Supplementary Information (SI) for CrystEngComm.

Crystal structures of potassium and cesium salts of adenine: the role of alkali cations

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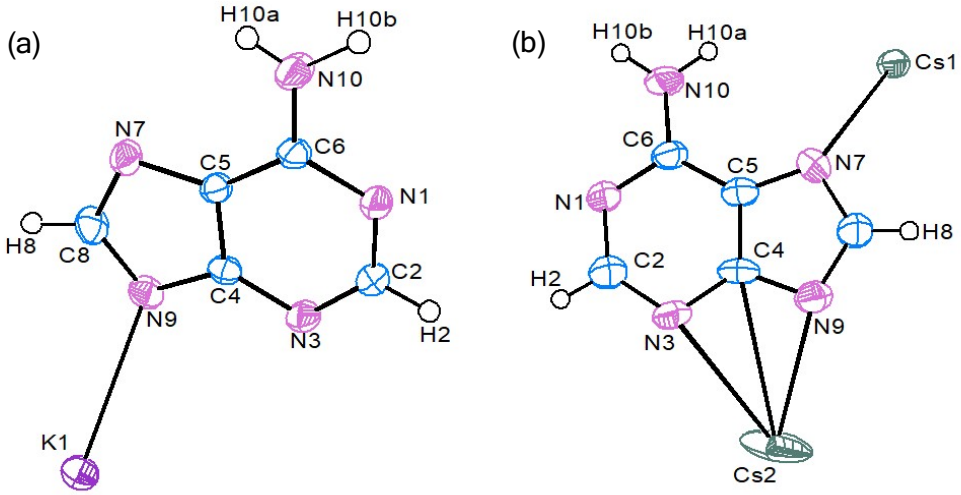

Figure S1. ORTEP drawings showing 50% probability ellipsoids of asymmetric units of (a) K-Adenine ($K^+C_5H_4N_5^-$) and, (b) Cs-Adenine ($Cs^+C_5H_4N_5^-$).

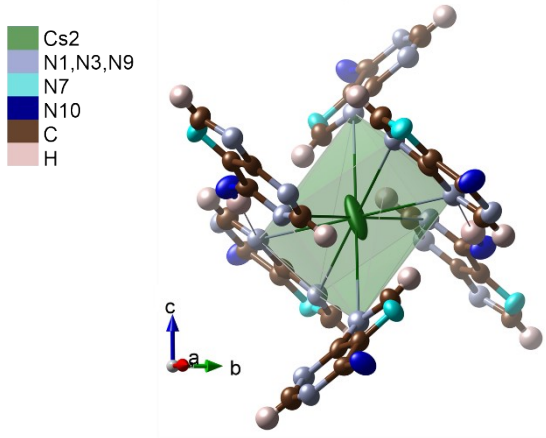

Figure S2. Anisotropic distortion and coordination environment of Cs2 in Cs-Adenine ($Cs^+C_5H_4N_5^-$).

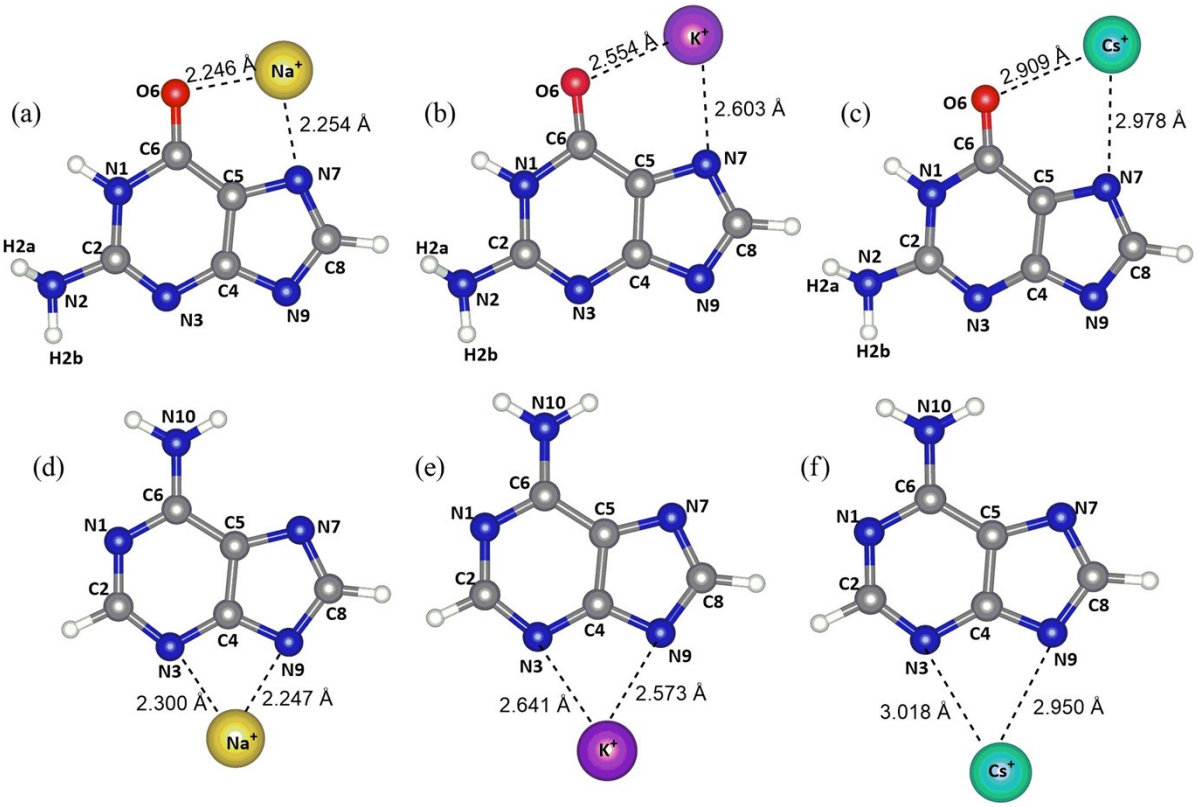

Figure S3. B3LYP-D3BJ/6-311+G(d) optimized geometries of (a) Na-Guanine, (b) K-Guanine, (c) Cs-Guanine, (d) Na-Adenine, (e) K-Adenine, and (f) Cs-Adenine.

