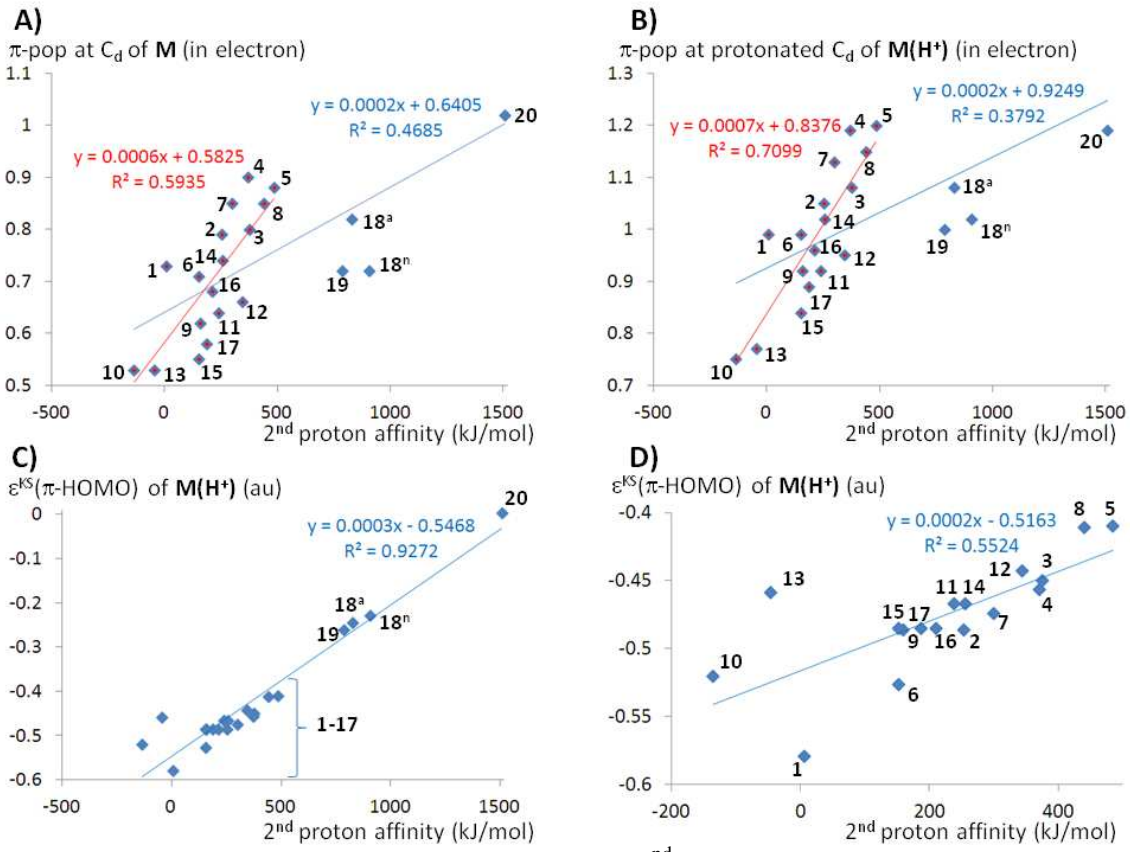

Figure S6. Plots of calculated B3LYP/aug-cc-pVTZ 2nd proton affinities versus A) the π-population at C_d in **1**-**20** (**1**-**17** in red); B) the π-population at the corresponding carbon center after protonation in **1**-**20** (**1**-**17** in red); C) the Kohn-Sham eigenvalues of the π-HOMO (which is the HOMO of $L(H^+)$, except for $\mathbf{18^a(H^+)}$ and $\mathbf{18^n(H^+)}$, where the π-HOMO is the HOMO-1) for compounds $\mathbf{1(H^+)}$-$\mathbf{20(H^+)}$ and; D) for compounds $\mathbf{1(H^+)}$-$\mathbf{17(H^+)}$.

