Electronic Supplementary Information

Interaction of myo-inositol hexakisphosphate with biogenic and synthetic polyamines†

Julia Torres,[a] Claudia Giorgi,[b] Nicolás Veiga,[a] Carlos Kremer,*[a] Antonio Bianchi*[b]

[a]*Cátedra de Química Inorgánica, Departamento Estrella Campos, Facultad de Química, Universidad de la República, Gral. Flores 2124, Montevideo, Uruguay. E-mail: ckremer@fq.edu.uy*

[b]*Department of Chemistry "Ugo Schiff", University of Florence, Sesto Fiorentino, Italy. E-mail: antonio.bianchi@unifi.it*

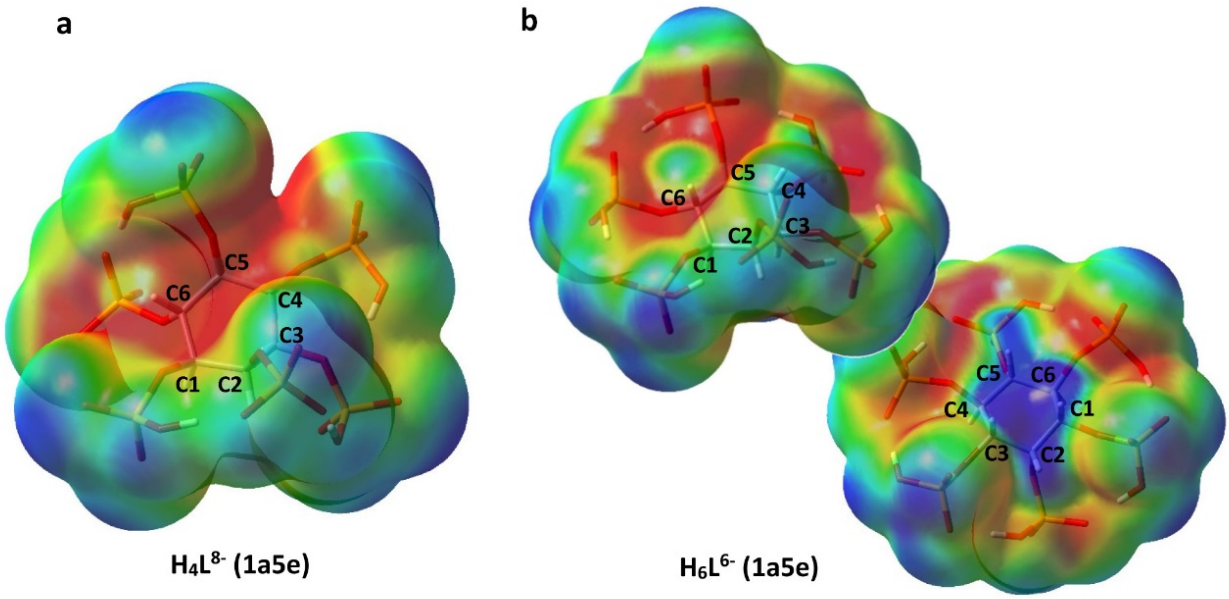
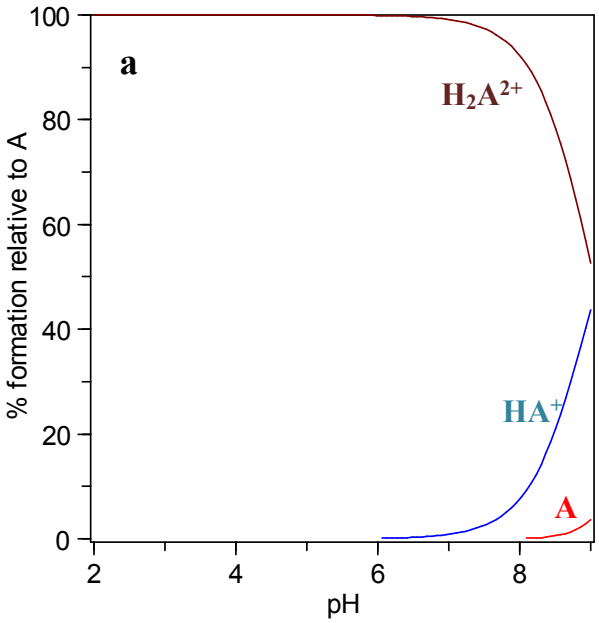