Table S1. Crystal data, data collection and structure refinement details

Chemical formula	$K^+C_5H_4N_5^-$	$Cs^+C_5H_4N_5^-$
M_r	173.23	267.04
Crystal system, space group	Monoclinic, $P2_1$	Orthorhombic, *Pbcn*
Temperature (K)	293(2)	293(2)
a (Å)	6.6480(6)	12.7149(8)
b (Å)	7.4057(5)	11.1762(8)
c (Å)	7.1220(7)	10.8144(9)
α (°)	90	90
β (°)	113.802(11)	90
γ (°)	90	90
Volume (Å^3)	320.81(5)	1536.77(19)
Z	2	8
Radiation type	Mo Kα (λ = 0.71073 Å)	Mo Kα (λ = 0.71073 Å)
μ (mm^{-1})	0.753	4.757
ρ_{calc} g/cm^3	1.793	2.308
Crystal size/mm^3	0.4 × 0.25 × 0.1	0.5 × 0.5 × 0.3
Data Collection		
2Θ range for data collection/°	6.252 to 52.652	6.144 to 52.712
Index ranges	$-8 \le h \le 8$, $-9 \le k \le 9$, $-8 \le l \le 8$	$-15 \le h \le 15$, $-13 \le k \le 13$, $-13 \le l \le 13$
Reflections collected	3436	8275
Independent reflections	1286 [R_{int} = 0.0242, R_{sigma} = 0.0296]	1571 [R_{int} = 0.0365, R_{sigma} = 0.0258]
Data/restraints/parameters	1286/1/112	1571/0/108
Goodness-of-fit on F^2	1.064	1.113
Final R indexes [I>=2σ (I)]	R_1 = 0.0244, wR_2 = 0.0644	R_1 = 0.0551, wR_2 = 0.1358
Final R indexes [all data]	R_1 = 0.0265, wR_2 = 0.0650	R_1 = 0.0625, wR_2 = 0.1415
Largest diff. peak/hole / e Å^{-3}	0.21/-0.19	2.78/-3.40

Table S2. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $K^+C_5H_4N_5^-$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
N1	2301(4)	3385(4)	3548(3)	27.0(5)
C2	4496(5)	3138(5)	288(4)	27.2(6)
N3	6018(4)	3444(3)	6141(4)	26.6(5)
C4	5149(4)	4079(4)	7459(4)	21.6(6)
C5	2896(4)	4301(4)	6914(4)	21.7(6)
C6	1471(5)	3965(4)	4898(5)	24.2(6)
N7	2585(4)	4936(4)	8614(4)	28.1(5)
C8	4661(5)	5076(4)	10007(5)	28.5(6)
N9	6293(4)	4583(3)	9437(4)	26.3(5)
N10	-716(4)	4250(5)	4152(4)	40.3(8)
K11	10099.4(9)	6883.0(11)	10565.3(8)	29.66(19)

Table S3. Hydrogen Atom Coordinates ($Å \times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $K^+C_5H_4N_5^-$.

Atom	x	y	z	U(eq)
H2	5070(60)	2670(50)	3350(60)	36
H8	4940(60)	5530(50)	11320(60)	36
H10A	-1230(60)	4490(50)	4950(70)	36
H10B	-1690(60)	3850(50)	2730(60)	36

Table S4. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for $K^+C_5H_4N_5^-$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	21.8(12)	39.6(14)	20.1(10)	-3.8(11)	9.0(10)	-2.4(11)
C2	24.4(14)	32.1(15)	28.0(15)	-4.3(12)	13.7(13)	-1.9(12)
N3	19.6(12)	32.1(13)	28.6(12)	-0.8(11)	10.4(10)	1.8(10)
C4	17.5(13)	21.5(12)	23.9(14)	1.7(11)	6.3(12)	0.1(10)
C5	18.8(13)	26.0(13)	20.8(14)	0.4(10)	8.6(12)	-0.1(11)
C6	16.9(13)	34.4(16)	19.8(13)	-0.7(12)	5.8(11)	-1.3(11)
N7	23.2(12)	40.0(14)	19.9(11)	-4.6(12)	7.4(10)	0.6(11)
C8	27.2(15)	33.4(14)	19.9(12)	-1.0(13)	4.4(12)	2.1(12)
N9	20.1(12)	30.3(13)	23.6(12)	0.4(10)	3.6(11)	-0.5(10)
N10	16.1(12)	81(2)	21.8(13)	-9.2(13)	5.5(11)	1.0(14)
K11	23.8(3)	31.6(3)	30.3(3)	-0.7(3)	7.6(2)	-2.3(3)

Table S5. Bond Lengths for $K^+C_5H_4N_5^-$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C2	1.349(4)	C8	N9	1.353(4)
N1	C6	1.357(3)	C8	$K11^5$	3.481(3)
N1	$K11^1$	2.931(2)	N9	$K11^3$	3.123(2)
N1	$K11^2$	3.295(3)	N9	K11	2.883(2)
C2	N3	1.319(4)	N10	$K11^2$	3.426(3)
N3	C4	1.369(4)	K11	$N1^6$	3.295(3)
N3	$K11^3$	2.935(3)	K11	$N1^7$	2.931(2)
C4	C5	1.397(4)	K11	$N3^8$	2.935(3)
C4	N9	1.355(4)	K11	$C4^8$	3.319(3)
C4	$K11^3$	3.319(3)	K11	$N7^9$	3.079(3)