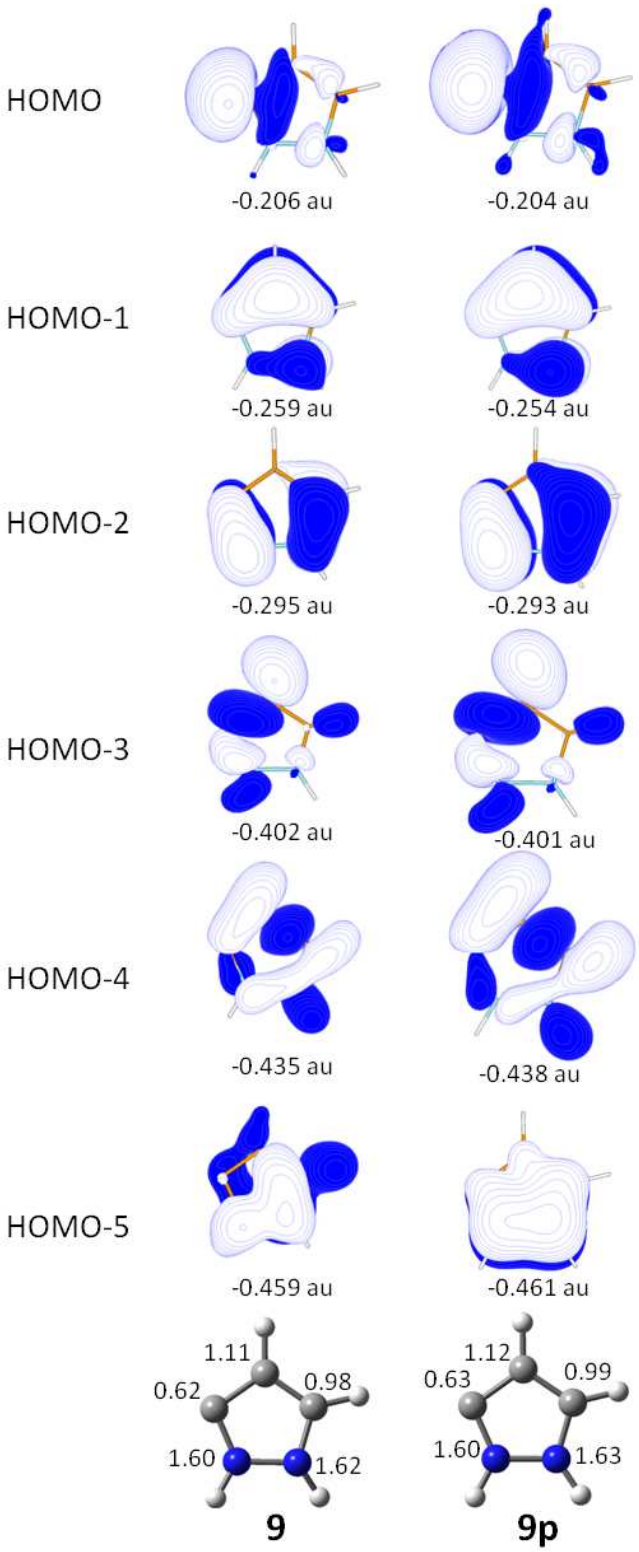

Figure S7. π-electron population from NPA in **9** and its planar constrained geometry **9p** (bottom) and their Kohn-Sham MOs (top) computed at the B3LYP/aug-cc-pVTZ level.

Table S1. Computed electronic and chemical properties of compounds **1**-**20** from absolute electronic energies.

	1^{st} PA (kJ/mol)	2^{nd} PA (kJ/mol)	$\Delta E^{vert}_{S\rightarrow T}$ (kJ/mol)	NPA π-spin-pop[(a)] (electron)	NPA π-pop [(b)] (electron)	ε^{KS}(σ-LP) (au)
1	1125	6	-20	-0.10	0.73	-0.19645
2	1203	254	267	-0.04	0.79	-0.1797
3	1237	375	257	-0.05	0.80	-0.17336
4	1140	371	348	-0.06	0.90	-0.21156
5	1218	485	308	-0.06	0.88	-0.18363
6	1179	153	45	-0.09	0.71	-0.18425
7	1131	300	253	-0.08	0.85	-0.20904
8	1238	440	253	-0.07	0.85	-0.1692
9	1135	160	307	0.45	0.62	-0.20605
10	1084	-135	355	0.72	0.53	-0.21157
11	1089	239	411	0.67	0.64	-0.22266
12	1125	344	409	0.64	0.66	-0.21599
13	1100	-46	376	0.71	0.53	-0.21217
14	1168	256	355	0.14	0.74	-0.19337
15	1218	153	119	0.49	0.55	-0.16679
16	1212	211	154	0.02	0.68	-0.17068
17	1151	188	215	0.42	0.58	-0.19605
18^{n}	1567	907	254 [(c)]	-	0.72	-0.05176
18^{a}	1646	828	254 [(c)]	-	0.82	-0.00775
19	1713	788	174	0.07	0.72	0.01878
20	2164	1509	-41 [(c)]	-	1.02	0.14322

[(a)] π-spin density population at C_d from NPA analysis based on DFT calculations for the triplet state. [(b)] π-population at C_d from NPA analysis based on DFT calculations for the singlet state. [(c)] These structures show no π-spin density.

Table S2. Computed PA of compounds **1**-**20** including zero-point and thermal corrections without scaling factor.

	1st PA[a] (kJ/mol)	2nd PA[a] (kJ/mol)	1st PA[b] (kJ/mol)	2nd PA[b] (kJ/mol)
1	1099	-8	1097	-10
2	1163	229	1164	228
3	1199	349	1199	350
4	1108	342	1107	342
5	1184	453	1183	453
6	1139	141	1139	139
7	1097	278	1097	276
8	1198	411	1200	410
9	1097	137	1097	137
10	1044	-146	1044	-146
11	1053	211	1053	211
12	1088	316	1088	316
13	1062	-52	1062	-53
14	1131	230	1131	230
15	1179	136	1179	135
16	1172	191	1173	189
17	1113	166	1114	165
18[n]	1532	825	1532	825
18[a]	1610	799	1610	798
19	1673	762	1673	760
20	2126	1473	2126	1473
R^2(PA)[c]	0.9998	0.9998	0.9999	0.9998
$R^2(\varepsilon(\sigma\text{-LP}))$[d]	0.9914		0.9915	
$R^2(\varepsilon(\pi\text{-MO}^{Cd\neq0}))$[e]		0.9517		0.9512

[(a)] PA including zero-point energy correction. [(b)] PA including thermal corrections at 298.15 K. [(c)] Correlation coefficient for the comparison with PA data from electronic energies. [(d)] Correlation coefficient for the comparison with ε(σ-LP) (Figure 2). [(e)] Correlation coefficient for the comparison with $\varepsilon(\pi\text{-MO}^{Cd\neq0})$ (Figure 6).

Table S3. Absolute electronic energies of all compounds.

L	E (u.a) of **L**	E (u.a.) of **$L(H^+)$**	E (u.a.) of **$L(H^+)_2$**	E (u.a) of **$L_{triplet}$**
1	-116.585779	-117.014122	-117.016374	-116.593494
1'	-116.707909	-	-	-
1[a]	-116.583935	-117.006485	-	-
2	-226.184494	-226.642733	-226.739363	-226.082859
3	-304.856863	-305.328112	-305.470988	-304.758843
4	-376.724229	-377.158542	-377.299966	-376.591671
5	-336.973527	-337.437256	-337.622007	-336.856292
6	-194.059886	-194.509040	-194.567248	-194.042915
6'	-194.065486	-	-	-
7	-344.642147	-345.073053	-345.187176	-344.545924
8	-304.897078	-305.368678	-305.536397	-304.790097
9	-226.210387	-226.642733	-226.703494	-226.093471
9p	-226.210164	-	-	-
10	-150.037649	-150.450408	-150.398858	-149.902515
11	-226.263944	-226.678649	-226.769772	-226.107339
12	-304.910636	-305.339146	-305.470008	-304.755007
13	-227.468706	-227.887720	-227.870102	-227.325523
14	-226.233771	-226.678649	-226.776247	-226.098564
15	-248.281578	-248.745465	-248.803719	-248.236178
16	-248.284019	-248.745465	-248.825977	-248.225291
17	-248.307134	-248.745465	-248.817018	-248.225063
18[n]	-225.637010	-226.233771	-226.560133	-225.540296
18[a]	-225.637010	-226.263944	-226.579333	-225.540296
19	-231.683122	-232.335571	-232.635702	-231.616738
20	-192.776963	-193.601164	-194.176082	-192.792772

Table S4. Computed zero-point energy correction (a.u.) of **1**-**20** and their protonated analogues.

