

Supporting Information

For

**A Lead-Filled G-Quadruplex:**

**Insight into the G-Quartet's Selectivity for Pb<sup>+2</sup> over K<sup>+</sup>**

010065120

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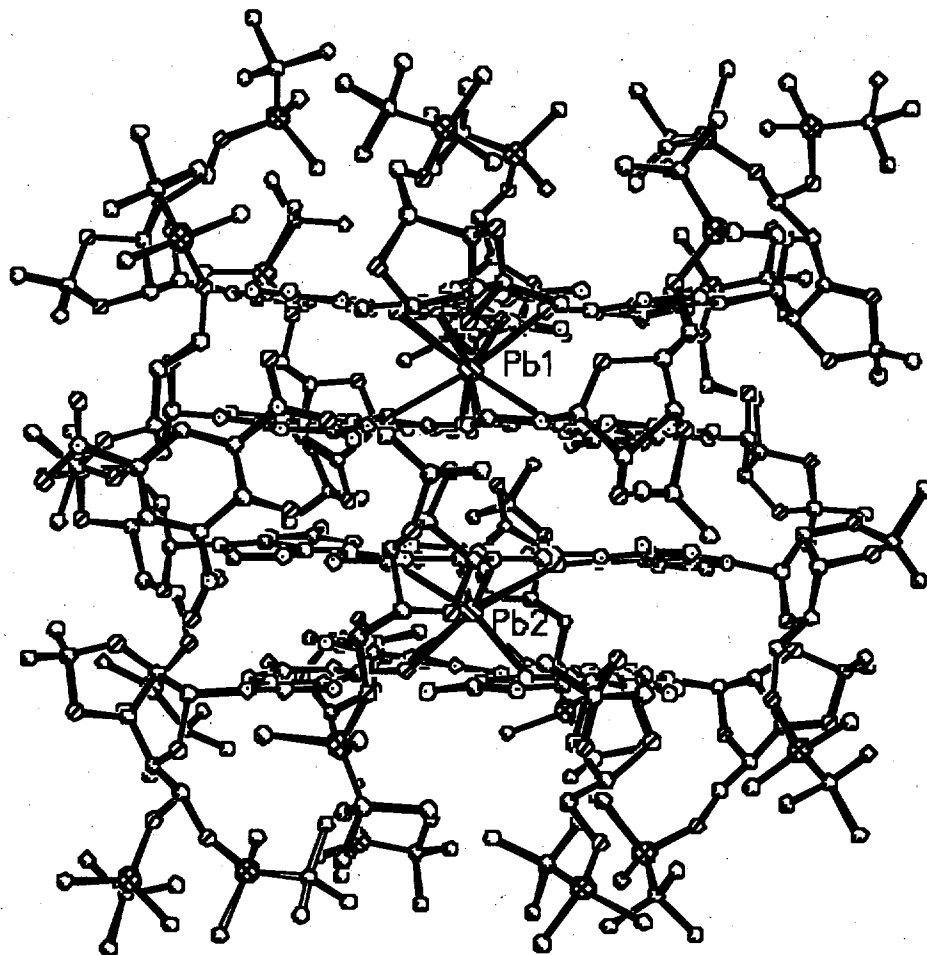
**UM624 Write-up**

A yellow crystalline block with dimensions 0.776 x 0.148 x 0.141 mm<sup>3</sup> was optically centered on the Bruker SMART CCD system at -80° C. The initial unit cell was indexed using a least-squares analysis of a random set of reflections collected from three series of 0.3° wide  $\omega$  scans (25 frames/series) that were well distributed in reciprocal space. Data frames were collected [MoK $\alpha$ ] with 0.3° wide  $\omega$ -scans, 60 seconds per frame, 700 frames per series. Six complete series were collected with an additional 160 frames with a repeat of the first series for redundancy and decay purposes. A crystal to detector distance of 8.962 cm was used, providing a complete sphere of data to  $2\theta_{\max} = 40^\circ$ . A total of 524613 reflections were collected and corrected for Lorentz and polarization effects and absorption using Blessing's method as incorporated into the program SADABS<sup>1,2</sup> with 88730 unique reflections [R(int)=0.1642].

**Structure Determination and Refinement.** Calculations were performed on a PC with dual Pentium 450 MHz processors and 384 MB of memory. The SHELXTL<sup>3</sup> program was used to determine the acentric orthorhombic space group P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub> (no. 19), and apply the absorption correction. The structure was determined by Patterson interpretation using the program XS<sup>4</sup>. Refinement with XL<sup>5</sup> and XH<sup>5</sup> and subsequent difference-Fourier maps and refinement cycles revealed atom locations. Disorder was modeled in a variety of locations within the G-quadruplexes. Disorder was prevalent in the solvent. Many of the sidechain t-butyltrimethylsilyl groups required construction via a series of DFIX<sup>5</sup> commands. During convergence, lead, silicon and chlorine atoms were refined anisotropically while the remainder of the ensemble was refined isotropically. Reasons for not expanding the number of atoms refined anisotropically included the size of the complex and time required per refinement cycle. Due to the large number of variables, 4989, refinement was performed in two BLOCs<sup>5</sup>, in order to use a least-squares full-matrix approach on F<sup>2</sup>. The entire ensemble refined to convergence. This produced the residuals R(F)=16.19%, wR(F<sup>2</sup>)=24.35% and GOF=1.037 for 88730 unique reflections [R(F)=8.75%, wR(F<sup>2</sup>)=21.40% for those 54223 data with Fo > 4 $\sigma$ (Fo)]. A final difference-Fourier map possessed many background peaks, with one as large as  $|\Delta\rho| \leq 0.932 \text{ e}\text{\AA}^{-3}$ , indicating that the structure is correct and complete. The function minimized during the full-matrix least-squares refinement was  $\sum w(F_o^2 - F_c^2)^2$  where  $w = 1/[\sigma^2(F_o^2) + (0.1412 * P)^2 + 0 * P]$  and  $P = (\max(F_o^2, 0) + 2 * F_c^2)/3$ . An empirical correction for extinction was applied to the data in the form  $(F_c^2, \text{corr}) = k[1 + 0.001 * x * F_c^2 * \lambda^3 / \sin(2\theta)]^{-1/4}$ , where k=0.05200 is the scale factor. The value determined for x was 0.011(4).

1. "An Empirical Correction for Absorption Anisotropy, Blessing." R. H. (1995). Acta Cryst. A51, 33.
2. Sheldrick, G.M., SADABS 'Siemens Area Detector Absorption Correction' Universität Göttingen: Göttingen, Germany, 1996.
3. Sheldrick, G.M., (1994). SHELXTL/PC. Version 5.03. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
4. Phase Annealing in SHELX-90: Direct Methods for Larger Structures, Sheldrick, G. M., (1990). Acta Cryst. A46, 467-473.
5. Sheldrick, G.M., (1993). Shelx93 Program for the Refinement of Crystal Structures. University of Göttingen, Germany.

Ball-and-stick model of [(G 1)8-Pb<sup>+2</sup>]<sub>2</sub>



**Table 1. Crystal data and structure refinement.**

Identification code	UM624fn	
Empirical formula	C <sub>169.81</sub> H <sub>270.06</sub> Cl <sub>1.31</sub> N <sub>48.63</sub> O <sub>58.63</sub> Pb Sig	
Formula weight	4409.35	
Temperature	193(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	
Unit cell dimensions	a = 25.5691(13) Å	α = 90°
	b = 44.385(2) Å	β = 90°
	c = 83.840(4) Å	γ = 90°
Volume	95149(8) Å <sup>3</sup>	
Z	16	
Density (calculated)	1.231 Mg/m <sup>3</sup>	
Absorption coefficient	0.845 mm <sup>-1</sup>	
F(000)	37034	
Crystal size	0.776 x 0.148 x 0.141 mm <sup>3</sup>	
Theta range for data collection	1.30 to 20.00°	
Index ranges	-24 ≤ h ≤ 24, -42 ≤ k ≤ 42, -80 ≤ l ≤ 80	
Reflections collected	524,613	
Independent reflections	88,730 [R(int) = 0.1642]	
Completeness to theta = 25.00°	99.8%	
Absorption correction	Empirical, SADABS	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	88,730 / 578 / 4989	
Goodness-of-fit on F <sup>2</sup>	1.037	
Final R indices [I > 2σ(I)]	R1 = 0.0875, wR2 = 0.2140	
R indices (all data)	R1 = 0.1619, wR2 = 0.2435	
Absolute structure parameter	0.011(4)	
Largest diff. peak and hole	0.932 and -0.765 eÅ <sup>-3</sup>	

**Table 2.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for  $[(G\ 1)_8\text{-Pb}^{+2}]_2$ .  $U(\text{eq})$  is one third the trace of orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
<b>Cations</b>				
Pb(1)	-2653(1)	4788(1)	5418(1)	42(1)
Pb(2)	-2660(1)	5259(1)	4684(1)	48(1)
Pb(3)	1440(1)	2218(1)	2537(1)	43(1)
Pb(4)	2803(1)	3468(1)	2529(1)	42(1)
<b>Guanosine 1</b>				
O(1)	-2608(4)	4214(3)	5507(1)	62(3)
N(1)	-1735(5)	4100(3)	5491(2)	56(4)
C(1)	-1306(7)	3916(4)	5455(2)	57(5)
C(2)	-1886(8)	3543(4)	5407(2)	69(6)
N(2)	-827(6)	4022(4)	5467(2)	74(5)
O(2)	-1693(6)	2818(4)	5490(2)	112(5)
C(3)	-2322(8)	3725(4)	5435(2)	70(5)
O(3)	-1239(8)	2891(5)	5104(2)	152(7)
N(3)	-1371(5)	3612(3)	5418(2)	59(4)
N(4)	-2776(7)	3565(4)	5412(2)	102(6)
O(4)	-862(6)	2567(4)	5264(2)	119(5)
C(4)	-2233(7)	4021(4)	5477(2)	57(5)
N(5)	-2077(7)	3270(4)	5357(2)	91(5)
C(5)	-2600(10)	3273(6)	5367(3)	111(8)
C(6)	-1825(10)	2947(6)	5339(3)	123(9)
C(7)	-1234(9)	3018(6)	5270(3)	114(8)
C(8)	-862(9)	2829(6)	5355(3)	102(8)
C(9)	-837(11)	2654(6)	5100(3)	116(9)
C(10)	-370(13)	2774(7)	5034(4)	173(12)
C(11)	-1166(15)	2409(9)	5011(5)	221(17)
C(12)	-1128(11)	2761(7)	5494(3)	138(10)
C(13)	-917(15)	2940(9)	5658(5)	209(16)
Si(1)	-254(7)	2697(3)	5891(2)	115(5)
O(5)	-449(12)	2765(7)	5706(3)	123(11)
C(14)	108(19)	3022(10)	5969(5)	170(30)
C(15)	-854(18)	2644(16)	6012(5)	240(40)
C(16)	162(17)	2394(9)	5860(7)	270(50)
C(17)	540(30)	2316(17)	6003(9)	260(40)
C(18)	-100(30)	2084(7)	5830(8)	200(30)
C(19)	612(19)	2443(15)	5735(7)	200(30)
C(13A)	-917(15)	2940(9)	5658(5)	209(16)
Si(1A)	-1468(9)	3144(5)	5907(3)	210(10)
O(5A)	-1310(14)	2934(9)	5749(4)	162(15)
C(14A)	-1530(20)	2865(10)	6080(5)	300(50)
C(15A)	-2164(11)	3261(9)	5876(5)	133(19)
C(16A)	-1061(13)	3434(8)	5979(4)	180(30)
C(17A)	-1170(30)	3518(13)	6161(4)	280(50)
C(18A)	-472(12)	3335(12)	5979(8)	250(40)
C(19A)	-1142(17)	3721(7)	5881(5)	310(30)

**Guanosine 2**

Si(2)	-236(6)	4623(4)	6199(2)	241(6)
O(21)	-1763(4)	4705(2)	5589(1)	49(3)
C(21)	-1182(6)	5368(3)	5754(2)	37(4)
N(21)	-1536(5)	5152(3)	5705(2)	51(4)
C(22)	-553(6)	5072(4)	5673(2)	48(5)
N(22)	-1397(5)	5622(3)	5818(1)	47(4)
O(22)	672(5)	4981(3)	5815(2)	93(4)
C(23)	-869(6)	4846(4)	5622(2)	40(4)
N(23)	-679(5)	5334(3)	5740(2)	46(4)
O(23)	934(6)	5583(3)	5662(2)	100(5)
C(24)	-1388(6)	4870(3)	5637(2)	40(4)
N(24)	-591(5)	4611(3)	5554(2)	57(4)
O(24)	924(6)	5665(4)	5927(2)	110(5)
C(25)	-107(7)	4710(4)	5564(2)	66(6)
N(25)	-45(5)	4989(3)	5640(2)	54(4)
O(25)	228(10)	4853(6)	6128(3)	229(12)
C(26)	471(7)	5126(4)	5682(2)	67(6)
C(27)	437(8)	5439(5)	5712(2)	74(6)
C(28)	480(8)	5478(5)	5893(2)	82(6)
C(29)	1130(8)	5779(5)	5785(2)	75(6)
C(30)	1667(11)	5772(7)	5784(3)	146(11)
C(31)	890(12)	6095(7)	5748(4)	164(12)
C(32)	565(11)	5177(6)	5950(3)	128(9)
C(33)	88(11)	5076(7)	6065(4)	145(11)
C(34)	120(20)	4318(10)	6311(6)	590(70)
C(35)	-537(17)	4423(10)	6023(5)	410(40)
C(36)	-670(11)	4826(6)	6305(3)	216(17)
C(37)	-1095(13)	4999(9)	6198(5)	290(20)
C(38)	-439(18)	5056(11)	6429(5)	460(50)
C(39)	-1058(19)	4619(11)	6415(6)	530(60)

**Guanosine 3**

Si(3)	-3195(2)	5377(1)	6391(1)	76(2)
C(41)	-3946(6)	5421(4)	5777(2)	44(5)
N(41)	-3547(4)	5235(3)	5726(1)	37(3)
O(41)	-2669(4)	5138(2)	5685(1)	39(3)
C(42)	-3376(6)	5747(3)	5856(2)	33(4)
N(42)	-4425(5)	5308(3)	5757(2)	52(4)
O(42)	-3428(4)	6228(2)	6170(1)	52(3)
C(43)	-2938(6)	5599(3)	5813(2)	35(4)
N(43)	-3878(5)	5685(3)	5848(1)	37(3)
O(43)	-4144(5)	6629(3)	5974(1)	70(4)
C(44)	-3027(6)	5316(3)	5742(2)	37(4)
N(44)	-2491(5)	5756(3)	5840(2)	47(4)
O(44)	-4672(4)	6408(3)	6154(1)	70(4)
C(45)	-2646(7)	6014(4)	5907(2)	55(5)
N(45)	-3178(5)	6026(3)	5917(1)	39(3)
O(45)	-3489(4)	5701(2)	6375(1)	70(4)
C(46)	-3451(6)	6268(4)	6003(2)	42(4)
C(47)	-4009(6)	6310(4)	5963(2)	48(5)
C(48)	-4313(6)	6162(4)	6103(2)	56(5)
C(49)	-4629(7)	6640(4)	6041(2)	62(5)
C(50)	-5091(7)	6605(4)	5922(2)	75(6)
C(51)	-4681(9)	6938(5)	6135(3)	98(7)

C(52)	-3910(6)	6097(4)	6227(2)	46(5)
C(53)	-3855(7)	5763(4)	6256(2)	64(5)
C(54)	-3691(10)	5071(5)	6374(3)	198(15)
C(55)	-2729(9)	5346(6)	6224(3)	166(12)
C(56)	-2875(7)	5373(4)	6576(2)	97(7)
C(57)	-2598(13)	5674(6)	6614(4)	270(20)
C(58)	-3291(11)	5308(8)	6719(3)	260(20)
C(59)	-2463(8)	5113(5)	6593(3)	132(10)

