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金属离子(Na^+、K^+、Ca^{2+}、Mg^{2+}、Zn^{2+})与鸟嘌呤异构体配合物的稳定性

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Stability of Complexes Combined by Metal Ions (Na^+, K^+, Ca^{2+}, Mg^{2+}, Zn^{2+}) and Guanine Isomers

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表 S1　各模型相对能量值

Table S1　Various relative energy obtained by different models

	PCM						COSMORS
	UAO	UAHF	UFF	PAULING	BONDI	KLAMT	KLAMT
$aG1Na^+$	0	0	0	0	0	0	0
$aG2Na^+$	5.64	17.8	4.8	9.9	31.9	15.8	14.4
$aG3Na^+$	16.3	19.1	18.3	16.6	20.6	19.1	17.9
$aG4Na^+$	28	28.8	31.9	25.6	22.9	28.7	26.2
$aG5Na^+$	34.7	39.3	34.7	26.3	29.1	34.9	36.0
$aG6Na^+$	37.8	46.6	37.1	47.3	62.6	46.9	47.1

Energy in $kJ \cdot mol^{-1}$

表 S2 液气两相中 Gn_xM^+配合物的各项能量

Table S2 Various energy of G and its complexes aGn_xM^+ and gGn_xM^+ (in parentheses)

M		***Na*$^+$**			***K*$^+$**		***G***	
	E_s	E_b	E_d	E_s	E_b	E_d	ΔE	E_s
$G1_xM^+$	-421.7	-12.1(-249.4 -220.5[a] -227.6[b])	0.8 (12.1)	-377.4	-11.7(-190.4 -176.6[b])	2.5 (7.1)	0.0/0.0[d] (2.1)	-156.5
$G2_xM^+$	-410.9	-8.4(-204.2 -184.9[a]-187.9[b])	0.4 (7.5)	-366.1	-7.5(-148.5 137.2[b])	0.4 (4.2)	3.4/2.2[d] (0)	-162.0
$G3_xM^+$	-411.3	-12.9(-233.0 -204.2[a])	0.8 (10.9)	-365.7	-10.5 (-175.3)	0.4 (6.7)	17.2 (26.4)	-174.5
$G4_xM^+$	-412.5	-16.3(-271.5 -241.4[a])	1.2 (13.4)	-368.2	-14.6 (-210.5)	0.4 (8.7)	31.1 (80.6)	-213.4
$G5_xM^+$	-411.3	-16.3(-272.8 -246.9[a])	0.4 (9.2)	-364.0	-12.6 (-212.1)	0.4 (6.3)	39.7 (81.2)	-207.1
$G6_xM^+$	-409.2	-5.9(-197.1 -176.6[a] -179.1[b])	0.4 (6.3)	-366.5	-7.5(-145.6 130.5[b])	0.4 (4.2)	31.1/29.3[d] (11.3)	-143.1
$G7_xM^+$	-410.5	-6.3(-214.6 -197.9[a])	1.3 (6.3)	-365.3	-6.7(-160.7 144.3[b])	0.4 (4.2)	36.5/35.3[d] (22.6)	-150.2
$G8_xM^+$	-410.5	-2.5(-173.6 -153.6[a] -158.2[b])	0.4 (6.3)	-362.1	-4.2(-125.1 111.8[b])	0.4 (4.2)	37.4 (14.2)	-141.4
$G9_xM^+$	-415.1	-1.7 (-211.3)	0.4 (6.7)	-361.5	-6.7 (-178.2)	0.4 (4.2)	55.8 (53.6)	-168.2
$G10_xM^+$	-416.3	-2.5 (-161.9)	0.4 6.3)	-363.6	-4.2 (-120.9)	0.1 (5.6)	59.8 (62.3)	-165.3
$G11_xM^+$	-411.3	-6.7 (-216.7)	0.4 (7.5)	-366.1	-7.1 (-162.8)	0.4 (5.0)	76.1 (92.1)	-178.2
$G12_xM^+$	-377.4	-13.4 (-217.2)	4.2 (7.9)	-364.7	-10.0 (-168.2)	0.3 (5.4)	55.6 (69.9)	-176.9
$G13_xM^+$	-403.3	-8.4 (180.7)	7.1 (9.2)	-366.1	-7.1 (-120.9)	0.4 (4.6)	76.6 (93.3)	-179.5

[a] values from Ref [12], [b] values from Ref[15], [d] values from Ref[24]. E_s, E_b and E_d indicate the energy values of solute-solvent interaction energy, binding energy and deformation energy, ΔE is the relative energy of guanine isomers. Energy in kJ•mol^{-1}