L	L	$L(H^+)$	$L(H^+)_2$
1	0.05846	0.068144	0.07363
2	0.068807	0.084197	0.09374
3	0.123805	0.138444	0.14837
4	0.080198	0.092455	0.10374
5	0.104565	0.117461	0.1295
6	0.088512	0.10368	0.10808
7	0.102756	0.115755	0.12407
8	0.126265	0.141397	0.15266
9	0.069568	0.084197	0.09279
10	0.057218	0.072289	0.07627
11	0.071355	0.085121	0.09579
12	0.126208	0.140186	0.15072
13	0.093615	0.107968	0.10998
14	0.070842	0.085121	0.09498
15	0.087869	0.102815	0.10912
16	0.087605	0.102815	0.11063
17	0.088562	0.102815	0.111
18^n	0.057563	0.070842	0.08292
18^a	0.057563	0.071355	0.08247
19	0.08514	0.100355	0.11023
20	0.06393	0.078504	0.09226

Table S5. Computed thermal corrections (a.u.) of **1**-**20** and their protonated analogues.

L	L	$L(H^+)$	$L(H^+)_2$
1	0.061649	0.071984	0.078059
2	0.073286	0.088184	0.097838
3	0.131627	0.146309	0.155871
4	0.08593	0.09868	0.109895
5	0.110979	0.124284	0.136374
6	0.092845	0.108174	0.11338
7	0.108827	0.121883	0.130812
8	0.133503	0.148093	0.159484
9	0.073727	0.088184	0.096952
10	0.061104	0.076036	0.080278
11	0.075144	0.088881	0.09972
12	0.133206	0.147348	0.157991
13	0.0984	0.112758	0.115435
14	0.074645	0.088881	0.098972
15	0.092439	0.107174	0.114122
16	0.092312	0.107174	0.11557
17	0.092971	0.107174	0.115967
18^n	0.061358	0.074645	0.086964
18^a	0.061358	0.075144	0.086515
19	0.089584	0.104738	0.115234
20	0.068207	0.082506	0.096397

Table S6. xyz coordinates of all compounds.

Below are given the optimized geometries of the structures discussed in the text at the B3LYP/aug-cc-pVTZ level of theory and the number of imaginary frequencies (NIm).

Structure of **1**. NIm = 1
C 0.000000 0.000000 0.664391
H 0.000000 2.128826 0.232395
H 0.000000 1.055767 -1.262622
H 0.000000 -2.128826 0.232395
H 0.000000 -1.055767 -1.262622
C 0.000000 1.113531 -0.160491
C 0.000000 -1.113531 -0.160491

Structure of **1**($\mathbf{H^+}$). NIm = 0
C 0.000000 0.492397 0.000000
H 0.000001 1.574468 0.000001
C -1.184410 -0.210426 0.000002
H -2.144771 0.293256 -0.000001
H -1.192487 -1.295121 -0.000001
C 1.184409 -0.210427 -0.000003
H 2.144770 0.293257 0.000002
H 1.192487 -1.295122 0.000003

Structure of **1**($\mathbf{H^+}$)$_\mathbf{2}$. NIm = 0
C 0.000000 0.439427 0.000000
C -1.270643 -0.257892 0.000005
H -2.200661 0.320576 0.000000
H -1.357155 -1.349486 -0.000003
C 1.270643 -0.257892 -0.000007
H 2.200661 0.320576 -0.000002
H 1.357155 -1.349485 0.000002
H -0.000003 1.257985 -0.784676
H 0.000003 1.257978 0.784685

Structure of **1'**. NIm = 0
C 0.000000 0.000001 0.000000
C -1.297321 -0.005552 0.084958
H -1.802127 -0.393805 0.961118
H -1.915369 0.377896 -0.717670
C 1.297321 0.005551 -0.084958
H 1.837117 -0.833339 -0.506988
H 1.880378 0.849246 0.263539

Structure of **1**$^\mathbf{a}$.
C 0.000000 0.000000 0.714602
H 0.000000 2.113674 0.169591
H 0.000000 0.977109 -1.269035
H 0.000000 -2.113674 0.169591
H 0.000000 -0.977109 -1.269035
C 0.000000 1.078763 -0.174061
C 0.000000 -1.078763 -0.174061

Structure of **1**$^\mathbf{a}$($\mathbf{H^+}$).
C 0.000000 0.594361 0.000001
H 0.000001 1.672945 0.000003
C -1.109075 -0.240612 0.000015
H -2.126723 0.140267 -0.000002
H -1.001505 -1.316145 -0.000007
C 1.109074 -0.240613 -0.000018
H 2.126723 0.140268 0.000008
H 1.001505 -1.316146 0.000014

Structure of **2**. NIm = 0
C 1.076758 -0.469534 0.000001
C -0.000007 -1.356537 0.000000
C -1.076763 -0.469524 0.000000
N -0.674538 0.834015 -0.000001
N 0.674547 0.834008 0.000001
H 2.140965 -0.655458 0.000000
H -1.184625 1.704154 0.000006
H 1.184642 1.704143 -0.000005
H -2.140972 -0.655437 0.000000

Structure of **2**($\mathbf{H^+}$). NIm = 0
H -2.304384 0.000001 0.000138
C -1.229701 0.000000 0.000074
C -0.395379 1.108203 0.000037
N 0.871145 0.673412 -0.000045
H -0.617276 -2.161903 0.000019
H 1.732838 1.200321 -0.000102
H 1.732837 -1.200322 -0.000113
H -0.617275 2.161903 0.000060
N 0.871144 -0.673413 -0.000063
C -0.395380 -1.108203 0.000014

Structure of **2**($\mathbf{H^+}$)$_\mathbf{2}$. NIm = 0
C 1.241154 -0.000019 0.000000
C 0.313193 -1.150824 -0.000001
N -0.897890 -0.700050 0.000001
H -1.784962 -1.215393 0.000002

H -1.784925 1.215447 -0.000001
N -0.897868 0.700077 -0.000001
C 0.313228 1.150814 0.000000
H 0.534854 -2.214995 -0.000001
H 1.932486 -0.000029 -0.865255
H 1.932482 -0.000030 0.865259
H 0.534922 2.214979 0.000000