**Guanosine 4**

Si(4)	-4878(4)	3945(2)	5993(1)	161(4)
C(61)	-4085(7)	3953(4)	5487(2)	59(5)
N(61)	-3709(6)	4184(3)	5520(2)	62(4)
O(61)	-3527(4)	4667(2)	5588(1)	50(3)
C(62)	-4740(6)	4277(4)	5521(2)	48(5)
N(62)	-3875(6)	3679(4)	5447(2)	86(5)
O(62)	-6093(6)	4287(3)	5597(2)	102(5)
C(63)	-4414(6)	4512(4)	5563(2)	42(4)
N(63)	-4570(5)	3994(3)	5484(2)	48(4)
O(63)	-6167(5)	3854(3)	5343(2)	85(4)
C(64)	-3884(7)	4473(4)	5564(2)	56(5)
N(64)	-4706(5)	4771(3)	5588(2)	59(4)
O(64)	-6204(6)	3526(4)	5555(2)	108(5)
C(65)	-5215(8)	4684(4)	5564(2)	71(6)
N(65)	-5222(5)	4383(3)	5522(2)	54(4)
O(65)	-5302(6)	4057(4)	5850(2)	117(5)
C(66)	-5743(7)	4247(4)	5475(2)	67(6)
C(67)	-5703(9)	3900(5)	5446(3)	94(7)
C(68)	-5830(8)	3763(5)	5592(3)	85(7)
C(69)	-6341(8)	3553(5)	5397(3)	89(7)
C(70)	-6105(10)	3330(6)	5294(3)	123(9)
C(71)	-6931(8)	3570(5)	5372(3)	110(8)
C(72)	-6086(10)	4020(6)	5698(3)	107(8)
C(73)	-5879(9)	4052(6)	5856(3)	132(10)
C(74)	-5111(10)	3580(5)	6072(3)	158(12)
C(75)	-4233(7)	3882(6)	5892(3)	153(11)
C(76)	-4853(11)	4246(5)	6122(3)	235(19)
C(77)	-4632(12)	4543(5)	6043(3)	191(14)
C(78)	-5375(11)	4335(8)	6203(4)	260(20)
C(79)	-4459(14)	4171(8)	6269(3)	290(20)

**Guanosine 5**

Si(5)	725(4)	3819(3)	5569(1)	187(5)
C(81)	-821(6)	4581(4)	5148(2)	44(5)
N(81)	-1341(5)	4622(3)	5179(1)	44(4)
O(81)	-2200(4)	4486(2)	5188(1)	49(3)
C(82)	-1001(7)	4127(4)	5075(2)	59(5)
N(82)	-496(5)	4808(3)	5176(1)	52(4)
O(82)	-178(5)	3644(3)	5144(2)	86(4)
C(83)	-1537(7)	4152(4)	5092(2)	60(5)
N(83)	-625(5)	4314(3)	5095(2)	52(4)
O(83)	7(5)	3720(3)	4739(2)	90(4)
C(84)	-1718(6)	4418(4)	5153(2)	43(5)
N(84)	-1794(5)	3871(3)	5051(2)	58(4)
O(84)	687(5)	3555(3)	4888(2)	83(4)
C(85)	-1410(7)	3690(4)	5011(2)	57(5)



N(85)	-924(6)	3825(3)	5015(2)	64(4)
O(85)	354(5)	3917(3)	5412(2)	101(5)
C(86)	-404(7)	3688(5)	4991(2)	72(6)
C(87)	-44(7)	3855(5)	4895(2)	69(6)
C(88)	463(7)	3810(4)	4972(2)	64(6)
C(89)	512(8)	3587(5)	4729(2)	75(6)
C(90)	423(10)	3264(6)	4653(3)	134(10)
C(91)	829(9)	3768(5)	4628(3)	113(8)
C(92)	376(8)	3714(5)	5140(2)	88(7)
C(93)	457(9)	4006(5)	5250(2)	95(7)
C(94)	218(10)	3812(7)	5745(3)	204(16)
C(95)	1106(11)	4179(6)	5629(4)	210(16)
C(96)	1100(12)	3514(6)	5556(4)	380(40)
C(97)	1592(11)	3569(7)	5439(4)	209(16)
C(98)	1356(17)	3415(10)	5720(4)	370(30)
C(99)	812(18)	3222(7)	5491(7)	570(60)
C(93A)	-4706(11)	6869(6)	4383(3)	142(10)
O(85A)	-4948(15)	6706(11)	4222(5)	50(15)
Si(5A)	-4454(11)	6676(6)	4095(3)	82(9)
C(94A)	-3830(17)	6750(20)	4194(11)	350(150)
C(95A)	-4550(40)	6946(14)	3931(7)	210(60)
C(96A)	-4464(18)	6293(10)	4017(5)	50(20)
C(97A)	-4970(30)	6253(14)	3908(9)	240(60)
C(98A)	-3990(30)	6231(12)	3913(8)	110(40)
C(99A)	-4520(20)	6064(8)	4152(5)	0(14)
<b>Guanosine 6</b>				
Si(6)	-996(3)	6395(1)	6104(1)	82(2)
C(101)	-2004(7)	5894(4)	5457(2)	54(5)
N(101)	-2131(5)	5583(3)	5398(1)	46(4)
O(101)	-1893(4)	5135(2)	5307(1)	51(3)
C(102)	-1159(7)	5782(4)	5427(2)	51(5)
N(102)	-2432(5)	6055(3)	5492(1)	55(4)
O(102)	-450(4)	6124(3)	5657(1)	60(3)
C(103)	-1226(6)	5494(4)	5360(2)	40(4)
N(103)	-1524(5)	5991(3)	5467(2)	53(4)
O(103)	-217(6)	6512(3)	5290(2)	101(5)
C(104)	-1733(7)	5408(4)	5352(2)	55(5)
N(104)	-774(5)	5376(3)	5329(2)	51(4)
O(104)	11(6)	6720(4)	5528(2)	107(5)
C(105)	-419(7)	5583(4)	5369(2)	53(5)
N(105)	-636(5)	5835(3)	5426(1)	41(3)
O(105)	-1087(4)	6257(3)	5920(1)	70(4)
C(106)	-369(7)	6108(4)	5482(2)	59(5)
C(107)	-579(7)	6398(4)	5416(2)	65(5)
C(108)	-543(8)	6617(5)	5548(2)	74(6)
C(109)	161(11)	6741(6)	5364(3)	120(9)
C(110)	670(10)	6662(6)	5328(3)	132(10)
C(111)	-67(11)	7027(6)	5299(3)	143(10)
C(112)	-575(8)	6428(4)	5703(2)	76(6)
C(113)	-1073(7)	6439(4)	5781(2)	70(6)
C(114)	-381(7)	6608(5)	6114(3)	133(10)
C(115)	-1553(8)	6638(5)	6151(3)	165(12)
C(116)	-986(7)	6074(4)	6233(2)	107(8)
C(117)	-888(8)	6166(5)	6408(2)	116(8)

C(118)	-1520(7)	5899(5)	6231(3)	128(9)
C(119)	-548(8)	5850(5)	6184(3)	128(9)
<b>Guanosine 7</b>				
Si(7)	-6085(3)	5390(1)	5910(1)	82(2)
C(121)	-4512(7)	5274(4)	5291(2)	57(5)
N(121)	-3988(5)	5199(3)	5297(1)	42(3)
O(121)	-3120(4)	5283(2)	5350(1)	43(3)
C(122)	-4300(6)	5713(4)	5397(2)	40(4)
N(122)	-4853(5)	5074(3)	5227(2)	55(4)
O(122)	-5090(4)	5987(2)	5646(1)	54(3)
C(123)	-3779(6)	5664(3)	5403(2)	36(4)
N(123)	-4696(5)	5543(3)	5346(2)	46(4)
O(123)	-5366(7)	6476(4)	5356(2)	132(6)
C(124)	-3594(6)	5384(3)	5349(2)	31(4)
N(124)	-3484(5)	5893(3)	5469(1)	42(3)
O(124)	-6129(5)	6218(3)	5426(2)	76(4)
C(125)	-3868(7)	6073(4)	5505(2)	54(5)
N(125)	-4370(5)	5996(3)	5475(2)	45(4)
O(125)	-5596(4)	5483(3)	5787(1)	70(4)
C(126)	-4851(7)	6147(5)	5518(2)	76(6)
C(127)	-5238(7)	6169(4)	5384(2)	62(5)
C(128)	-5718(6)	6013(4)	5439(2)	40(4)
C(129)	-5925(8)	6510(5)	5400(2)	77(6)
C(130)	-6004(12)	6699(7)	5543(4)	163(12)
C(131)	-6163(12)	6649(7)	5248(4)	166(12)
C(132)	-5604(6)	5918(4)	5605(2)	44(5)
C(133)	-5677(7)	5582(4)	5628(2)	58(5)
C(134)	-6700(9)	5579(5)	5865(3)	112(8)
C(135)	-6190(9)	4967(5)	5892(3)	105(8)
C(136)	-5871(8)	5516(5)	6102(2)	75(6)
C(137)	-5324(8)	5377(5)	6150(3)	97(7)
C(138)	-6235(12)	5404(7)	6245(4)	175(13)
C(139)	-5786(9)	5856(5)	6106(3)	104(8)
<b>Guanosine 8</b>				
Si(8)	-4182(4)	2755(2)	5441(1)	158(4)
C(141)	-3301(7)	3892(4)	5065(2)	58(5)
N(141)	-3159(5)	4194(3)	5120(2)	55(4)
O(141)	-3392(4)	4659(2)	5218(1)	46(3)
C(142)	-4117(7)	4015(4)	5083(2)	55(5)
N(142)	-2891(6)	3731(4)	5026(2)	79(5)
O(142)	-4832(5)	3487(4)	5168(2)	100(5)
C(143)	-4051(7)	4308(4)	5135(2)	57(5)
N(143)	-3767(7)	3804(4)	5045(2)	75(5)
O(143)	-5132(5)	3565(3)	4768(2)	86(4)
C(144)	-3555(6)	4405(4)	5159(2)	42(4)
N(144)	-4523(5)	4444(3)	5154(2)	49(4)
O(144)	-5157(8)	3083(5)	4876(3)	164(7)
C(145)	-4868(7)	4236(4)	5134(2)	53(5)
N(145)	-4646(6)	3982(4)	5079(2)	67(4)
O(145)	-4156(5)	3074(3)	5347(2)	102(5)
C(146)	-4942(8)	3685(5)	5043(2)	76(6)
C(147)	-4735(9)	3556(5)	4886(3)	97(7)
C(148)	-4665(9)	3213(5)	4963(3)	98(7)
C(149)	-5281(14)	3234(8)	4715(5)	170(13)

C(150)	-5928(13)	3254(8)	4723(4)	194(14)
C(151)	-5007(18)	3167(11)	4572(6)	280(20)
C(152)	-4673(10)	3172(6)	5119(3)	110(8)
C(153)	-4139(8)	3089(5)	5192(2)	87(7)
C(154)	-3571(8)	2531(6)	5398(3)	170(12)
C(155)	-4767(8)	2549(5)	5379(3)	147(11)
C(156)	-4189(10)	2840(6)	5650(3)	198(15)
C(157)	-3669(9)	3000(6)	5707(3)	173(13)
C(158)	-4673(10)	3038(7)	5692(3)	209(16)
C(159)	-4212(12)	2536(6)	5748(3)	215(16)

**Guanosine 9**

Si(9)	-2499(4)	3576(3)	3938(1)	173(4)
C(161)	-2700(8)	4045(4)	4662(2)	64(5)
N(161)	-2610(5)	4358(3)	4705(2)	53(4)
O(161)	-2094(4)	4767(3)	4749(1)	60(3)
C(162)	-1847(7)	3987(4)	4636(2)	47(5)
N(162)	-3201(7)	3952(4)	4675(2)	101(6)
O(162)	-1479(5)	3604(3)	4350(2)	92(4)
C(163)	-1706(6)	4295(4)	4679(2)	43(4)
N(163)	-2316(6)	3868(3)	4630(2)	67(4)
O(163)	-1187(8)	3064(5)	4584(3)	163(7)
C(164)	-2130(6)	4481(4)	4711(2)	46(5)
N(164)	-1184(5)	4344(3)	4668(2)	56(4)
O(164)	-1912(6)	2892(4)	4453(2)	109(5)
C(165)	-982(8)	4090(5)	4616(2)	76(6)
N(165)	-1376(6)	3873(3)	4596(2)	69(4)
O(165)	-2276(6)	3685(3)	4115(2)	111(5)
C(166)	-1290(8)	3581(4)	4511(2)	74(6)
C(167)	-1550(8)	3316(5)	4592(3)	92(7)
C(168)	-1953(8)	3219(5)	4471(2)	82(6)
C(169)	-1398(12)	2844(7)	4482(4)	136(10)
C(170)	-1036(14)	2826(9)	4350(4)	211(16)
C(171)	-1364(13)	2559(8)	4609(4)	188(14)
C(172)	-1871(8)	3380(5)	4327(2)	76(6)
C(173)	-2372(9)	3538(5)	4257(3)	106(8)
C(174)	-2748(15)	3177(6)	3970(4)	310(30)
C(175)	-3039(13)	3808(10)	3869(5)	450(40)
C(176)	-1959(9)	3574(6)	3819(3)	171(13)
C(177)	-1746(14)	3910(6)	3799(5)	290(20)
C(178)	-1490(11)	3377(8)	3874(4)	280(20)
C(179)	-2109(14)	3468(9)	3641(3)	270(20)

**Guanosine 10**

Si(10)	996(4)	5773(3)	4361(1)	165(4)
C(181)	-704(7)	5103(4)	4837(2)	51(5)
N(181)	-1245(5)	5142(3)	4842(1)	48(4)
O(181)	-1971(4)	5423(2)	4898(1)	42(3)
C(182)	-604(6)	5551(4)	4929(2)	46(5)
N(182)	-551(5)	4831(3)	4792(2)	62(4)
O(182)	343(5)	5897(3)	4806(2)	82(4)
C(183)	-1117(6)	5613(4)	4946(2)	41(4)
N(183)	-357(5)	5309(3)	4881(2)	58(4)
C(184)	-1489(6)	5402(3)	4899(2)	31(4)
N(184)	-1187(5)	5910(3)	5017(2)	53(4)
O(185)	590(5)	5639(3)	4502(2)	106(5)

C(185)	-708(7)	6012(4)	5029(2)	55(5)
N(185)	-336(5)	5813(3)	4981(2)	55(4)
C(186)	236(7)	5888(5)	4969(2)	71(6)
O(184)	1420(10)	5638(7)	4993(3)	285(15)
O(183)	771(9)	5693(5)	5197(2)	196(9)
C(188)	938(9)	5546(6)	4927(3)	121(9)
C(187)	539(8)	5671(5)	5039(3)	102(8)
C(189)	1292(11)	5790(7)	5147(4)	232(18)
C(190)	1606(10)	5602(7)	5259(3)	161(12)
C(191)	1450(20)	6105(8)	5150(7)	600(70)
C(192)	834(8)	5723(5)	4775(2)	77(6)
C(193)	709(8)	5511(4)	4651(2)	76(6)
C(194)	860(12)	6196(4)	4353(3)	184(14)
C(195)	1675(8)	5709(9)	4413(5)	360(30)
C(196)	835(12)	5629(6)	4169(3)	270(20)
C(197)	950(16)	5286(6)	4154(4)	320(30)
C(198)	266(10)	5702(8)	4123(4)	215(16)
C(199)	1216(14)	5801(9)	4045(3)	310(30)

**Guanosine 11**

Si(11)	-2879(3)	7466(2)	4800(1)	108(3)
C(201)	-2575(6)	6159(3)	5099(2)	38(4)
N(201)	-2673(5)	5878(3)	5025(1)	40(3)
O(201)	-3210(4)	5526(2)	4908(1)	47(3)
C(202)	-3414(6)	6239(3)	5096(2)	38(4)
N(202)	-2091(5)	6228(3)	5138(1)	49(4)
O(202)	-3747(4)	6898(3)	5051(1)	57(3)
C(203)	-3554(6)	5964(4)	5019(2)	42(4)
N(203)	-2968(4)	6337(3)	5128(1)	29(3)
C(204)	-3159(6)	5783(3)	4981(2)	33(4)
N(204)	-4102(5)	5950(3)	4998(2)	51(4)
C(205)	-4279(7)	6217(4)	5045(2)	58(5)
N(205)	-3903(5)	6391(3)	5114(1)	43(4)
O(205)	-2822(5)	7139(3)	4898(2)	85(4)
C(206)	-3951(6)	6707(4)	5168(2)	45(5)
O(203)	-4054(4)	6785(2)	5454(1)	56(3)
O(204)	-3889(5)	7270(3)	5362(1)	76(4)
C(207)	-3682(7)	6766(4)	5328(2)	61(5)
C(208)	-3475(6)	7079(4)	5303(2)	57(5)
C(209)	-4095(7)	7110(4)	5496(2)	64(6)
C(210)	-4664(7)	7177(5)	5495(2)	90(7)
C(211)	-3848(8)	7171(5)	5650(2)	91(7)
C(212)	-3431(6)	7121(4)	5121(2)	49(5)
C(213)	-2868(6)	7106(4)	5074(2)	62(5)
C(214)	-3584(7)	7479(5)	4731(3)	133(10)
C(215)	-2780(11)	7785(5)	4942(3)	196(14)
C(216)	-2437(8)	7476(6)	4639(3)	167(12)
C(217)	-2502(9)	7193(5)	4530(3)	134(10)
C(218)	-1867(7)	7498(6)	4700(3)	172(12)
C(219)	-2566(11)	7765(5)	4531(3)	179(13)