Fig. S1 RHF/3-21+G* geometries for the 1a5e conformer of two InsP_6 species: H_4L^{8-} (a) and H_6L^{6-} (b), taken from reference [1]. In all cases, the electrostatic potential is mapped on an isodensity surface (isodensity value = 0.0004 e, scale: -0.75 V (red) to -0.65 V (blue) for a, and -0.56 V (red) to -0.51 V (blue) for b). Color code: C (grey), H (white), O (red), P (orange).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4
6
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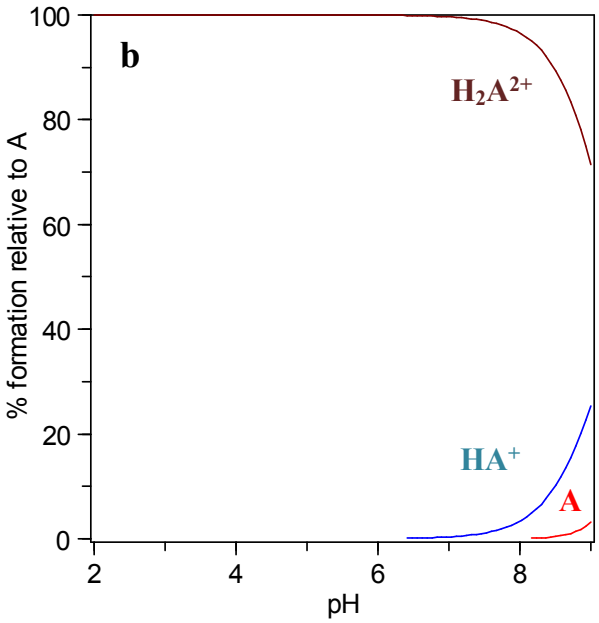
HA+
A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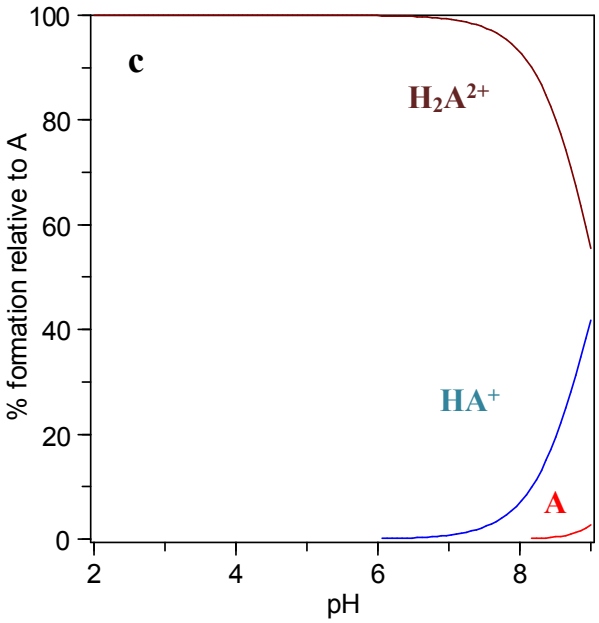
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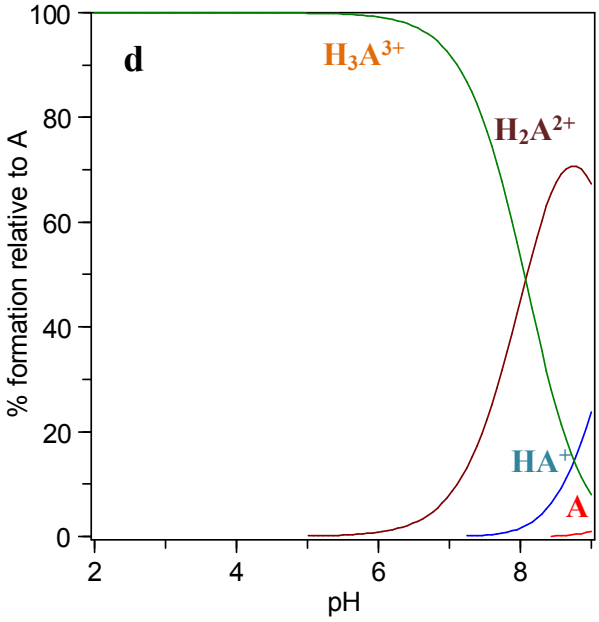
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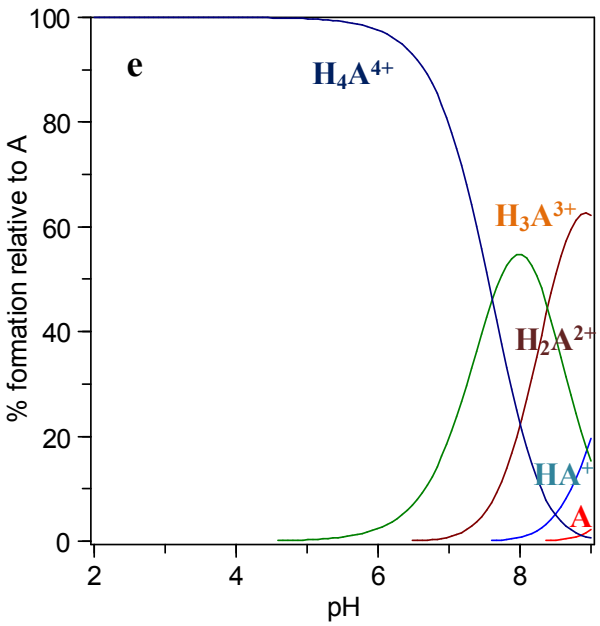
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HA^{+}
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% fomation relative to A
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6
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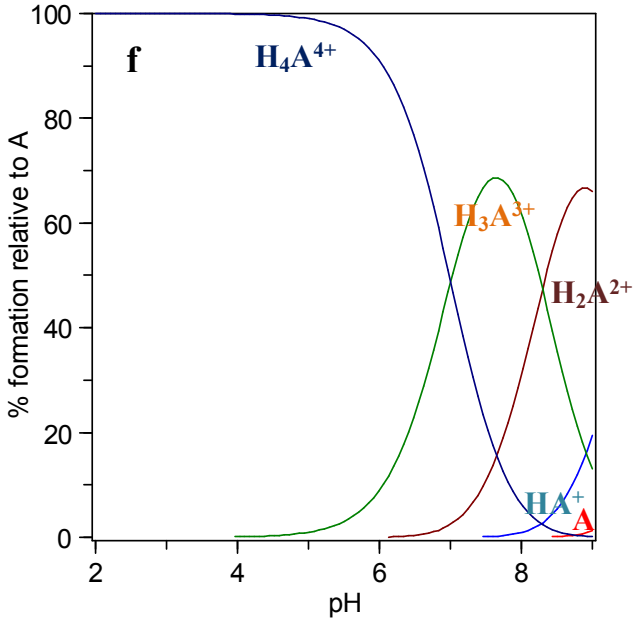
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% fomation relative to A
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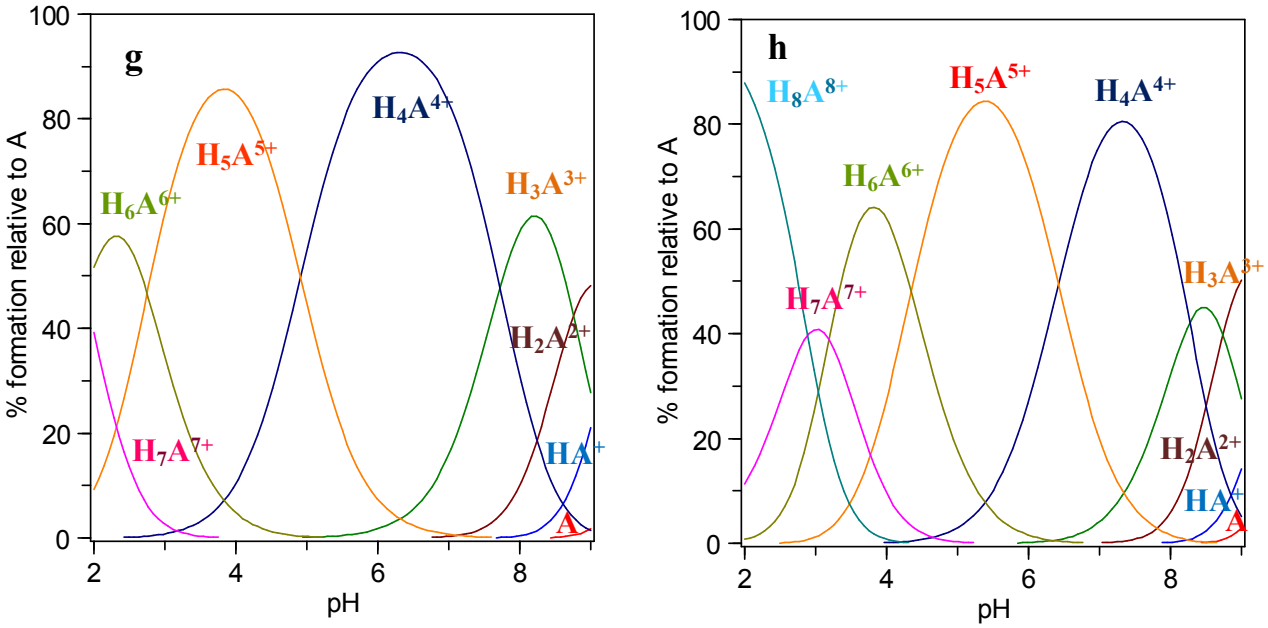
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HA^{+}
A
H_8A^{8+}

