Structural Chemistry

Crystal structure and vibrational spectra of salts of 1H-pyrazole-1-carboxamidine and its protonation route

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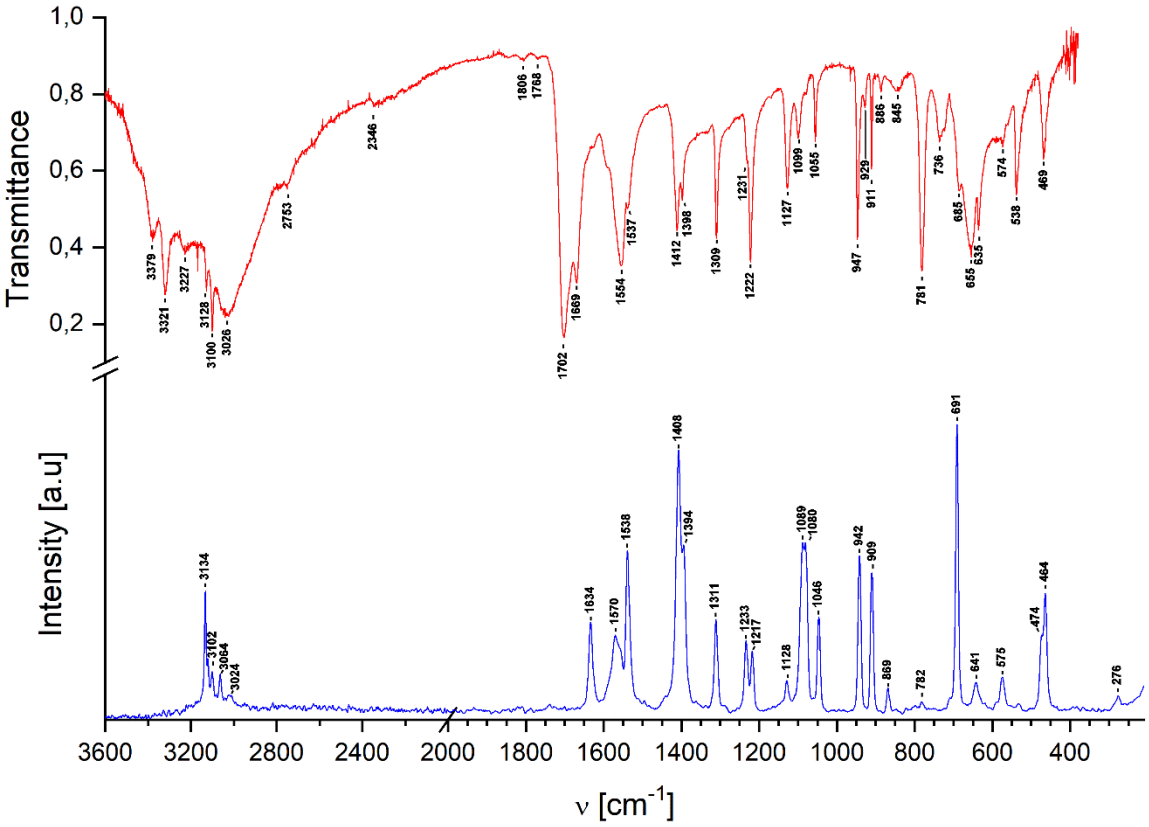

Figure S1. FT-IR and FT Raman spectra for (HPyCA)Cl (**1**).

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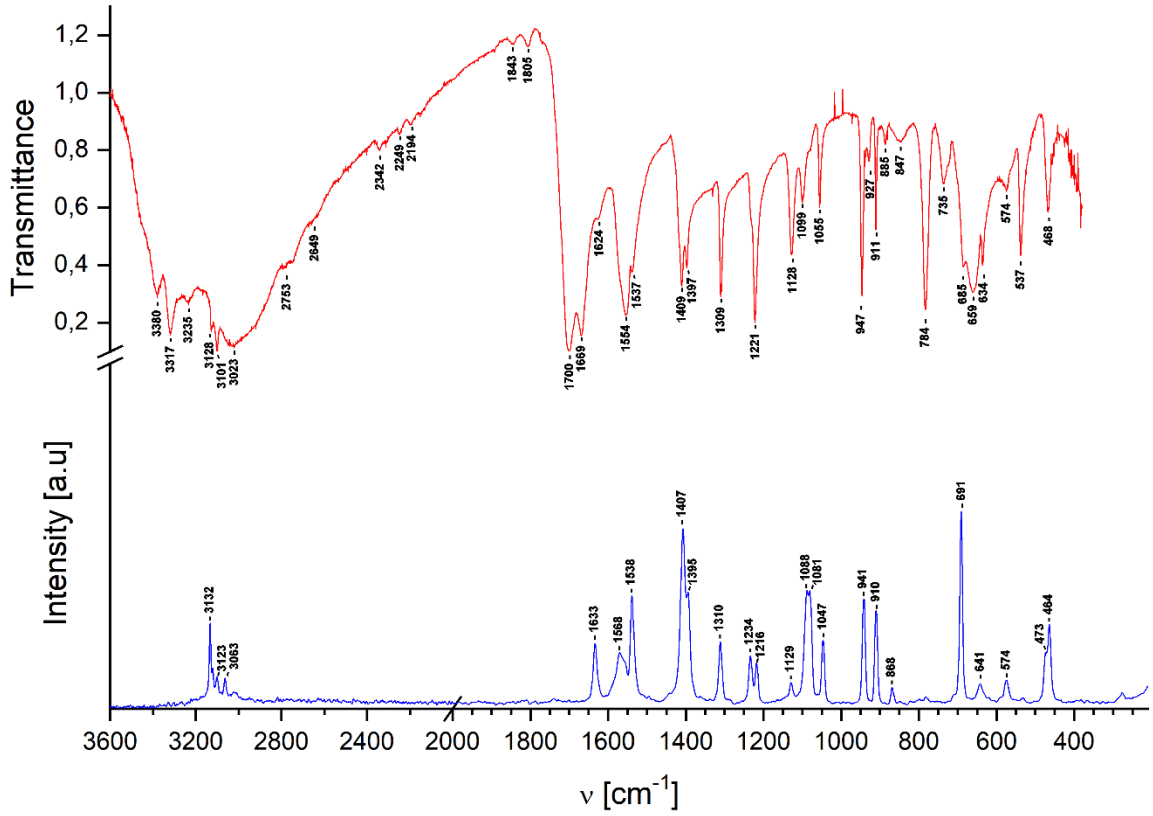


Figure S2. FT-IR and FT Raman spectra for (HPyCA)Cl·H_2O (**2**).