**Guanosine 12**

Si(12)	-6432(3)	5259(2)	4317(1)	114(2)
C(221)	-4571(6)	5171(4)	4846(2)	40(4)
N(221)	-4047(5)	5130(3)	4841(1)	45(4)
O(221)	-3323(5)	4851(3)	4778(1)	59(3)

C(222)	-4684(7)	4706(4)	4776(2)	60(5)
N(222)	-4749(6)	5454(3)	4897(2)	69(5)
O(222)	-5729(5)	4576(3)	4591(2)	85(4)
C(223)	-4187(7)	4639(4)	4763(2)	61(5)
N(223)	-4916(5)	4968(3)	4820(2)	51(4)
O(223)	-5994(6)	4268(3)	4968(2)	103(5)
C(224)	-3800(7)	4857(4)	4789(2)	50(5)
N(224)	-4110(6)	4334(3)	4709(2)	67(4)
O(224)	-6680(6)	4407(3)	4812(2)	99(5)
C(225)	-4582(8)	4240(5)	4691(2)	77(6)
N(225)	-4962(6)	4440(3)	4726(2)	65(4)
O(225)	-5994(4)	5137(3)	4441(1)	70(4)
C(226)	-5545(8)	4407(5)	4718(2)	87(7)
C(227)	-5819(8)	4529(5)	4864(2)	75(6)
C(228)	-6307(7)	4658(5)	4801(2)	76(6)
C(229)	-6571(9)	4233(6)	4952(3)	103(8)
C(230)	-6610(12)	3929(7)	4908(4)	165(12)
C(231)	-6845(9)	4341(5)	5088(3)	110(8)
C(232)	-6186(7)	4737(4)	4630(2)	64(5)
C(233)	-6092(8)	5063(4)	4602(2)	83(6)
C(234)	-6988(8)	4986(5)	4293(3)	155(11)
C(235)	-6730(10)	5602(5)	4408(3)	174(13)
C(236)	-6120(8)	5331(5)	4135(2)	125(9)
C(237)	-5842(10)	5032(5)	4070(3)	171(12)
C(238)	-5696(9)	5579(5)	4144(3)	148(11)
C(239)	-6525(11)	5424(7)	4000(3)	220(17)
<b>Guanosine 13</b>				
Si(13)	-976(5)	5061(2)	3793(1)	187(5)
C(241)	-1806(7)	4495(4)	4279(2)	55(5)
N(241)	-1998(5)	4768(3)	4356(2)	63(4)
O(241)	-1890(4)	5210(3)	4476(1)	63(3)
C(242)	-1001(7)	4664(4)	4313(2)	60(5)
N(242)	-2184(6)	4313(3)	4236(2)	71(5)
O(242)	78(6)	4549(3)	4094(2)	102(5)
C(243)	-1128(7)	4934(4)	4388(2)	49(5)
N(243)	-1304(6)	4451(3)	4262(2)	60(4)
O(243)	122(7)	3933(4)	4288(2)	130(6)
C(244)	-1661(8)	4984(5)	4410(2)	76(6)
N(244)	-715(6)	5107(4)	4429(2)	74(5)
O(244)	100(6)	3865(4)	4022(2)	115(5)
C(245)	-318(10)	4929(5)	4387(3)	97(7)
N(245)	-476(6)	4677(3)	4318(2)	63(4)
O(245)	-586(7)	4764(4)	3827(2)	162(7)
C(246)	-77(8)	4455(5)	4246(2)	77(6)
C(247)	-286(9)	4159(5)	4232(3)	101(8)
C(248)	-305(10)	4088(6)	4053(3)	109(8)
C(249)	234(11)	3693(6)	4170(3)	117(9)
C(250)	-139(11)	3462(7)	4186(3)	156(11)
C(251)	816(11)	3651(7)	4169(3)	156(11)
C(252)	-208(9)	4381(5)	3980(3)	93(7)
C(253)	-725(11)	4516(7)	3909(3)	146(11)
C(254)	-1251(17)	5157(10)	3993(4)	400(40)
C(255)	-530(16)	5375(7)	3734(6)	390(40)
C(256)	-1426(14)	4963(9)	3650(4)	450(40)

C(257)	-1170(20)	4858(15)	3489(4)	460(50)
C(258)	-1800(20)	4699(14)	3707(7)	670(90)
C(259)	-1810(20)	5228(13)	3600(7)	490(50)
<b>Guanosine 14</b>				
Si(14)	-746(4)	7014(3)	4130(1)	160(4)
C(261)	-952(7)	5906(4)	4574(2)	62(5)
N(261)	-1451(5)	5795(3)	4569(2)	48(4)
O(261)	-2337(4)	5827(2)	4617(1)	51(3)
C(262)	-1240(7)	6307(4)	4688(2)	56(5)
N(262)	-583(6)	5734(3)	4518(2)	66(4)
O(262)	-824(6)	7054(4)	4733(2)	106(5)
C(263)	-1766(6)	6231(4)	4696(2)	49(5)
N(263)	-841(6)	6176(3)	4637(2)	65(4)
O(263)	105(5)	6790(3)	4888(2)	88(4)
C(264)	-1876(7)	5938(4)	4625(2)	50(5)
N(264)	-2085(5)	6435(3)	4770(2)	58(4)
O(264)	389(6)	6919(4)	4650(2)	111(5)
C(265)	-1732(7)	6641(4)	4815(2)	65(6)
N(265)	-1242(5)	6586(3)	4775(2)	57(4)
O(265)	-578(7)	6969(4)	4317(2)	151(7)
C(266)	-774(8)	6774(5)	4821(2)	77(6)
C(267)	-283(7)	6664(4)	4790(2)	64(6)
C(268)	-107(8)	6776(5)	4628(3)	89(7)
C(269)	572(9)	6838(5)	4802(3)	84(7)
C(270)	897(10)	6605(6)	4800(3)	136(10)
C(271)	767(10)	7142(6)	4870(3)	133(10)
C(272)	-497(8)	7020(5)	4590(3)	91(7)
C(273)	-875(10)	6935(6)	4454(3)	131(10)
C(274)	-1454(7)	7125(7)	4115(3)	190(14)
C(275)	-376(10)	7329(5)	4044(3)	184(14)
C(276)	-663(12)	6669(5)	4034(4)	320(30)
C(277)	-77(12)	6585(9)	4015(6)	410(40)
C(278)	-973(16)	6412(6)	4124(4)	290(20)
C(279)	-899(16)	6679(8)	3860(3)	290(20)
<b>Guanosine 15</b>				
Si(15)	-4575(4)	7425(2)	4189(1)	123(4)
C(281)	-3525(7)	6351(4)	4678(2)	51(5)
N(281)	-3358(5)	6061(3)	4636(1)	50(4)
O(281)	-3470(4)	5569(3)	4547(1)	63(3)
C(282)	-4343(8)	6202(4)	4625(2)	67(6)
N(282)	-3183(6)	6530(3)	4731(2)	66(4)
O(282)	-5387(6)	6582(4)	4494(2)	106(5)
C(283)	-4211(7)	5905(4)	4570(2)	60(5)
N(283)	-4019(5)	6431(3)	4673(2)	53(4)
O(283)	-5488(6)	6738(4)	4862(2)	115(5)
C(284)	-3659(7)	5829(4)	4582(2)	59(5)
N(284)	-4639(6)	5727(3)	4533(2)	66(4)
O(284)	-5445(7)	7151(4)	4711(2)	134(6)
C(285)	-5031(9)	5917(5)	4565(2)	92(7)
N(285)	-4878(7)	6198(4)	4609(2)	93(6)
C(286)	-5275(9)	6452(6)	4645(3)	107(8)
C(287)	-5061(9)	6678(5)	4751(3)	98(7)
C(288)	-4998(9)	6974(5)	4658(3)	93(7)
C(289)	-5577(13)	7039(8)	4878(4)	144(10)

C(290)	-5213(16)	7196(9)	4983(5)	229(18)
C(291)	-6156(12)	7097(7)	4889(4)	172(13)
C(292)	-5134(10)	6858(6)	4482(3)	106(8)
C(293)	-4706(11)	6869(6)	4383(3)	142(10)
O(285)	-4465(8)	7187(5)	4343(2)	138(8)
C(294)	-4721(12)	7190(7)	4009(3)	165(15)
C(295)	-5207(8)	7621(6)	4236(3)	139(13)
C(296)	-4048(7)	7663(5)	4163(3)	101(9)
C(297)	-3503(8)	7494(6)	4145(4)	139(12)
C(298)	-3937(13)	7894(6)	4304(3)	182(17)
C(299)	-4082(10)	7873(5)	4010(3)	119(11)

**Guanosine 16**

Si(16)	-4172(6)	4719(3)	3733(2)	239(6)
C(301)	-4413(7)	4931(4)	4400(2)	61(5)
N(301)	-3901(5)	5022(3)	4420(2)	50(4)
O(301)	-3015(4)	4951(3)	4424(1)	57(3)
C(302)	-4103(9)	4474(5)	4325(2)	82(6)
N(302)	-4781(6)	5122(3)	4424(2)	65(4)
O(302)	-4528(7)	3963(5)	4070(2)	148(7)
C(303)	-3598(7)	4546(4)	4352(2)	60(5)
N(303)	-4540(6)	4647(4)	4345(2)	73(5)
O(303)	-5374(7)	3811(4)	4312(2)	120(5)
C(304)	-3459(7)	4849(4)	4401(2)	61(5)
N(304)	-3252(6)	4312(4)	4315(2)	74(5)
O(304)	-5755(7)	4060(4)	4096(2)	139(6)
C(305)	-3612(10)	4091(6)	4284(3)	114(8)
N(305)	-4114(7)	4177(4)	4286(2)	87(5)
O(305)	-4462(10)	4464(6)	3838(3)	219(11)
C(306)	-4545(9)	3983(6)	4244(3)	96(7)
C(307)	-5033(9)	4078(5)	4280(3)	95(7)
C(308)	-5275(11)	4231(7)	4128(3)	138(10)
C(309)	-5857(12)	3890(7)	4220(4)	135(10)
C(310)	-6219(13)	4012(8)	4344(4)	182(13)
C(311)	-6081(12)	3560(7)	4176(4)	172(13)
C(312)	-4888(14)	4212(9)	4000(4)	176(13)
C(313)	-4725(17)	4508(11)	3980(5)	240(20)
C(314)	-3753(12)	4524(7)	3579(4)	243(19)
C(315)	-4667(12)	4932(8)	3608(4)	280(20)
C(316)	-3784(12)	4988(7)	3834(4)	510(50)
C(317)	-4107(13)	5185(7)	3957(4)	260(20)
C(318)	-3329(10)	4833(7)	3928(4)	208(16)
C(319)	-3546(15)	5226(8)	3710(4)	340(30)

**Guanosine 17**

Si(17)	-1967(4)	1676(2)	2403(1)	135(3)
C(321)	-186(6)	2356(4)	2168(2)	48(5)
N(321)	124(5)	2250(3)	2286(2)	45(4)
O(321)	382(4)	2197(2)	2549(1)	48(3)
C(322)	-718(7)	2563(4)	2349(2)	53(5)
N(322)	-61(5)	2307(3)	2019(2)	54(4)
O(322)	-2022(5)	2639(3)	2358(2)	73(4)
C(323)	-423(7)	2456(4)	2480(2)	64(5)
N(323)	-640(5)	2514(3)	2199(2)	45(4)
O(323)	-1843(5)	3191(3)	2152(2)	77(4)
C(324)	42(6)	2292(3)	2449(2)	43(4)

N(324)	-626(5)	2547(3)	2619(2)	57(4)
O(324)	-2255(6)	2857(3)	2010(2)	92(4)
C(325)	-1049(7)	2689(4)	2584(2)	68(6)
N(325)	-1116(6)	2708(3)	2423(2)	71(5)
O(325)	-2131(6)	1995(3)	2339(2)	124(6)
C(326)	-1598(7)	2849(5)	2359(2)	76(6)
C(327)	-1530(8)	2924(4)	2175(2)	68(6)
C(328)	-1834(7)	2682(4)	2086(2)	68(6)
C(329)	-2088(8)	3164(5)	2007(2)	71(6)
C(330)	-1766(7)	3222(4)	1863(2)	77(6)
C(331)	-2570(9)	3342(6)	2006(3)	120(9)
C(332)	-2076(8)	2494(5)	2219(2)	83(7)
C(333)	-1857(9)	2165(5)	2214(3)	98(7)
C(334)	-1395(11)	1713(8)	2545(4)	290(20)
C(335)	-1766(11)	1420(6)	2241(3)	183(14)
C(336)	-2522(8)	1536(6)	2511(3)	181(13)
C(337)	-2992(11)	1480(9)	2393(4)	290(20)
C(338)	-2420(14)	1227(6)	2596(4)	270(20)
C(339)	-2708(13)	1760(7)	2641(4)	250(20)

**Guanosine 18**

Si(18)	390(4)	769(3)	1875(1)	178(4)
C(341)	2051(6)	1472(4)	2081(2)	53(5)
N(341)	1745(5)	1617(3)	2194(2)	46(4)
O(341)	1093(4)	1932(2)	2276(1)	53(3)
C(342)	1541(6)	1678(4)	1895(2)	48(5)
N(342)	2444(5)	1290(3)	2132(2)	71(5)
O(342)	1134(6)	1411(4)	1534(2)	117(5)
C(343)	1221(6)	1827(4)	1993(2)	50(5)
N(343)	1946(5)	1496(3)	1927(2)	61(4)
O(343)	2253(5)	1576(3)	1416(2)	79(4)
C(344)	1337(6)	1796(4)	2164(2)	39(4)
N(344)	864(5)	2010(3)	1919(2)	50(4)
O(344)	2166(7)	1083(4)	1407(2)	124(6)
C(345)	978(7)	1941(4)	1768(2)	65(6)
N(345)	1384(5)	1762(3)	1751(2)	53(4)
O(345)	696(10)	924(5)	1720(2)	198(9)
C(346)	1513(7)	1653(4)	1578(2)	72(6)
C(347)	2023(7)	1497(4)	1568(2)	58(5)
C(348)	1919(9)	1148(5)	1555(3)	96(7)
C(349)	2533(8)	1310(5)	1351(3)	87(7)
C(350)	3023(10)	1272(6)	1416(3)	121(9)
C(351)	2440(9)	1323(6)	1175(3)	118(9)
C(352)	1361(10)	1128(6)	1546(3)	114(8)
C(353)	1224(12)	946(8)	1714(4)	172(13)
C(354)	136(16)	394(6)	1817(5)	360(30)
C(355)	846(12)	738(9)	2042(3)	270(20)
C(356)	-134(9)	1019(5)	1920(3)	170(13)
C(357)	-453(13)	900(8)	2070(4)	270(20)
C(358)	-2(12)	1349(5)	1952(4)	206(16)
C(359)	-533(13)	1019(10)	1776(4)	360(30)

**Guanosine 19**

Si(19)	2096(5)	280(3)	2697(2)	233(6)
C(361)	2402(6)	1455(4)	2906(2)	45(5)
N(361)	2079(5)	1559(3)	2791(2)	48(4)



O(361)	1852(4)	1652(2)	2531(1)	47(3)
C(362)	2893(7)	1245(4)	2723(2)	56(5)
N(362)	2286(6)	1523(3)	3063(2)	72(4)
O(362)	3631(7)	596(4)	2724(2)	130(6)
C(363)	2603(7)	1349(4)	2599(2)	54(5)
N(363)	2814(5)	1285(3)	2879(2)	50(4)
O(363)	4384(6)	935(3)	2927(2)	97(5)
C(364)	2171(6)	1525(4)	2628(2)	51(5)
N(364)	2812(5)	1255(3)	2449(2)	49(4)
O(364)	4029(8)	606(4)	3091(2)	137(6)
C(365)	3215(7)	1097(4)	2493(2)	65(5)
N(365)	3308(5)	1076(3)	2656(2)	53(4)
O(365)	2695(10)	300(9)	2770(4)	314(17)
C(366)	3751(7)	911(4)	2730(2)	64(6)
C(367)	3843(7)	968(5)	2899(2)	71(6)
C(368)	3606(9)	732(5)	2988(3)	92(7)
C(369)	4440(11)	791(6)	3078(3)	118(9)
C(370)	4418(11)	1028(7)	3219(3)	156(11)
C(371)	4955(9)	600(6)	3063(3)	121(9)
C(372)	3470(10)	502(6)	2870(3)	115(8)
C(373)	2790(17)	470(10)	2901(5)	250(20)
C(374)	1620(16)	258(11)	2860(5)	430(40)
C(375)	1937(15)	597(7)	2566(4)	290(20)
C(376)	2323(13)	-34(6)	2608(4)	284(11)
C(377)	2950(13)	-5(11)	2573(7)	470(30)
C(378)	2290(20)	-328(7)	2720(6)	420(30)
C(379)	2070(20)	-134(11)	2446(5)	430(30)