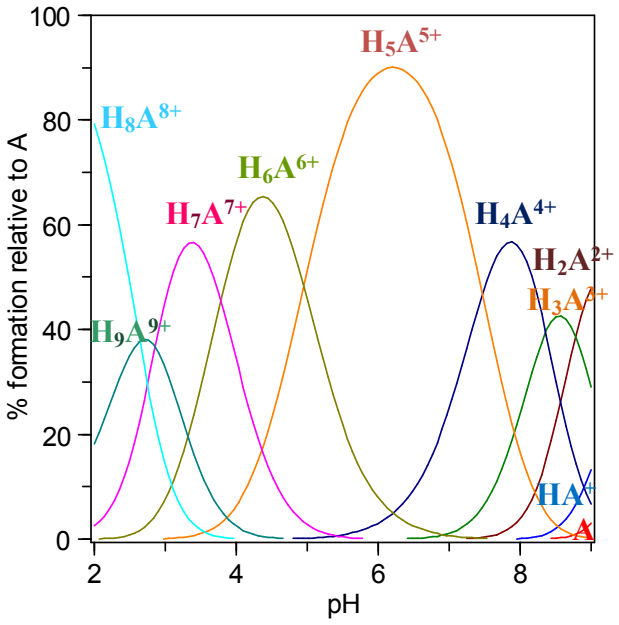

Fig. S2 Speciation of the amines (labelled as A): a) put; b) cad; c) agm; d) spd; e) spm; f) 3,3,3-tet; g) Me_2hexaen; h) Me_2heptaen; i) Me_2octaen.