Structure of **3**. NIm = 0
C 0.000000 -1.096983 -0.000002
C 1.084869 -0.218830 -0.025174
N 0.679457 1.091546 -0.064524
H 1.188033 1.912191 0.233422
H -1.188034 1.912191 -0.233419
N -0.679457 1.091545 0.064523
C -1.084869 -0.218830 0.025172
C 2.546824 -0.518620 0.004044
H 3.140182 0.230750 -0.523609
H 2.911533 -0.577334 1.032897
H 2.713203 -1.490772 -0.453856
C -2.546824 -0.518620 -0.004041
H -3.140184 0.230770 0.523581
H -2.911527 -0.577374 -1.032893
H -2.713208 -1.490754 0.453896

Structure of **3(H$^+$)**. NIm = 0
H 0.000000 -2.059391 -0.028411
C 0.000000 -0.984229 -0.016293
C -1.124399 -0.163654 -0.009257
N -0.676897 1.104704 -0.000001
H -1.200510 1.966556 -0.009753
H 1.200510 1.966556 -0.009754
N 0.676897 1.104703 -0.000002
C 1.124398 -0.163655 -0.009259
C -2.573057 -0.494673 0.010589
H -2.898521 -0.698591 1.032258
H -3.179239 0.318657 -0.384959
H -2.760398 -1.387198 -0.582443
C 2.573057 -0.494674 0.010589
H 3.179213 0.318545 -0.385227
H 2.898589 -0.698303 1.032294
H 2.760357 -1.387364 -0.582205

Structure of **3(H$^+$)$_2$**. NIm = 0
C 0.000000 1.028387 -0.000001
C 1.178496 0.104902 0.000000
N 0.698844 -1.107251 0.000000
H 1.204325 -1.993796 0.000000
H -1.204325 -1.993796 0.000000
N -0.698844 -1.107251 0.000000
C -1.178496 0.104902 0.000000
C 2.603720 0.440063 0.000000
H 2.827475 1.063359 0.874275
H 3.247344 -0.437016 -0.000006
H 2.827473 1.063371 -0.874267
C -2.603720 0.440063 0.000000
H -3.247345 -0.437016 -0.000009
H -2.827476 1.063356 0.874277
H -2.827472 1.063373 -0.874266
H 0.000000 1.699885 0.870622
H 0.000000 1.699885 -0.870622

Structure of **4**. NIm = 0
C 1.045583 0.216891 -0.035277
C 0.000000 1.113597 0.000000
C -1.045583 0.216891 0.035277
N -0.692508 -1.120570 0.108585
N 0.692508 -1.120570 -0.108585
O -2.362678 0.448896 -0.002173
O 2.362678 0.448896 0.002173
H -1.204913 -1.797639 -0.442855
H 1.204913 -1.797639 0.442855
H -2.462956 1.408326 -0.070248
H 2.462956 1.408326 0.070248

Structure of **4(H$^+$)**. NIm = 0
C 1.103555 0.178588 -0.025196
C 0.000000 1.026228 0.000001
C -1.103555 0.178588 0.025196
N -0.684577 -1.103996 0.066958
N 0.684577 -1.103996 -0.066958
O -2.400144 0.387918 -0.004174
O 2.400144 0.387918 0.004174
H 0.000000 2.101308 0.000001
H -1.220927 -1.902622 -0.243780
H 1.220927 -1.902622 0.243780
H -2.628065 1.326379 -0.041821
H 2.628065 1.326379 0.041821

Structure of **4(H$^+$)$_2$**. NIm = 0
C -1.164587 -0.128611 0.000003
C 0.000000 -1.084960 0.000001
C 1.164587 -0.128611 0.000000
N 0.696347 1.100744 -0.000002
N -0.696347 1.100744 0.000003
O 2.420907 -0.332850 -0.000002
O -2.420907 -0.332850 -0.000003
H 1.219643 1.977349 0.000011

H -1.219643 1.977349 -0.000013
H 2.730301 -1.259159 0.000002
H -2.730301 -1.259159 0.000001
H 0.000002 -1.734047 0.885547
H -0.000002 -1.734053 -0.885540

Structure of **5**. NIm = 0
C 1.059073 0.227676 0.024040
C 0.000000 1.117239 0.000000
C -1.059074 0.227676 -0.024040
N -0.702171 -1.129996 -0.087692
N 0.702171 -1.129996 0.087692
N -2.393024 0.507441 0.067684
N 2.393024 0.507441 -0.067684
H -1.157078 -1.740962 0.581352
H 1.157078 -1.740961 -0.581354
H -2.603448 1.488875 -0.012167
H -3.045165 -0.107805 -0.391106
H 3.045164 -0.107804 0.391111
H 2.603448 1.488875 0.012167

Structure of **5(H$^+$)**. NIm = 0
C -0.000005 -1.011803 0.000015
C 1.111935 -0.175954 -0.029803
N 0.697167 1.131347 -0.088909
H 1.179148 1.833107 0.458666
H -1.179143 1.833125 -0.458633
N -0.697150 1.131344 0.088911
C -1.111934 -0.175927 0.029809
H -0.000030 -2.086596 0.000020
N 2.409734 -0.482423 0.025401
H 2.698114 -1.444705 0.058410
H 3.122092 0.203467 -0.158333
N -2.409744 -0.482415 -0.025440
H -3.122118 0.203445 0.158373
H -2.698090 -1.444714 -0.058365

Structure of **5(H$^+$)$_2$**. NIm = 0
C 0.000000 1.057493 0.000001
C -1.175595 0.111090 -0.000003
N -0.700496 -1.127058 -0.000004
H -1.195693 -2.012350 0.000003
H 1.195693 -2.012350 0.000007
N 0.700496 -1.127058 0.000003
C 1.175595 0.111091 0.000003
N -2.432411 0.451311 0.000001
H -2.707236 1.426204 0.000001
H -3.188771 -0.224577 -0.000001
N 2.432411 0.451312 -0.000002
H 3.188768 -0.224579 -0.000003
H 2.707233 1.426205 0.000000
H -0.000006 1.701923 0.884575
H 0.000005 1.701927 -0.884570