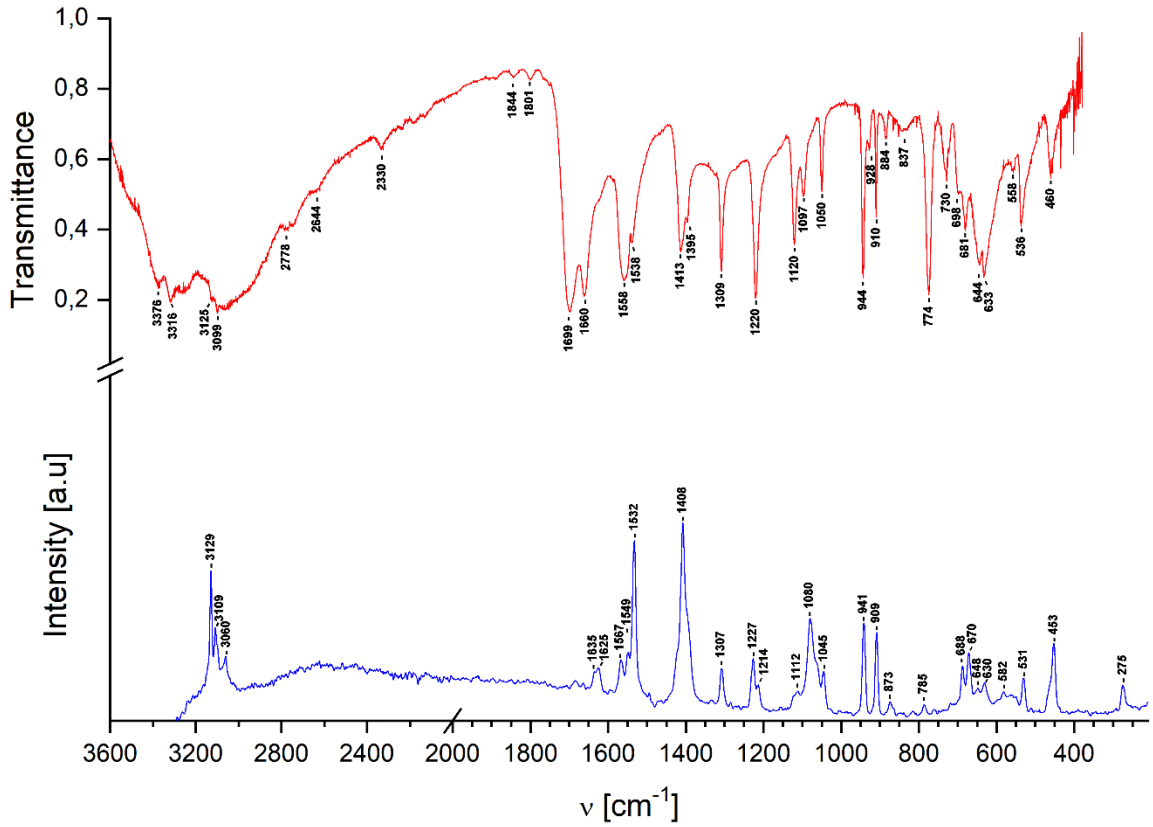


Figure S3. FT-IR and FT Raman spectra for (HPyCA)Br (**3**).