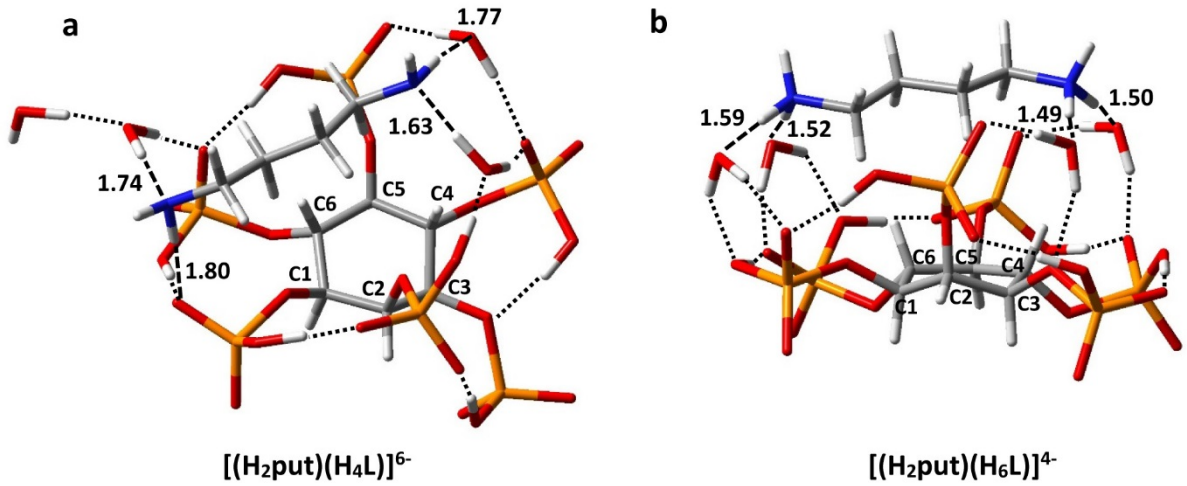

Fig. S3 RB3LYP/LANL2DZ geometries for $[(H_2put)H_4L]^{6-}$ (a) and $[(H_2put)H_6L]^{4-}$ (b) species. The O-H···N and O-H···O hydrogen bonds are shown as dashed and dotted lines, respectively, with the associated distances for the former in Å. Color code: C (grey), H (white), O (red), P (orange), N (blue).

Table S1 Relative formation constants of 1:1 complexes of InsP_6 (L^{12-}) with polyamines (A) calculated from Tables 1 and 2.

	put	cad	agm	spd	spm	3,3,3-tet	Me_2hexaen	Me_2heptaen	Me_2octaen
$HA^{+} + H_3L^{9-} \rightarrow [(HA)(H_3L)]^{8-}$	3.50(4)	3.90(6)	3.16(6)	2.7(3)	4.43(6)				
$H_2A^{2+} + H_3L^{9-} \rightarrow [(H_2A)(H_3L)]^{7-}$	4.39(4)	4.43(5)	3.7(2)	4.28(4)	5.30(1)	4.66(5)	4.0(2)	5.0(1)	5.6(1)
$H_2A^{2+} + H_4L^{8-} \rightarrow [(H_2A)(H_4L)]^{6-}$	4.02(6)	3.8(1)	3.6(1)	5.04(6)	6.43(6)	5.84(5)	5.86(6)	6.61(6)	7.12(7)
$H_2A^{2+} + H_5L^{7-} \rightarrow [(H_2A)(H_5L)]^{5-}$	3.72(8)	3.6(1)	4.5(1)						
$H_3A^{3+} + H_4L^{8-} \rightarrow [(H_3A)(H_4L)]^{5-}$				4.78(6)	7.03(5)	6.90(5)	6.34(7)	7.38(7)	8.18(7)
$H_3A^{3+} + H_5L^{7-} \rightarrow [(H_3A)(H_5L)]^{4-}$				3.78(9)					
$H_4A^{4+} + H_4L^{8-} \rightarrow [(H_4A)(H_4L)]^{4-}$					6.75(6)	7.48(6)	5.88(8)	6.86(8)	7.90(7)
$H_4A^{4+} + H_5L^{7-} \rightarrow [(H_4A)(H_5L)]^{3-}$					5.42(6)	6.10(6)	5.07(7)	6.39(8)	
$H_4A^{4+} + H_6L^{6-} \rightarrow [(H_4A)(H_6L)]^{2-}$					3.85(7)	4.60(8)	4.0(1)		
$H_5A^{5+} + H_4L^{8-} \rightarrow [(H_5A)(H_4L)]^{3-}$									7.15(7)
$H_5A^{5+} + H_5L^{7-} \rightarrow [(H_5A)(H_5L)]^{2-}$								5.1(1)	5.73(8)
$H_5A^{5+} + H_6L^{6-} \rightarrow [(H_5A)(H_6L)]^{-}$							3.90(8)	4.3(1)	5.06(7)

Table S2 Structural parameters for some of the 1:1 and 2:1 amine-InsP_6 species.

