

Supporting Information
For

**A Lead-Filled G-Quadruplex:
Insight into the G-Quartet's Selectivity for Pb^{+2} over K^{+}**

ol0065120

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UM624 Write-up

A yellow crystalline block with dimensions 0.776 x 0.148 x 0.141 mm³ 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 ω scans (25 frames/series) that were well distributed in reciprocal space. Data frames were collected [MoK α] with 0.3° wide ω -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^{1,2} 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 SHELXTL³ program was used to determine the acentric orthorhombic space group P2₁2₁2₁ (no. 19), and apply the absorption correction. The structure was determined by Patterson interpretation using the program XS⁴. Refinement with XL⁵ and XH⁵ 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-butyl dimethylsilyl groups required construction via a series of DFIX⁵ 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 BLOCs⁵, in order to use a least-squares full-matrix approach on F². The entire ensemble refined to convergence. This produced the residuals R(F)=16.19%, wR(F²)=24.35% and GOF=1.037 for 88730 unique reflections [R(F)=8.75%, wR(F²)=21.40% for those 54223 data with Fo > 4 σ (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 $w = 1/[\sigma^2(F_o^2) + (0.1412 \cdot P)^2 + 0 \cdot P]$ and $P = (\max(F_o^2, 0) + 2 \cdot F_c^2)/3$. An empirical correction for extinction was applied to the data in the form $(F_c^2, \text{corr}) = k[1 + 0.001 \cdot x \cdot F_c^2 \cdot \lambda^3 / \sin(2\theta)]^{-1/4}$, 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⁺²]₂

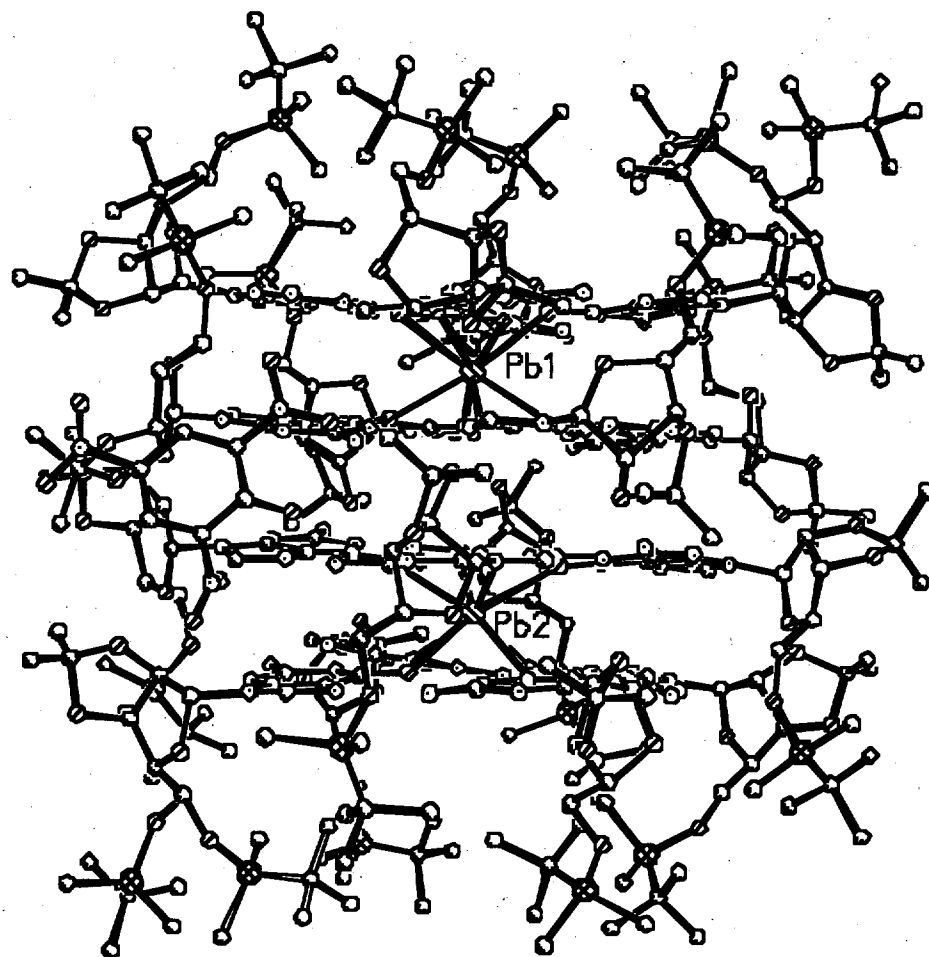


Table 1. Crystal data and structure refinement.