C5	C6	1.387(4)	K11	N7[10]	2.932(2)
C5	N7	1.389(4)	K11	C8[10]	3.481(3)
C6	N10	1.348(4)	K11	N9[8]	3.123(3)
N7	C8	1.340(4)	K11	N10[6]	3.426(3)
N7	K11[4]	3.079(3)	K11	K11[3]	3.7804(3)
N7	K11[5]	2.932(2)	K11	K11[8]	3.7804(3)

[1]1-X,-1/2+Y,1-Z; [2]-1+X,+Y,-1+Z; [3]2-X,-1/2+Y,2-Z; [4]1-X,-1/2+Y,2-Z; [5]1+X,+Y,+Z; [6]1+X,+Y,1+Z; [7]1-X,1/2+Y,1-Z; [8]2-X,1/2+Y,2-Z; [9]1-X,1/2+Y,2-Z; [10]1+X,+Y,+Z

Table S6. Bond Angles for $K^+C_5H_4N_5^-$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	N1	C6	116.8(2)	N1[6]	K11	K11[8]	57.13(5)
C2	N1	K11[1]	119.20(19)	N3[8]	K11	N1[7]	77.05(6)
C2	N1	K11[2]	113.94(17)	N3[8]	K11	C4[8]	24.30(7)
C6	N1	K11[1]	90.36(17)	N3[8]	K11	N7[10]	87.08(7)
C6	N1	K11[2]	127.96(18)	N3[8]	K11	C8[9]	73.56(7)
K11[2]	N1	K11[1]	74.52(6)	N3[8]	K11	N9[8]	47.18(7)
N3	C2	N1	129.8(2)	N3[8]	K11	N10[7]	88.92(7)
C2	N3	C4	112.3(2)	N3[8]	K11	K11[8]	74.23(5)
C2	N3	K11[3]	143.54(19)	N3[8]	K11	K11[3]	120.00(6)
C4	N3	K11[3]	93.76(17)	C4[8]	K11	C8[9]	60.85(7)
N3	C4	C5	123.5(3)	C4[8]	K11	N10[7]	111.89(7)
N3	C4	K11[3]	61.94(15)	C4[8]	K11	K11[3]	121.05(5)
C5	C4	K11[3]	154.90(19)	C4[8]	K11	K11[8]	63.62(5)
N9	C4	N3	126.3(2)	N7[1]	K11	N1[7]	126.55(6)
N9	C4	C5	110.2(2)	N7[9]	K11	N1[7]	74.35(6)
N9	C4	K11[3]	69.86(15)	N7[9]	K11	N3[8]	95.20(7)
C6	C5	C4	118.3(2)	N7[9]	K11	C4[8]	79.63(7)
C6	C5	N7	133.1(2)	N7[10]	K11	C4[8]	94.87(7)
N7	C5	C4	108.5(3)	N7[9]	K11	N7[10]	158.74(7)
N1	C6	C5	119.2(2)	N7[9]	K11	C8[9]	22.06(7)
N10	C6	N1	116.9(3)	N7[10]	K11	C8[9]	154.46(8)
N10	C6	C5	123.9(3)	N7[9]	K11	N9[8]	74.62(7)
C5	N7	K11[4]	152.87(19)	N7[10]	K11	N9[8]	91.95(7)
C5	N7	K11[5]	102.63(18)	N7[10]	K11	N10[7]	89.90(7)
C8	N7	C5	101.5(2)	N7[9]	K11	N10[7]	111.25(8)
C8	N7	K11[5]	114.8(2)	N7[9]	K11	K11[3]	52.78(5)
C8	N7	K11[4]	102.71(18)	N7[9]	K11	K11[8]	111.02(6)
K11[4]	N7	K11[5]	77.91(6)	N7[10]	K11	K11[8]	49.31(5)
N7	C8	N9	117.9(3)	N7[10]	K11	K11[3]	141.87(5)
N7	C8	K11[4]	55.24(15)	C8[9]	K11	K11[8]	108.02(6)
N9	C8	K11[4]	168.2(2)	C8[9]	K11	K11[3]	63.66(6)
C4	N9	K11[3]	86.10(16)	N9	K11	N1[6]	83.28(7)
C4	N9	K11	120.90(17)	N9	K11	N1[7]	80.03(7)
C8	N9	C4	101.8(2)	N9[8]	K11	N1[7]	111.23(6)
C8	N9	K11	118.47(19)	N9	K11	N3[8]	147.73(7)
C8	N9	K11[3]	151.9(2)	N9	K11	C4[8]	170.40(7)
K11	N9	K11[3]	77.91(6)	N9[8]	K11	C4[8]	24.04(6)
C6	N10	K11[1]	85.00(18)	N9	K11	N7[10]	88.63(7)
N1[6]	K11	N1[7]	149.74(8)	N9	K11	N7[9]	100.16(7)
N1[6]	K11	N3[8]	126.70(8)	N9[8]	K11	C8[9]	62.71(7)
N1[7]	K11	C4[8]	90.73(7)	N9	K11	C8[9]	116.63(8)
N1[6]	K11	C4[8]	106.19(7)	N9	K11	N9[8]	165.05(3)
N1[6]	K11	N7[9]	84.06(7)	N9	K11	N10[7]	59.09(7)
N1[6]	K11	N7[10]	77.74(6)	N9[8]	K11	N10[7]	135.84(7)
N1[6]	K11	C8[9]	100.36(7)	N9[8]	K11	K11[8]	48.21(5)
N1[7]	K11	C8[9]	65.83(7)	N9	K11	K11[8]	124.62(6)
N1[6]	K11	N9[8]	82.24(7)	N9[8]	K11	K11[3]	126.00(5)

N1[7]	K11	N10[7]	40.06(6)	N9	K11	K11[3]	53.88(5)
N1[6]	K11	N10[7]	140.80(7)	N10[7]	K11	C8[9]	105.87(8)
N1[6]	K11	K11[3]	101.58(6)	N10[7]	K11	K11[8]	135.55(6)
N1[7]	K11	K11[3]	48.36(4)	N10[7]	K11	K11[3]	66.35(6)
N1[7]	K11	K11[8]	151.12(5)	K11[3]	K11	K11[8]	156.76(3)

