

## Supplementary Material

### X-ray evidence for the relationship between pyridyl side chain basicity and the *Z/E* preferences of 5-halogen substituted (pyridin-2-yl)aminomethane-1,1-diphosphonic acids; implications for metal ions coordination in solution

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**Dedicated to Prof. Pawel Kafarski to honor the achievements within his career**

**Table S1.** Geometry of hydrogen bonds and close contacts for **1-a**, **2-a** and **3-a** (Å, deg) (all data)

Compound	<i>D</i> –H··· <i>A</i>	<i>D</i> –H (Å)	H··· <i>A</i> (Å)	<i>D</i> ··· <i>A</i> (Å)	<i>D</i> –H··· <i>A</i> (deg)
<b>1-a</b>	O2–H2···O3 <sup>i</sup>	0.83	1.96	2.546 (2)	127
	O3–H3···O2 <sup>i</sup>	0.83	1.73	2.546 (2)	168
	O5–H5···O6 <sup>ii</sup>	0.83	1.75	2.555 (2)	162
	O6–H6···O5 <sup>ii</sup>	0.83	1.73	2.555 (2)	169
	N11–H11···O3	0.87	2.26	2.928 (3)	134
	N11–H11···O6	0.87	2.12	2.798 (3)	135
	N41–H41A···O5 <sup>iii</sup>	0.87	1.95	2.764 (3)	156
	N41–H41B···O2 <sup>iv</sup>	0.87	2.10	2.804 (3)	138
	N12–H12···O1	0.87	2.53	3.125 (4)	126
	N12–H12···O4	0.87	2.15	2.890 (3)	142
	N42–H42B···O1W	0.87	2.04	2.892 (4)	168
	N42–H42A···O2W	0.87	2.25	3.099 (7)	165
	O1W–H1W···O3W	0.84	1.99	2.814 (3)	166
	O1W–H2W···O4W	0.84	1.96	2.797 (9)	174
	O2W–H3W···O3W <sup>v</sup>	0.84	2.10	2.836 (5)	146
	O2W–H4W···O4 <sup>iii</sup>	0.84	2.04	2.763 (4)	144

	O3W–H5W…O1 <sup>iv</sup>	0.84	1.88	2.722 (3)	174
	O3W–H6W…O2W <sup>vi</sup>	0.84	2.12	2.960 (10)	174
	O4W–H7W…O1 <sup>vii</sup>	0.84	1.97	2.804 (7)	170
	C6–H16…N2 <sup>viii</sup>	0.94	2.50	3.348 (3)	151
	C21–H21…O6	0.94	2.58	3.038 (3)	110
	C62–H62…O1	0.94	2.53	3.136 (4)	123
<b>2-a</b>	O2–H2…O3 <sup>i</sup>	0.83	1.75	2.549 (2)	161
	O3–H3…O2 <sup>i</sup>	0.83	1.73	2.549 (2)	168
	O6–H6…O5 <sup>ii</sup>	0.83	1.75	2.571 (2)	171
	N11–H11…O3	0.87	2.21	2.905 (3)	137
	N11–H11…O6	0.87	2.18	2.845 (3)	132
	N41–H41A…O5 <sup>iii</sup>	0.87	1.94	2.762 (3)	156
	N41–H41B…O2 <sup>iv</sup>	0.87	2.12	2.825 (3)	138
	N12–H12…O1	0.87	2.58	3.166 (4)	125
	N12–H12…O4	0.87	2.13	2.883 (3)	144
	N42–H42A…O1W	0.87	2.06	2.913 (4)	168
	N42–H42B…O2W	0.87	2.31	3.146 (9)	162
	O1W–H1W…O3W	0.84	2.04	2.835 (3)	159
	O1W–H2W…O4W	0.84	1.95	2.786 (8)	174
	O2W–H3W…O3W <sup>v</sup>	0.84	2.15	2.835 (5)	138
	O2W–H4W…O4 <sup>iii</sup>	0.84	2.05	2.769 (5)	144
	O3W–H5W…O1 <sup>iv</sup>	0.84	1.88	2.721 (2)	174
	O3W–H6W…O2W <sup>vi</sup>	0.84	2.12	2.954 (14)	175
	O4W–H7W…O1 <sup>vii</sup>	0.84	1.95	2.792 (6)	176
	C6–H16…N2 <sup>viii</sup>	0.94	2.49	3.355 (3)	154
	C21–H21…O6	0.94	2.55	3.043 (3)	113
	C62–H62…O1	0.94	2.53	3.163 (4)	124
<b>3-a</b>	O3–H3…O2 <sup>i</sup>	0.84	1.74	2.581 (2)	175
	O6–H6…O5 <sup>ii</sup>	0.84	1.74	2.559 (2)	164
	N1–H1N…O2 <sup>i</sup>	0.88	2.60	3.179 (2)	124
	N11–H11…O3	0.88	2.53	3.110 (3)	124
	N11–H11…O5	0.88	1.95	2.734 (2)	148
	N41–H41A…O6 <sup>iii</sup>	0.88	2.09	2.898 (2)	152
	N41–H41B…O2 <sup>iv</sup>	0.88	1.96	2.753 (2)	150
	N12–H12…O4	0.88	1.94	2.746 (2)	152

	N42-H42B...O1W	0.88	2.04	2.871 (3)	157
	N42-H42A...O2W	0.88	2.30	2.951 (2)	130
	O1W-H1W...O3W	0.84	2.10	2.915 (2)	163
	O1W-H2W...O4W	0.84	1.87	2.698 (8)	170
	O2W-H3W...O3W <sup>v</sup>	0.84	2.06	2.803 (2)	147
	O2W-H30W...O4W <sup>v</sup>	0.84	2.04	2.842 (7)	161
	O2W-H4W...O4 <sup>iii</sup>	0.84	1.95	2.766 (2)	164
	O3W-H5W...O1 <sup>iv</sup>	0.84	1.98	2.776 (2)	157
	O3W-H60W...O3W <sup>ix</sup>	0.84	2.02	2.856 (3)	173
	O4W-H7W...O1 <sup>vii</sup>	0.84	1.91	2.748 (7)	173
	O4W-H8W...O4W <sup>v</sup>	0.84	2.46	3.199 (18)	147
	C6-H16...N2 <sup>viii</sup>	0.95	2.51	3.376 (3)	152
	C22-H22...O1W <sup>x</sup>	0.95	2.44	3.231 (3)	140
	C61-H61...O3	0.95	2.48	3.103 (3)	123
	C62-H62...O1	0.95	2.44	3.158 (3)	132

**Symmetry codes:** (i)  $-x, -y+1, -z+1$ ; (ii)  $-x+1, -y+1, -z+1$ ; (iii)  $x, y+1, z$ ; (iv)  $x+1, y+1, z$ ; (v)  $-x+2, -y+3, -z+2$ ; (vi)  $x+1, y, z$ ; (vii)  $-x+1, -y+2, -z+2$ ; (viii)  $-x, -y, -z+1$ ; (ix)  $-x+3, -y+3, -z+2$ ; (x)  $-x+2, -y+2, -z+2$ .