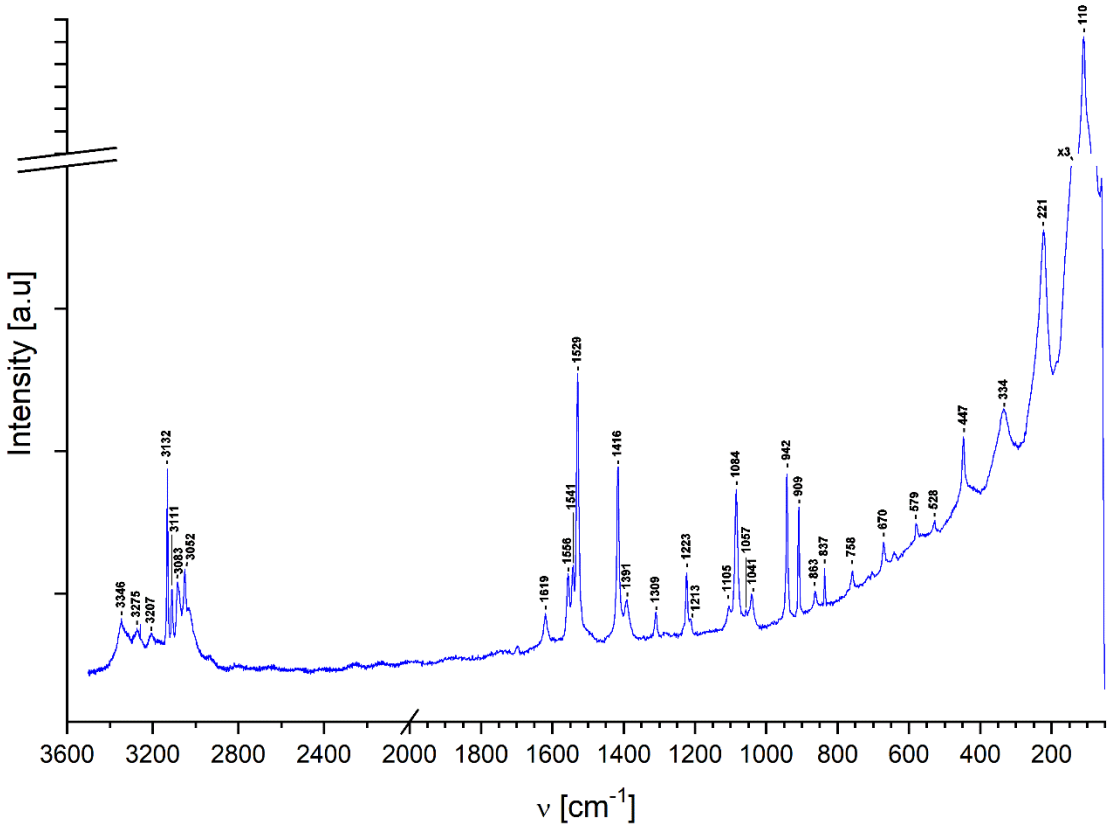


Figure S4. FT Raman spectrum for $(HPyCA)_2(I)I_3$ (**4**).

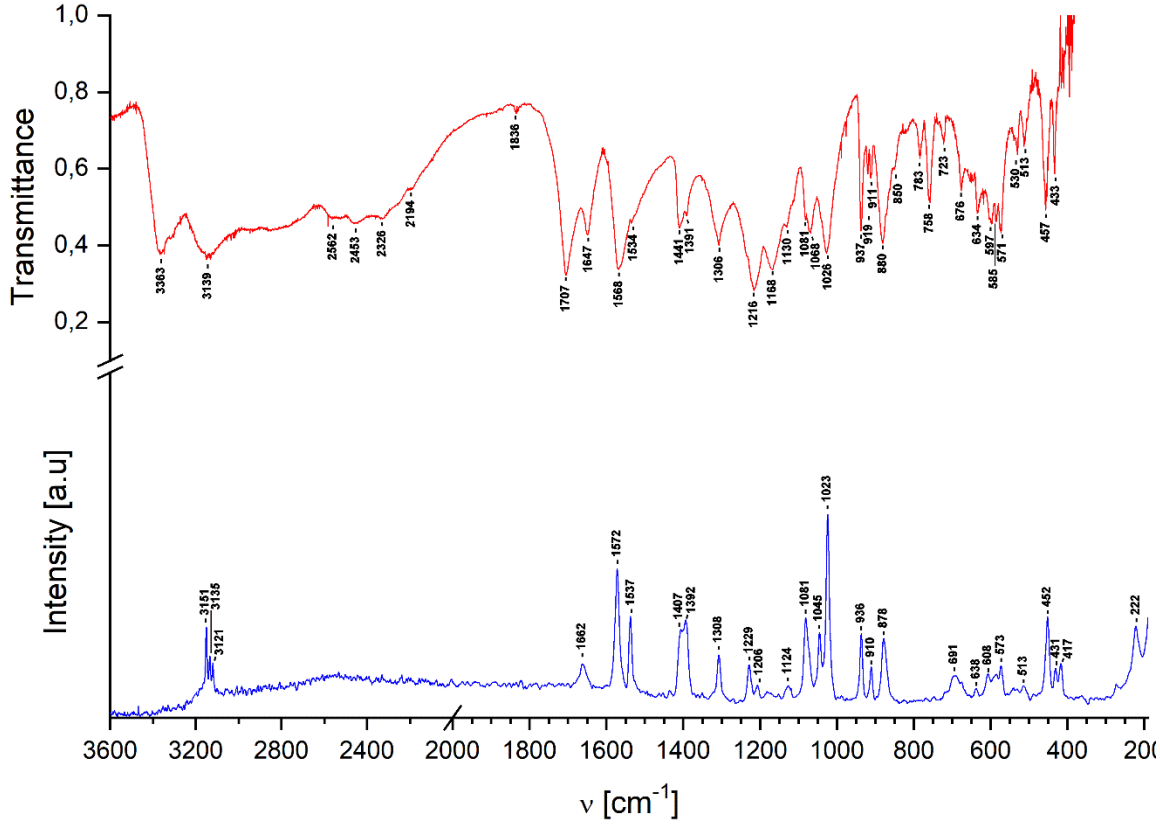


Figure S5. FT-IR and FT Raman spectra for $(HPyCA)HSO_4$ (**5**).

Table S1. Geometry parameters for selected hydrogen bonds of $C_4H_7N_4 \cdot Cl$, $C_4H_7N_4 \cdot HSO_4$, $C_4H_7N_4 \cdot Br$, $2(C_4H_7N_4) \cdot I_3 \cdot I$, and $C_4H_7N_4 \cdot Cl \cdot H_2O$