[1]-1+X,+Y,-1+Z; [2]1-X,-1/2+Y,1-Z; [3]2-X,-1/2+Y,2-Z; [4]-1+X,+Y,+Z; [5]1-X,-1/2+Y,2-Z; [6]1-X,1/2+Y,1-Z; [7]1+X,+Y,1+Z; [8]2-X,1/2+Y,2-Z; [9]1+X,+Y,+Z; [10]1-X,1/2+Y,2-Z

Table S7. Torsion Angles for $K^+C_5H_4N_5^-$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C2	N3	C4	1.2(5)	C6	C5	N7	K11[4]	-22.1(7)
N1	C2	N3	K11[1]	133.6(3)	N7	C5	C6	N1	178.0(3)
N1	C6	N10	K11[2]	-52.5(3)	N7	C5	C6	N10	0.8(6)
C2	N1	C6	C5	1.3(4)	N7	C8	N9	C4	0.4(4)
C2	N1	C6	N10	178.6(3)	N7	C8	N9	K11	135.6(2)
C2	N3	C4	C5	2.5(4)	N7	C8	N9	K11[1]	-103.8(4)
C2	N3	C4	N9	-177.3(3)	N9	C4	C5	C6	175.8(2)
C2	N3	C4	K11[1]	153.9(3)	N9	C4	C5	N7	-1.2(3)
N3	C4	C5	C6	-4.1(4)	K11[5]	N1	C2	N3	-171.2(3)
N3	C4	C5	N7	179.0(3)	K11[2]	N1	C2	N3	103.8(3)
N3	C4	N9	C8	-179.6(3)	K11[2]	N1	C6	C5	-122.1(2)
N3	C4	N9	K11	46.5(3)	K11[5]	N1	C6	C5	167.4(2)
N3	C4	N9	K11[1]	-26.9(3)	K11[2]	N1	C6	N10	55.3(3)
C4	C5	C6	N1	1.9(4)	K11[5]	N1	C6	N10	-15.2(4)
C4	C5	C6	N10	-175.2(3)	K11[1]	N3	C4	C5	-151.4(2)
C4	C5	N7	C8	1.3(3)	K11[1]	N3	C4	N9	28.8(3)
C4	C5	N7	K11[3]	-117.7(2)	K11[1]	C4	C5	C6	-98.8(5)
C4	C5	N7	K11[4]	154.2(3)	K11[1]	C4	C5	N7	84.2(5)
C5	C4	N9	C8	0.5(3)	K11[1]	C4	N9	C8	-152.7(2)
C5	C4	N9	K11	-133.36(19)	K11[1]	C4	N9	K11	73.41(13)
C5	C4	N9	K11[1]	153.2(2)	K11[4]	N7	C8	N9	-168.8(2)
C5	C6	N10	K11[2]	124.7(3)	K11[3]	N7	C8	N9	108.8(3)
C5	N7	C8	N9	-1.0(4)	K11[3]	N7	C8	K11[4]	-82.38(13)
C5	N7	C8	K11[4]	167.7(3)	K11[4]	C8	N9	C4	-51.2(11)
C6	N1	C2	N3	-3.1(5)	K11[4]	C8	N9	K11[1]	-155.3(8)
C6	C5	N7	C8	-175.1(3)	K11[4]	C8	N9	K11	84.1(11)
C6	C5	N7	K11[3]	66.0(4)					

[1]2-X,-1/2+Y,2-Z; [2]-1+X,+Y,-1+Z; [3]1-X,-1/2+Y,2-Z; [4]-1+X,+Y,+Z; [5]1-X,-1/2+Y,1-Z

Table S8. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for $Cs^+C_5H_4N_5^-$. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
N1	3652(5)	2535(6)	19(7)	37.6(15)
C2	2607(6)	2688(8)	-50(8)	42.4(19)
N3	1861(5)	2093(6)	549(7)	37.5(15)
C4	2260(5)	1252(7)	1339(7)	33.6(17)
C5	3328(6)	1026(7)	1494(7)	34.2(16)
C6	4040(6)	1690(7)	792(7)	34.3(16)

N7	3486(6)	134(6)	2330(7)	42.2(17)
C8	2477(7)	-111(8)	2657(8)	42.9(19)
N9	1708(5)	519(6)	2084(7)	39.6(15)
N10	5104(5)	1527(8)	839(8)	48.3(19)
Cs11	5000	-2088.5(6)	2500	33.2(2)
Cs12	0	0	0	99.8(6)

Table S9. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for $Cs^+C_5H_4N_5^-$.

Atom	x	y	z	U(eq)
H2	2376.51	3285.73	-583.54	51
H8	2320.55	-687.33	3249.34	51
H10A	5400(80)	960(90)	1380(90)	58
H10B	5620(80)	1970(80)	440(90)	58

Table S10. Anisotropic Displacement Parameters (Å^2×10^3) for $Cs^+C_5H_4N_5^-$. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N1	25(3)	42(4)	45(4)	7(3)	3(3)	2(3)
C2	30(4)	47(5)	51(5)	4(4)	3(4)	3(4)
N3	21(3)	47(4)	45(4)	-1(3)	1(3)	0(3)
C4	21(3)	38(4)	42(4)	-13(3)	-6(3)	6(3)
C5	24(3)	38(4)	41(4)	-4(3)	-1(3)	3(3)
C6	23(3)	46(4)	34(4)	-1(3)	1(3)	-1(3)
N7	37(4)	43(4)	46(4)	12(3)	-5(3)	4(3)
C8	33(4)	44(5)	51(5)	9(4)	3(4)	3(4)
N9	30(3)	43(4)	46(4)	0(3)	-3(3)	-3(3)
N10	20(3)	71(5)	54(5)	14(4)	2(3)	2(3)
Cs11	26.5(4)	36.4(4)	36.7(4)	0	-1.5(3)	0
Cs12	58.2(6)	42.2(5)	199.0(15)	-38.9(7)	-74.9(8)	12.7(4)