Structure of **6**. NIm = 1
C 0.000000 -1.431994 -0.000002
C 1.076825 -0.538680 -0.000001
H 1.199787 1.421778 0.871917
H -1.199787 1.421780 -0.871913
C -1.076825 -0.538680 -0.000001
C 0.762621 0.923259 0.000001
C -0.762621 0.923259 0.000002
H 1.199787 1.421780 -0.871914
H -1.199787 1.421777 0.871918
H -2.118456 -0.855053 -0.000001
H 2.118456 -0.855053 -0.000002

Structure of **6(H$^+$)**. NIm = 0
C -1.283351 0.000000 -0.000001
C -0.468146 -1.119684 -0.000001
H 1.463842 -1.209731 0.865534
H 1.463842 1.209731 -0.865533
C -0.468146 1.119684 0.000002
H -2.362221 0.000000 -0.000002
C 0.956627 -0.764779 0.000001
C 0.956626 0.764779 0.000000
H 1.463844 -1.209731 -0.865531
H 1.463843 1.209731 0.865532
H -0.827408 2.141838 0.000001
H -0.827407 -2.141838 -0.000002

Structure of **6(H$^+$)$_2$**. NIm = 0
C 1.281155 0.000000 0.000001
C 0.390416 1.166851 -0.000005
H -1.518509 1.264952 0.841405
H -1.518509 -1.264952 -0.841406
C 0.390416 -1.166851 0.000005
C -0.985063 0.767731 0.000002
C -0.985063 -0.767731 -0.000003
H -1.518515 1.264955 -0.841396
H -1.518515 -1.264955 0.841394
H 0.739108 -2.199637 0.000005
H 0.739108 2.199637 -0.000006
H 2.022331 -0.000003 -0.835581
H 2.022326 0.000002 0.835587

Structure of **6'**. NIm = 0
C 0.000000 -1.000068 -0.000002

C 1.096430 -0.206010 0.132181
H 1.368734 1.908518 0.469207
H -1.368733 1.908521 -0.469198
C -1.096429 -0.206009 -0.132183
C 0.775073 1.238692 -0.157041
C -0.775073 1.238692 0.157046
H 0.931375 1.551051 -1.194215
H -0.931374 1.551045 1.194223
H -2.039645 -0.499966 -0.578857
H 2.039645 -0.499969 0.578856

Structure of **7**. NIm = 0
C -0.000001 -1.109238 0.000014
C 1.062033 -0.228852 0.000002
H 1.199800 1.734321 0.876304
H -1.199805 1.734329 -0.876297
C -1.062035 -0.228848 0.000003
H 2.353439 -1.558096 -0.000005
H -2.353425 -1.558099 -0.000001
C 0.766994 1.247707 -0.000001
C -0.766994 1.247708 0.000002
H 1.199799 1.734324 -0.876305
H -1.199794 1.734320 0.876312
O -2.341299 -0.586999 -0.000009
O 2.341300 -0.586996 -0.000007

Structure of **7(H$^+$)**. NIm = 0
C -0.000001 -1.017430 0.000042
C 1.116502 -0.193454 0.000006
H 1.201271 1.743976 0.875016
H -1.201302 1.744014 -0.874971
C -1.116502 -0.193453 0.000003
H 2.520549 -1.492221 -0.000018
H -2.520549 -1.492220 -0.000018
C 0.768055 1.256082 0.000001
C -0.768053 1.256081 0.000002
H 1.201311 1.744015 -0.874967
H -1.201277 1.743978 0.875011
H 0.000004 -2.097433 0.000067
O -2.370569 -0.533816 -0.000027
O 2.370567 -0.533816 -0.000028

Structure of **7(H$^+$)$_2$**. NIm = 0
C 0.000001 -1.089059 0.000154
C 1.176119 -0.151902 0.000013
H 1.218835 1.771975 0.866959
H -1.218863 1.772029 -0.866866
C -1.176119 -0.151907 -0.000002
H 2.630964 -1.425519 -0.000118
H -2.630950 -1.425525 -0.000116
C 0.769917 1.267776 0.000021
C -0.769927 1.267771 0.000025
H 1.218853 1.772016 -0.866878
H -1.218848 1.771952 0.866970
O -2.389994 -0.473965 -0.000118
O 2.390002 -0.473960 -0.000120
H -0.000017 -1.754559 0.878077
H 0.000020 -1.755034 -0.877393

Structure of **8**. NIm = 0
C 0.000000 1.113932 0.000000
C 1.080204 0.245148 0.000001
H 1.186101 -1.739063 -0.878039
H -1.186102 -1.739062 0.878039
C -1.080204 0.245149 -0.000001
N 2.366030 0.640974 -0.000004
H 2.557398 1.628660 0.000002
H 3.134044 -0.004725 0.000012
N -2.366028 0.640975 0.000003
H -2.557398 1.628660 0.000001
H -3.134042 -0.004724 -0.000006
C 0.766376 -1.240887 0.000003
C -0.766378 -1.240887 -0.000003
H 1.186091 -1.739059 0.878051
H -1.186093 -1.739058 -0.878052

Structure of **8(H$^+$)**. NIm = 0
C 0.000000 -1.005995 0.000006
C 1.132349 -0.200926 0.000001
H 1.185565 1.755232 0.877372
H -1.185568 1.755239 -0.877365
C -1.132349 -0.200926 0.000000
N 2.389389 -0.607869 -0.000003
H 2.629811 -1.586421 0.000000
H 3.152829 0.048628 -0.000008
H 0.000000 -2.085400 0.000008
N -2.389389 -0.607869 -0.000003
H -2.629812 -1.586421 -0.000003
H -3.152830 0.048628 -0.000010
C 0.769682 1.258108 0.000000
C -0.769682 1.258108 0.000001
H 1.185568 1.755236 -0.877369
H -1.185563 1.755229 0.877376

Structure of **8(H$^+$)$_2$**. NIm = 0
C -0.000002 -1.079689 0.000104
C 1.185721 -0.151774 0.021800
H 0.956269 1.588611 1.182066

H -0.956273 1.588659 -1.182016
C -1.185719 -0.151770 -0.021784
N 2.401421 -0.550777 -0.051539
H 2.656751 -1.533547 -0.118696
H 3.180490 0.104941 -0.038697
N -2.401430 -0.550771 0.051393
H -2.656771 -1.533538 0.118538
H -3.180496 0.104949 0.038434
C 0.756958 1.273587 0.149790
C -0.756945 1.273593 -0.149757
H 1.332359 1.942320 -0.491537
H -1.332336 1.942302 0.491606
H -0.008816 -1.738637 0.877427
H 0.008805 -1.738898 -0.877016

Structure of **9**. NIm = 0
C 0.731793 0.871849 -0.003917
C 1.141815 -0.436376 0.008722
C -0.001903 -1.307144 0.004654
N -1.014383 -0.441314 0.021227
N -0.623662 0.898939 -0.059970
H 1.282570 1.797843 0.010789
H -1.993928 -0.645551 -0.080071
H -1.219274 1.639147 0.278155
H 2.166717 -0.764794 0.005573

Structure of **9(H$^+$) = 2(H$^+$)**.