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
$C_4H_7N_4 \cdot Cl$				
N3—H3A···Cl1	0.86	2.44	3.210 (2)	149.0
N3—H3B···N2^{i}	0.86	2.26	3.028 (3)	149.5
N4—H4A···Cl1	0.86	2.37	3.159 (2)	151.9
N4—H4B···Cl1^{ii}	0.86	2.33	3.1547 (19)	161.9
C1—H1···Cl1^{ii}	0.93	2.76	3.625 (3)	155.2
C2—H2···Cl1^{iii}	0.93	2.94	3.770 (2)	149.4
$C_4H_7N_4 \cdot HSO_4$				
O1—H1O···O4^{iv}	0.83	1.76	2.5969 (19)	176.8
N3—H3A···O2	0.86	2.06	2.904 (2)	168.2
N3—H3B···O4^{v}	0.86	2.18	2.936 (2)	146.0
N4—H4A···O3	0.86	2.06	2.886 (2)	159.7
N4—H4B···O3^{vi}	0.86	2.17	2.923 (2)	146.7
N4—H4B···O2^{vii}	0.86	2.58	3.148 (2)	124.5
C1—H1···O1^{viii}	0.93	2.57	3.394 (2)	148.5
$C_4H_7N_4 \cdot Br$				
N3—H3A···Br1^{ix}	0.86	2.68	3.342 (3)	134.5
N3—H3B···N2^{x}	0.86	2.30	3.065 (4)	148.3
N4—H4A···Br1	0.86	2.64	3.391 (3)	146.9
N4—H4B···Br1^{xi}	0.86	2.52	3.344 (3)	160.7
C1—H1···Br1^{xii}	0.93	3.12	3.807 (4)	132.3
C2—H2···Br1^{xiii}	0.93	3.01	3.793 (4)	143.2
C3—H3···Br1^{xi}	0.93	2.88	3.752 (3)	155.9
$2(C_4H_7N_4) \cdot I_3 \cdot I$				
N13—H13B···I3^{v}	0.86	3.05	3.768 (5)	142.9
N13—H13A···I4	0.86	2.84	3.635 (4)	154.1
N14—H14B···I1	0.86	3.19	3.752 (4)	125.0
N14—H14A···I4	0.86	2.88	3.664 (4)	152.4
N14—H14B···I4^{i}	0.86	3.04	3.770 (5)	143.9
N23—H23B···I3^{xiv}	0.86	3.22	4.025 (4)	156.2
N23—H23A···I4	0.86	2.87	3.644 (5)	151.5
N24—H24A···I1^{v}	0.86	3.26	3.744 (4)	117.9
N24—H24A···I4	0.86	2.91	3.679 (4)	149.9
N24—H24B···I4^{xv}	0.86	3.07	3.803 (4)	143.9
C11—H11···N12^{xvi}	0.93	2.66	3.296 (7)	126.0
C13—H13···I1^{xvii}	0.93	3.25	3.824 (5)	122.2
C13—H13···I4^{i}	0.93	3.32	3.997 (5)	131.5
C23—H23···I1^{xviii}	0.93	3.25	4.049 (6)	145.1
C23—H23···I2^{xviii}	0.93	3.31	3.943 (5)	126.8
$C_4H_7N_4 \cdot Cl \cdot H_2O$				
N3—H3A···O1	0.86	1.95	2.800 (3)	171.2
N3—H3B···N2^{xvii}	0.86	2.26	3.020 (3)	147.5
N4—H4A···Cl1	0.86	2.37	3.217 (2)	167.7
N4—H4B···Cl1^{xix}	0.86	2.39	3.223 (2)	164.5
O1—H1O···Cl1^{xx}	0.833 (19)	2.38 (2)	3.180 (2)	161 (4)
O1—H2O···Cl1	0.816 (19)	2.54 (3)	3.261 (2)	148 (4)
C1—H1···O1^{xvii}	0.93	2.64	3.529 (3)	159.1
C2—H2···Cl1^{xxi}	0.93	2.90	3.815 (3)	167.4
C3—H3···Cl1^{xix}	0.93	2.70	3.573 (3)	157.7

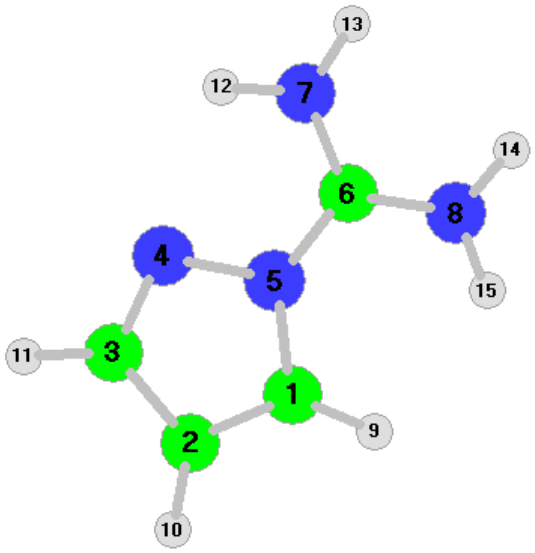
Symmetry code(s): (i) $-x+2, -y+1, -z+1$; (ii) $x-1/2, -y+1/2, z-1/2$; (iii) $-x+1/2, y+1/2, -z+1/2$; (iv) $x, -y+1/2, z-1/2$; (v) $-x+1, -y+1, -z+1$; (vi) $-x+1, -y, -z+1$; (vii) $-x+1, y-1/2, -z+1/2$; (viii) $x+1, -y+1/2, z-1/2$; (ix) $x-1, y, z$; (x) $-x, -y+1, -z$; (xi) $-x+2, y+1/2, -z+1/2$; (xii) $-x+1, -y+1, -z$; (xiii) $x, y+1, z$; (xiv) $-x+1, -y+1, -z+2$; (xv) $-x+1, -y+2, -z+1$; (xvi) $-x+2, -y+1, -z$; (xvii) $-x+2, -y, -z+1$; (xviii) $x-1, y+1, z$; (xix) $-x, -y+1, -z+1$; (xx) $x+1, y, z$; (xxi) $x, y-1, z+1$.

Table S2. Theoretical frequencies for the $(HPyCA)^+$ ion scaled by $\nu_{sc} = 0.9614 \cdot \nu_{calc} + 17.8$ equation (ν_{sc}), mode symmetry (S), PED (%) and assignment. Frequencies in cm^{-1}.