**Guanosine 20**

Si(20)	-707(3)	1209(2)	3215(1)	123(3)
C(381)	54(6)	2280(4)	3000(2)	41(4)
N(381)	397(5)	2159(3)	2884(2)	57(4)
O(381)	1152(4)	1936(2)	2804(1)	47(3)
C(382)	617(7)	2128(4)	3188(2)	50(5)
N(382)	-377(5)	2413(3)	2949(2)	62(4)
O(382)	456(5)	1841(3)	3563(2)	86(4)
C(383)	983(7)	2009(4)	3088(2)	61(5)
N(383)	158(5)	2249(3)	3156(2)	54(4)
O(383)	142(5)	2455(3)	3658(2)	82(4)
C(384)	878(7)	2025(4)	2914(2)	56(5)
N(384)	1427(6)	1887(3)	3161(2)	60(4)
O(384)	-569(6)	2150(3)	3658(2)	98(5)
C(385)	1287(7)	1940(4)	3312(2)	66(6)
N(385)	845(5)	2072(3)	3340(2)	53(4)
O(385)	-580(6)	1444(3)	3364(2)	102(5)
C(386)	631(7)	2130(4)	3511(2)	71(6)
C(387)	126(7)	2294(4)	3500(2)	70(6)
C(388)	-308(8)	2081(5)	3509(2)	79(6)
C(389)	-380(8)	2427(5)	3719(3)	84(7)
C(390)	-694(11)	2678(7)	3652(3)	150(11)
C(391)	-351(9)	2400(6)	3896(3)	115(8)
C(392)	-66(8)	1780(5)	3532(3)	85(7)
C(393)	-87(9)	1568(6)	3378(3)	109(8)
C(394)	-703(10)	1425(6)	3026(2)	155(11)
C(395)	-180(8)	924(5)	3210(3)	151(11)

C(396)	-1327(8)	1051(5)	3250(3)	163(12)
C(397)	-1514(10)	830(6)	3115(3)	165(12)
C(398)	-1340(12)	878(7)	3410(3)	216(17)
C(399)	-1765(10)	1302(6)	3266(4)	215(17)

**Guanosine 21**

Si(21)	-1908(3)	2688(2)	3135(1)	115(3)
C(401)	261(6)	3088(4)	2765(2)	44(5)
N(401)	670(5)	2909(3)	2719(2)	46(4)
O(401)	1381(4)	2612(2)	2773(1)	46(3)
C(402)	474(6)	3014(4)	3014(2)	39(4)
N(402)	-30(5)	3216(3)	2648(2)	51(4)
O(402)	-419(5)	3020(3)	3276(1)	72(4)
C(403)	892(6)	2841(4)	2987(2)	49(5)
N(403)	131(5)	3148(3)	2918(2)	43(4)
O(403)	89(5)	3728(3)	3334(2)	86(4)
C(404)	1002(6)	2774(4)	2822(2)	45(5)
N(404)	1150(5)	2756(3)	3127(1)	39(3)
O(404)	-781(5)	3687(3)	3374(2)	83(4)
C(405)	844(6)	2874(4)	3239(2)	55(5)
N(405)	429(5)	3035(3)	3184(2)	49(4)
O(405)	-1291(5)	2791(3)	3094(2)	93(4)
C(406)	36(6)	3201(4)	3276(2)	47(5)
C(407)	-98(6)	3502(4)	3220(2)	50(5)
C(408)	-672(7)	3526(4)	3227(2)	59(5)
C(409)	-362(8)	3901(5)	3390(3)	85(7)
C(410)	-257(10)	3986(6)	3558(3)	136(10)
C(411)	-454(9)	4163(5)	3285(3)	111(8)
C(412)	-869(7)	3218(4)	3241(2)	70(6)
C(413)	-1126(9)	3095(5)	3083(2)	91(7)
C(414)	-2057(12)	2784(7)	3350(2)	228(18)
C(415)	-2352(9)	2904(6)	3014(3)	159(11)
C(416)	-1905(11)	2298(5)	3111(3)	226(18)
C(417)	-1824(14)	2205(7)	2935(3)	233(18)
C(418)	-1478(11)	2157(6)	3223(3)	190(14)
C(419)	-2447(11)	2157(7)	3170(4)	270(20)

**Guanosine 22**

Si(22)	-638(2)	2210(1)	1544(1)	82(2)
C(421)	1143(6)	2751(4)	1991(2)	42(4)
N(421)	1242(5)	2686(3)	2150(1)	42(4)
O(421)	1065(4)	2717(2)	2417(1)	47(3)
C(422)	448(6)	3007(3)	2060(2)	34(4)
N(422)	1484(5)	2644(3)	1883(2)	48(4)
O(422)	-467(4)	2995(3)	1830(1)	60(3)
C(423)	529(5)	2963(3)	2222(2)	21(4)
N(423)	737(5)	2910(3)	1942(1)	39(3)
O(423)	56(4)	3719(3)	1775(1)	57(3)
C(424)	949(5)	2781(3)	2271(2)	34(4)
N(424)	138(5)	3109(3)	2312(2)	52(4)
O(424)	-495(4)	3526(3)	1589(1)	55(3)
C(425)	-179(7)	3228(4)	2201(2)	56(5)
N(425)	8(5)	3170(3)	2047(2)	44(4)
O(425)	-338(5)	2454(3)	1663(1)	72(4)
C(426)	-260(7)	3250(4)	1898(2)	53(5)
C(427)	115(7)	3400(4)	1776(2)	50(5)

C(428)	-117(6)	3301(4)	1624(2)	42(4)
C(429)	-246(7)	3803(4)	1639(2)	67(6)
C(430)	75(7)	3938(4)	1518(2)	58(5)
C(431)	-693(7)	4017(4)	1694(2)	78(6)
C(432)	-376(7)	3007(4)	1661(2)	57(5)
C(433)	-65(7)	2728(4)	1619(2)	60(5)
C(434)	-241(9)	1858(4)	1538(3)	143(10)
C(435)	-696(8)	2367(5)	1342(2)	103(8)
C(436)	-1262(7)	2145(5)	1631(2)	118(9)
C(437)	-1221(8)	1987(5)	1798(2)	111(8)
C(438)	-1590(9)	2437(5)	1661(3)	156(11)
C(439)	-1602(9)	1923(6)	1523(3)	175(13)

**Guanosine 23**

Si(23)	3425(4)	578(2)	1984(1)	149(4)
C(441)	3288(7)	1932(4)	2307(2)	53(5)
N(441)	2836(5)	2079(3)	2350(2)	54(4)
O(441)	2061(4)	2338(2)	2298(1)	45(3)
C(442)	3060(6)	1989(4)	2059(2)	47(5)
N(442)	3608(5)	1851(3)	2419(2)	60(4)
O(442)	3356(4)	1489(3)	1816(1)	66(3)
C(443)	2604(6)	2149(3)	2084(2)	33(4)
N(443)	3406(5)	1877(3)	2150(2)	45(4)
O(443)	4260(5)	2007(3)	1705(2)	87(4)
C(444)	2477(5)	2207(3)	2250(2)	35(4)
N(444)	2339(5)	2228(3)	1943(1)	45(3)
O(444)	4521(7)	1534(5)	1695(2)	142(6)
C(445)	2628(6)	2112(3)	1834(2)	38(4)
N(445)	3066(5)	1964(3)	1888(2)	49(4)
O(445)	3350(6)	955(3)	1997(2)	101(5)
C(446)	3449(6)	1790(4)	1788(2)	55(5)
C(447)	3987(7)	1864(4)	1830(2)	66(6)
C(448)	4252(8)	1535(5)	1843(2)	76(6)
C(449)	4690(9)	1813(5)	1655(3)	84(7)
C(450)	5184(9)	1906(6)	1728(3)	117(9)
C(451)	4679(11)	1841(7)	1476(3)	152(11)
C(452)	3832(7)	1328(4)	1849(2)	60(5)
C(453)	3761(8)	1169(5)	2012(3)	93(7)
C(454)	4050(11)	500(9)	1867(5)	370(30)
C(455)	3469(14)	410(7)	2174(3)	226(18)
C(456)	2940(10)	447(7)	1852(3)	209(16)
C(457)	3037(17)	584(10)	1679(3)	390(40)
C(458)	2392(9)	506(8)	1909(4)	250(20)
C(459)	3016(12)	93(6)	1826(4)	218(17)

**Guanosine 24**

Si(24)	2331(3)	1234(2)	3542(1)	120(3)
C(461)	2470(6)	2357(3)	3078(2)	39(4)
N(461)	2291(5)	2358(3)	2918(1)	38(3)
O(461)	2387(4)	2241(2)	2653(1)	42(3)
C(462)	3145(6)	2085(4)	3008(2)	41(4)
N(462)	2146(5)	2504(3)	3187(2)	67(4)
O(462)	3494(5)	1609(3)	3249(2)	78(4)
C(463)	3022(6)	2074(3)	2847(2)	35(4)
N(463)	2880(5)	2217(3)	3128(1)	43(3)
O(463)	4463(5)	2158(3)	3297(2)	75(4)

C(464)	2565(6)	2234(4)	2797(2)	50(5)
N(464)	3403(5)	1918(3)	2757(2)	53(4)
O(464)	4272(7)	1866(4)	3513(2)	120(6)
C(465)	3724(6)	1822(4)	2868(2)	50(5)
N(465)	3588(5)	1913(3)	3022(2)	53(4)
O(465)	2536(5)	1493(3)	3410(2)	91(4)
C(466)	3809(7)	1828(4)	3167(2)	67(6)
C(467)	3920(7)	2084(4)	3284(2)	66(6)
C(468)	3751(7)	1959(5)	3455(2)	74(6)
C(469)	4657(11)	2081(7)	3459(3)	118(9)
C(470)	4640(14)	2328(8)	3557(4)	191(14)
C(471)	5168(13)	1884(8)	3424(4)	182(14)
C(472)	3405(7)	1678(5)	3421(2)	77(6)
C(473)	2844(6)	1745(4)	3449(2)	63(5)
C(474)	2931(10)	1065(7)	3644(4)	243(19)
C(475)	1953(8)	1403(5)	3701(2)	105(8)
C(476)	2022(9)	948(5)	3429(3)	190(14)
C(477)	2392(10)	801(6)	3302(3)	180(13)
C(478)	1516(8)	1073(6)	3352(3)	142(10)
C(479)	1843(12)	676(6)	3547(3)	228(18)

**Guanosine 25**

Si(25)	3291(3)	4156(2)	3655(1)	117(3)
C(481)	2670(6)	3126(3)	3126(2)	40(4)
N(481)	2601(5)	3172(3)	2961(2)	45(4)
O(481)	2124(4)	3354(2)	2751(1)	51(3)
C(482)	1967(6)	3375(3)	3173(2)	35(4)
N(482)	3104(5)	2970(3)	3163(2)	59(4)
O(482)	1870(5)	3777(3)	3489(1)	69(4)
C(483)	1814(6)	3433(3)	3022(2)	35(4)
N(483)	2380(5)	3232(3)	3239(1)	39(3)
O(483)	1175(5)	3112(3)	3579(2)	77(4)
C(484)	2172(6)	3316(4)	2901(2)	48(5)
N(484)	1360(5)	3591(3)	3008(2)	49(4)
O(484)	1390(5)	3442(3)	3778(2)	83(4)
C(485)	1240(6)	3642(3)	3156(2)	41(4)
N(485)	1568(5)	3519(3)	3263(2)	53(4)
O(485)	2900(5)	3934(3)	3540(2)	88(4)
C(486)	1512(7)	3556(4)	3441(2)	60(5)
C(487)	1627(7)	3269(4)	3529(2)	54(5)
C(488)	1861(8)	3387(5)	3683(2)	76(6)
C(489)	1030(8)	3204(5)	3738(2)	80(6)
C(490)	473(8)	3328(5)	3735(3)	104(8)
C(491)	1094(8)	2951(5)	3853(2)	89(7)
C(492)	2121(7)	3678(5)	3632(2)	73(6)
C(493)	2709(7)	3657(4)	3600(2)	74(6)
C(494)	2964(10)	4204(6)	3853(3)	137(10)
C(495)	3957(11)	3960(6)	3689(3)	147(11)
C(496)	3389(10)	4490(5)	3547(3)	111(8)
C(497)	2865(9)	4629(6)	3479(3)	116(9)
C(498)	3786(12)	4389(7)	3398(4)	175(13)
C(499)	3698(15)	4720(9)	3664(5)	231(18)

**Guanosine 26**

Si(26)	405(4)	5197(2)	2491(2)	170(5)
C(501)	809(6)	3758(4)	2602(2)	48(5)

N(501)	1294(5)	3612(3)	2562(2)	53(4)
O(501)	1923(4)	3431(2)	2393(1)	49(3)
C(502)	689(5)	3819(3)	2336(2)	31(4)
N(502)	694(5)	3781(3)	2746(2)	54(4)
O(502)	101(5)	4411(3)	2213(1)	73(4)
C(503)	1145(6)	3678(3)	2294(2)	39(4)
N(503)	522(5)	3873(3)	2487(2)	57(4)
O(503)	-883(5)	3893(3)	2183(2)	76(4)
C(504)	1498(6)	3561(3)	2405(2)	31(4)
N(504)	1191(5)	3671(3)	2128(2)	47(4)
O(504)	-1136(5)	4353(3)	2266(2)	92(4)
C(505)	776(6)	3818(4)	2083(2)	44(5)
N(505)	450(5)	3912(3)	2196(2)	41(4)
O(505)	415(5)	4838(3)	2440(2)	97(4)
C(506)	-37(7)	4098(4)	2170(2)	67(6)
C(507)	-463(7)	3998(4)	2281(2)	67(6)
C(508)	-664(7)	4292(4)	2361(2)	67(6)
C(509)	-1343(8)	4078(5)	2213(2)	74(6)
C(510)	-1619(10)	4127(6)	2058(3)	137(10)
C(511)	-1686(9)	3926(6)	2339(3)	113(8)
C(512)	-257(7)	4524(4)	2330(2)	57(5)
C(513)	45(8)	4620(5)	2470(3)	92(7)
C(514)	-192(8)	5304(5)	2577(3)	107(8)
C(515)	925(16)	5267(10)	2685(5)	242(19)
C(516)	773(14)	5420(8)	2373(4)	184(14)
C(517)	1331(10)	5343(6)	2329(3)	141(10)
C(518)	843(13)	5754(8)	2417(4)	193(14)
C(519)	328(17)	5381(10)	2227(5)	250(20)
<b>Guanosine 27</b>				
Si(27)	3468(2)	3918(1)	1369(1)	74(2)
C(521)	2252(6)	3206(3)	1943(2)	37(4)
N(521)	2387(5)	3184(3)	2103(1)	38(3)
O(521)	2923(4)	3038(2)	2311(1)	42(3)
C(522)	2956(6)	2913(3)	1884(2)	37(4)
N(522)	1825(5)	3344(3)	1909(2)	49(4)
O(522)	3514(4)	3051(2)	1571(1)	55(3)
C(523)	3112(6)	2886(3)	2039(2)	36(4)
N(523)	2551(5)	3071(3)	1829(2)	46(4)
O(523)	2818(4)	2385(3)	1484(1)	67(4)
C(524)	2830(6)	3034(3)	2157(2)	37(4)
N(524)	3553(5)	2719(3)	2048(1)	43(4)
O(524)	3171(5)	2656(3)	1282(1)	71(4)
C(525)	3680(6)	2653(4)	1896(2)	45(5)
N(525)	3310(5)	2768(3)	1794(2)	51(4)
O(525)	3260(4)	3667(3)	1500(1)	66(4)
C(526)	3343(7)	2749(4)	1622(2)	62(5)
C(527)	2856(6)	2684(4)	1533(2)	49(5)
C(528)	2879(7)	2879(4)	1381(2)	63(5)
C(529)	2969(7)	2371(4)	1317(2)	62(5)
C(530)	2472(7)	2300(5)	1218(2)	83(7)
C(531)	3400(8)	2139(5)	1297(3)	98(7)
C(532)	3216(6)	3138(4)	1425(2)	50(5)
C(533)	2930(6)	3419(4)	1458(2)	59(5)
C(534)	3904(9)	3728(5)	1220(3)	110(8)