Structure of **9(H$^+$)$_2$**. NIm = 0
C 0.417253 1.165289 0.000073
C 1.195058 -0.068516 0.000031
N 0.195275 -1.098118 -0.000045
H -1.830455 1.406659 -0.000008
H 0.311257 -2.117464 -0.000090
H -1.822921 -1.114802 -0.000101
N -0.965070 -0.540699 -0.000049
C -0.922419 0.816594 0.000001
H 0.831502 2.167625 0.000131
H 1.879889 -0.175292 0.870727
H 1.879942 -0.175210 -0.870632

Structure of **9p**. NIm = 1
N 0.000000 1.085201 0.000000
C 1.098751 0.302624 0.000000
C 0.688012 -1.010122 0.000000
C -0.744015 -1.075110 0.000000
N -1.084372 0.215641 0.000000
H 2.077867 0.751989 0.000000
H -2.008026 0.612497 0.000000
H -0.080798 2.087618 0.000000
H 1.345076 -1.862353 0.000000

Structure of **10**. NIm = 0
C 0.000000 -0.595804 -0.000001
H 2.004362 -0.326949 0.000003
H 1.141837 1.156311 0.000006
H -2.004362 -0.326949 -0.000002
H -1.141837 1.156311 0.000002
N 1.115720 0.136864 0.000001
N -1.115720 0.136864 -0.000001

Structure of **10(H$^+$)**. NIm = 0
C 0.000002 0.426043 0.000000
H -2.011362 0.370261 -0.000020
H -1.263759 -1.180310 0.000016
H 2.011360 0.370260 0.000010
H 1.263750 -1.180313 -0.000004
H 0.000007 1.509006 0.000009
N -1.162403 -0.174653 0.000001
N 1.162402 -0.174656 -0.000003

Structure of **10(H$^+$)$_2$**. NIm = 0
C 0.000000 0.292857 0.000001
H -2.044759 0.373015 0.000015
H -1.366081 -1.224731 -0.000004
H 2.044759 0.373015 -0.000014
H 1.366081 -1.224731 -0.000001
N -1.203317 -0.211065 0.000003
N 1.203317 -0.211065 -0.000004
H -0.000003 1.450600 -0.482034
H 0.000003 1.450598 0.482040

Structure of **11**. NIm = 0
H -1.376511 1.748836 0.000155
C -0.675086 0.934991 0.000082
C 0.675087 0.934990 0.000021
N 1.048711 -0.402869 -0.000027
H 1.376514 1.748834 0.000042
C -0.000001 -1.271450 -0.000088
H -1.999457 -0.724349 -0.000006
H 1.999456 -0.724351 -0.000050
N -1.048711 -0.402868 -0.000006

Structure of **11(H$^+$)**. NIm = 0
H -1.383699 1.785515 0.000151
C -0.678211 0.975229 0.000081
C 0.678211 0.975229 0.000051
N 1.070305 -0.348102 -0.000045

H 1.383699 1.785516 0.000090
C 0.000000 -1.138308 -0.000077
H -2.024839 -0.678251 -0.000005
H 2.024839 -0.678250 -0.000085
H 0.000000 -2.213989 -0.000150
N -1.070304 -0.348103 -0.000002

Structure of **11**$(\mathbf{H^+})_2$. NIm = 0
H 1.406340 1.833714 -0.000151
C 0.737281 0.978006 -0.000082
C -0.737282 0.978006 -0.000034
N -1.115947 -0.252598 0.000042
C 0.000000 -1.181938 0.000070
H 2.092948 -0.565592 -0.000018
H -2.092948 -0.565593 0.000084
N 1.115947 -0.252598 -0.000013
H 0.000022 -1.822106 0.895197
H -1.406340 1.833714 -0.000065
H -0.000022 -1.822210 -0.894983

Structure of **12**. NIm = 0
C 0.000000 -0.976548 0.000004
N -1.061262 -0.121741 -0.000002
C -0.675746 1.210202 0.000001
C 0.675747 1.210202 0.000001
N 1.061262 -0.121741 -0.000002
C 2.441022 -0.570756 0.000000
C -2.441022 -0.570756 -0.000001
H -1.374446 2.027730 0.000006
H 1.374447 2.027729 -0.000007
H 2.434478 -1.656170 -0.000043
H 2.964637 -0.213169 -0.887613
H 2.964612 -0.213240 0.887657
H -2.434478 -1.656170 -0.000046
H -2.964613 -0.213242 0.887656
H -2.964637 -0.213167 -0.887613

Structure of **12**$(\mathbf{H^+})$. NIm = 0
C 0.155542 8.716582 12.080087
N 0.485047 9.346628 10.952307
C 1.495883 8.638475 10.337680
C 1.767518 7.565572 11.123374
N 0.919118 7.631239 12.208232
C 0.867574 6.668128 13.314166
C -0.122444 10.583629 10.448216
H 1.930428 8.953272 9.406536
H 2.482570 6.772273 11.003641
H 0.106038 6.982162 14.021244
H 0.618129 5.683891 12.925685
H 1.833589 6.636725 13.811812
H -0.890010 10.909373 11.143378
H 0.640702 11.353260 10.363844
H -0.569998 10.396624 9.475300
H -0.603209 9.032431 12.773719