表 S3 液相中配合物 aGn_xM^+的各项相对能

Table S3 Various relative energy of G and its complexes aGn_xM^+

M											
				***Na*$^+$**					***K*$^+$**		aGn
	ΔE_s	ΔE_b	ΔE_d	ΔE_{bsd}	ΔE	ΔE_s	ΔE_b	ΔE_d	ΔE_{bsd}	ΔE	ΔE_G
$aG1_xM^+$	0	0	0	0	0	0	0	0	0	0	0
$aG2_xM^+$	10.8	3.7	-0.4	17.5	6.4	11.3	4.2	-2.1	16.8	7.0	3.4
$aG3_xM^+$	10.4	-0.8	0	26.8	17.2	11.7	1.2	-2.1	28.0	18.8	17.2
$aG4_xM^+$	9.2	-4.2	0.4	36.5	28.0	9.2	-2.9	-2.1	35.3	27.9	31.1
$aG5_xM^+$	10.4	-4.2	-0.4	45.5	36.8	13.4	-0.9	-2.1	50.1	39.5	39.7
$aG6_xM^+$	12.5	6.2	-0.4	49.4	37.3	10.9	4.2	-2.1	44.1	34.7	31.1
$aG7_xM^+$	11.2	5.8	0.5	54.0	41.1	12.1	5.0	-2.1	51.5	41.0	36.5
$aG8_xM^+$	11.2	9.6	-0.4	57.8	46.4	15.3	7.5	-2.1	58.1	48.1	37.4
$aG9_xM^+$	6.6	10.4	-0.4	72.4	57.7	15.9	5.0	-2.1	74.6	57.3	55.8
$aG10_xM^+$	5.4	9.6	-0.4	74.4	68.2	13.8	7.5	-2.4	78.7	74.1	59.8
$aG11_xM^+$	10.4	5.4	-0.4	91.5	85.4	11.3	4.6	-2.1	89.9	85.1	76.1
$aG12_xM^+$	44.3	-1.3	3.4	102.0	91.6	12.7	1.7	-2.2	67.8	61.9	55.6
$aG13_xM^+$	18.4	3.7	6.3	105.0	92.1	11.3	4.6	-2.1	90.4	85.8	76.5

ΔE_s, ΔE_b, and ΔE_d indicate the relative values of solute-solvent interaction energy, binding energy and deformation energy, respectively. ΔE and ΔE_G are the relative energy of complexes aGn_xM^+ and guanine isomers. $\Delta E_{bsd} = \Delta E_s + \Delta E_b + \Delta E_d + \Delta E_G$. Energy in $kJ \cdot mol^{-1}$

表 S4 液气两相中 Gn_xM^{2+}配合物的各项能量

Table S4 Various energy of complexes aGn_xM^{2+} and gGn_xM^{2+} (in parentheses)

M		***Ca^{2+}***			***Mg^{2+}***			***Zn^{2+}***	
	E_s	***E_b***	***E_d***	***E_s***	***E_b***	***E_d***	***E_s***	***E_b***	***E_d***
$G1_xM^{2+}$	-1225.1	-6.7(-662.7 -645.7[c])	2.1 (34.7)	-1341.8	-53.9(-896.2 -790.8[a] -879.0[c])	6.3 (55.6)	-1512.9	-56.5(-1087.0 -936.8[a])	10.0 (66.1)
$G2_xM^{2+}$	-1208.2	8.8(-565.7 555.6[c])	-21.7 (-21.8)	-1310.0	-28.0(-785.4 -713.8[a] -767.0[c])	9.2 (36.4)	-1514.2	-58.5(-975.7 -852.3[a])	4.2 (48.1)
$G3_xM^{2+}$	-1197.4	10.9 (-63.2)	0.4 (32.2)	-1332.4	-59.8(-856.0 -756.0[a])	10.5 (49.4)	-1501.6	-62.3(1043.9 -896.2[a])	12.6 (57.7)
$G4_xM^{2+}$	-1226.0	-17.2 (-717.6)	4.2 (38.5)	-1331.8	-63.2(-953.1 -847.7[a])	9.6 (57.7)	-1481.9	-66.1(-1148.1 -998.7[a])	11.7 (67.8)
$G5_xM^{2+}$	1215.5	-19.7 (-703.3)	2.9 (29.3)	-1325.5	-73.6(-942.7 -847.7[a])	10.5 (45.6)	-1493.3	-81.2(-1138.5 -994.5[a])	12.6 (52.7)
$G6_xM^{2+}$	-1211.2	-6.7(-540.1 -528.0[c])	56.1 (21.8)	-1335.9	-20.9(-758.1 -672.8[a] -739.6[c])	2.5 (40.6)	-1432.6	-43.9(-938.5 -807.1[a])	5.0 (52.3)
$G7_xM^{2+}$	-1229.1	1.0(-589.1 -579.1[c])	40.5 (21.8)	-1323.8	-27.6(-809.6 -733.5[a] -794.4[c])	8.2 (36.8)	-1381.5	-38.1(-1004.2 -873.2[a])	6.7 (48.5)
$G8_xM^{2+}$	-1187.9	-3.0(-503.8 -484.4[c])	48.9 (23.8)	-1271.9	-10.8(-705.0 -614.2[a] -689.6[c])	8.8 (39.7)	-1358.9	-16.7(-955.6 -789.9[a])	7.5 (91.2)
$G9_xM^{2+}$	-1217.1	5.0 (-578.2)	16.5 (22.6)	-1233.5	-9.2 (-803.7)	10.0 (38.5)	-1425.4	-57.7 (-1000.4)	5.0 (50.6)
$G10_xM^{2+}$	-1227.1	10.6 (-463.2)	18.0 (33.1)	-1302.5	-39.7 (-807.5)	-0.8 (53.9)	-1417.4	-66.1 (-1005.2)	1.9 (66.1)
$G11_xM^{2+}$	-1181.8	14.6 (-598.7)	53.2 (25.9)	-1297.9	-50.6 (-817.1)	2.9 (41.8)	-1398.7	-81.2 (1015.5)	5.4 (55.6)
$G12_xM^{2+}$	-1173.8	0 (-584.1)	-15.1 (-25.1)	-1311.3	-41.4 (-)	2.5 (-)	-1393.2	-34.3 (-1005.4)	63.6 (58.6)
$G13_xM^{2+}$	-1189.1	5.9 (-606.6)	7.5 (71.9)	-1247.2	-53.1 (-825.9)	9.6 (87.0)	-1360.2	-82.8 (1007.2)	12.6 (101.4)

