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. Paweł 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	*D*–H···*A*	*D*–H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*–H···*A* (deg)
1-a	O2–H2···O3^{i}	0.83	1.96	2.546 (2)	127
	O3–H3···O2^{i}	0.83	1.73	2.546 (2)	168
	O5–H5···O6^{ii}	0.83	1.75	2.555 (2)	162
	O6–H6···O5^{ii}	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–H41*A*···O5^{iii}	0.87	1.95	2.764 (3)	156
	N41–H41*B*···O2^{iv}	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–H42*B*···O1*W*	0.87	2.04	2.892 (4)	168
	N42–H42*A*···O2*W*	0.87	2.25	3.099 (7)	165
	O1*W*–H1*W*···O3*W*	0.84	1.99	2.814 (3)	166
	O1*W*–H2*W*···O4*W*	0.84	1.96	2.797 (9)	174
	O2*W*–H3*W*···O3*W*^{v}	0.84	2.10	2.836 (5)	146
	O2*W*–H4*W*···O4^{iii}	0.84	2.04	2.763 (4)	144

	O3*W*–H5*W*···O1^{iv}	0.84	1.88	2.722 (3)	174
	O3*W*–H6*W*···O2*W*^{vi}	0.84	2.12	2.960 (10)	174
	O4*W*–H7*W*···O1^{vii}	0.84	1.97	2.804 (7)	170
	C6–H16···N2^{viii}	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
2-a	O2–H2···O3^{i}	0.83	1.75	2.549 (2)	161
	O3–H3···O2^{i}	0.83	1.73	2.549 (2)	168
	O6–H6···O5^{ii}	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–H41*A*···O5^{iii}	0.87	1.94	2.762 (3)	156
	N41–H41*B*···O2^{iv}	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–H42*A*···O1*W*	0.87	2.06	2.913 (4)	168
	N42–H42*B*···O2*W*	0.87	2.31	3.146 (9)	162
	O1*W*–H1*W*···O3*W*	0.84	2.04	2.835 (3)	159
	O1*W*–H2*W*···O4*W*	0.84	1.95	2.786 (8)	174
	O2*W*–H3*W*···O3*W*^{v}	0.84	2.15	2.835 (5)	138
	O2*W*–H4*W*···O4^{iii}	0.84	2.05	2.769 (5)	144
	O3*W*–H5*W*···O1^{iv}	0.84	1.88	2.721 (2)	174
	O3*W*–H6*W*···O2*W*^{vi}	0.84	2.12	2.954 (14)	175
	O4*W*–H7*W*···O1^{vii}	0.84	1.95	2.792 (6)	176
	C6–H16···N2^{viii}	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
3-a	O3–H3···O2^{i}	0.84	1.74	2.581 (2)	175
	O6–H6···O5^{ii}	0.84	1.74	2.559 (2)	164
	N1–H1*N*···O2^{i}	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–H41*A*···O6^{iii}	0.88	2.09	2.898 (2)	152
	N41–H41*B*···O2^{iv}	0.88	1.96	2.753 (2)	150
	N12–H12···O4	0.88	1.94	2.746 (2)	152

	N42–H42*B*···O1*W*	0.88	2.04	2.871 (3)	157
	N42–H42*A*···O2*W*	0.88	2.30	2.951 (2)	130
	O1*W*–H1*W*···O3*W*	0.84	2.10	2.915 (2)	163
	O1*W*–H2*W*···O4*W*	0.84	1.87	2.698 (8)	170
	O2*W*–H3*W*···O3*W*^{v}	0.84	2.06	2.803 (2)	147
	O2*W*–H30*W*···O4*W*^{v}	0.84	2.04	2.842 (7)	161
	O2*W*–H4*W*···O4^{iii}	0.84	1.95	2.766 (2)	164
	O3*W*–H5*W*···O1^{iv}	0.84	1.98	2.776 (2)	157
	O3*W*–H60*W*···O3*W*^{ix}	0.84	2.02	2.856 (3)	173
	O4*W*–H7*W*···O1^{vii}	0.84	1.91	2.748 (7)	173
	O4*W*–H8*W*···O4*W*^{v}	0.84	2.46	3.199 (18)	147
	C6–H16···N2^{viii}	0.95	2.51	3.376 (3)	152
	C22–H22···O1*W*^{x}	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.