Structure of **12**$(\mathbf{H^+})_2$. NIm = 0
C 0.2329448 8.8384145 12.2180820
N 0.4832559 9.3717614 10.8770916
C 1.2239306 8.5276946 10.1966550
C 1.5151773 7.3754826 11.0432071
N 0.9415860 7.5564902 12.2102522
C 0.9671880 6.6511770 13.3710836
C -0.0451987 10.6686479 10.4214264
H 1.5527981 8.6968452 9.1563217
H 2.1122264 6.4842540 10.7822302
H -0.0736821 6.3571004 13.6242116
H 1.5677533 5.7579789 13.1217153
H 1.4118861 7.1846115 14.2380479
H -1.1538981 10.6528082 10.4884615
H 0.3444812 11.4716697 11.0827999
H 0.2733090 10.8436286 9.3780948
H 0.6336325 9.5192831 13.0075091
H -0.8596102 8.6980952 12.4019069

Structure of **13**. NIm = 0
H -1.092980 -1.310362 -1.036863
C -0.766172 -0.931899 -0.065417
C 0.766172 -0.931899 0.065417
N 1.062317 0.509846 -0.066875
H 1.092980 -1.310361 1.036863
C 0.000000 1.327542 0.000000
H -1.998339 0.865936 0.020794
H 1.998339 0.865936 -0.020792
N -1.062317 0.509846 0.066875
H 1.253838 -1.515724 -0.713924
H -1.253838 -1.515723 0.713925

Structure of **13**$(\mathbf{H^+})$. NIm = 0
H 1.453548 1.195680 0.885936
C 0.982224 0.777294 0.000002
C 0.982347 -0.777140 -0.000002
N -0.464332 -1.090836 0.000002
H 1.453737 -1.195452 -0.885936
C -1.189014 -0.000093 0.000000
H -0.848325 2.022244 -0.000002
H -0.848006 -2.022377 0.000001
H -2.269747 -0.000179 0.000000
N -0.464504 1.090764 -0.000002

H 1.453744 -1.195457 0.885925
H 1.453555 1.195685 -0.885925

Structure of **13(H^+)$_2$**. NIm = 0
H -1.495783 1.242977 -0.879176
C -1.020105 0.787767 0.000010
C -1.020106 -0.787766 -0.000010
N 0.404165 -1.118409 0.000012
H -1.495784 -1.242976 0.879176
C 1.171075 0.000000 0.000000
H 0.782855 2.068388 -0.000002
H 0.782854 -2.068389 0.000002
N 0.404166 1.118408 -0.000012
H -1.495742 -1.242953 -0.879232
H -1.495741 1.242954 0.879232
H 1.986918 0.000004 0.800893
H 1.986919 -0.000006 -0.800892

Structure of **14**. NIm = 0
H -2.129760 -0.723217 -0.000129
C -1.080964 -0.485332 -0.000068
C 0.017304 -1.321024 -0.000039
N 1.057672 -0.375916 0.000045
C 0.647398 0.898812 0.000068
H -1.273337 1.669279 -0.000034
H 2.029404 -0.634790 0.000089
N -0.682858 0.853485 -0.000020
H 1.247574 1.791002 0.000130

Structure of **14(H^+) = 11(H^+)**.

Structure of **14(H^+)$_2$**. NIm = 0
H 1.282727 -1.882348 0.000128
C 0.662558 -0.989063 0.000068
C -0.803335 -0.908518 0.000035
N -1.011697 0.539211 -0.000048
C 0.108999 1.165808 -0.000062
H 2.140671 0.476605 0.000013
H -1.929414 0.992044 -0.000091
N 1.146821 0.225878 0.000009
H -1.257092 -1.396140 0.881261
H 0.264967 2.241096 -0.000118
H -1.257059 -1.396237 -0.881155

Structure of **15**. NIm = 0
C 1.182059 -0.762426 0.000001
C 1.181349 0.609369 -0.000001
C -1.181349 0.609369 0.000000
C -1.182059 -0.762426 -0.000001
C 0.000000 -1.554650 0.000000
H 2.155616 -1.243541 0.000002
H 2.068027 1.230543 -0.000002
H 0.000000 2.279668 0.000001
H -2.068028 1.230543 0.000002
H -2.155616 -1.243541 -0.000001
N 0.000000 1.272987 0.000000

Structure of **15(H^+)**. NIm = 0
C -0.713642 -1.206531 0.000000
C 0.663556 -1.184994 0.000000
C 0.663575 1.184984 0.000000
C -0.713621 1.206543 0.000000
C -1.409021 0.000011 0.000000
H -1.230101 -2.154415 0.000000
H 1.279703 -2.071173 0.000000
H 2.317344 -0.000019 0.000000
H 1.279739 2.071151 0.000000
H -1.230067 2.154434 0.000000
H -2.490213 0.000022 0.000000
N 1.304073 -0.000011 0.000000

Structure of **15(H^+)$_2$**. NIm = 0
C -0.664018 1.243098 -0.000011
C 0.725891 1.205337 0.000000
C 0.725904 -1.205329 -0.000001
C -0.664005 -1.243105 -0.000011
C -1.397079 -0.000007 -0.000005
H -1.184716 2.194945 -0.000015
H 1.360467 2.083096 0.000001
H 2.356429 0.000012 0.000011
H 1.360490 -2.083082 0.000000
H -1.184693 -2.194957 -0.000013
H -2.188379 -0.000010 -0.800942
N 1.329782 0.000007 0.000004
H -2.188227 -0.000012 0.801100

Structure of **16**. NIm = 0
C 1.117109 0.792129 -0.000001
C -0.154932 1.315715 0.000000
C -1.023962 -0.896383 -0.000001
C 0.213411 -1.526525 0.000000
C 1.277232 -0.598666 0.000000
H 1.962331 1.468840 -0.000002
H -0.384720 2.369610 0.000001
H -2.131033 0.838692 0.000002
H -1.969541 -1.431138 -0.000002
H 2.299957 -0.969233 0.000003
N -1.192878 0.457944 0.000001

Structure of **16(H^+) = 15(H^+)**.