C(535)	2901(10)	4107(6)	1271(3)	130(10)
C(536)	3863(7)	4169(4)	1477(2)	75(6)
C(537)	4344(9)	4019(6)	1547(3)	121(9)
C(538)	3584(10)	4316(6)	1629(3)	119(9)
C(539)	4042(10)	4450(6)	1378(3)	120(9)
<b>Guanosine 28</b>				
Si(28)	6507(2)	2892(2)	2509(1)	83(2)
C(541)	4090(6)	2547(4)	2469(2)	48(5)
N(541)	3661(5)	2733(3)	2506(2)	50(4)
O(541)	3139(4)	2989(2)	2682(1)	49(3)
C(542)	4261(6)	2523(4)	2728(2)	40(4)
N(542)	4153(5)	2480(3)	2319(2)	50(4)
O(542)	5443(5)	2476(3)	2820(1)	68(4)
C(543)	3842(6)	2691(4)	2777(2)	44(5)
N(543)	4417(6)	2429(3)	2581(2)	64(4)
O(543)	5091(6)	1729(3)	2880(2)	88(4)
C(544)	3514(6)	2813(4)	2661(2)	48(5)
N(544)	3848(5)	2720(3)	2940(2)	53(4)
O(544)	5905(6)	1814(4)	2801(2)	106(5)
C(545)	4263(6)	2569(4)	2990(2)	51(5)
N(545)	4533(5)	2443(3)	2865(2)	58(4)
O(545)	5911(5)	2788(3)	2561(1)	71(4)
C(546)	5043(6)	2284(4)	2879(2)	52(5)
C(547)	5029(8)	1990(4)	2765(2)	73(6)
C(548)	5573(8)	1985(5)	2694(3)	88(7)
C(549)	5569(9)	1611(5)	2870(3)	92(7)
C(550)	5828(14)	1503(8)	3019(4)	196(15)
C(551)	5523(10)	1314(6)	2768(3)	129(9)
C(552)	5765(7)	2317(4)	2702(2)	63(5)
C(553)	5744(7)	2502(4)	2540(2)	74(6)
C(554)	6978(9)	2661(6)	2622(3)	117(9)
C(555)	6600(8)	2845(5)	2294(2)	89(7)
C(556)	6569(8)	3288(4)	2563(3)	86(7)
C(557)	6456(10)	3332(6)	2737(3)	120(9)
C(558)	6179(9)	3497(5)	2477(3)	112(8)
C(559)	7117(9)	3405(5)	2518(3)	114(8)
<b>Guanosine 29</b>				
Si(29)	2583(5)	5281(3)	2966(1)	187(5)
C(561)	2472(7)	4056(4)	3066(2)	56(5)
N(561)	2605(5)	3988(3)	2905(2)	51(4)
O(561)	2439(4)	4003(2)	2634(1)	48(3)
C(562)	1782(7)	4302(4)	2975(2)	51(5)
N(562)	2800(5)	3956(3)	3176(2)	48(4)
O(562)	972(6)	4895(3)	3089(2)	97(5)
C(563)	1859(7)	4232(4)	2818(2)	67(6)
N(563)	2051(5)	4212(3)	3101(2)	55(4)
O(563)	799(5)	4559(3)	3390(2)	76(4)
C(564)	2307(6)	4067(3)	2781(2)	44(4)
N(564)	1460(6)	4362(3)	2721(2)	71(5)
O(564)	1483(6)	4858(3)	3477(2)	107(5)
C(565)	1125(7)	4482(4)	2828(2)	63(5)
N(565)	1295(6)	4449(3)	2981(2)	65(4)
O(565)	2041(8)	5086(5)	3031(2)	154(7)
C(566)	1035(8)	4589(4)	3118(2)	66(6)

C(567)	1207(8)	4542(5)	3270(2)	75(6)
C(568)	1544(8)	4799(5)	3305(2)	80(6)
C(569)	1049(9)	4675(5)	3523(3)	93(7)
C(570)	1252(9)	4436(5)	3638(3)	100(8)
C(571)	693(10)	4859(6)	3611(3)	130(9)
C(572)	1344(10)	5048(6)	3190(3)	113(8)
C(573)	1680(13)	5254(8)	3118(4)	176(13)
C(574)	2989(13)	5419(8)	3131(4)	195(15)
C(575)	2426(15)	5586(9)	2816(5)	224(17)
C(576)	2864(13)	5034(7)	2844(4)	170(13)
C(577)	3385(14)	5191(9)	2736(4)	208(16)
C(578)	2528(11)	4925(6)	2690(3)	148(11)
C(579)	3112(11)	4735(7)	2963(3)	146(10)

**Guanosine 30**

Si(30)	3172(3)	5116(2)	1962(1)	138(3)
C(581)	1709(7)	4349(4)	2279(2)	61(5)
N(581)	2109(5)	4173(3)	2322(2)	45(4)
O(581)	2799(4)	3851(2)	2277(1)	47(3)
C(582)	1914(6)	4258(4)	2032(2)	45(5)
N(582)	1401(5)	4475(3)	2390(2)	62(4)
O(582)	1865(4)	4721(3)	1706(1)	68(3)
C(583)	2318(7)	4079(4)	2062(2)	48(5)
N(583)	1593(5)	4408(3)	2123(2)	48(4)
O(583)	687(5)	4599(3)	1700(2)	75(4)
C(584)	2445(6)	4010(4)	2224(2)	48(5)
N(584)	2560(5)	3957(3)	1923(2)	58(4)
O(584)	798(5)	5075(3)	1791(2)	79(4)
C(585)	2298(7)	4099(4)	1808(2)	57(5)
N(585)	1874(5)	4270(3)	1860(2)	53(4)
O(585)	2609(6)	5111(3)	1870(2)	98(5)
C(586)	1566(6)	4454(4)	1748(2)	52(5)
C(587)	1056(7)	4561(4)	1826(2)	62(5)
C(588)	1195(7)	4907(4)	1873(2)	65(6)
C(589)	390(9)	4881(5)	1736(3)	91(7)
C(590)	-30(8)	4830(5)	1851(3)	100(7)
C(591)	232(10)	4992(6)	1572(3)	122(9)
C(592)	1712(7)	4975(5)	1804(2)	74(6)
C(593)	2124(7)	5044(4)	1934(2)	70(6)
C(594)	3304(10)	4714(6)	2052(3)	137(10)
C(595)	3671(11)	5183(7)	1808(3)	151(11)
C(596)	3238(16)	5402(8)	2099(4)	185(14)
C(597)	2860(14)	5330(9)	2247(4)	210(16)
C(598)	3107(18)	5697(11)	2028(6)	270(20)
C(599)	3824(14)	5361(8)	2175(4)	206(16)

**Guanosine 31**

Si(31)	5848(6)	4130(3)	2024(2)	221(6)
C(601)	3805(6)	3494(3)	1982(2)	35(4)
N(601)	3676(4)	3547(3)	2135(1)	35(3)
O(601)	3776(4)	3494(2)	2408(1)	47(3)
C(602)	4502(6)	3241(4)	2066(2)	42(4)
N(602)	3491(5)	3600(3)	1871(2)	50(4)
O(602)	5698(5)	3174(3)	1906(2)	84(4)
C(603)	4388(6)	3287(4)	2226(2)	48(5)
N(603)	4231(5)	3351(3)	1940(2)	51(4)

O(603)	5206(5)	2722(3)	1677(2)	80(4)
C(604)	3941(6)	3440(4)	2265(2)	39(4)
N(604)	4752(5)	3139(3)	2320(2)	47(4)
O(604)	5395(5)	3134(3)	1528(1)	69(4)
C(605)	5081(7)	3019(4)	2216(2)	63(5)
N(605)	4946(5)	3077(3)	2060(2)	54(4)
O(605)	5803(7)	3827(4)	1921(2)	128(6)
C(606)	5279(7)	2971(4)	1924(2)	60(5)
C(607)	4993(7)	2966(4)	1773(2)	59(5)
C(608)	5167(7)	3256(4)	1686(2)	70(6)
C(609)	5241(7)	2842(4)	1515(2)	63(5)
C(610)	4704(7)	2809(5)	1438(2)	81(6)
C(611)	5657(8)	2671(5)	1434(2)	86(7)
C(612)	5597(7)	3383(4)	1787(2)	70(6)
C(613)	5407(10)	3701(6)	1841(3)	116(9)
C(614)	6515(9)	4086(8)	2136(4)	213(16)
C(615)	6008(19)	4460(7)	1882(5)	490(50)
C(616)	5366(11)	4254(7)	2146(4)	330(30)
C(617)	5218(10)	3978(6)	2246(3)	148(11)
C(618)	5560(20)	4526(9)	2255(6)	610(70)
C(619)	4925(14)	4394(11)	2034(5)	380(40)

**Guanosine 32**

Si(32)	5319(7)	4297(4)	3023(2)	270(7)
C(621)	4660(7)	3262(4)	2769(2)	56(5)
N(621)	4210(4)	3402(3)	2718(2)	39(3)
O(621)	3431(4)	3653(2)	2764(1)	48(3)
C(622)	4441(7)	3373(4)	3012(2)	59(5)
N(622)	4947(5)	3141(3)	2656(2)	51(4)
O(622)	5192(8)	3541(5)	3334(2)	144(7)
C(623)	3980(7)	3513(4)	2978(2)	52(5)
N(623)	4799(5)	3242(3)	2922(2)	58(4)
O(623)	5478(5)	2899(3)	3358(2)	91(4)
C(624)	3823(6)	3537(4)	2818(2)	40(4)
N(624)	3721(6)	3616(3)	3117(2)	63(4)
O(624)	6185(7)	3109(5)	3248(2)	132(6)
C(625)	4053(7)	3523(4)	3229(2)	66(6)
N(625)	4479(6)	3386(4)	3185(2)	75(5)
O(625)	5564(11)	3995(6)	3113(4)	258(14)
C(626)	4911(8)	3281(5)	3296(3)	83(7)
C(627)	5280(8)	3060(5)	3220(2)	75(6)
C(628)	5766(11)	3267(7)	3178(4)	135(10)
C(629)	6043(12)	2850(7)	3315(4)	137(10)
C(630)	6105(15)	2580(9)	3203(5)	215(17)
C(631)	6268(12)	2827(7)	3477(4)	162(12)
C(632)	5659(12)	3543(7)	3254(3)	132(10)
C(633)	5640(20)	3731(10)	3071(6)	270(20)
C(634)	5359(15)	4627(7)	3152(4)	290(20)
C(635)	4579(9)	4220(9)	3002(4)	270(20)
C(636)	5564(13)	4299(9)	2834(3)	540(60)
C(637)	5299(17)	4023(9)	2733(4)	310(30)
C(638)	6159(12)	4274(12)	2818(5)	390(40)
C(639)	5370(20)	4594(10)	2740(5)	500(50)



**Picrate Anions**

C(711)	-6150(5)	5468(3)	5113(2)	81(6)
C(712)	-6294(6)	5748(4)	5052(1)	96(7)
C(713)	-6678(6)	5917(3)	5129(2)	108(8)
C(714)	-6917(5)	5805(3)	5265(2)	71(6)
C(715)	-6773(5)	5526(3)	5326(1)	83(6)
C(716)	-6390(6)	5357(3)	5249(2)	95(7)
N(712)	-6046(11)	5862(6)	4917(3)	133(8)
N(714)	-7275(7)	6006(5)	5365(2)	96(6)
N(716)	-6270(8)	5061(5)	5316(3)	107(6)
O(711)	-5758(5)	5335(3)	5042(2)	96(5)
O(712)	-5612(9)	5942(5)	4935(2)	159(8)
O(713)	-6306(13)	5959(7)	4816(4)	254(14)
O(714)	-7358(7)	6248(4)	5302(2)	136(6)
O(715)	-7372(7)	5895(4)	5485(2)	121(5)
O(716)	-6380(7)	5001(4)	5452(2)	133(6)
O(717)	-6014(7)	4871(4)	5239(2)	138(6)
C(721)	-2049(5)	6899(2)	5479(1)	62(5)
C(722)	-2216(4)	6971(3)	5632(1)	58(5)
C(723)	-2073(5)	7244(3)	5701(1)	104(8)
C(724)	-1763(6)	7445(2)	5616(2)	109(8)
C(725)	-1595(5)	7374(3)	5463(2)	99(7)
C(726)	-1738(5)	7101(3)	5395(1)	53(5)
N(722)	-2549(6)	6777(4)	5725(2)	69(5)
N(724)	-1731(15)	7759(5)	5670(4)	261(18)
N(726)	-1550(7)	7035(5)	5240(2)	88(5)
O(721)	-2215(5)	6659(3)	5411(1)	78(4)
O(722)	-2847(5)	6611(3)	5665(2)	80(4)
O(723)	-2496(5)	6794(3)	5866(2)	103(5)
O(724)	-1782(13)	7801(7)	5819(4)	265(14)
O(725)	-1379(9)	7912(5)	5607(3)	181(8)
O(726)	-1591(7)	7237(5)	5136(2)	145(6)
O(727)	-1396(6)	6786(4)	5208(2)	96(4)
C(731)	923(4)	4714(3)	4930(2)	61(5)
C(732)	1128(5)	4732(3)	4776(1)	76(6)
C(733)	1645(5)	4818(3)	4754(1)	66(6)
C(734)	1958(4)	4886(3)	4884(2)	80(6)
C(735)	1754(5)	4868(3)	5038(1)	84(7)
C(736)	1236(5)	4782(3)	5060(1)	76(6)
N(732)	810(8)	4649(4)	4637(2)	97(6)
N(734)	2465(7)	5029(4)	4860(3)	95(6)
N(736)	1014(9)	4775(5)	5227(3)	116(7)
O(731)	428(5)	4654(3)	4960(1)	76(4)
O(732)	407(6)	4517(3)	4649(2)	102(5)
O(733)	1004(8)	4735(5)	4513(3)	173(8)
O(734)	2619(7)	5044(4)	4717(2)	126(6)
O(735)	2721(7)	5104(4)	4966(2)	132(6)
O(736)	1285(9)	4670(5)	5322(3)	167(8)
O(737)	660(7)	4938(4)	5248(2)	113(5)
C(741)	-3194(6)	3075(3)	4693(2)	111(8)
C(742)	-3376(6)	3038(3)	4539(2)	123(9)
C(743)	-3278(6)	2771(4)	4457(2)	133(10)
C(744)	-2997(6)	2542(3)	4531(2)	110(8)
C(745)	-2814(6)	2579(3)	4686(2)	105(8)

C(746)	-2913(6)	2846(4)	4767(2)	95(7)
N(742)	-3607(12)	3300(7)	4436(4)	179(12)
N(744)	-2932(17)	2254(6)	4456(4)	290(20)
N(746)	-2787(12)	2865(8)	4935(4)	174(11)
O(741)	-3310(7)	3308(4)	4781(2)	146(7)
O(742)	-3943(10)	3466(6)	4536(3)	195(9)
O(743)	-3633(12)	3249(7)	4318(4)	228(13)
O(744)	-2972(11)	2290(7)	4312(3)	237(12)
O(745)	-2639(11)	2076(7)	4516(3)	240(12)
O(746)	-2750(18)	2709(10)	5022(5)	330(20)
O(747)	-2451(12)	3091(7)	4946(3)	239(12)