ν_{sc}	S	PED**(HPyCA+)**	Assingnment
3585	A'	s1(98)	$\nu_{as}NH_2$
3555	A'	s2(88) s4(11)	$\nu_{as}NH_2$
3478	A'	s3(98)	$\nu_{s}NH_2$
3403	A'	s4(88) s2(11)	$\nu_{s}NH_2$
3171	A'	s5(94)	$\nu_{s}CH$
3154	A'	s6(92)	$\nu_{as}CH$
3140	A'	s7(93)	νCH
1684	A'	s8(65) s12(17) s32(10)	$\nu CN_{(gua)}$
1633	A'	s9(60) s29(10)	$\delta_{s}NH_2$
1567	A'	s10(50) s9(15)	$\nu CN_{(gua)}$
1548	A'	s11(54) s9(11)	νCC + νCN
1518	A'	s12(65) s8(10)	$\nu_{s}NH_2$
1422	A'	s13(69)	νCC + νCN
1376	A'	s14(65)	δCH
1292	A'	s15(37) s14(14) s16(13)	νCC + νCN + δCH
1210	A'	s16(65)	δCH
1197	A'	s17(56)	νNN
1092	A'	s10(15) s18(15) s20(15) s19(14) s21(13)	δCH + ρNH_2
1066	A'	s29(42) s19(21) s21(15)	ρNH_2
1034	A'	s21(34) s18(18) s15(13)	ρNH_2 + δCH
1026	A'	s19(30) s20(28) s15(11)	ρNH_2 + δCH
933	A"	s22(95)	γCH
918	A'	s23(63) s21(13) s15(10)	νCN + νCC
911	A'	s24(77)	ring breathing

875	A"	s25(97)	γCH
733	A"	s26(91)	γCH
701	A"	s27(83)	γCN
667	A"	s33(77)	γNH
661	A'	s18(19) s11(13) s29(12) s19(11) s21(11)	δCN
636	A"	s30(88)	γCN + γNN
581	A"	s31(86)	γCN
526	A'	s32(70) s17(13)	δCN
484	A"	s28(47) s36(41)	ωNH_2
437	A'	s34(65) s20(11)	δCN
372	A"	s36(49) s28(30) s35(11)	ωNH_2
346	A"	s35(74)	δNH
268	A'	s37(95)	δCN
167	A"	s38(95)	γCN

Table S3. The definitions of local modes calculated for the $HPyCA^{+}$ ion and a numbering scheme used in calculations by VEDA program.



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	1.00		7	12	NH	1.015184
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	1.00		1	9	CH	1.077107
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	-1.00		4	3	NC	1.309797
	1.00		1	2	CC	1.358595
	1.00		2	3	CC	1.431619
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	1.00		11	3	4	HCN 119.71
	1.00		1	5	4	CNN 111.56
	1.00		2	1	5	CCN 106.16
k 15	1.00	STRE	5	1	NC	1.390807
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         1.00            1    5    4   CNN   111.56
         1.00            9    1    2   HCC   130.62
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        -1.00            2    3    4    5   CCNN     0.00
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         1.00           10    2    3    4   HCCN  -180.00
        -1.00           10    2    1    5   HCCN  -180.00
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        -1.00            5    6    7   NCN   117.05
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k 39     1.00   TORS     1    5    6    8   CNCN     0.00
         1.00            8    6    5    4   NCNN  -180.00
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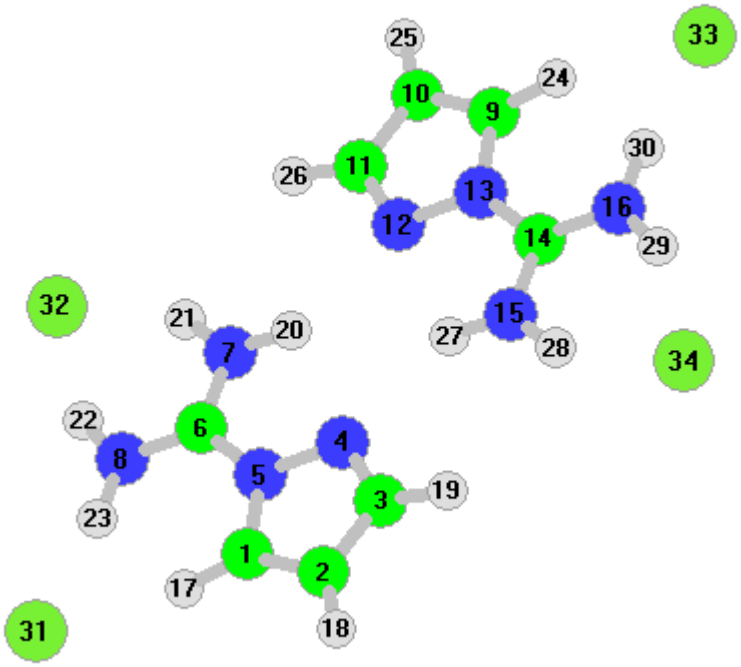
Table S4. The definitions of local modes calculated for the $[(HPyCA)_2Cl_4]^{2-}$ ion and a numbering scheme used in calculations by VEDA program.



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       -1.00           5    1   NC    1.374209
        1.00           2    3   CC    1.418708
        1.00          10   11   CC    1.418708
s 21    1.00   STRE    1    2   CC    1.371019  f1589 10  f1572 51  f1252 13
f1116 10
        1.00          12   11   NC    1.320529
s 22   -1.00   STRE    5    6   NC    1.403081  f1566 44  f1548 13  f1143 14
f1116 12
       -1.00          13   14   NC    1.403081
        1.00           8    6   NC    1.306150
        1.00          16   14   NC    1.306150
        1.00           1    2   CC    1.371019
        1.00           9   10   CC    1.371019
        1.00          15   14   NC    1.322169
        1.00           7    6   NC    1.322169
s 23   -1.00   BEND   20    7   21   HNH   123.48  f1754 13  f1548 64
       -1.00          27   15   28   HNH   123.48
        1.00          21    7    6   HNC   115.82
        1.00          28   15   14   HNC   115.82
       -1.00          23    8    6   HNC   126.17
       -1.00          30   16   14   HNC   126.17
s 24    1.00   BEND   27   15   28   HNH   123.48  f1753 14  f1589 12  f1545 58
        1.00          22    8   23   HNH   118.63
s 25    1.00   BEND   19    3    2   HCC   128.59  f1446 17  f1262 13  f1249 34
        1.00          18    2    1   HCC   126.63
        1.00          26   11   10   HCC   128.59
       -1.00          17    1    2   HCC   132.30
```