Structure of **16(H^+)$_2$**. NIm = 0
C 0.069940 1.453171 0.000000
C -1.142550 0.790322 0.000000
C -0.146375 -1.360906 0.000000
C 1.175988 -0.757977 0.000000
C 1.234029 0.701161 0.000000
H 0.085353 2.536096 -0.000001
H -2.098813 1.304111 0.000001
H -2.139114 -1.022781 -0.000001
H -0.291304 -2.438404 -0.000002
H 1.781008 -1.187295 -0.833396
N -1.210405 -0.591512 0.000000
H 2.208512 1.181523 -0.000001
H 1.781004 -1.187293 0.833399

Structure of **17**. NIm = 0
C -0.100536 1.365115 0.000000
C 1.109072 0.732753 0.000000
C 0.100407 -1.502537 0.000000
C -1.141569 -0.808827 0.000000
C -1.255082 0.564821 0.000000
H -0.152632 2.443300 0.000000
H 2.056963 1.252641 0.000001
H 2.067102 -1.044586 0.000000
H -2.044050 -1.407368 0.000001
H -2.229372 1.039877 0.000000
N 1.146891 -0.627402 0.000000

Structure of **17(H^+) = 15(H^+)**.

Structure of **17(H^+)$_2$**. NIm = 0
C 1.048332 0.985775 0.000000
C -0.359510 1.344128 0.000000
C -0.959100 -0.987588 0.000000
C 0.449638 -1.319474 0.000000
C 1.444634 -0.332895 0.000000
H 1.772006 1.795057 0.000001
H -0.676375 2.383078 0.000000
H -2.253542 0.686800 0.000000
H -1.466825 -1.482178 0.856753
N -1.265087 0.419895 0.000000
H 2.494155 -0.603632 0.000000
H 0.709046 -2.375890 0.000000
H -1.466826 -1.482178 -0.856753

Structure of **18**. NIm = 0
C -0.381422 1.231354 0.000059
C 0.893624 0.727982 0.000038
N 0.847745 -0.686939 -0.000034
H 1.842997 1.241322 0.000066
C -0.423364 -1.164339 -0.000060
H -2.121059 0.006042 0.000002
H 1.640452 -1.302449 -0.000064
N -1.118518 0.013382 0.000002

Structure of **18^n(H^+) = 14**.

Structure of **18^a(H^+) = 11**.

Structure of **18^n(H^+)$_2$**. NIm = 0
H -2.145426 -0.714884 -0.000144
C -1.104854 -0.418931 -0.000073
C 0.083745 -1.342338 -0.000038
N 1.054997 -0.460250 0.000047
C 0.697189 0.952888 0.000071
H -1.372533 1.624887 -0.000026
H 2.031152 -0.736779 0.000095
N -0.749063 0.821837 -0.000015
H 1.044309 1.477097 -0.893941
H 1.044206 1.477040 0.894156

Structure of **18^a(H^+)$_2$**. NIm = 0
H -1.101287 1.492672 -0.882761
C -0.721259 0.965406 0.000082
C 0.747837 0.885664 0.000040
N 1.083808 -0.358183 -0.000044
H 1.449315 1.709981 0.000073
C -0.049009 -1.299328 -0.000077
H -2.007231 -0.789407 0.000006
H 2.037600 -0.705202 -0.000089
N -1.051843 -0.456738 0.000002
H -1.101241 1.492561 0.883010

Structure of **19**. NIm = 0
C -0.000005 1.362403 -0.000004
C -1.196268 0.646659 -0.000001
C -1.175360 -0.752030 0.000005
C 0.000008 -1.537424 0.000001
C 1.175365 -0.752022 -0.000005
C 1.196261 0.646671 0.000002
H -0.000013 2.447358 0.000002
H -2.144561 1.183790 0.000006
H -2.147871 -1.250258 -0.000011
H 2.147883 -1.250237 0.000004
H 2.144553 1.183805 0.000013

Structure of **19**($\mathbf{H^+}$). NIm = 0
C -0.000001 1.391006 0.000000
C -1.204648 0.695501 0.000000
C -1.204648 -0.695507 0.000000
C 0.000001 -1.391006 0.000000
C 1.204648 -0.695501 0.000000
C 1.204648 0.695507 0.000000
H -0.000005 2.472878 0.000000
H -2.141578 1.236433 0.000000
H -2.141576 -1.236443 0.000000
H 0.000005 -2.472878 0.000000
H 2.141578 -1.236433 0.000000
H 2.141576 1.236443 0.000000

Structure of **19**($\mathbf{H^+})_\mathbf{2}$. NIm = 0
C -1.409387 0.011384 0.000003
C -0.748039 -1.229782 -0.000005
C 0.616578 -1.254681 -0.000002
C 1.390466 -0.011231 0.000004
C 0.636816 1.244575 0.000000
C -0.728031 1.241689 0.000001
H -2.492820 0.020155 0.000009
H -1.322922 -2.144478 -0.000006
H 1.156630 -2.192706 0.000006
H 1.191902 2.173784 -0.000016
H -1.288099 2.165532 -0.000001
H 2.102438 -0.017017 0.845797
H 2.102450 -0.016997 -0.845788

Structure of **20**. NIm = 0
C -0.000844 -1.275530 0.034604
C -1.144530 -0.441351 -0.017369
C -0.707938 0.909980 -0.003951
C 0.709471 0.908920 -0.003445
H 2.174706 -0.776207 -0.025587
H -2.175695 -0.773983 -0.024985
H -1.336814 1.800132 0.048291
H 1.340794 1.797822 0.048149
C 1.143343 -0.443313 -0.017483

Structure of **20**($\mathbf{H^+}$). NIm = 0
C 0.000000 1.200995 0.000000
C 1.142214 0.371128 0.000000
C 0.705927 -0.971625 0.000000
C -0.705927 -0.971625 0.000000
H -2.172344 0.705837 0.000000
H 0.000000 2.284137 0.000000
H 2.172344 0.705837 0.000000
H 1.342582 -1.847906 0.000000
H -1.342582 -1.847906 0.000000
C -1.142214 0.371128 0.000000

Structure of **20**($\mathbf{H^+})_\mathbf{2}$. NIm = 0
C 0.000602 -1.213322 -0.000001
C -1.176261 -0.281244 -0.000011
C -0.732982 0.987389 0.000000
C 0.732001 0.988113 -0.000001
H 2.205560 -0.604709 -0.000024
H -2.204953 -0.606891 0.000018
H -1.346157 1.876663 0.000012
H 1.344295 1.877995 -0.000010
C 1.176540 -0.280078 0.000012
H 0.000954 -1.874112 -0.874466
H 0.000905 -1.874091 0.874480