	Hydrogen bond mean distance		**Number of hydrogen bonds**	
	$d_{H\cdots O}$ (Å)[a]		**n[a]**	
Species	**A = N**	**A = O**	**A = N**	**A = O**
$[(H_2put)(H_4L)]^{6-}$	1.73	1.57	4	11
$[(H_2cad)(H_4L)]^{6-}$	1.80	1.63	5	12
$[(H_2agm)(H_4L)]^{6-}$	2.03	1.63	7	13
$[(H_3spd)(H_4L)]^{5-}$	1.96	1.72	4	15
$[(H_2put)_2(H_6L)]^{2-}$	1.54	1.70	8	20
$[(H_2cad)_2(H_6L)]^{2-}$	1.53	1.66	8	20
$[(H_2agm)_2(H_6L)]^{2-}$	1.82	1.62	11	21

a) $d_{H\cdots O}$ and n represent the average distance (proton-acceptor) and number of A-H···O hydrogen bonds, respectively, with A = N or O.

Table S3 Protonation data of polyamines (A) at 310.1 ± 0.1 K in 0.15 M Me_4NCl.

		log *K*	Δ*G*° (kJ/mol)	Δ*H*° (kJ/mol)	*T*Δ*S*° (kJ/mol)
put	$A + H^+ \rightarrow HA^+$	10.076(3)	-59.80(2)	-57.10(5)	2.70(5)
	$HA^+ + H^+ \rightarrow H_2A^{2+}$	9.080(7)	-53.89(4)	-57.81(5)	-3.92(6)
cad	$A + H^+ \rightarrow HA^+$	9.90(1)	-58.76(6)	-56.53(3)	2.23(7)
	$HA^+ + H^+ \rightarrow H_2A^{2+}$	9.45(2)	-56.1(6)	-56.10(6)	0.0(6)
agm	$A + H^+ \rightarrow HA^+$	10.179(7)	-60.42(4)	-54.73(5)	5.69(6)
	$HA^+ + H^+ \rightarrow H_2A^{2+}$	9.14(7)	-54.3(4)	-55.04(5)	-0.7(4)
spd	$A + H^+ \rightarrow HA^+$	10.369(8)	-61.54(5)	-50.88(2)	10.66(5)
	$HA^+ + H^+ \rightarrow H_2A^{2+}$	9.45(1)	-56.09(6)	-55.14(4)	0.95(7)
	$H_2A^{2+} + H^+ \rightarrow H_3A^{3+}$	8.07(3)	-47.9(2)	-49.04(4)	-1.14(2)
spm	$A + H^+ \rightarrow HA^+$	9.95(1)	-59.06(6)	-51.06(6)	8.00(8)
	$HA^+ + H^+ \rightarrow H_2A^{2+}$	9.50(2)	-56.4(1)	-52.15(5)	4.3(1)
	$H_2A^{2+} + H^+ \rightarrow H_3A^{3+}$	8.39(2)	-49.8(1)	-51.33(6)	-1.5(1)
	$H_3A^{3+} + H^+ \rightarrow H_4A^{4+}$	7.61(4)	-45.2(2)	-48.63(6)	-3.4(2)
3,3,3-tet	$A + H^+ \rightarrow HA^+$	10.157(4)	-60.29(2)	-52.4(1)	7.9(1)
	$HA^+ + H^+ \rightarrow H_2A^{2+}$	9.532(7)	-56.58(4)	-54.4(1)	2.2(1)
	$H_2A^{2+} + H^+ \rightarrow H_3A^{3+}$	8.30(1)	-49.26(6)	-54.0(1)	-4.7(1)
	$H_3A^{3+} + H^+ \rightarrow H_4A^{4+}$	7.01(2)	-41.6(1)	-50.3(1)	-8.7(1)
Me_2hexaen	$A + H^+ \rightarrow HA^+$	10.09(1)	-59.89(6)	-36.17(6)	23.72(8)
	$HA^+ + H^+ \rightarrow H_2A^{2+}$	9.36(3)	-55.6(2)	-43.25(5)	12.4(2)
	$H_2A^{2+} + H^+ \rightarrow H_3A^{3+}$	8.76(5)	-52.0(3)	-41.90(5)	10.1(3)
	$H_3A^{3+} + H^+ \rightarrow H_4A^{4+}$	7.72(8)	-45.8(5)	-42.87(5)	2.9(5)
	$H_4A^{4+} + H^+ \rightarrow H_5A^{5+}$	4.6(1)	-27.3(6)	-36.11(5)	-8.8(6)
	$H_5A^{5+} + H^+ \rightarrow H_6A^{6+}$	3.1 (2)	-18(1)	-31.67(6)	-14(1)
	$H_6A^{6+} + H^+ \rightarrow H_7A^{7+}$	2.2(2)	-13(1)	-25.79(7)	-13(1)
Me_2heptaen	$A + H^+ \rightarrow HA^+$	9.69(2)	-57.5(1)	-36.22(6)	21.3(1)
	$HA^+ + H^+ \rightarrow H_2A^{2+}$	9.55(4)	-56.7(2)	-43.75(5)	13.0(2)
	$H_2A^{2+} + H^+ \rightarrow H_3A^{3+}$	8.74(6)	-51.9(2)	-38.76(5)	13.1(3)
	$H_3A^{3+} + H^+ \rightarrow H_4A^{4+}$	8.3(1)	-49.3(6)	-42.77(5)	6.5(6)
	$H_4A^{4+} + H^+ \rightarrow H_5A^{5+}$	6.4(2)	-38(1)	-35.82(5)	2(1)
	$H_5A^{5+} + H^+ \rightarrow H_6A^{6+}$	4.4(3)	-26(2)	-28.66(5)	-3(2)
	$H_6A^{6+} + H^+ \rightarrow H_7A^{7+}$	3.2(3)	-19(2)	-31.85(6)	-13(2)
	$H_7A^{7+} + H^+ \rightarrow H_8A^{8+}$	2.9(4)	-17(2)	-26.3(1)	-9(2)
Me_2octaen	$A + H^+ \rightarrow HA^+$	9.65(2)	-57.3(1)	-42.92(6)	14.4(6)
	$HA^+ + H^+ \rightarrow H_2A^{2+}$	9.56(3)	-56.7(2)	-44.4(1)	12.3(2)
	$H_2A^{2+} + H^+ \rightarrow H_3A^{3+}$	8.78(4)	-52.1(2)	-44.40(9)	7.7(2)
	$H_3A^{3+} + H^+ \rightarrow H_4A^{4+}$	8.36(6)	-49.6(4)	-47.35(8)	2.3(4)
	$H_4A^{4+} + H^+ \rightarrow H_5A^{5+}$	7.47(8)	-44.3(5)	-45.30(8)	-1.0(5)
	$H_5A^{5+} + H^+ \rightarrow H_6A^{6+}$	5.0(1)	-29.7(6)	-37.00(9)	-7.3(6)
	$H_6A^{6+} + H^+ \rightarrow H_7A^{7+}$	3.8(2)	-23(1)	-37.1(1)	-14(1)
	$H_7A^{7+} + H^+ \rightarrow H_8A^{8+}$	2.9(2)	-17(1)	-32.5(1)	-16(1)
	$H_8A^{8+} + H^+ \rightarrow H_9A^{9+}$	2.6(3)	-15(2)	-27.2(2)	-12(2)