Table S11. Bond Lengths for $Cs^+C_5H_4N_5^-$.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
N1	C2	1.343(10)	N10	$Cs11^1$	3.668(8)
N1	C6	1.354(10)	Cs11	$N1^1$	3.257(7)
N1	$Cs11^1$	3.257(7)	Cs11	$N1^4$	3.257(7)
N1	$Cs12^2$	3.245(7)	Cs11	$N3^5$	3.299(6)
C2	N3	1.327(10)	Cs11	$N3^6$	3.299(6)
N3	C4	1.367(10)	Cs11	$C4^5$	3.644(7)
N3	$Cs11^3$	3.299(6)	Cs11	$C4^6$	3.644(7)
N3	Cs12	3.380(6)	Cs11	$N7^7$	3.148(7)
C4	C5	1.391(10)	Cs11	$N9^6$	3.474(7)
C4	N9	1.347(10)	Cs11	$N9^5$	3.474(7)
C4	$Cs11^3$	3.644(7)	Cs11	$N10^1$	3.668(8)
C4	Cs12	3.509(7)	Cs11	$N10^4$	3.668(8)
C5	C6	1.396(11)	Cs12	$N1^8$	3.245(7)
C5	N7	1.361(10)	Cs12	$N1^6$	3.245(7)
C6	N10	1.365(9)	Cs12	$N3^9$	3.380(6)
C6	$Cs11^1$	3.790(8)	Cs12	$C4^9$	3.509(7)
N7	C8	1.358(11)	Cs12	$N9^9$	3.183(7)
N7	Cs11	3.148(7)	Cs12	$Cs11^{10}$	4.2306(6)
C8	N9	1.355(11)	Cs12	$Cs11^3$	4.2306(6)

C8	Cs11	3.899(9)	Cs12	Cs12[11]	5.4072(5)
N9	Cs11[3]	3.474(7)	Cs12	Cs12[12]	5.4072(5)
N9	Cs12	3.183(7)			

[1]1-X,-Y,-Z; [2]1/2+X,1/2-Y,-Z; [3]-1/2+X,1/2+Y,1/2-Z; [4]+X,-Y,1/2+Z; [5]1/2+X,-1/2+Y,1/2-Z; [6]1/2-X,-1/2+Y,+Z; [7]1-X,+Y,1/2-Z; [8]-1/2+X,1/2-Y,-Z; [9]-X,-Y,-Z; [10]1/2-X,-1/2-Y,-1/2+Z; [11]-X,+Y,1/2-Z; [12]-X,+Y,-1/2-Z

Table S12. Bond Angles for $Cs^{+}C_5H_4N_5^{-}$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	N1	C6	119.0(7)	N7	Cs11	C4[5]	84.20(18)
C2	N1	Cs11[1]	119.6(5)	N7[7]	Cs11	C4[6]	84.20(18)
C2	N1	Cs12[2]	114.5(5)	N7	Cs11	C4[6]	154.72(19)
C6	N1	Cs11[1]	102.6(5)	N7[7]	Cs11	N7	75.8(3)
C6	N1	Cs12[2]	113.8(5)	N7	Cs11	N9[5]	102.55(17)
Cs12[2]	N1	Cs11[1]	81.19(15)	N7[7]	Cs11	N9[5]	175.72(18)
N3	C2	N1	128.0(8)	N7	Cs11	N9[6]	175.72(18)
C2	N3	C4	112.6(7)	N7[7]	Cs11	N9[6]	102.55(17)
C2	N3	Cs11[3]	133.3(5)	N7	Cs11	N10[4]	86.82(18)
C2	N3	Cs12	139.6(6)	N7	Cs11	N10[1]	77.60(18)
C4	N3	Cs11[3]	93.3(4)	N7[7]	Cs11	N10[1]	86.82(18)
C4	N3	Cs12	83.9(4)	N7[7]	Cs11	N10[4]	77.60(18)
Cs11[3]	N3	Cs12	78.59(13)	N9[6]	Cs11	C4[6]	21.65(17)
N3	C4	C5	124.2(7)	N9[5]	Cs11	C4[6]	98.38(17)
N3	C4	Cs11[3]	64.7(4)	N9[6]	Cs11	C4[5]	98.38(17)
N3	C4	Cs12	73.3(4)	N9[5]	Cs11	C4[5]	21.65(17)
C5	C4	Cs11[3]	145.1(5)	N9[5]	Cs11	N9[6]	79.3(2)
C5	C4	Cs12	141.0(5)	N9[5]	Cs11	N10[4]	106.36(17)
N9	C4	N3	126.8(7)	N9[6]	Cs11	N10[1]	106.36(17)
N9	C4	C5	109.0(7)	N9[6]	Cs11	N10[4]	88.96(17)
N9	C4	Cs11[3]	72.1(4)	N9[5]	Cs11	N10[1]	88.96(17)
N9	C4	Cs12	65.0(4)	N10[4]	Cs11	N10[1]	160.3(3)
Cs12	C4	Cs11[3]	72.50(13)	N1[5]	Cs12	N1[8]	180.00(18)
C4	C5	C6	118.1(7)	N1[5]	Cs12	N3[9]	77.48(15)
N7	C5	C4	110.9(7)	N1[8]	Cs12	N3[9]	102.52(15)
N7	C5	C6	130.9(7)	N1[8]	Cs12	N3	77.48(15)
N1	C6	C5	118.0(7)	N1[5]	Cs12	N3	102.52(15)
N1	C6	N10	118.5(7)	N1[5]	Cs12	C4	84.46(16)
N1	C6	Cs11[1]	57.0(4)	N1[8]	Cs12	C4[9]	84.46(16)
C5	C6	Cs11[1]	141.5(5)	N1[5]	Cs12	C4[9]	95.54(16)
N10	C6	C5	123.5(8)	N1[8]	Cs12	C4	95.54(16)
N10	C6	Cs11[1]	74.5(5)	N1[8]	Cs12	Cs11[10]	130.47(12)
C5	N7	Cs11	135.0(5)	N1[5]	Cs12	Cs11[3]	130.47(12)
C8	N7	C5	100.4(7)	N1[8]	Cs12	Cs11[3]	49.53(12)
C8	N7	Cs11	113.8(5)	N1[5]	Cs12	Cs11[10]	49.53(12)
N7	C8	Cs11	47.6(4)	N1[5]	Cs12	Cs12[11]	90.36(12)
N9	C8	N7	117.2(7)	N1[8]	Cs12	Cs12[12]	90.36(12)
N9	C8	Cs11	150.3(6)	N1[5]	Cs12	Cs12[12]	89.64(12)
C4	N9	C8	102.3(6)	N1[8]	Cs12	Cs12[11]	89.64(12)
C4	N9	Cs11[3]	86.3(4)	N3[9]	Cs12	N3	180.0
C4	N9	Cs12	92.4(4)	N3	Cs12	C4	22.80(17)
C8	N9	Cs11[3]	142.4(6)	N3[9]	Cs12	C4	157.20(17)
C8	N9	Cs12	136.2(6)	N3[9]	Cs12	C4[9]	22.80(17)
Cs12	N9	Cs11[3]	78.78(15)	N3	Cs12	C4[9]	157.20(17)
C6	N10	Cs11[1]	84.5(5)	N3[9]	Cs12	Cs11[10]	49.86(11)
N1[1]	Cs11	N1[4]	162.4(2)	N3[9]	Cs12	Cs11[3]	130.14(11)