```
s 26    1.00   STRE   10   11   CC    1.418708  f1446 19  f1439 13  f1066 31
f80 13
       -1.00           2    3   CC    1.418708
        1.00          31   23   ClH    2.048053
        1.00          33   30   ClH    2.048053
       -1.00           9   10   CC    1.371019
        1.00          12   13   NN    1.368870
        1.00           4    3   NC    1.320529
s 27   -1.00   BEND   18    2    1   HCC   126.63  f1439 48  f1261 11  f1116 10
       -1.00          24    9   10   HCC   132.30
        1.00          17    1    2   HCC   132.30
       -1.00          25   10   11   HCC   127.85
s 28    1.00   STRE    2    3   CC    1.418708  f1446 12  f1438 39  f1067 22
        1.00          10   11   CC    1.418708
       -1.00           5    1   NC    1.374209
       -1.00          13    9   NC    1.374209
       -1.00           9   10   CC    1.371019
       -1.00           1    2   CC    1.371019
        1.00           7    6   NC    1.322169
        1.00          15   14   NC    1.322169
s 29    1.00   STRE    5    1   NC    1.374209  f1343 57
        1.00           4    3   NC    1.320529
       -1.00           5    6   NC    1.403081
        1.00          15   14   NC    1.322169
s 30   -1.00   STRE    5    1   NC    1.374209  f1343 51
       -1.00          13    9   NC    1.374209
       -1.00          12   11   NC    1.320529
       -1.00           4    3   NC    1.320529
       -1.00           2    3   CC    1.418708
       -1.00          10   11   CC    1.418708
        1.00          12   13   NN    1.368870
        1.00           4    5   NN    1.368870
        1.00           7    6   NC    1.322169
        1.00          15   14   NC    1.322169
s 31   -1.00   STRE    5    1   NC    1.374209  f1446 23  f1262 54
       -1.00          13    9   NC    1.374209
        1.00          12   13   NN    1.368870
        1.00           4    5   NN    1.368870
        1.00           1    2   CC    1.371019
        1.00           9   10   CC    1.371019
        1.00           4    3   NC    1.320529
        1.00          12   11   NC    1.320529
s 32    1.00   STRE   13    9   NC    1.374209  f1446 10  f1261 57
        1.00           4    5   NN    1.368870
       -1.00           9   10   CC    1.371019
        1.00           4    3   NC    1.320529
s 33    1.00   BEND   19    3    2   HCC   128.59  f1446 14  f1261 10  f1252 30
       -1.00          26   11   10   HCC   128.59
        1.00          18    2    1   HCC   126.63
       -1.00          17    1    2   HCC   132.30
        1.00          25   10   11   HCC   127.85
k 34    1.00   STRE    4    5   NN    1.368870  f1249 36  f1116 11
        1.00          12   13   NN    1.368870
       -1.00           5    6   NC    1.403081
       -1.00          13   14   NC    1.403081
       -1.00           4    3   NC    1.320529
       -1.00          10   11   CC    1.418708
       -1.00           2    3   CC    1.418708
        1.00          13    9   NC    1.374209
        1.00           5    1   NC    1.374209
       -1.00           7    6   NC    1.322169
s 35    1.00   BEND   29   16   14   HNC   115.21  f1167 50  f1116 14
s 36    1.00   BEND   22    8    6   HNC   115.21  f1566 13  f1249 10  f1166 34
f1116 13
```

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         1.00           29   16   14   HNC   115.21
s 37    -1.00   BEND   20    7    6   HNC   120.70  f1154 57
         1.00           21    7    6   HNC   115.82
s 38    -1.00   BEND   20    7    6   HNC   120.70  f1566 12  f1143 61
        -1.00           27   15   14   HNC   120.70
         1.00           21    7    6   HNC   115.82
         1.00           28   15   14   HNC   115.82
s 39     1.00   BEND   17    1    2   HCC   132.30  f1580 12  f1438 37  f1116 15
         1.00           24    9   10   HCC   132.30
s 40     1.00   STRE    5    6   NC    1.403081  f1446 11  f1154 10  f1116 23
f704 25
         1.00           1    2   CC    1.371019
        -1.00           13   14   NC    1.403081
         1.00           7    6   NC    1.322169
        -1.00           15   14   NC    1.322169
         1.00           4    3   NC    1.320529
        -1.00           16   14   NC    1.306150
s 41     1.00   BEND   25   10   11   HCC   127.85  f1446 10  f1067 52  f964 19
        -1.00           24    9   10   HCC   132.30
s 42     1.00   BEND   25   10   11   HCC   127.85  f1066 51  f963 10
         1.00           18    2    1   HCC   126.63
s 43     1.00   BEND   11   12   13   CNN   104.55  f964 52
         1.00           10    9   13   CCN   105.89
         1.00           2    1    5   CCN   105.89
         1.00           1    5    4   CNN   112.26
         1.00           9   13   12   CNN   112.26
        -1.00           27    4    3   HNC   103.54
        -1.00           27    4    5   HNN   151.91
k 44    -1.00   STRE    4    5   NN    1.368870  f1252 10  f963 54
         1.00           12   13   NN    1.368870
         1.00           13    9   NC    1.374209
s 45    -1.00   TORS   17    1    2    3   HCCC  -179.98  f959 81
         1.00           24    9   13   14   HCNC     0.02
         1.00           25   10   11   26   HCCH     0.00
         1.00           17    1    5    6   HCNC    -0.02
        -1.00           24    9   10   25   HCCH    -0.02
        -1.00           17    1    2   18   HCCH     0.02
s 46    -1.00   TORS   17    1    2   18   HCCH     0.02  f959 84
         1.00           17    1    5    6   HCNC    -0.02
         1.00           24    9   10   11   HCCC  -180.02
        -1.00           25   10   11   26   HCCH     0.00
s 47    -1.00   BEND   25   10    9   HCC   126.63  f946 88
         1.00           18    2    3   HCC   127.85
         1.00           18    2    1   HCC   126.63
        -1.00           25   10   11   HCC   127.85
         1.00           26   11   10   HCC   128.59
        -1.00           19    3    4   HCN   119.63
        -1.00           19    3    2   HCC   128.59
         1.00           26   11   12   HCN   119.63
         1.00           24    9   13   HCN   121.81
        -1.00           17    1    5   HCN   121.81
         1.00           24    9   10   HCC   132.30
        -1.00           17    1    2   HCC   132.30
s 48     1.00   BEND    2    3    4   CCN   111.78  f946 82
        -1.00           1    2    3   CCC   105.52
         1.00           10   11   12   CCN   111.78
s 49     1.00   TORS   19    3    2    1   HCCC  -180.00  f909 87
        -1.00           26   11   10    9   HCCC  -180.00
        -1.00           24    9   10   11   HCCC  -180.02
         1.00           17    1    2    3   HCCC  -179.98
s 50     1.00   TORS   17    1    2    3   HCCC  -179.98  f909 89
         1.00           19    3    2    1   HCCC  -180.00
         1.00           24    9   10   11   HCCC  -180.02
         1.00           26   11   10    9   HCCC  -180.00
```