[a] Values in parentheses are standard deviation on the last significant figures.

Table S4 Thermodynamic data for the formation of InsP_6 (L^{12-}) complexes with cadaverine (A). 0.10 M Me_4NCl, 37.0 ± 0.1 °C.

Equilibrium	log*K*	Δ*G*° (kJ/mol)	Δ*H*° (kJ/mol)	*T*Δ*S*° (kJ/mol)
$HA^+ + H_3L^{9-} \rightarrow [(HA)(H_3L)]^{8-}$	3.90(6) [a]	-23.1(4)	-25.1(6)	-2.0(7)
$H_2A^{2+} + H_3L^{9-} \rightarrow [(H_2A)(H_3L)]^{7-}$	4.43(3)	-26.3(2)	77.8(5)	104.1(5)
$H_2A^{2+} + H_4L^{8-} \rightarrow [(H_2A)(H_4L)]^{6-}$	3.8(1)	-22.6(6)	79.8(5)	102.4(8)
$H_2A^{2+} + H_5L^{7-} \rightarrow [(H_2A)(H_5L)]^{5-}$	3.65(1)	-21.66(6)	89.0(5)	110.7(5)

[a] Values in parentheses are standard deviation on the last significant figures

Table S5 Thermodynamic data for the formation of InsP_6 (L^{12-}) complexes with agmatine (A). 0.10 M Me_4NCl, 37.0 ± 0.1 °C.

Equilibrium	log*K*	Δ*G*° (kJ/mol)	Δ*H*° (kJ/mol)	*T*Δ*S*° (kJ/mol)
$HA^{+} + H_3L^{9-} \rightarrow [(HA)(H_3L)]^{8-}$	3.16(6) [a]	-18.8(4)	-31.7(6)	-12.9(7)
$H_2A^{2+} + H_3L^{9-} \rightarrow [(H_2A)(H_3L)]^{7-}$	3.7(2)	-22(1)	37.9(5)	60(1)
$H_2A^{2+} + H_4L^{8-} \rightarrow [(H_2A)(H_4L)]^{6-}$	3.6(1)	-21.4(6)	27.5(5)	48.9(8)
$H_2A^{2+} + H_5L^{7-} \rightarrow [(H_2A)(H_5L)]^{5-}$	4.5(1)	-26.7(6)	19.8(5)	46.5(8)

[a] Values in parentheses are standard deviation on the last significant figures

Table S6 Thermodynamic data for the formation of InsP_6 (L^{12-}) complexes with spermidine (A). 0.10 M Me_4NCl, 37.0 ± 0.1 °C.