N1[4]	Cs11	N3[5]	96.61(16)	N3	Cs12	Cs11[3]	49.86(11)
N1[1]	Cs11	N3[5]	78.47(16)	N3	Cs12	Cs11[10]	130.14(11)
N1[1]	Cs11	N3[6]	96.61(16)	N3	Cs12	Cs12[11]	100.12(12)
N1[4]	Cs11	N3[6]	78.47(16)	N3[9]	Cs12	Cs12[11]	79.88(12)
N1[1]	Cs11	C4[5]	92.79(16)	N3[9]	Cs12	Cs12[12]	100.12(12)
N1[4]	Cs11	C4[6]	92.79(16)	N3	Cs12	Cs12[12]	79.88(12)
N1[4]	Cs11	C4[5]	78.20(16)	C4[9]	Cs12	C4	180.0
N1[1]	Cs11	C4[6]	78.20(16)	C4	Cs12	Cs11[3]	55.22(11)
N1[1]	Cs11	N9[5]	95.91(17)	C4[9]	Cs12	Cs11[10]	55.22(11)
N1[1]	Cs11	N9[6]	70.21(17)	C4	Cs12	Cs11[10]	124.78(11)
N1[4]	Cs11	N9[5]	70.21(17)	C4[9]	Cs12	Cs11[3]	124.78(11)
N1[4]	Cs11	N9[6]	95.91(17)	C4[9]	Cs12	Cs12[12]	114.37(13)
N1[1]	Cs11	N10[1]	38.88(16)	C4[9]	Cs12	Cs12[11]	65.63(13)
N1[4]	Cs11	N10[4]	38.88(16)	C4	Cs12	Cs12[12]	65.63(13)
N1[1]	Cs11	N10[4]	146.18(15)	C4	Cs12	Cs12[11]	114.37(13)
N1[4]	Cs11	N10[1]	146.18(15)	N9	Cs12	N1[5]	77.88(17)
N3[5]	Cs11	N3[6]	147.8(2)	N9	Cs12	N1[8]	102.12(17)
N3[5]	Cs11	C4[6]	130.15(17)	N9[9]	Cs12	N1[5]	102.12(17)
N3[5]	Cs11	C4[5]	22.00(17)	N9[9]	Cs12	N1[8]	77.88(17)
N3[6]	Cs11	C4[5]	130.15(17)	N9	Cs12	N3	43.27(17)
N3[6]	Cs11	C4[6]	22.00(17)	N9[9]	Cs12	N3	136.73(17)
N3[6]	Cs11	N9[5]	108.52(16)	N9	Cs12	N3[9]	136.73(17)
N3[6]	Cs11	N9[6]	108.52(16)	N9[9]	Cs12	N3[9]	43.27(17)
N3[6]	Cs11	N9[6]	41.89(17)	N9[9]	Cs12	C4[9]	22.55(18)
N3[5]	Cs11	N9[5]	41.89(17)	N9[9]	Cs12	C4	157.45(18)
N3[5]	Cs11	N10[1]	52.56(16)	N9	Cs12	C4	22.55(18)
N3[5]	Cs11	N10[4]	134.66(15)	N9	Cs12	C4[9]	157.45(18)
N3[6]	Cs11	N10[1]	134.66(15)	N9	Cs12	N9[9]	180.0
N3[6]	Cs11	N10[4]	52.56(16)	N9	Cs12	Cs11[10]	126.35(13)
C4[5]	Cs11	C4[6]	118.8(2)	N9	Cs12	Cs11[3]	53.65(13)
C4[6]	Cs11	N10[4]	73.70(17)	N9[9]	Cs12	Cs11[3]	126.35(13)
C4[6]	Cs11	N10[1]	117.06(16)	N9[9]	Cs12	Cs11[10]	53.65(13)
C4[5]	Cs11	N10[1]	73.70(17)	N9[9]	Cs12	Cs12[11]	44.92(13)
C4[5]	Cs11	N10[4]	117.06(16)	N9	Cs12	Cs12[11]	135.08(13)
N7[7]	Cs11	N1[4]	113.18(18)	N9[9]	Cs12	Cs12[12]	135.08(13)
N7[7]	Cs11	N1[1]	81.25(18)	N9	Cs12	Cs12[12]	44.92(13)
N7	Cs11	N1[1]	113.18(18)	Cs11[3]	Cs12	Cs11[10]	180.0
N7	Cs11	N1[4]	81.25(18)	Cs11[3]	Cs12	Cs12[11]	129.722(7)
N7[7]	Cs11	N3[6]	75.09(18)	Cs11[3]	Cs12	Cs12[12]	50.278(7)
N7	Cs11	N3[5]	75.09(18)	Cs11[10]	Cs12	Cs12[11]	50.278(7)
N7	Cs11	N3[6]	134.02(18)	Cs11[10]	Cs12	Cs12[12]	129.722(7)
N7[7]	Cs11	N3[5]	134.02(18)	Cs12[12]	Cs12	Cs12[11]	180.0
N7[7]	Cs11	C4[5]	154.72(19)				