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s 51   -1.00   TORS    6    8   22   32   CNHCl     0.00  f875 52  f840 22  f51
14
       -1.00          14   16   29   34   CNHCl     0.00
        1.00          22    8    6    5   HNCN  -179.97
        1.00          29   16   14   13   HNCN  -180.03
s 52    1.00   TORS   28   15   27    4   HNHN    -0.09  f871 80
        1.00           3    4   27   15   CNHN     0.03
        1.00          21    7    6    5   HNCN  -180.03
        1.00          23    8   22   32   HNHCl  -179.98
        1.00          29   16   14   13   HNCN  -180.03
s 53    1.00   TORS   17   31   23    8   HClHN  -180.22  f840 57  f737 16
        1.00          24   33   30   16   HClHN  -179.78
       -1.00          22    8   23   31   HNHCl     0.16
       -1.00          29   16   30   33   HNHCl    -0.16
s 54   -1.00   TORS    6    8   22   32   CNHCl     0.00  f839 78
        1.00          14   16   29   34   CNHCl     0.00
       -1.00           6    8   23   31   CNHCl  -179.81
s 55    1.00   TORS   18    2    1    5   HCCN  -180.00  f793 88
        1.00          25   10    9   13   HCCN  -180.00
s 56    1.00   TORS   25   10   11   12   HCCN  -180.00  f793 88
        1.00          18    2    1    5   HCCN  -180.00
s 57    1.00   TORS   21    7    6    5   HNCN  -180.03  f737 65
        1.00          22    8    6    5   HNCN  -179.97
s 58    1.00   TORS   21    7    6    5   HNCN  -180.03  f734 65
        1.00          22    8    6    5   HNCN  -179.97
       -1.00          29   16   14   13   HNCN  -180.03
        1.00           3    4   27   15   CNHN     0.03
        1.00          28   15   27    4   HNHN    -0.09
       -1.00          27   15   14   13   HNCN    -0.05
s 59    1.00   OUT     7    5    8    6   NNNC     0.00  f715 77
        1.00          16   13   15   14   NNNC     0.00
s 60    1.00   OUT     7    5    8    6   NNNC     0.00  f715 75
       -1.00          16   13   15   14   NNNC     0.00
s 61   -1.00   BEND    7    6    8   NCN   122.80  f706 61  f475 13
       -1.00          15   14   16   NCN   122.80
        1.00           1    5    4   CNN   112.26
        1.00           9   13   12   CNN   112.26
s 62   -1.00   BEND    7    6    8   NCN   122.80  f1446 10  f704 56
        1.00           1    5    4   CNN   112.26
s 63    1.00   TORS   10   11   12   13   CCNN     0.00  f657 86
        1.00           1    2    3    4   CCCN     0.00
        1.00           1    5    4    3   CNNC     0.00
s 64    1.00   TORS    3    4   27   15   CNHN     0.03  f655 80
       -1.00           9   13   12   11   CNNC     0.00
       -1.00          27    4    5    1   HNNC  -180.13
       -1.00           5    4   27   15   NNHN  -179.84
s 65    1.00   TORS    2    1    5    4   CCNN     0.00  f606 86
       -1.00          10    9   13   12   CCNN     0.00
s 66    1.00   TORS    2    1    5    4   CCNN     0.00  f606 84
       -1.00          11   10    9   13   CCCN     0.00
s 67   -1.00   TORS    3    4   27   15   CNHN     0.03  f577 68
        1.00          27   15   14   13   HNCN    -0.05
s 68   -1.00   BEND    5    6    8   NCN   119.99  f1754 10  f539 71
        1.00          13   14   15   NCN   117.21
        1.00           9   13   14   CNC   127.89
s 69    1.00   BEND   13   14   15   NCN   117.21  f1753 10  f535 69
        1.00           5    6    8   NCN   119.99
       -1.00           1    5    6   CNC   127.89
        1.00           9   13   14   CNC   127.89
s 70    1.00   TORS   21    7   20   12   HNHN     0.09  f509 82
       -1.00          28   15   27    4   HNHN    -0.09
s 71   -1.00   BEND   15   14   16   NCN   122.80  f963 11  f475 53
        1.00           1    5    4   CNN   112.26
s 72    1.00   BEND    7    6    8   NCN   122.80  f475 59
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         1.00           15   14   16   NCN   122.80
         1.00            1    5    4   CNN   112.26
         1.00            9   13   12   CNN   112.26
s 73    -1.00   BEND     9   13   14   CNC   127.89  f293 70
         1.00            1    5    6   CNC   127.89
         1.00           13   14   15   NCN   117.21
         1.00            5    6    8   NCN   119.99
s 74     1.00   BEND    16   29   34   NHCl   153.59  f289 59
         1.00            8   22   32   NHCl   153.59
         1.00            1    5    6   CNC   127.89
         1.00            9   13   14   CNC   127.89
s 75    -1.00   OUT      6    1    4    5   CCNN     0.00  f182 75
         1.00           14    9   12   13   CCNN     0.00
s 76     1.00   TORS     2    1    5    6   CCNC  -180.01  f180 83
s 77     1.00   STRE    31   23   ClH    2.048053  f179 76
         1.00           33   30   ClH    2.048053
         1.00           32   22   ClH    2.155887
         1.00           34   29   ClH    2.155887
s 78     1.00   STRE    33   30   ClH    2.048053  f178 82
s 79    -1.00   STRE    32   22   ClH    2.155887  f475 15  f173 73