Equilibrium	log*K*	Δ*G*° (kJ/mol)	Δ*H*° (kJ/mol)	*T*Δ*S*° (kJ/mol)
$HA^{+} + H_3L^{9-} \rightarrow [(HA)(H_3L)]^{8-}$	2.7(3) [a]	-16(2)	b	b
$H_2A^{2+} + H_3L^{9-} \rightarrow [(H_2A)(H_3L)]^{7-}$	4.28(4)	-25.4(2)	-18.2(3)	7.2(3)
$H_2A^{2+} + H_4L^{8-} \rightarrow [(H_2A)(H_4L)]^{6-}$	5.04(6)	-29.9(4)	-42.7(3)	-12.8(5)
$H_3A^{3+} + H_4L^{8-} \rightarrow [(H_3A)(H_4L)]^{5-}$	4.78(6)	-28.4(4)	8.4(3)	36.8(5)
$H_3A^{3+} + H_5L^{7-} \rightarrow [(H_3A)(H_5L)]^{4-}$	3.78(9)	-22.4(5)	5.8(3)	28.2(6)

[a] Values in parentheses are standard deviation on the last significant figures. [b] Not determined.

Table S7 Thermodynamic data for the formation of InsP_6 (L^{12-}) complexes with spermine (A). 0.10 M Me_4NCl, 37.0 ± 0.1 °C.

Equilibrium	log*K*	Δ*G*° (kJ/mol)	Δ*H*° (kJ/mol)	*T*Δ*S*° (kJ/mol)
$HA^{+} + H_3L^{9-} \rightarrow [(HA)(H_3L)]^{8-}$	4.43(6) [a]	-26.3(4)	-15.0(7)	11.3(8)
$H_2A^{2+} + H_3L^{9-} \rightarrow [(H_2A)(H_3L)]^{7-}$	5.30(4)	-31.5(2)	-13.7(7)	17.8(7)
$H_2A^{2+} + H_4L^{8-} \rightarrow [(H_2A)(H_4L)]^{6-}$	6.43(6)	-38.2(4)	-88.2(9)	-50(1)
$H_3A^{3+} + H_4L^{8-} \rightarrow [(H_3A)(H_4L)]^{5-}$	7.03(5)	-41.7(3)	-42.8(7)	-1.1(8)
$H_4A^{4+} + H_4L^{8-} \rightarrow [(H_4A)(H_4L)]^{4-}$	6.75(6)	-40.1(4)	-5.9(7)	34.2(8)
$H_4A^{4+} + H_5L^{7-} \rightarrow [(H_4A)(H_5L)]^{3-}$	5.42(6)	-32.2(4)	8.5(7)	40.7(8)
$H_4A^{4+} + H_6L^{6-} \rightarrow [(H_4A)(H_6L)]^{2-}$	3.85(7)	-22.9(4)	-2.0(6)	20.9(7)

[a] Values in parentheses are standard deviation on the last significant figures.

Table S8 Thermodynamic data for the formation of InsP_6 (L^{12-}) complexes with Me_2heptaen (A). 0.10 M Me_4NCl, 37.0 ± 0.1 °C.

Equilibrium	log*K*	Δ*G*° (kJ/mol)	Δ*H*° (kJ/mol)	*T*Δ*S*° (kJ/mol)
$H_2A^{2+} + H_3L^{9-} \rightarrow [(H_2A)(H_3L)]^{7-}$	5.0(1) [a]	-29.7(6)	-43.5(6)	-13.8(8)
$H_2A^{2+} + H_4L^{8-} \rightarrow [(H_2A)(H_4L)]^{6-}$	6.61(6)	-39.2(4)	-76.1(5)	-36.9(6)
$H_3A^{3+} + H_4L^{8-} \rightarrow [(H_3A)(H_4L)]^{5-}$	7.38(7)	-43.8(4)	-63.2(5)	-19.4(6)
$H_4A^{4+} + H_4L^{8-} \rightarrow [(H_4A)(H_4L)]^{4-}$	6.86(8)	-40.7(5)	-58.1(5)	-17.4(7)
$H_4A^{4+} + H_5L^{7-} \rightarrow [(H_4A)(H_5L)]^{3-}$	6.39(8)	-37.9(5)	-64.3(5)	-26.4(7)
$H_5A^{5+} + H_5L^{7-} \rightarrow [(H_5A)(H_5L)]^{2-}$	5.1(1)	-30.3(6)	-14.0(4)	16.3(7)
$H_5A^{5+} + H_6L^{6-} \rightarrow [(H_5A)(H_6L)]^{-}$	4.3(1)	-25.5(6)	-44.0(5)	-18.5(8)

[a] Values in parentheses are standard deviation on the last significant figures.

Table S9 Thermodynamic data for the formation of InsP_6 (L^{12-}) complexes with Me_2octaen (A). 0.10 M Me_4NCl, 37.0 ± 0.1 °C.