Identification code	UM624fn		
Empirical formula	C _{169.81} H _{270.06} Cl _{1.31} N _{48.63} O _{58.63} Pb Si ₈		
Formula weight	4409.35		
Temperature	193(2) K		
Wavelength	0.71073 Å		
Crystal system	Orthorhombic		
Space group	P2 ₁ 2 ₁ 2 ₁		
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 ³		
Z	16		
Density (calculated)	1.231 Mg/m ³		
Absorption coefficient	0.845 mm ⁻¹		
F(000)	37034		
Crystal size	0.776 x 0.148 x 0.141 mm ³		
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 ²		
Data / restraints / parameters	88,730 / 578 / 4989		
Goodness-of-fit on F ²	1.037		
Final R indices [I>2sigma(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 ⁻³		

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)
Cations				
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)
Guanosine 1				
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)

Guanosine 6

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)
Guanosine 7				
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)
Guanosine 8				
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)

Guanosine 13

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)

Guanosine 14

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)

Guanosine 15

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)

Guanosine 27

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)

Guanosine 28

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)

Guanosine 29

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)

Table 3. Pb-O bond lengths [Å] for [(G 1)₈Pb⁺²]₂ [Å].

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⁺²]₂ [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

Symmetry transformations used to generate equivalent atoms:

#1 -x-1/2,-y+1,z+1/2 #2 -x-1/2,-y+1,z-1/2 #3 -x,y+1/2,-z+1/2

#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

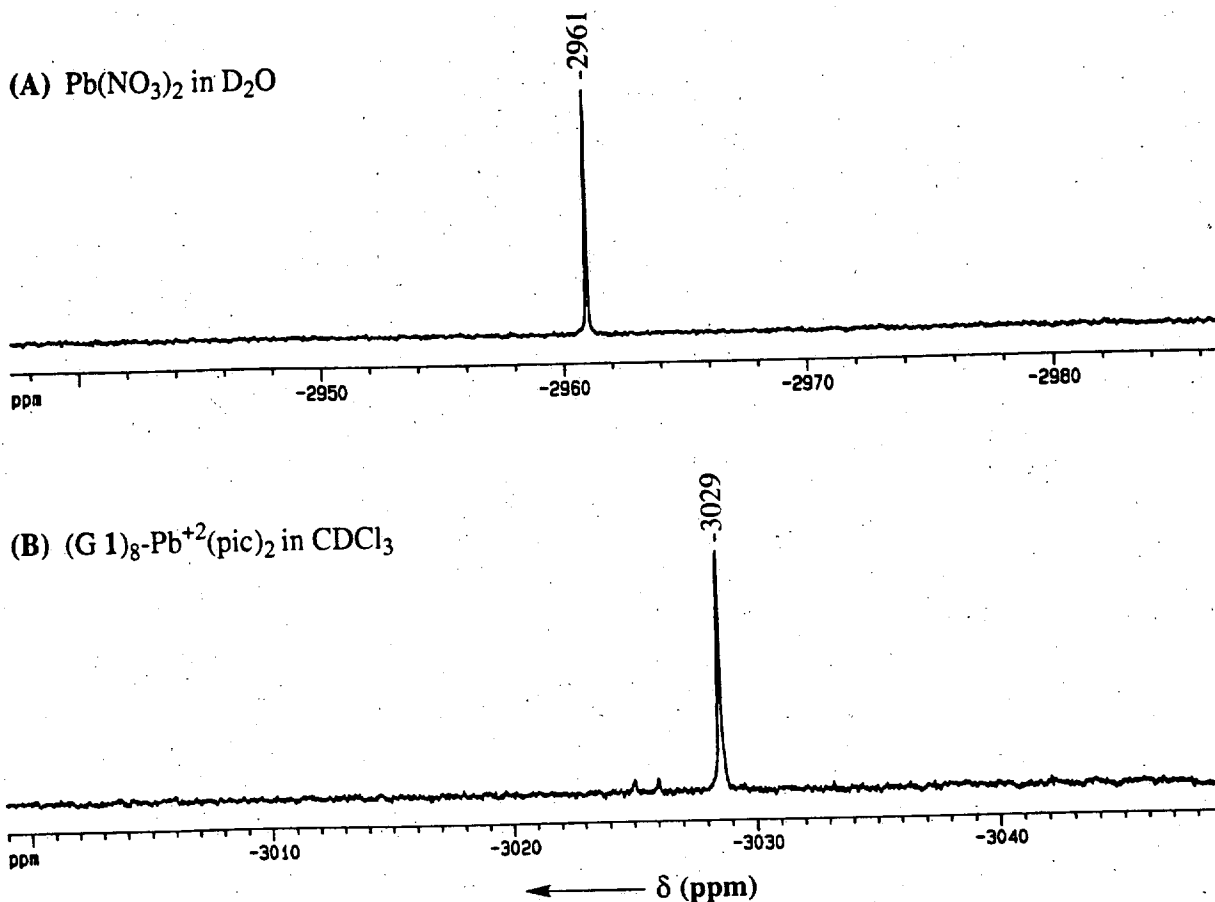


Figure 1. One dimensional ^{207}Pb NMR. Spectra were recorded on a Bruker DRX 500 MHz spectrometer at 25 °C operating at 104.63 MHz for ^{207}Pb . A total of 16,000 data points were collected with an acquisition time of 1.6 s for both experiments. A sweep width of 5 kHz was used. Fourier transformation 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% D_2O 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 CDCl_3 . The sample was 50 mM in octamer. A total of 1000 transients were collected with a 0.5 s relaxation delay.

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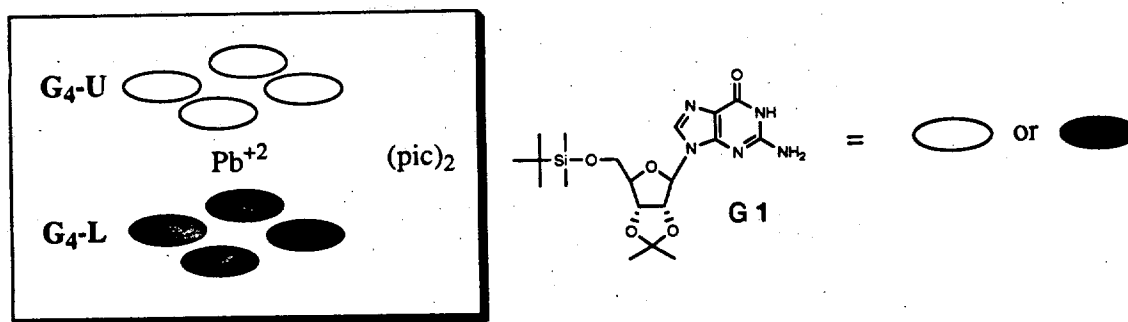


Figure 2A. Schematic for identification of inequivalent G₄-quartets. From the crystal structure of (G 1)₈-Pb⁺²(pic)₂, it is apparent that the N2 H_B protons of one G₄-quartet are hydrogen bonded to the 5'-oxygens of the other G₄-quartet. The G₄-quartet containing the N2 H_B protons (hydrogen bond donors) is arbitrarily defined as the upper quartet (G₄-U). Conversely, the quartet containing the hydrogen bonding acceptor 5'-oxygens is defined as the lower quartet (G₄-L).