**Solvent Molecules**

C(751)	1365(5)	3115(3)	1463(1)	64(5)
C(752)	1458(5)	3399(2)	1400(1)	60(5)
C(753)	1494(4)	3438(2)	1236(1)	60(5)
C(754)	1438(5)	3193(3)	1134(1)	63(5)
C(755)	1345(5)	2908(2)	1197(1)	76(6)
C(756)	1308(4)	2869(2)	1361(1)	51(5)
N(752)	1507(6)	3660(4)	1497(2)	68(4)
N(754)	1483(8)	3231(6)	961(2)	107(6)
N(756)	1233(7)	2569(4)	1420(2)	83(5)
O(751)	1355(4)	3067(2)	1619(1)	57(3)
O(752)	1767(6)	3878(4)	1439(2)	99(5)
O(753)	1307(5)	3674(3)	1625(2)	78(4)
O(754)	1505(6)	3482(4)	917(2)	103(5)
O(755)	1479(7)	3010(4)	885(2)	122(6)
O(756)	891(7)	2406(4)	1354(2)	119(5)
O(757)	1488(6)	2474(3)	1532(2)	95(4)
C(761)	-899(6)	3930(4)	2790(2)	83(6)
C(762)	-1367(8)	3776(3)	2769(2)	101(8)
C(763)	-1839(6)	3917(5)	2803(2)	200(15)
C(764)	-1843(7)	4212(5)	2859(3)	187(14)
C(765)	-1375(9)	4366(3)	2880(2)	219(17)
C(766)	-903(7)	4225(4)	2845(2)	110(8)
N(762)	-1400(9)	3512(5)	2701(3)	129(7)
N(764)	-2330(12)	4369(9)	2883(7)	360(20)
N(766)	-423(14)	4417(9)	2870(4)	189(12)
O(761)	-458(6)	3796(4)	2766(2)	115(5)
O(762)	-1116(7)	3432(4)	2582(2)	122(6)
O(763)	-1739(9)	3324(5)	2746(3)	168(8)
O(764)	-2260(20)	4652(12)	2851(7)	290(20)
O(765)	-2450(19)	4424(12)	3023(6)	240(20)
O(74A)	-2794(19)	4099(11)	2931(6)	142(17)
O(75A)	-2680(20)	4373(13)	2751(7)	170(20)
O(766)	-438(13)	4683(9)	2878(4)	255(14)
O(767)	-35(8)	4276(5)	2902(2)	147(7)
C(771)	2839(5)	2689(3)	3627(1)	70(6)
C(772)	2449(4)	2557(3)	3719(2)	62(5)
C(773)	2459(5)	2589(3)	3884(2)	71(6)
C(774)	2858(6)	2752(3)	3957(1)	106(8)
C(775)	3248(5)	2883(3)	3864(2)	101(8)
C(776)	3238(5)	2851(3)	3699(2)	88(7)
N(772)	2042(7)	2394(4)	3655(2)	97(6)
N(774)	2854(11)	2788(5)	4142(3)	132(8)

N(776)	3651(10)	3022(6)	3600(3)	135(8)
O(771)	2852(5)	2647(3)	3471(2)	94(4)
O(772)	1843(6)	2483(3)	3523(2)	103(5)
O(773)	1828(7)	2198(4)	3734(2)	126(6)
O(774)	2468(9)	2675(5)	4203(3)	175(8)
O(775)	3269(9)	2888(5)	4183(2)	157(7)
O(776)	3990(11)	3119(6)	3685(3)	193(9)
O(777)	3747(10)	2923(6)	3477(4)	211(11)
C(781)	5043(5)	1713(3)	2253(2)	75(6)
C(782)	5445(6)	1842(3)	2164(2)	85(7)
C(783)	5849(5)	1663(4)	2107(2)	140(10)
C(784)	5852(6)	1355(4)	2138(2)	181(14)
C(785)	5450(7)	1226(3)	2226(2)	127(9)
C(786)	5045(5)	1405(4)	2284(2)	87(7)
N(782)	5478(8)	2158(4)	2120(2)	89(6)
N(784)	6218(14)	1157(7)	2058(5)	310(20)
N(786)	4648(8)	1268(6)	2392(3)	116(7)
O(781)	4687(5)	1879(3)	2308(2)	78(4)
O(782)	5076(8)	2288(4)	2106(2)	130(6)
O(783)	5889(8)	2254(4)	2091(2)	138(6)
O(784)	6626(11)	1275(6)	2016(3)	217(11)
O(785)	6267(15)	897(8)	2107(4)	301(17)
O(786)	4506(8)	1034(6)	2355(2)	161(8)
O(787)	4494(7)	1388(4)	2506(2)	125(6)
N(791)	-2720(20)	9573(13)	6350(7)	360(20)
C(791)	-2893(14)	9816(9)	6210(5)	176(13)
C(792)	-2909(14)	9960(8)	6095(4)	189(15)
N(795)	-7554(10)	6530(6)	5703(3)	177(10)
C(795)	-7676(11)	6599(6)	5901(4)	134(9)
C(796)	-7777(9)	6679(5)	6026(3)	101(7)
N(797)	-8207(10)	4047(6)	4972(3)	171(10)
C(797)	-8014(16)	4088(9)	4810(5)	202(16)
C(798)	-7757(12)	4130(7)	4664(4)	161(11)
N(799)	2474(12)	3502(8)	4029(4)	84(10)
C(799)	2301(15)	3497(9)	4148(5)	71(11)
C(800)	2124(19)	3449(12)	4300(6)	122(17)
N(801)	-2782(14)	7748(8)	5379(4)	94(11)
C(801)	-3008(13)	7838(8)	5472(4)	54(10)
C(802)	-3395(16)	7998(10)	5582(5)	92(14)
N(803)	-3521(17)	10451(10)	5884(5)	112(14)
C(803)	-3330(30)	10615(18)	5832(9)	160(30)
C(804)	-2970(40)	10750(20)	5737(11)	270(50)
N(805)	1004(16)	2631(9)	5040(5)	120(14)
C(805)	850(20)	2543(12)	5214(7)	121(18)
C(806)	600(20)	2534(12)	5342(6)	130(19)
N(807)	-2250(30)	1991(14)	4974(7)	190(20)
C(807)	-2310(20)	8154(11)	-30(6)	109(16)
C(808)	1790(20)	3185(14)	5039(7)	160(20)
N(809)	-3467(18)	6868(10)	6406(5)	129(15)
C(809)	-3070(20)	6664(13)	6443(6)	116(17)
C(810)	-2792(18)	6450(10)	6470(5)	97(15)
N(813)	-5688(15)	4662(10)	2444(5)	246(18)
C(813)	-5944(17)	4484(10)	2463(5)	184(15)
C(814)	-6304(12)	4256(7)	2506(4)	163(12)

N(817)	4690(20)	259(12)	2561(6)	157(19)
C(817)	5020(20)	360(12)	2518(6)	105(16)
C(818)	5340(30)	581(18)	2507(10)	230(30)
N(821)	-4719(19)	3448(12)	3770(6)	150(17)
C(821)	-4260(40)	3630(20)	3690(11)	220(30)
C(822)	-3850(30)	3795(18)	3612(9)	230(40)
N(823)	-1660(11)	7384(6)	6826(3)	62(9)
C(823)	-1930(30)	7150(20)	6658(10)	210(30)
C(824)	-2100(20)	6941(13)	6558(6)	140(20)
N(825)	-3178(19)	7617(12)	5982(6)	139(17)
C(825)	-3100(30)	7390(20)	6045(10)	190(30)
C(826)	-3090(30)	7105(16)	6159(8)	180(30)
N(827)	-7470(30)	4270(20)	5723(11)	300(40)
C(827)	-7400(20)	4146(13)	5907(7)	132(19)
C(828)	-7130(30)	4158(18)	6115(9)	230(40)
C(831)	-7830(30)	4978(16)	5597(11)	170(30)
C(832)	-8010(20)	4925(14)	5726(8)	160(20)
N(831)	-7623(18)	4896(11)	5444(6)	310(20)
C(833)	-7360(40)	4540(20)	5545(12)	230(40)
C(834)	-7390(20)	4395(12)	5445(6)	124(18)
C(851)	-2366(9)	5558(5)	890(3)	79(8)
Cl(51)	-1830(6)	5421(4)	983(2)	233(7)
Cl(52)	-2891(7)	5433(6)	987(2)	368(17)
Cl(53)	-2184(8)	5922(3)	890(2)	252(9)
C(861)	-541(12)	6393(7)	2427(3)	74(12)
Cl(61)	37(9)	6463(4)	2517(6)	390(30)
Cl(62)	-840(5)	6139(2)	2543(2)	113(5)
Cl(63)	-587(8)	6241(4)	2239(2)	181(9)
C(871)	-2509(16)	4014(10)	3171(6)	240(40)
Cl(71)	-2002(11)	3801(7)	3227(4)	295(16)
Cl(72)	-2828(14)	4166(10)	3324(5)	380(20)
Cl(73)	-2838(13)	3704(8)	3189(6)	400(30)
O(900)	-25(16)	6461(10)	2363(4)	119(14)
O(901)	-1080(30)	8467(17)	5916(9)	300(30)
O(902)	-2950(40)	8420(20)	5935(12)	400(50)
O(903)	-3480(40)	8370(20)	6075(10)	350(40)
O(907)	-890(30)	1063(16)	1366(8)	280(30)
O(908)	-1040(50)	670(30)	1483(14)	240(50)
O(909)	-300(20)	1003(13)	1383(7)	230(20)
O(910)	-3129(13)	5750(7)	4164(4)	110(10)
O(911)	-2670(17)	5647(9)	4190(5)	152(14)
O(912)	-1973(15)	5804(9)	4173(4)	147(14)
O(913)	6880(40)	2340(20)	3900(13)	210(40)
O(914)	6590(40)	2200(30)	3770(14)	230(40)
O(915)	-6680(30)	6590(15)	1561(8)	270(30)
O(916)	-6800(20)	3196(12)	6336(6)	210(20)
O(917)	-6510(20)	3444(12)	6220(6)	210(20)
O(918)	-2824(12)	7854(7)	389(4)	115(10)
O(919)	-2650(20)	8196(15)	372(7)	260(30)
O(920)	-6630(30)	3072(15)	5852(7)	250(30)
O(921)	-7009(18)	3253(10)	5825(5)	168(16)
O(922)	2608(17)	5062(10)	1445(5)	165(15)
O(923)	2860(30)	5423(16)	1443(8)	280(30)
O(924)	5361(19)	1027(11)	1699(6)	195(18)

O(925)	5250(30)	947(15)	1866(8)	270(30)
O(926)	-2090(40)	8630(30)	5745(13)	220(40)
O(927)	-2100(50)	4400(30)	3205(16)	260(50)
O(928)	-3030(20)	8972(15)	6656(7)	250(30)
O(929)	-2720(20)	8721(13)	6818(7)	240(20)
O(930)	-2010(40)	7570(30)	6216(14)	210(40)
O(931)	7020(30)	2280(20)	1339(12)	180(30)
O(932)	5930(30)	597(19)	1478(9)	150(30)
O(933)	-6200(30)	5850(20)	3600(10)	170(30)
O(934)	-2683(16)	6152(10)	4260(5)	161(14)
O(935)	-2502(16)	6470(10)	4306(5)	169(16)
O(936)	2370(30)	5877(17)	4789(9)	150(30)
O(937)	-6100(20)	6105(13)	1608(7)	240(20)
O(938)	5500(16)	363(10)	1703(5)	173(16)
O(939)	3060(20)	5062(12)	1008(7)	220(20)
O(940)	-2120(20)	7976(13)	6878(7)	230(20)
O(941)	2350(20)	712(14)	3847(7)	110(20)
O(942)	-6870(40)	2630(30)	6062(13)	230(50)
O(943)	2670(30)	4975(19)	1108(10)	160(30)
O(944)	3080(60)	6450(40)	4790(18)	310(70)
O(945)	-2640(50)	8780(30)	6196(14)	260(50)
O(946)	-2590(50)	8470(30)	5718(13)	230(40)
O(947)	2160(50)	5260(30)	1386(14)	250(50)
O(948)	-2948(12)	5835(7)	910(4)	9(8)

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Table 3. Pb-O bond lengths [Å] for [(G 1)<sub>8</sub>-Pb<sup>+2</sup>]<sub>2</sub> [Å].

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Pb(1)-O(121)	2.565(10)
Pb(1)-O(141)	2.588(10)
Pb(1)-O(81)	2.618(10)
Pb(1)-O(101)	2.648(11)
Pb(1)-O(1)	2.659(11)
Pb(1)-O(61)	2.707(10)
Pb(1)-O(21)	2.717(10)
Pb(1)-O(41)	2.723(9)
Pb(2)-O(221)	2.604(11)
Pb(2)-O(181)	2.617(10)
Pb(2)-O(201)	2.627(10)
Pb(2)-O(241)	2.640(11)
Pb(2)-O(161)	2.678(12)
Pb(2)-O(261)	2.711(10)
Pb(2)-O(301)	2.727(11)
Pb(2)-O(281)	2.740(12)
Pb(3)-O(441)	2.608(10)
Pb(3)-O(461)	2.611(10)
Pb(3)-O(421)	2.612(10)
Pb(3)-O(401)	2.648(10)
Pb(3)-O(381)	2.667(10)
Pb(3)-O(341)	2.678(11)
Pb(3)-O(321)	2.709(10)
Pb(3)-O(361)	2.723(10)
Pb(4)-O(501)	2.526(10)
Pb(4)-O(481)	2.598(11)
Pb(4)-O(541)	2.625(11)
Pb(4)-O(521)	2.656(10)
Pb(4)-O(621)	2.672(10)
Pb(4)-O(601)	2.689(10)
Pb(4)-O(561)	2.698(10)
Pb(4)-O(581)	2.709(10)

Table 4. Selected hydrogen bond lengths and angles for [(G 1)g-Pb<sup>+2</sup>]<sub>2</sub> [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1)-H(1)...O(21)	0.88	1.96	2.809(18)	161.2
N(2)-H(2A)...N(24)	0.88	1.90	2.78(2)	173.7
N(21)-H(21)...O(41)	0.88	2.07	2.903(17)	157.5
N(22)-H(22B)...N(44)	0.88	1.99	2.864(18)	169.7
N(41)-H(41)...O(61)	0.88	1.94	2.778(16)	159.4
N(42)-H(42B)...N(64)	0.88	2.00	2.86(2)	168.0
N(61)-H(61)...O(1)	0.88	1.98	2.822(18)	160.0
N(62)-H(62B)...N(4)	0.88	2.00	2.87(3)	168.8
N(81)-H(81)...O(101)	0.88	2.04	2.886(17)	160.9
N(82)-H(82B)...N(104)	0.88	2.05	2.914(19)	167.2
N(101)-H(101)...O(121)	0.88	2.03	2.885(16)	165.2
N(102)-H(10E)...N(124)	0.88	1.93	2.791(18)	166.2
N(121)-H(121)...O(141)	0.88	2.09	2.916(16)	156.0
N(122)-H(12B)...N(144)	0.88	2.12	2.987(19)	167.3
N(141)-H(141)...O(81)	0.88	1.99	2.830(17)	159.4
N(142)-H(14E)...N(84)	0.88	2.02	2.88(2)	165.4
N(161)-H(161)...O(221)	0.88	2.07	2.910(18)	160.3
N(162)-H(16B)...N(224)	0.88	2.02	2.89(2)	166.9
N(181)-H(181)...O(161)	0.88	2.00	2.846(17)	159.5
N(182)-H(18E)...N(164)	0.88	2.03	2.89(2)	167.0
N(201)-H(201)...O(181)	0.88	2.07	2.906(16)	158.5
N(202)-H(20B)...N(184)	0.88	2.04	2.894(19)	162.3
N(221)-H(221)...O(201)	0.88	1.98	2.825(17)	160.4
N(222)-H(22D)...N(204)	0.88	2.01	2.88(2)	168.3
N(241)-H(241)...O(301)	0.88	1.93	2.784(18)	164.0
N(242)-H(24B)...N(304)	0.88	1.98	2.81(2)	158.1
N(261)-H(261)...O(241)	0.88	2.11	2.936(18)	156.3
N(262)-H(26B)...N(244)	0.88	2.04	2.90(2)	164.9
N(281)-H(281)...O(261)	0.88	1.97	2.814(17)	160.2
N(282)-H(28B)...N(264)	0.88	1.99	2.86(2)	167.1
N(301)-H(301)...O(281)	0.88	2.04	2.870(18)	156.9
N(302)-H(30A)...N(284)	0.88	1.99	2.86(2)	171.6
N(321)-H(321)...O(341)	0.88	2.01	2.852(17)	159.4
N(322)-H(32A)...N(344)	0.88	1.96	2.836(19)	172.9
N(341)-H(341)...O(361)	0.88	2.01	2.850(17)	159.5
N(342)-H(34E)...N(364)	0.88	1.96	2.82(2)	168.2
N(361)-H(361)...O(381)	0.88	2.07	2.903(17)	158.4
N(362)-H(36B)...N(384)	0.88	1.97	2.85(2)	173.6
N(381)-H(381)...O(321)	0.88	1.98	2.808(17)	156.6
N(382)-H(38B)...N(324)	0.88	2.03	2.89(2)	169.1
N(401)-H(401)...O(421)	0.88	2.03	2.858(17)	157.3
N(402)-H(40B)...N(424)	0.88	2.01	2.890(19)	174.0
N(421)-H(421)...O(441)	0.88	2.04	2.885(16)	160.9
N(422)-H(42B)...N(444)	0.88	2.04	2.907(18)	166.8
N(441)-H(441)...O(461)	0.88	2.05	2.876(17)	155.7
N(442)-H(44B)...N(464)	0.88	2.02	2.895(19)	172.3
N(461)-H(461)...O(401)	0.88	2.01	2.857(16)	160.7
N(462)-H(46B)...N(404)	0.88	1.97	2.827(19)	164.4