[1]1-X,-Y,-Z; [2]1/2+X,1/2-Y,-Z; [3]-1/2+X,1/2+Y,1/2-Z; [4]+X,-Y,1/2+Z; [5]1/2-X,-1/2+Y,+Z; [6]1/2+X,-1/2+Y,1/2-Z; [7]1-X,+Y,1/2-Z; [8]-1/2+X,1/2-Y,-Z; [9]-X,-Y,-Z; [10]1/2-X,-1/2-Y,-1/2+Z; [11]-X,+Y,-1/2-Z; [12]-X,+Y,1/2-Z

Table S13. Torsion Angles for $Cs^{+}C_5H_4N_5^{-}$.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N1	C2	N3	C4	1.6(13)	N7	C5	C6	Cs11[2]	108.6(10)
N1	C2	N3	Cs11[1]	120.1(8)	N7	C8	N9	C4	-1.2(10)
N1	C2	N3	Cs12	-106.5(10)	N7	C8	N9	Cs11[1]	-101.3(10)
N1	C6	N10	Cs11[2]	-37.4(7)	N7	C8	N9	Cs12	105.7(9)
C2	N1	C6	C5	-0.8(12)	N9	C4	C5	C6	179.5(7)
C2	N1	C6	N10	178.9(8)	N9	C4	C5	N7	0.8(9)
C2	N1	C6	Cs11[2]	134.6(8)	Cs11[2]	N1	C2	N3	126.1(8)
C2	N3	C4	C5	-0.7(11)	Cs11[2]	N1	C6	C5	-135.4(6)
C2	N3	C4	N9	179.0(8)	Cs11[2]	N1	C6	N10	44.3(8)
C2	N3	C4	Cs11[1]	140.2(7)	Cs11[1]	N3	C4	C5	-140.9(7)
C2	N3	C4	Cs12	-141.7(7)	Cs11[1]	N3	C4	N9	38.9(8)
N3	C4	C5	C6	-0.7(12)	Cs11[1]	N3	C4	Cs12	78.15(14)
N3	C4	C5	N7	-179.4(7)	Cs11[1]	C4	C5	C6	-94.8(11)
N3	C4	N9	C8	-179.6(8)	Cs11[1]	C4	C5	N7	86.5(10)
N3	C4	N9	Cs11[1]	-36.6(7)	Cs11[1]	C4	N9	C8	-143.0(6)
N3	C4	N9	Cs12	42.0(8)	Cs11[1]	C4	N9	Cs12	78.59(15)
C4	C5	C6	N1	1.5(11)	Cs11	N7	C8	N9	-148.5(6)
C4	C5	C6	N10	-178.2(8)	Cs11	C8	N9	C4	-52.3(13)
C4	C5	C6	Cs11[2]	-69.8(10)	Cs11	C8	N9	Cs11[1]	-152.4(6)
C4	C5	N7	C8	-1.4(9)	Cs11	C8	N9	Cs12	54.5(15)
C4	C5	N7	Cs11	138.5(6)	Cs12[3]	N1	C2	N3	-140.2(8)
C5	C4	N9	C8	0.2(9)	Cs12[3]	N1	C6	C5	138.8(6)
C5	C4	N9	Cs11[1]	143.2(6)	Cs12[3]	N1	C6	N10	-41.5(9)
C5	C4	N9	Cs12	-138.2(5)	Cs12[3]	N1	C6	Cs11[2]	-85.8(3)
C5	C6	N10	Cs11[2]	142.2(8)	Cs12	N3	C4	C5	141.0(7)
C5	N7	C8	N9	1.7(10)	Cs12	N3	C4	N9	-39.3(7)
C5	N7	C8	Cs11	150.2(8)	Cs12	N3	C4	Cs11[1]	-78.15(14)
C6	N1	C2	N3	-0.9(14)	Cs12	C4	C5	C6	106.0(9)
C6	C5	N7	C8	-179.8(9)	Cs12	C4	C5	N7	-72.7(11)
C6	C5	N7	Cs11	-39.9(13)	Cs12	C4	N9	C8	138.4(6)
N7	C5	C6	N1	179.8(8)	Cs12	C4	N9	Cs11[1]	-78.59(15)
N7	C5	C6	N10	0.2(14)					

[1]-1/2+X,1/2+Y,1/2-Z; [2]1-X,-Y,-Z; [3]1/2+X,1/2-Y,-Z

Table S14. Cartesian coordinates of adenylate anion

N	-1.222812	-1.444326	-0.006366
N	-2.137148	0.686607	0.011026
N	-0.021769	1.924784	0.001252
N	1.929042	0.495925	0.003409
N	1.815938	-1.845551	-0.072478
C	-0.216781	-0.507821	-0.021902
C	-0.780888	0.799597	-0.007686
C	1.174146	-0.610013	-0.019571
C	-2.314872	-0.657248	0.011176
C	1.280915	1.683710	0.007551
H	-3.312686	-1.085863	0.027254
H	1.932678	2.556362	0.023050
H	2.744314	-1.831870	0.326096
H	1.237815	-2.610053	0.248293