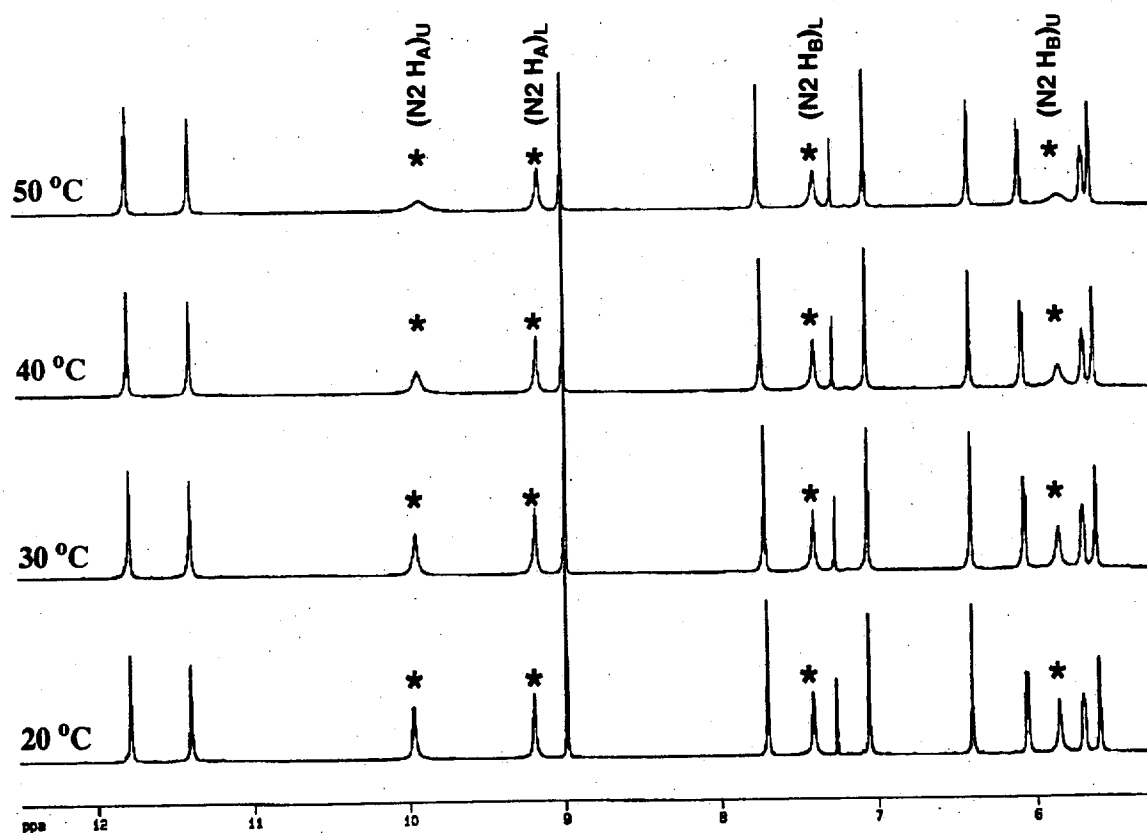


Figure 2B. Temperature-dependent ¹H NMR spectra of (G 1)₈-Pb⁺²(pic)₂. A series of one dimensional spectra were recorded in CDCl₃ at temperatures between 20 - 50 °C. The two sets of amino protons, N2 H_A and N2 H_B for both upper and lower G₄-quartets, are labeled with asterisks. Separate signals for these four amino protons are observed over this temperature range, indicating relatively slow C2-N2 bond rotation on the NMR chemical shift timescale.

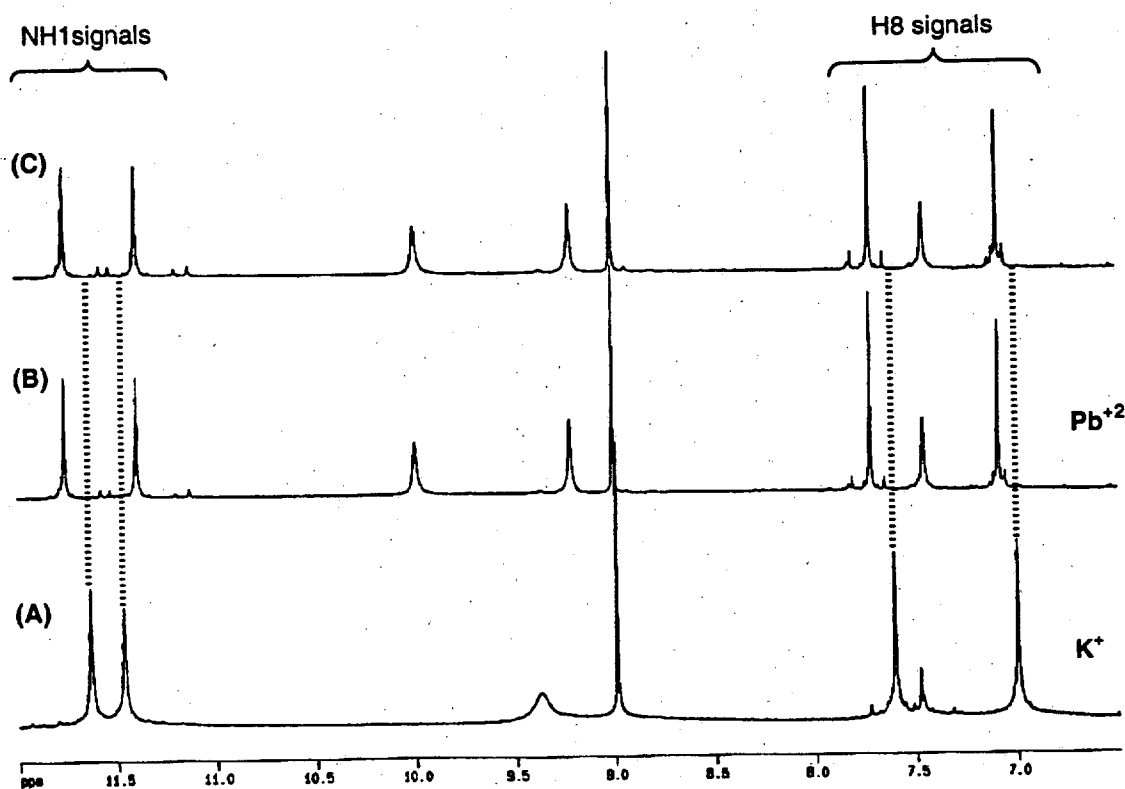


Figure 3. Extraction selectivity of Pb^{2+} vs. K^+ . Spectra were recorded at 25 °C in CD_2Cl_2 . (A) $(\text{G } 1)_8\text{-K}^+(\text{pic})$. (B) $(\text{G } 1)_8\text{-Pb}^{2+}(\text{pic})_2$. (C) the $(\text{G } 1)_8\text{-Pb}^{2+}(\text{pic})_2$ complex formed after extraction of salt from an aqueous phase containing 1 equiv of PbCl_2 and 10 equiv of K^+ picrate. The dashed lines in the ^1H NMR spectrum indicate that no K^+ , and only Pb^{2+} , was extracted from this mixture. See the experimental section for the details of the extraction procedure.