N(481)-H(481)...O(541)	0.88	2.01	2.834(17)	155.9
N(482)-H(48B)...N(544)	0.88	2.01	2.885(19)	170.4
N(501)-H(501)...O(481)	0.88	2.06	2.887(17)	156.4
N(502)-H(50B)...N(484)	0.88	2.04	2.905(19)	169.1
N(521)-H(521)...O(501)	0.88	2.07	2.914(16)	159.6
N(522)-H(52B)...N(504)	0.88	1.97	2.844(19)	169.9
N(541)-H(541)...O(521)	0.88	2.00	2.841(16)	159.5
N(542)-H(54B)...N(524)	0.88	2.07	2.941(18)	169.4
N(561)-H(561)...O(621)	0.88	2.00	2.842(17)	158.4
N(562)-H(56B)...N(624)	0.88	1.97	2.840(19)	172.0
N(581)-H(581)...O(561)	0.88	2.01	2.853(16)	160.4
N(582)-H(58A)...N(564)	0.88	1.96	2.83(2)	169.7
N(601)-H(601)...O(581)	0.88	2.04	2.876(16)	158.5
N(602)-H(60B)...N(584)	0.88	2.02	2.892(19)	169.8
N(621)-H(621)...O(601)	0.88	2.02	2.854(16)	158.1
N(622)-H(62D)...N(604)	0.88	1.99	2.859(19)	168.6

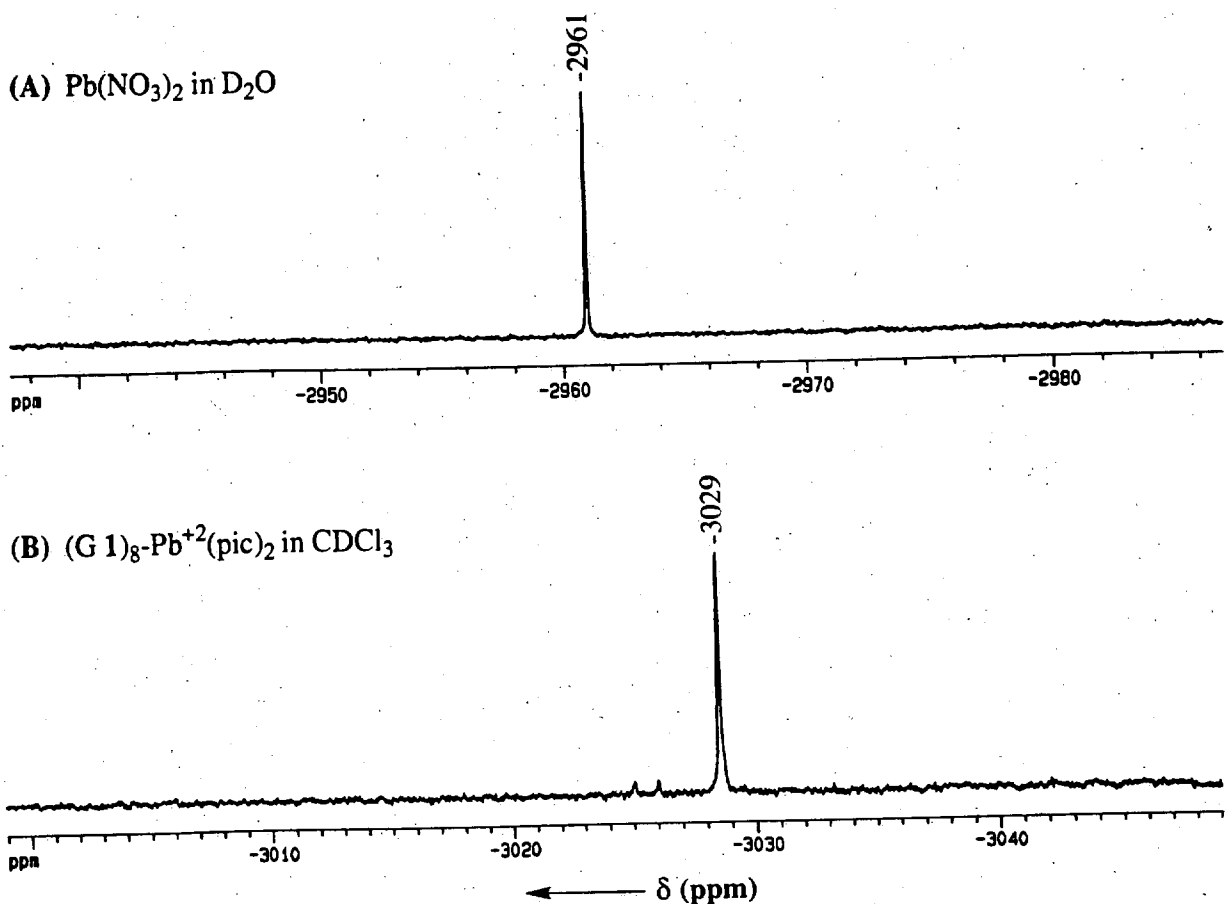
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Symmetry transformations used to generate equivalent atoms:

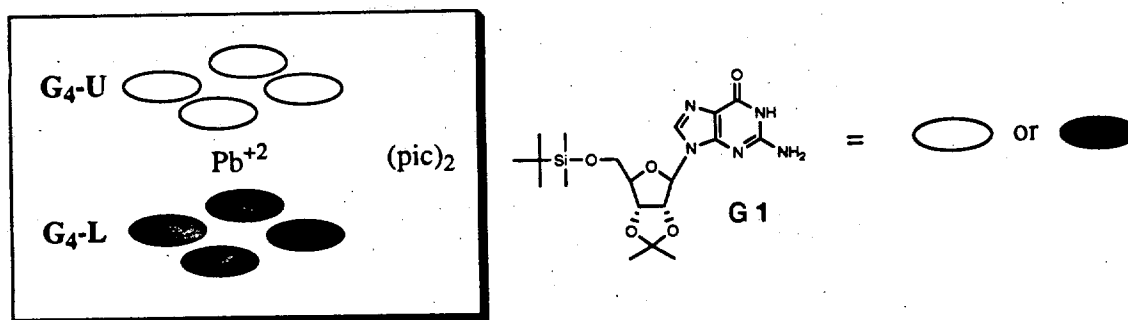
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#4 -x,y-1/2,-z+1/2 #5 -x+1/2,-y+1,z+1/2 #6 -x+1/2,-y+1,z-1/2

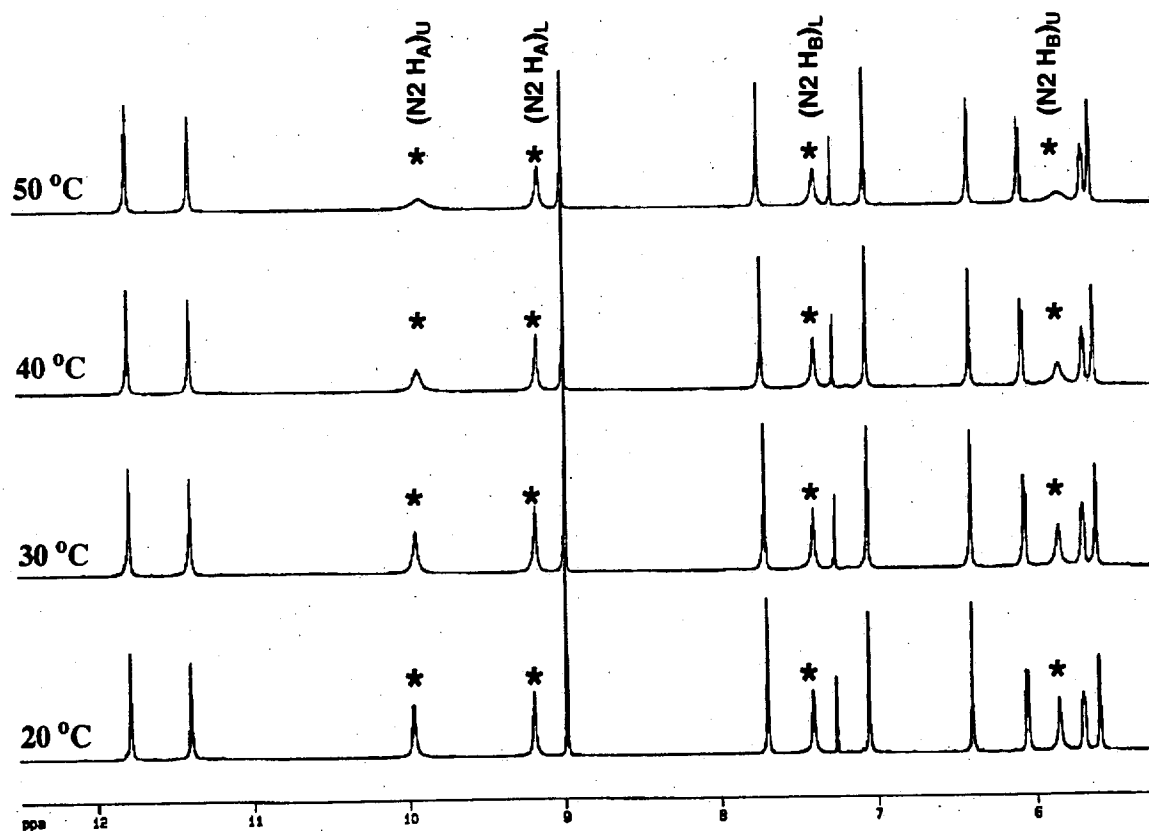




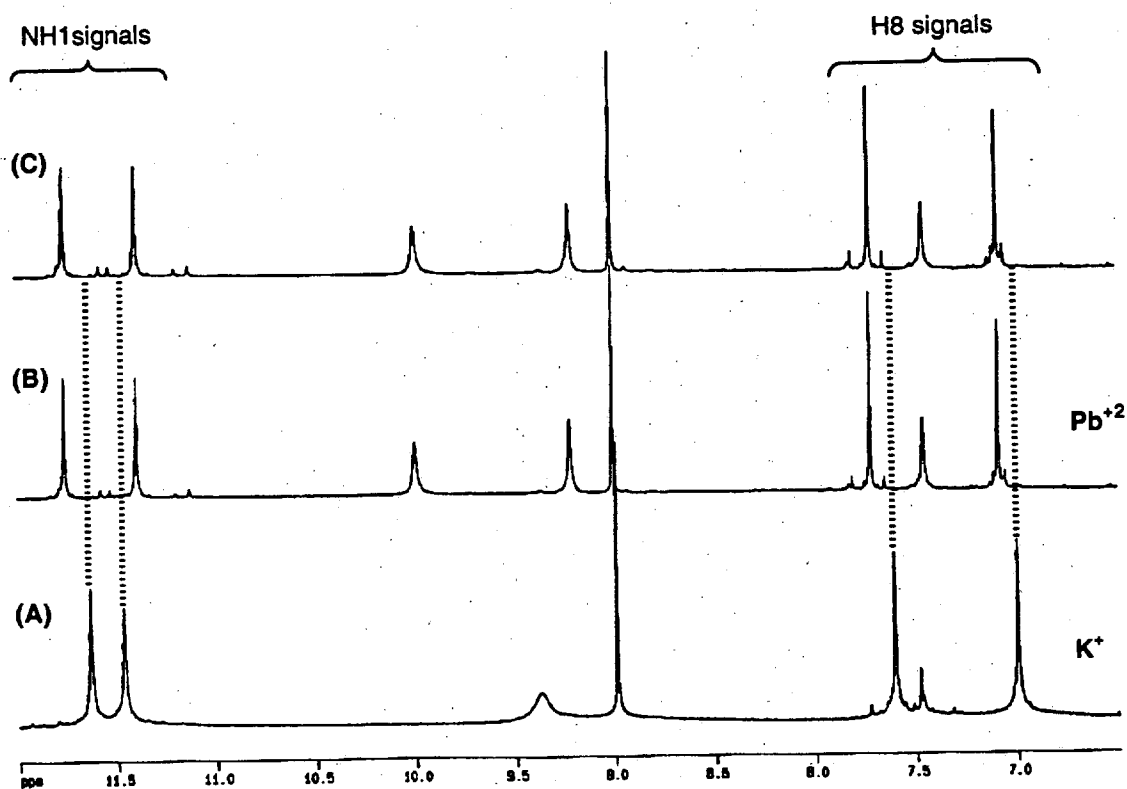
**Figure 1.** One dimensional  $^{207}\text{Pb}$  NMR. Spectra were recorded on a Bruker DRX 500 MHz spectrometer at 25 °C operating at 104.63 MHz for  $^{207}\text{Pb}$ . A total of 16,000 data points were collected with an acquisition time of 1.6 s for both experiments. A sweep width of 5 kHz was used. Fourier transformation was done with a line broadening of 3 Hz. (A) A 1.0 M solution of  $\text{Pb}(\text{NO}_3)_2$  in 99.9%  $\text{D}_2\text{O}$  at pH 3.3 was used as the external reference. Two transients were collected with a 2 s relaxation delay. The NMR signal at  $\delta = -2961$  ppm is relative to  $\text{Pb}(\text{CH}_3)_4$  at  $\delta = 0.0$  ppm. (B) The Pb octamer,  $(\text{G} 1)_8\text{-Pb}^{+2}(\text{pic})_2$ , in  $\text{CDCl}_3$ . The sample was 50 mM in octamer. A total of 1000 transients were collected with a 0.5 s relaxation delay.



**Figure 2A. Schematic for identification of inequivalent G<sub>4</sub>-quartets.** From the crystal structure of (G 1)<sub>8</sub>-Pb<sup>+2</sup>(pic)<sub>2</sub>, it is apparent that the N2 H<sub>B</sub> protons of one G<sub>4</sub>-quartet are hydrogen bonded to the 5'-oxygens of the other G<sub>4</sub>-quartet. The G<sub>4</sub>-quartet containing the N2 H<sub>B</sub> protons (hydrogen bond donors) is arbitrarily defined as the upper quartet (G<sub>4</sub>-U). Conversely, the quartet containing the hydrogen bonding acceptor 5'-oxygens is defined as the lower quartet (G<sub>4</sub>-L).



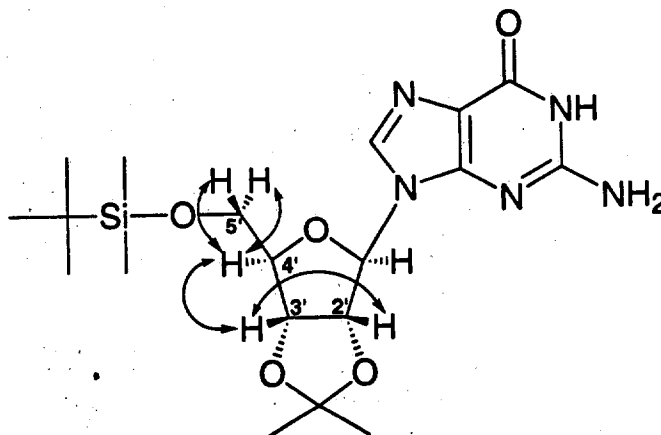
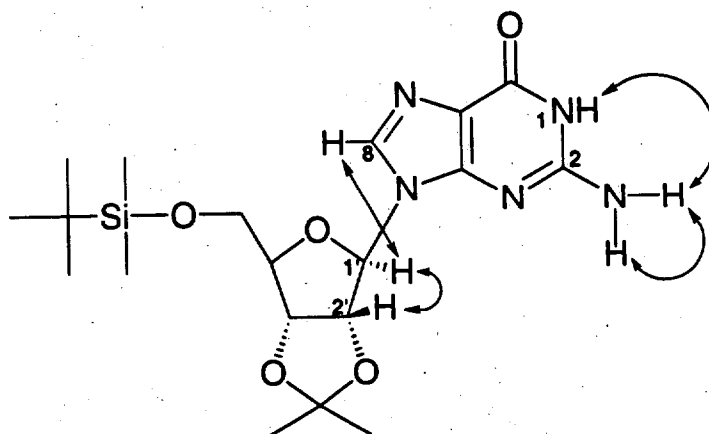
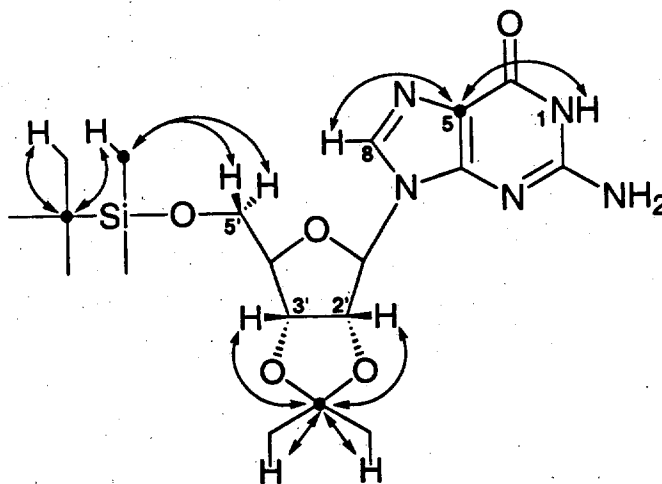
**Figure 2B. Temperature-dependent <sup>1</sup>H NMR spectra of (G 1)<sub>8</sub>-Pb<sup>+2</sup>(pic)<sub>2</sub>.** A series of one dimensional spectra were recorded in CDCl<sub>3</sub> at temperatures between 20 - 50 °C. The two sets of amino protons, N2 H<sub>A</sub> and N2 H<sub>B</sub> for both upper and lower G<sub>4</sub>-quartets, are labeled with asterisks. Separate signals for these four amino protons are observed over this temperature range, indicating relatively slow C2-N2 bond rotation on the NMR chemical shift timescale.