         1.00           34   29   ClH    2.155887
        -1.00           33   30   ClH    2.048053
        -1.00           32   21   ClH    2.176647
s 80     1.00   STRE    32   22   ClH    2.155887  f171 75
         1.00           34   29   ClH    2.155887
        -1.00           33   30   ClH    2.048053
        -1.00           31   23   ClH    2.048053
         1.00            5    6   NC    1.403081
         1.00           13   14   NC    1.403081
s 81    -1.00   STRE    33   24   ClH    2.418702  f119 84
         1.00           31   17   ClH    2.418702
         1.00           34   28   ClH    2.176647
s 82     1.00   STRE    31   17   ClH    2.418702  f116 72
         1.00           33   24   ClH    2.418702
        -1.00           32   21   ClH    2.176647
        -1.00           34   28   ClH    2.176647
         1.00           32   22   ClH    2.155887
s 83     1.00   TORS    12   13   14   15   NNCN    -0.04  f110 85
         1.00            4    5    6    8   NNCN  -179.96
         1.00            1    5    6    8   CNCN     0.05
s 84     1.00   TORS    12   13   14   15   NNCN    -0.04  f99 80
        -1.00            4    5    6    8   NNCN  -179.96
s 85     1.00   BEND    16   29   34   NHCl   153.59  f289 11  f80 48
         1.00            8   22   32   NHCl   153.59
        -1.00            9   13   14   CNC   127.89
         1.00           10    9   13   CCN   105.89
         1.00           11   12   13   CNN   104.55
         1.00            9   13   12   CNN   112.26
s 86    -1.00   STRE    31   17   ClH    2.418702  f77 74
         1.00           33   24   ClH    2.418702
        -1.00           34   29   ClH    2.155887
        -1.00           32   21   ClH    2.176647
         1.00           32   22   ClH    2.155887
        -1.00           33   30   ClH    2.048053
s 87    -1.00   TORS    23   31   17    1   HClHC     0.11  f73 76
        -1.00           19    3    4   27   HCNH     0.06
        -1.00           17    1    2    3   HCCC  -179.98
         1.00           24    9   10   11   HCCC  -180.02
s 88     1.00   TORS    30   33   24    9   HClHC    -0.11  f72 74
         1.00           23   31   17    1   HClHC     0.11
         1.00           17    1    2    3   HCCC  -179.98
         1.00           24    9   10   11   HCCC  -180.02
k 89     1.00   BEND     4   27   15   NHN   149.67  f62 63  f32 13
         1.00            7   20   12   NHN   149.67
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        1.00           8   23   31   NHCl   174.39
        1.00          27    4    5   HNN    151.91
        1.00          16   29   34   NHCl   153.59
        1.00           8   22   32   NHCl   153.59
        1.00          20    7   21   HNH    123.48
s 90    1.00   TORS   30   16   29   34   HNHCl  -180.02  f57 66  f25 13
        1.00          28   15   27    4   HNHN    -0.09
        1.00          21    7    6    5   HNCN  -180.03
       -1.00          22    8    6    5   HNCN  -179.97
        1.00           3    4   27   15   CNHN     0.03
s 91    1.00   TORS   14   16   29   34   CNHCl     0.00  f51 66
        1.00           6    8   22   32   CNHCl     0.00
        1.00          22    8    6    5   HNCN  -179.97
        1.00          29   16   14   13   HNCN  -180.03
        1.00          27   15   14   13   HNCN    -0.05
        1.00           5    4   27   15   NNHN  -179.84
       -1.00   OUT    14    9   12   13   CCNN     0.00
       -1.00           6    1    4    5   CCNN     0.00
s 92    1.00   STRE    4   27   NH    2.295113  f62 14  f32 68
        1.00          34   28   ClH    2.176647
        1.00          12   20   NH    2.295113
        1.00          32   21   ClH    2.176647
       -1.00          32   22   ClH    2.155887
s 93   -1.00   TORS   14   16   29   34   CNHCl     0.00  f26 63
        1.00           5    4   27   15   NNHN  -179.84
       -1.00           6    8   22   32   CNHCl     0.00
        1.00          23    8   22   32   HNHCl  -179.98
       -1.00          22    8    6    5   HNCN  -179.97
        1.00          30   16   29   34   HNHCl  -180.02
        1.00          27   15   14   13   HNCN    -0.05
       -1.00          29   16   14   13   HNCN  -180.03
        1.00   OUT    14    9   12   13   CCNN     0.00
       -1.00   TORS   12   13   14   15   NNCN    -0.04
       -1.00           4    5    6    8   NNCN  -179.96
       -1.00   OUT    16   13   15   14   NNNC     0.00
s 94   -1.00   TORS    5    4   27   15   NNHN  -179.84  f25 65
        1.00           3    4   27   15   CNHN     0.03
        1.00          27   15   14   13   HNCN    -0.05
s 95   -1.00   STRE    4   27   NH    2.295113  f22 88
        1.00          12   20   NH    2.295113
       -1.00          34   28   ClH    2.176647
s 96    1.00   TORS   14   15   27    4   CNHN  -180.01  f10 71
        1.00          27    4    5    1   HNNC  -180.13
```