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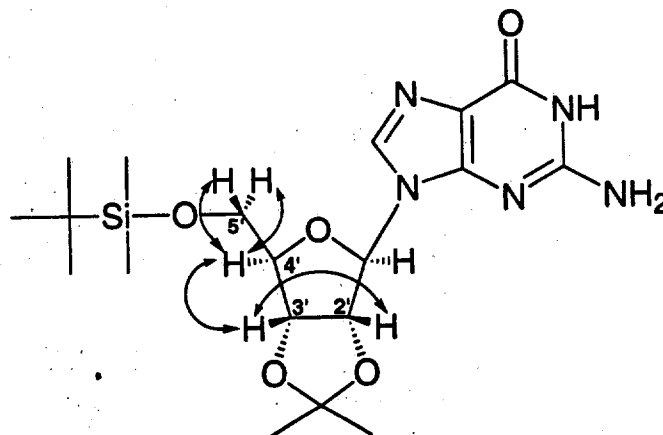
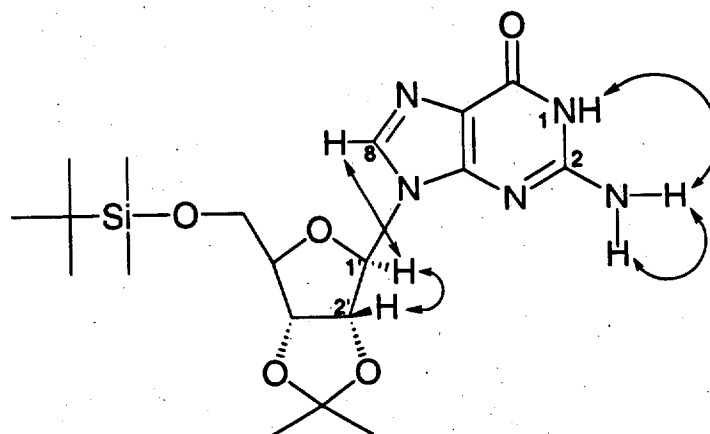
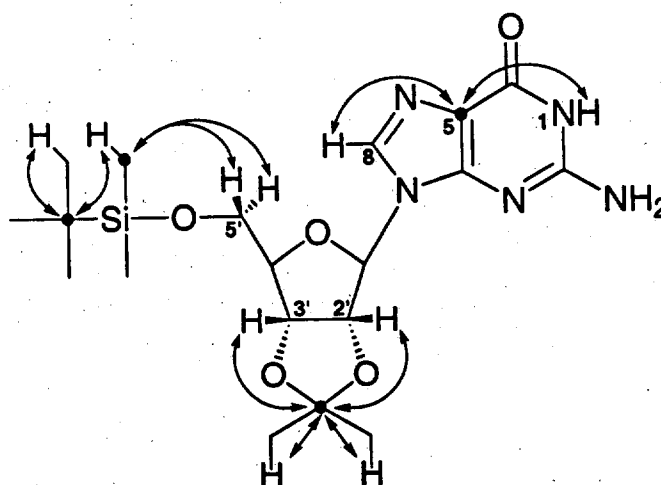
 ^1H - ^1H COSY ^1H - ^1H NOESY ^1H - ^{13}C HMBC

Figure 4. Assignment Strategy for ^1H and ^{13}C NMR resonances. The sugar protons ($\text{H}2'$, $3'$, $4'$, $5'$, and $5''$) were assigned to their respective G_4 -quartets based on a ^1H - ^1H COSY experiment. A ^1H - ^1H NOESY allowed for correlation of $\text{H}2'$ - $\text{H}1'$, $\text{H}1'$ - $\text{H}8$, and $\text{NH}1$ amide- $\text{N}2$ H_A and H_B amino protons. The carbon assignments were based on ^1H - ^{13}C HMQC and HMBC experiments. The HMBC experiment allowed for the correlations between $\text{C}5$ - $\text{H}8$ and $\text{C}5$ - $\text{NH}1$, 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.