Equilibrium	log*K*	Δ*G*° (kJ/mol)	Δ*H*° (kJ/mol)	*T*Δ*S*° (kJ/mol)
$H_2A^{2+} + H_3L^{9-} \rightarrow [(H_2A)(H_3L)]^{7-}$	5.6(1) [a]	-33.2(6)	-22.5(6)	10.7(8)
$H_2A^{2+} + H_4L^{8-} \rightarrow [(H_2A)(H_4L)]^{6-}$	7.12(7)	-42.3(4)	-67.8(5)	-25.5(6)
$H_3A^{3+} + H_4L^{8-} \rightarrow [(H_3A)(H_4L)]^{5-}$	8.18(7)	-48.6(4)	-66.9(4)	-18.3(6)
$H_4A^{4+} + H_4L^{8-} \rightarrow [(H_4A)(H_4L)]^{4-}$	7.90(7)	-46.9(4)	-56.3(4)	-9.4(6)
$H_5A^{5+} + H_4L^{8-} \rightarrow [(H_5A)(H_4L)]^{3-}$	7.15(7)	-42.4(4)	-23.1(5)	19.3(6)
$H_5A^{5+} + H_5L^{7-} \rightarrow [(H_5A)(H_5L)]^{2-}$	5.73(8)	-34.0(5)	-29.8(5)	4.2(7)
$H_5A^{5+} + H_6L^{6-} \rightarrow [(H_5A)(H_6L)]^{-}$	5.06(7)	-30.0(4)	-52.7(4)	-22.7(6)

[a] Values in parentheses are standard deviation on the last significant figures.

Table S10 Cumulative Δ*H*° values measured for the formation of InsP_6 (L^{12-}) complexes with polyamines in 0.10 M Me_4NCl at 37.0 ± 0.1 °C.

	1 1 4	1 1 5	1 1 6	1 1 7	1 1 8	1 1 9	1 1 10	1 1 11
put	-97.0(5) [a]	-116.3(4)	-96.3(3)	-110.6(3)				
cad	-106.0(5)	-59.2(4)	-56.5(4)	-45.5(4)				
agm	-110.8(5)	-96.2(5)	-105.9(4)	-11.8(4)				
spd		-148.6(2)	-172.4(2)	-170.3(2)	-171.1(2)			
spm	-90.4(6)	-141.3(6)	-215.1(8)	-221.0(6)	-232.7(6)	-216.5(6)	-217.7(5)	
Me_2hexaen		-173.5(4)	-174.6(2)	-210.5(2)	-223.8(3)	-227.9(3)	-233.2(3)	-240.6(3)
Me_2heptaen		-147.8(5)	-179.8(4)	-205.6(4)	-243.3(4)	-247.7(4)	-233.2(3)	-257.9(4)
Me_2octaen		-134.1(5)	-178.5(4)	-222.3(3)	-259.0(3)	-271.3(4)	276.1(4)	-293.6(3)

[a] Values in parentheses are standard deviation on the last significant figures.

Table S11 Cumulative $\Delta H°$ values measured for protonation of InsP_6 (L^{12-}) in 0.10 M Me_4NCl at 37.0 ± 0.1 °C.

	$\Delta H°$ (kJ/mol)
$L^{12-} + H^+$	9.90(8) [a]
$L^{12-} + 2H^+$	-20.23(8)
$L^{12-} + 3H^+$	-24.35(5)
$L^{12-} + 4H^+$	-23.68(7)
$L^{12-} + 5H^+$	-21.88(7)
$L^{12-} + 6H^+$	-16.53(5)
$L^{12-} + 7H^+$	-4.1(5)
$L^{12-} + 8H^+$	15.4(7)

[a] Values in parentheses are standard deviation on the last significant figures.

Table S12 Cumulative $\Delta H°$ values measured for protonation of polyamines in 0.10 M Me_4NCl at 37.0 ± 0.1 °C.

	1 1	1 2	1 3	1 4	1 5	1 6	1 7	1 8	1 9
Put	-57.10(5) [a]	-114.91(5)							
Cad	-56.53(3)	-112.63(3)							
Agm	-54.73(4)	-109.77(4)							
Spd	-50.88(2)	-106.02(2)	-155.06(2)						
Spm	-51.06(3)	-103.21(2)	-154.54(2)	-203.17(2					
3,3,3-tet	-52.4(1)	-106.8(1)	-160.8(1)	-211.1(1)					
Me_2hexaen	-36.17(6)	-79.41(5)	-121.31(5)	-164.18(5)	-200.30(5)	-231.96(5)	-257.75(6)		
Me_2heptaen	-36.22(6)	-79.97(5)	-118.73(5)	-161.50(5)	-197.33(5)	-225.99(5)	-257.84(6)	-284.1(1)	
Me_2octaen	-42.92(6)	-87.35(5)	-131.75(4)	-179.10(4)	-224.40(4)	-261.40(5)	-298.53(5)	-331.0(1)	-358.2(1)

[a] Values in parentheses are standard deviation on the last significant figures.

References

1 N. Veiga, J. Torres, I. Macho, K. Gomez, G. Gonzalez and C. Kremer, *Dalton Trans.*, 2014, **43**, 16238-16251.