Table S15. Cartesian coordinates of Na-adenylate

N	-0.480522	2.023126	0.001407
N	1.573933	0.986256	0.003343
N	0.794949	-1.313372	0.001223
N	-1.595099	-1.523437	0.005173
N	-3.048162	0.290927	-0.045475
C	-0.657132	0.658264	-0.005087
C	0.597757	0.033122	-0.001742
C	-1.775914	-0.186939	-0.006269
C	0.846491	2.144474	0.005133
C	-0.347850	-2.002878	0.005696
H	1.335431	3.110504	0.011054
H	-0.259248	-3.085701	0.013270
H	-3.800695	-0.351228	0.141913
H	-3.197318	1.271910	0.125937
Na	3.020547	-0.733295	-0.003477

Table S16. Cartesian coordinates of K-adenylate

N	-1.090084	1.988352	0.000415
N	1.082814	1.221486	0.007560
N	0.586190	-1.167925	0.004703
N	-1.766550	-1.661076	0.006095
N	-3.422695	-0.027183	-0.055311
C	-1.089797	0.613470	-0.006379
C	0.237099	0.148545	0.000126
C	-2.101002	-0.356227	-0.009000
C	0.211794	2.274533	0.008022
C	-0.468554	-1.984677	0.009400
H	0.572854	3.295867	0.015128
H	-0.252900	-3.050133	0.018813
H	-4.090130	-0.749321	0.162367
H	-3.676796	0.927843	0.139564
K	3.104316	-0.372300	-0.004900

Table S17. Cartesian coordinates of Cs-adenylate

N	-2.339699	1.945176	-0.001144
N	-0.107853	1.361244	0.013684
N	-0.414073	-1.066658	0.010718
N	-2.724968	-1.741898	0.006662
N	-4.502334	-0.237283	-0.067077
C	-2.223042	0.576210	-0.007920
C	-0.859104	0.220771	0.003727
C	-3.156151	-0.467433	-0.012261
C	-1.063625	2.334972	0.011071
C	-1.403102	-1.959969	0.013937
H	-0.788818	3.383461	0.019531
H	-1.106054	-3.006332	0.025912
H	-5.107025	-1.004690	0.178937
H	-4.819270	0.694046	0.151186
Cs	2.448615	-0.111234	-0.003033

Table S18. Cartesian coordinates of 9H-Guanylate anion

O	-0.174351	2.683351	0.009774
N	2.184259	0.684365	0.003171
N	-1.556988	0.843732	-0.006934
N	-0.718022	-1.428996	-0.008433
N	1.715921	-1.506024	0.005506
N	-2.991073	-0.970602	-0.075208
C	0.803857	0.502962	-0.005437
C	0.496067	-0.856292	-0.004455
C	-0.301327	1.453115	-0.002593
C	-1.674369	-0.476138	-0.017837
C	2.692454	-0.519278	0.006997
H	3.746252	-0.763228	0.012425
H	-3.079251	-1.885226	0.345225
H	-3.654234	-0.297248	0.281192
H	1.843271	-2.504646	-0.003799

Table S19. Cartesian coordinates of 1H-Guanylate anion

O	0.112449	2.680607	-0.012598
N	-2.259976	0.602844	0.021599
N	1.423546	0.808902	-0.003302
N	0.709409	-1.438399	0.001386
N	-1.712395	-1.640577	-0.011824
N	3.002476	-0.929718	-0.074006
C	-0.891983	0.466474	0.017148
C	-0.573029	-0.920133	-0.005618
C	0.138128	1.448652	0.003787
C	1.641921	-0.546447	-0.010915
C	-2.669306	-0.669622	0.003359
H	2.199588	1.439842	-0.144330
H	-3.724071	-0.926378	0.002393
H	3.049326	-1.939231	-0.006243
H	3.559756	-0.513997	0.665432

Table S20. Cartesian coordinates of Na-guanylate

O	-0.839810	-2.170535	-0.005273
N	-1.836094	0.721990	0.018293
N	1.265487	-1.231179	-0.004140
N	1.729413	1.095009	0.007171
N	-0.308121	2.439992	-0.010382
N	3.473125	-0.457077	-0.076604
C	-0.553014	0.207311	0.018209
C	0.370188	1.272296	-0.001893
C	-0.128289	-1.130800	0.007136
C	2.119649	-0.140508	-0.002836
C	-1.599953	2.047041	0.000905
H	1.639930	-2.162912	-0.121254
H	-2.409888	2.765807	-0.003672
H	4.040672	0.374954	0.012938
H	3.786398	-1.191080	0.545573
Na	-2.896072	-1.266881	-0.005536

Table S21. Cartesian coordinates of K-guanylate

O	-0.885757	-1.911647	0.004847
N	-1.336140	1.146533	0.026307
N	1.344811	-1.364983	-0.000925
N	2.238892	0.826956	0.002367
N	0.501310	2.532477	-0.012401
N	3.660140	-1.026764	-0.083109
C	-0.179756	0.387672	0.023387
C	0.935839	1.255198	-0.002791
C	-0.011122	-1.009278	0.013940
C	2.389356	-0.458930	-0.005772
C	-0.842669	2.397380	0.004484
H	1.534504	-2.350899	-0.118228
H	-1.495363	3.262235	0.000972
H	4.371925	-0.313419	0.001548
H	3.830744	-1.795734	0.552546
K	-3.145723	-0.723199	-0.010567

Table S22. Cartesian coordinates of Cs-guanylate

O	-0.078920	-1.691461	0.010083
N	-0.107826	1.420348	0.028995
N	2.198877	-1.445330	0.000139
N	3.388872	0.597338	-0.000543
N	1.911805	2.527775	-0.012738
N	4.539443	-1.437649	-0.086391
C	0.925164	0.501925	0.023771
C	2.155919	1.201873	-0.003881
C	0.898856	-0.908650	0.016372
C	3.358393	-0.695889	-0.008112
C	0.561031	2.584709	0.006757
H	2.248523	-2.447851	-0.117575
H	0.039928	3.535383	0.004767
H	5.341276	-0.826074	-0.007726
H	4.603910	-2.209490	0.565776
Cs	-2.591212	-0.222936	-0.004392