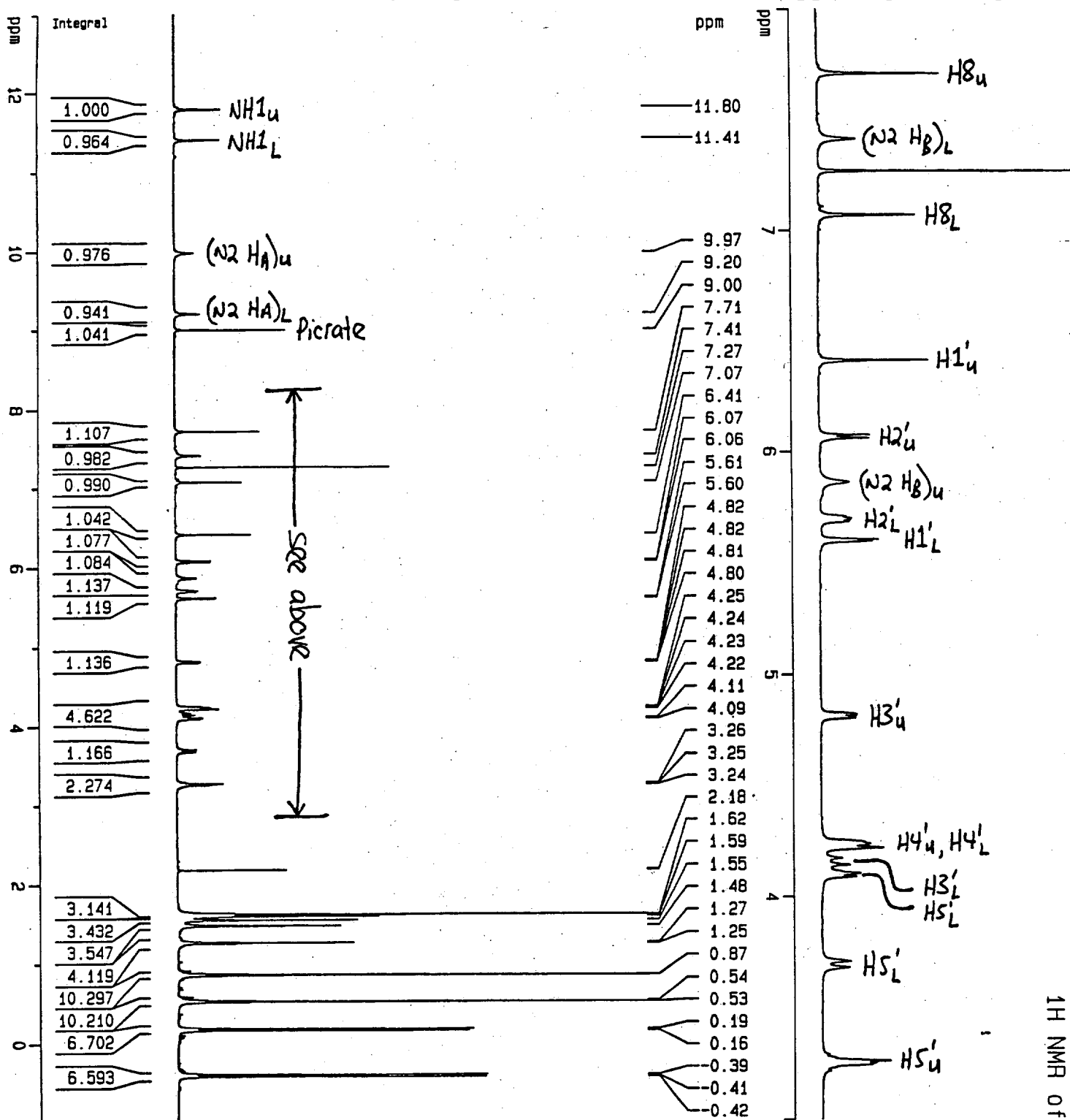
Table 1. ^1H NMR Assignments

	G₄-U	G₄-L
NH1	11.80	11.41
N2 H_A	9.97	9.20
N2 H_B	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}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. ^1H and ^{13}C NMR assignments for $(\text{G } 1)_8\text{-Pb}^{+2}(\text{pic})_2$. Assignments were based following the strategy described in Figure 4 of the Supporting Information.. Spectra were recorded at 25 °C in CDCl_3 . The abbreviations are: G₄-U = upper G₄-quartet, G₄-L = lower G₄-quartet, iP = isopropylidene, Bu = butyl, Me = methyl, quat = quaternary.