**Figure 3. Extraction selectivity of  $\text{Pb}^{2+}$  vs.  $\text{K}^+$ .** Spectra were recorded at 25 °C in  $\text{CD}_2\text{Cl}_2$ . (A)  $(\text{G } 1)_8\text{-K}^+(\text{pic})$ . (B)  $(\text{G } 1)_8\text{-Pb}^{2+}(\text{pic})_2$ . (C) the  $(\text{G } 1)_8\text{-Pb}^{2+}(\text{pic})_2$  complex formed after extraction of salt from an aqueous phase containing 1 equiv of  $\text{PbCl}_2$  and 10 equiv of  $\text{K}^+$  picrate. The dashed lines in the  $^1\text{H}$  NMR spectrum indicate that no  $\text{K}^+$ , and only  $\text{Pb}^{2+}$ , was extracted from this mixture. See the experimental section for the details of the extraction procedure.

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 $^1\text{H}$ - $^1\text{H}$  COSY $^1\text{H}$ - $^1\text{H}$  NOESY $^1\text{H}$ - $^{13}\text{C}$  HMBC

**Figure 4. Assignment Strategy for  $^1\text{H}$  and  $^{13}\text{C}$  NMR resonances.** The sugar protons (H2', 3', 4', 5', and 5'') were assigned to their respective G<sub>4</sub>-quartets based on a  $^1\text{H}$ - $^1\text{H}$  COSY experiment. A  $^1\text{H}$ - $^1\text{H}$  NOESY allowed for correlation of H2'-H1', H1'-H8, and NH1 amide-N2 H<sub>A</sub> and H<sub>B</sub> amino protons. The carbon assignments were based on  $^1\text{H}$ - $^{13}\text{C}$  HMQC and HMBC experiments. The HMBC experiment allowed for the correlations between C5-H8 and C5-NH1, as well as for the *t*-butyl-dimethylsilyl side chain and the isopropylidene. Arrows show key correlations obtained from the COSY, NOESY, and HMBC experiments.

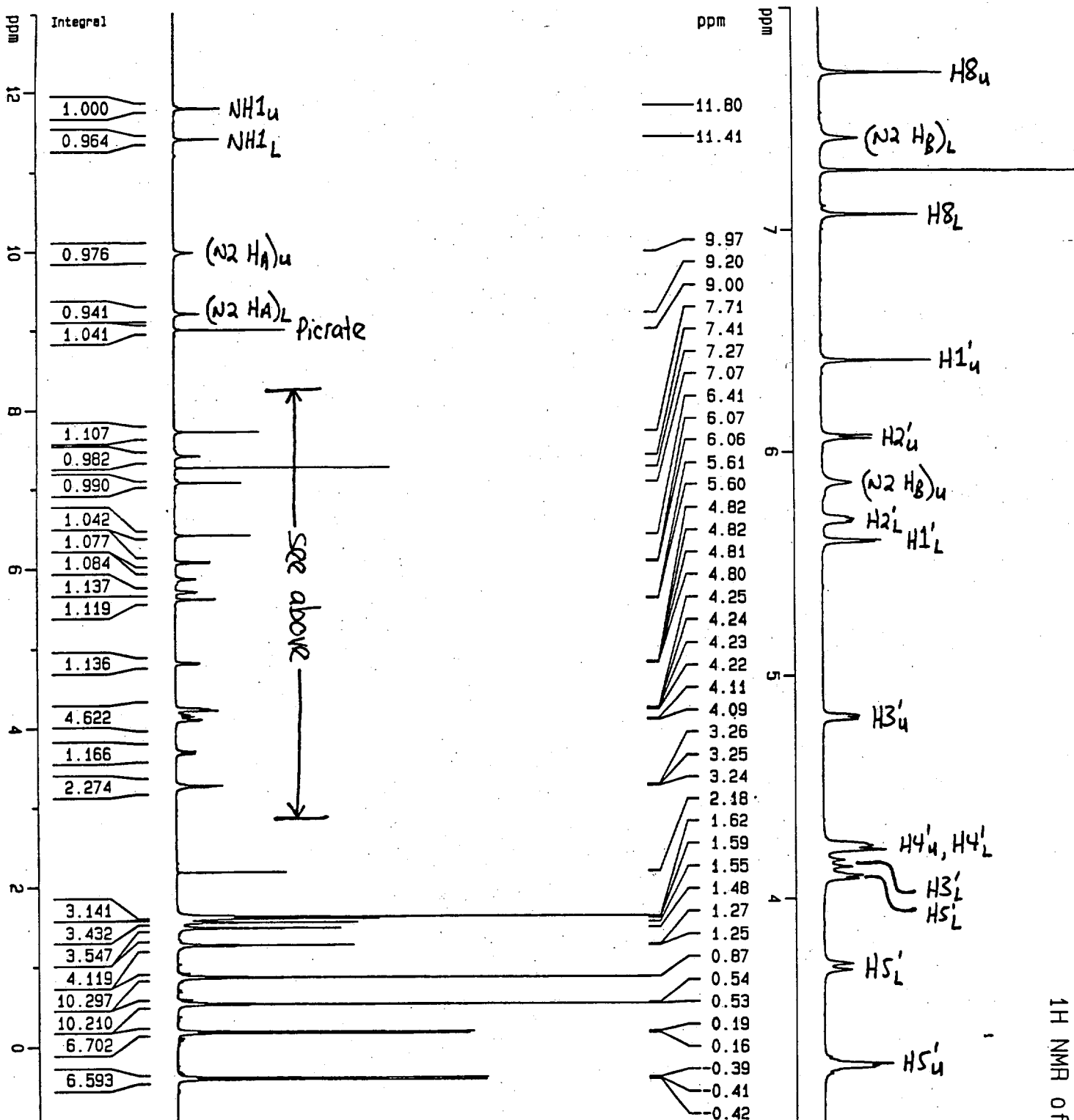
**Table 1.  $^1\text{H}$  NMR Assignments**

	$G_4\text{-U}$	$G_4\text{-L}$
NH1	11.80	11.41
N2 H <sub>A</sub>	9.97	9.20
N2 H <sub>B</sub>	5.86	7.41
H8	7.71	7.07
H1'	6.41	5.60
H2'	6.06	5.70
H3'	4.81	4.10
H4'	4.24	4.24
H5'	3.25	4.15, 3.69
iP	1.59, 1.48	1.55, 1.26
Si-t-Bu-Me	0.87	0.53
Si-Me's	0.17	-0.41
Picrate	9.00	

**Table 2.  $^{13}\text{C}$  NMR Assignments**

	U	L	Unassigned
C2	152.1	153.6	
C4			152.4
C5	115.3	114.9	
C6	160.1	159.4	
C8	140.3	137.0	
C1'	90.9	92.7	
C2'	82.1	81.2	
C3'			81.7
C4'	89.4	87.8	
C5'	63.4	64.3	
iP-quat	112.7	114.5	
iP-Me	24.4, 24.3	27.5, 26.9	
Si-Me's	-4.6, -4.8	-6.0, -6.2	
Si-t-Bu-quat	18.0	18.2	
Si-t-Bu-Me's	25.9	25.5	
Picrate			161.9, 141.6
			126.9, 126.7

Tables.  $^1\text{H}$  and  $^{13}\text{C}$  NMR assignments for  $(G\ 1)_8\text{-Pb}^{+2}(\text{pic})_2$ . Assignments were based following the strategy described in Figure 4 of the Supporting Information.. Spectra were recorded at 25 °C in  $\text{CDCl}_3$ . The abbreviations are:  $G_4\text{-U}$  = upper  $G_4$ -quartet,  $G_4\text{-L}$  = lower  $G_4$ -quartet, iP = isopropylidene, Bu = butyl, Me = methyl, quat = quaternary.



1H NMR of (G1) 8-Pb+2 (pic) 2

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DS 2  
 SWH 6775.068 Hz  
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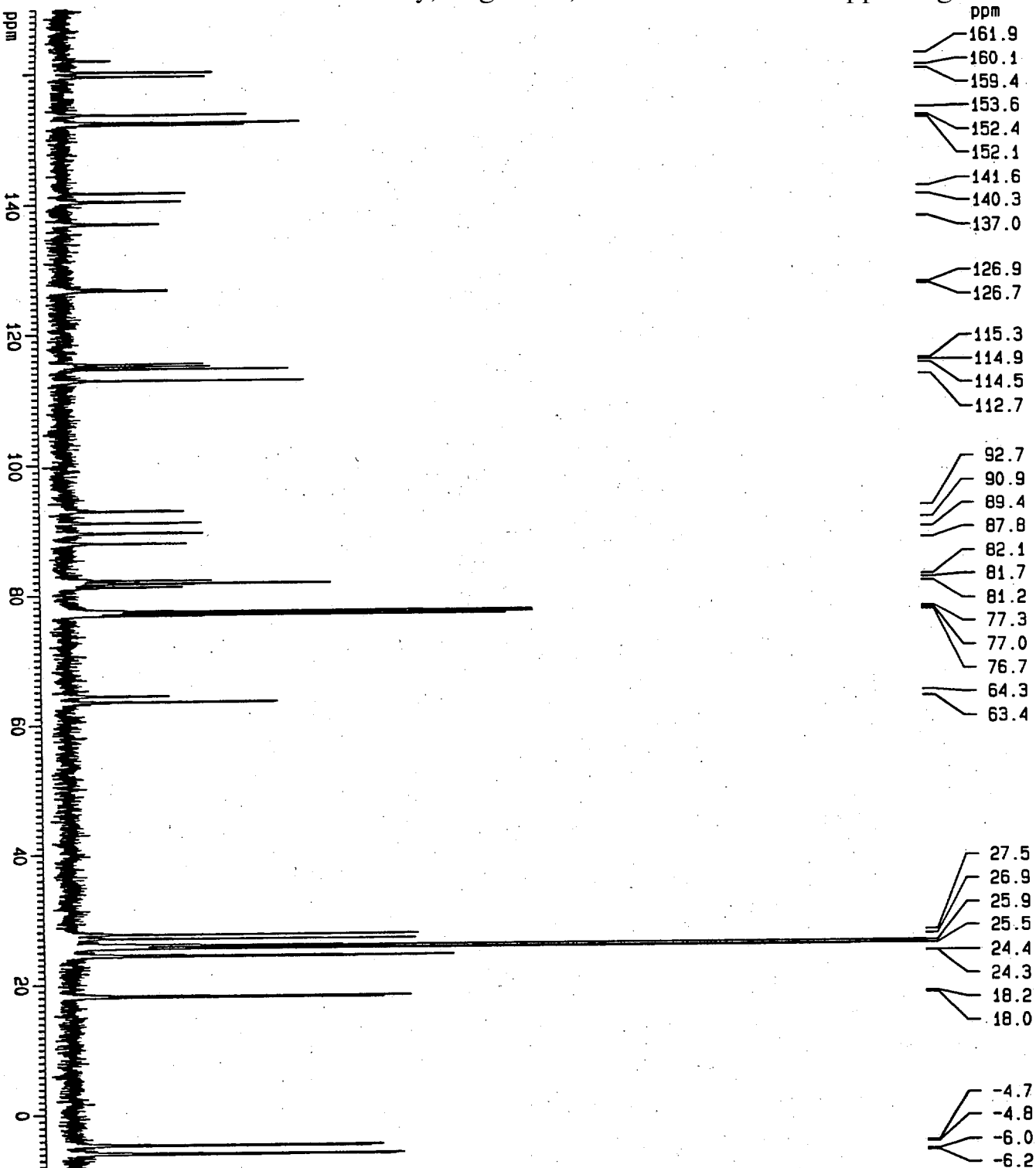
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1D NMR plot parameters

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13C NMR of (G1) 8-Pb+2 (pic) 2



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CHANNEL f2

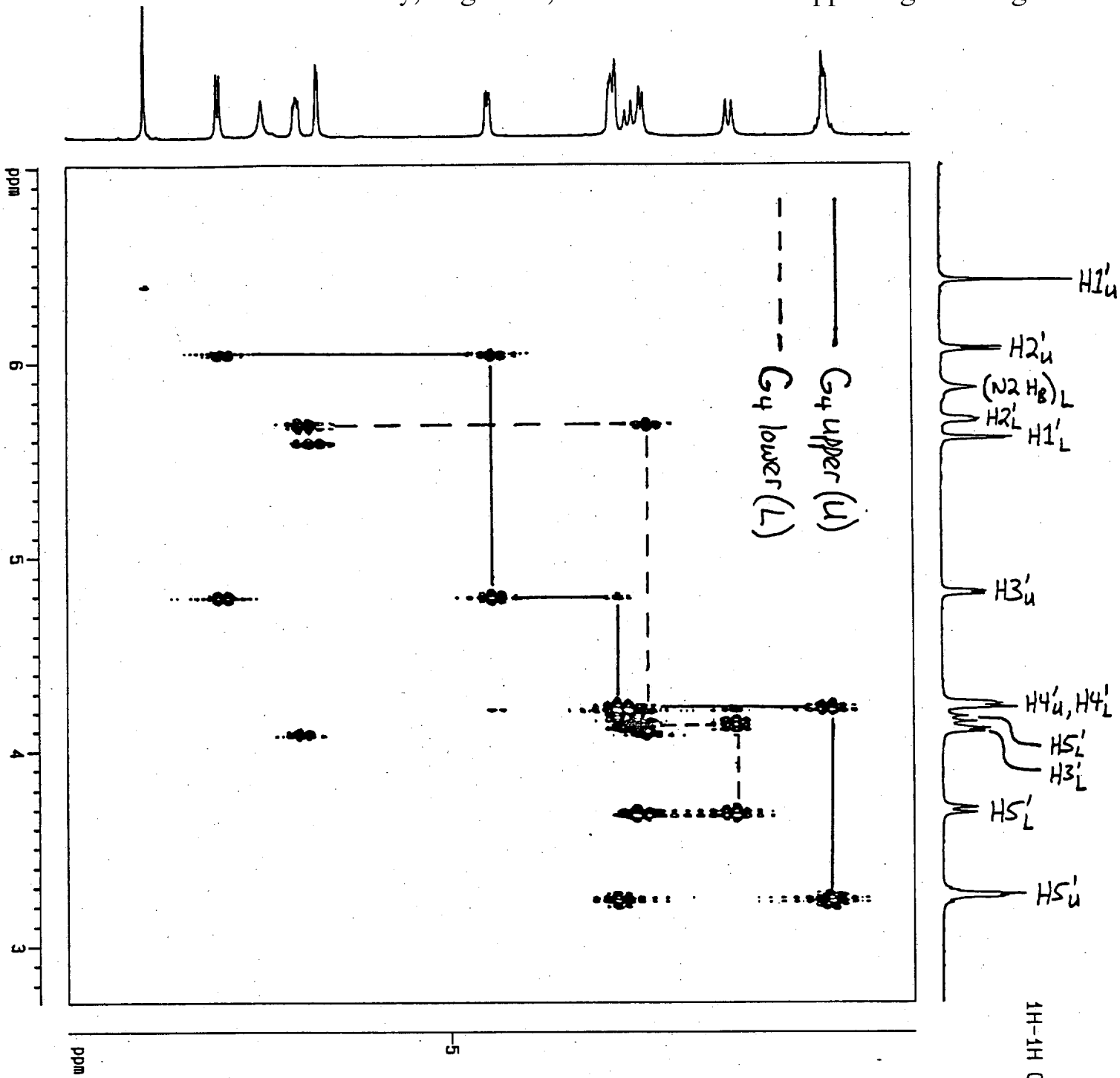
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1D NMR plot parameters

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1H-1H COSY of (G1) 8-Pd+2 (pic) 2

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