[a] values from Ref [12], [c] values from Ref [16]. ***E_s***, ***E_b*** and ***E_d*** indicate the energy values of solute-solvent interaction energy, binding energy and deformation energy, respectively. Energy in $kJ•mol^{-1}$

表 S5 液相中配合物 aGn_xM^{2+}的各项相对能.

Table S5 Various relative energy of complexes aGn_xM^{2+}

M			***Mg*$^{2+}$**					***Ca*$^{2+}$**					***Zn*$^{2+}$**		
	ΔE_s	ΔE_b	ΔE_d	ΔE_{bsd}	ΔE	ΔE_s	ΔE_b	ΔE_d	ΔE_{bsd}	ΔE	ΔE_s	ΔE_b	ΔE_d	ΔE_{bsd}	ΔE
$aG1_xM^{2+}$	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
$aG2_xM^{2+}$	31.8	25.9	2.9	64.0	20.4	16.9	15.5	-23.8	12.0	12.6	-1.3	-2.0	-5.8	-5.7	-15.7
$aG3_xM^{2+}$	9.4	-5.9	4.2	24.9	4.9	27.7	17.6	-1.7	60.8	30.9	11.3	-5.8	2.6	25.3	3.2
$aG4_xM^{2+}$	10.0	-9.3	3.3	35.1	13.6	-0.9	-11.0	2.1	21.8	20.9	31.0	-9.6	1.7	54.2	12.8
$aG5_xM^{2+}$	16.3	-19.7	4.2	40.5	14.6	9.6	-13.0	0.8	37.1	25.0	19.6	-25.0	2.6	37.2	6.3
$aG6_xM^{+}$	5.9	33.0	-3.8	66.2	49.5	13.9	0	54.0	99.0	84.1	80.3	12.6	-5.0	119.0	29.6
$aG7_xM^{2+}$	18.0	26.3	1.9	82.7	53.1	-4.0	7.7	38.4	78.6	45.1	131.4	18.4	-3.3	183.0	39.1
$aG8_xM^{2+}$	69.9	43.1	2.5	152.9	76.6	37.2	3.7	46.8	125.1	84.3	154.0	39.8	-2.5	228.7	70.3
$aG9_xM^{2+}$	108.3	44.7	3.7	212.5	84.9	8.0	11.7	14.4	89.9	62.3	87.5	-1.2	-5.0	137.1	36.8
$aG10_xM^{2+}$	39.3	14.2	-7.1	106.2	64.0	-2.0	17.3	15.9	91.0	71.1	95.5	-9.6	-8.1	137.6	38.9
$aG11_xM^{2+}$	43.9	3.3	-3.4	119.9	72.8	43.3	21.3	51.1	191.8	103.3	114.2	-25.0	-4.6	161.0	43.1
$aG12_xM^{2+}$	30.5	12.5	-3.8	94.8	62.3	51.3	6.7	-17.2	96.4	75.7	119.7	22.2	53.6	251.1	126.4
$aG13_xM^{2+}$	94.6	0.8	3.3	175.3	77.0	36.0	12.6	5.4	130.6	99.2	152.7	-26.0	2.6	205.6	48.1

ΔE_s, ΔE_b, and ΔE_d indicate the relative values of solute-solvent interaction energy, binding energy and deformation energy, respectively. ΔE is the relative energy of complexes aGn_xM^{2+}. ΔE_{bsd} $=\Delta E_s + \Delta E_b + \Delta E_d + \Delta E_G$. Energy in kJ•mol^{-1}