Current Data Parameters

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EXPNO 2

PROCNO 1

F2 - Acquisition Parameters

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Time 10.10

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PROBHD 5 mm QNP 1H

PULPROG zg

TD 30720

SOLVENT CD3CN

NS 32

DS 2

SWH 6775.068 Hz

FIDRES 0.220543 Hz

AQ 2.2671859 sec

RG 181

DM 73.800 usec

DE 8.00 usec

TE 305.0 K

D1 2.00000000 sec

----- CHANNEL f1 -----

NUC1 1H

P1 5.00 usec

PL1 -2.00 dB

SFO1 400.1330076 MHz

F2 - Processing parameters

SI 16384

SF 400.1300066 MHz

WDW EM

SSB 0

LB 0.40 Hz

GB 0

PC 1.00

1D NMR plot parameters

CX 20.00 cm

FAP 13.000 ppm

F1 5201.69 Hz

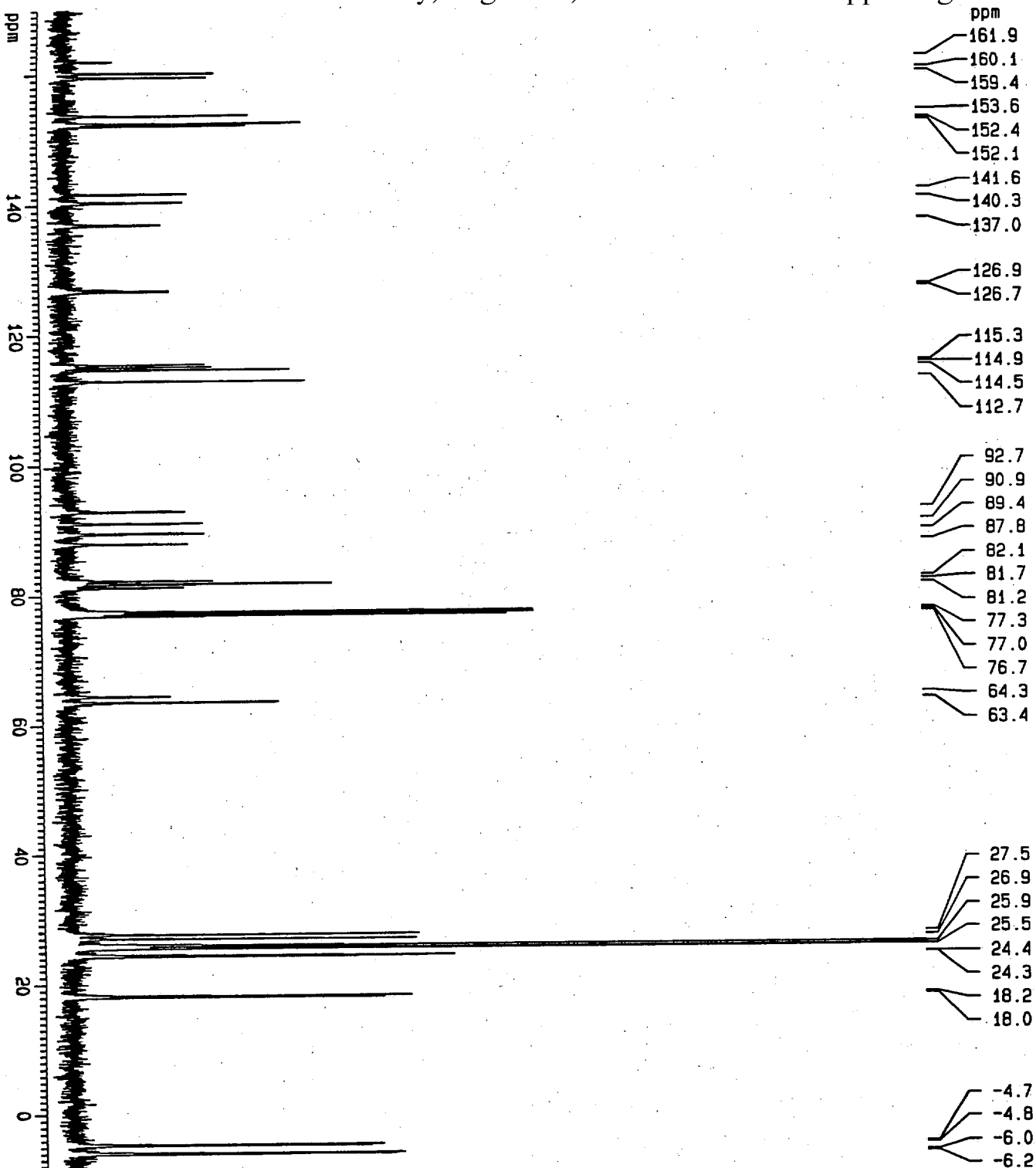
F2P -1.000 ppm

F2 -400.13 Hz

PPMCM 0.70000 ppm/cm

HZCM 280.09100 Hz/cm

¹³C NMR of (G1) 8-Pb+2 (pic) 2



Current Data Parameters

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PROCNO	1

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TD	65536
SOLVENT	CDCl3
NS	1464
DS	2
SWH	29498.525 Hz
FIDRES	0.450112 Hz
AQ	1.110851 sec
RG	11585.2
DM	16.950 usec
DE	24.21 usec
TE	300.0 K
D1	0.50000000 sec
d11	0.03000000 sec

CHANNEL f1 -----

NUC1	¹³ C
P1	7.00 usec
PL1	0.00 dB
SFO1	100.625153 MHz

CHANNEL f2 -----

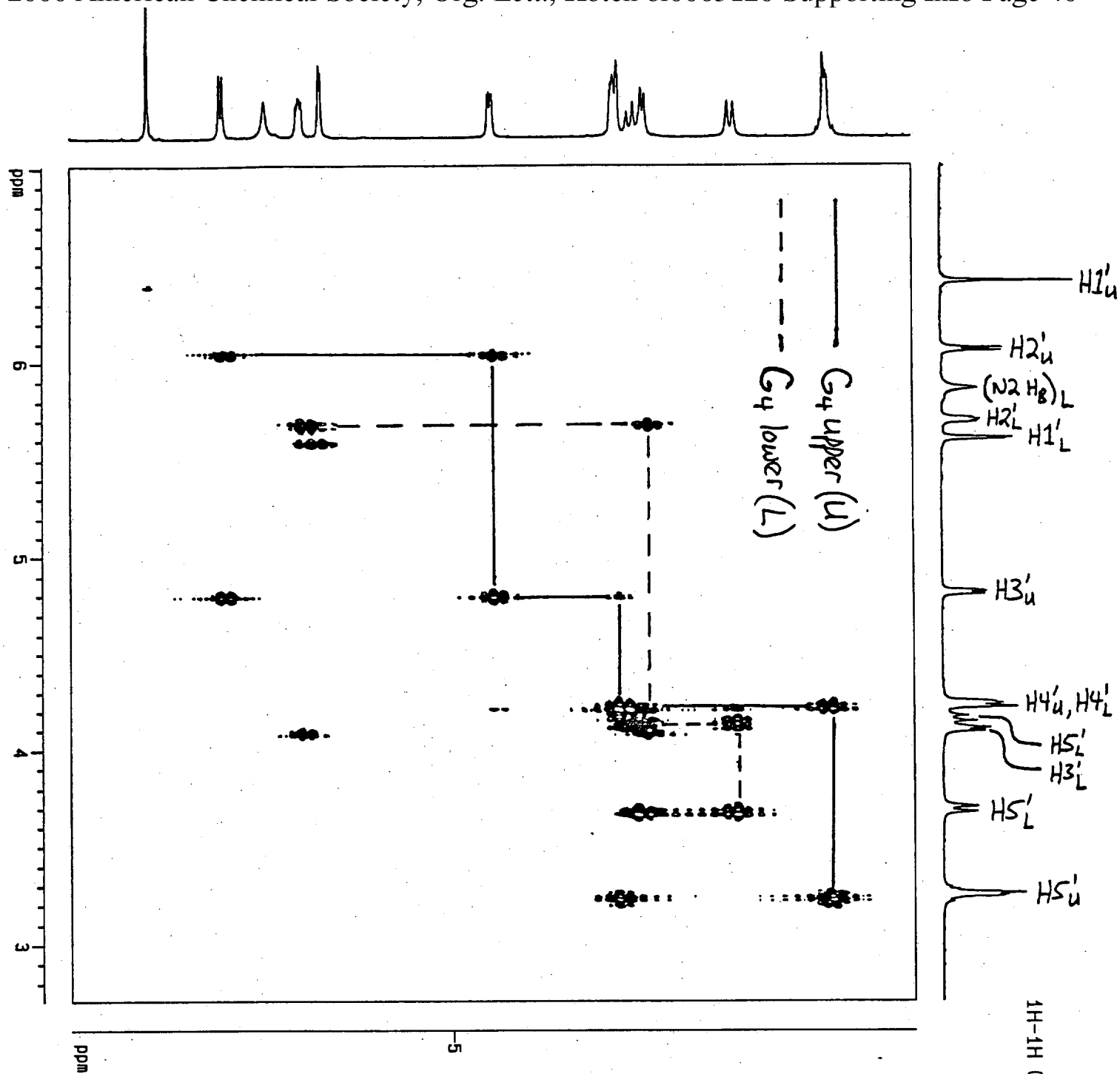
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NUC2	¹ H
PCPD2	100.00 usec
PL2	120.00 dB
PL12	21.00 dB
SFO2	400.1316005 MHz

F2 - Processing Parameters

SI	32768
SF	100.6127725 MHz
WDW	EM
SSB	0
LB	2.00 Hz
GB	0
PC	1.40

1D NMR plot parameters

CX	20.00 cm
F1P	170.000 ppm
F1	17104.17 Hz
F2P	-10.000 ppm
F2	-1006.13 Hz
PRGCM	9.00000 ppm/cm
HZCM	905.51495 Hz/cm



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

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