Engineering Crystalline Architecture with Diketopiperazines: An Interrogation of the Strength of Hydrogen-Bonded Tapes Based on the Cyclic Dipeptide of (S)-Aspartic Acid

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Supporting Material

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

Identification code	ZASPDKP
Empirical formula	$C_{22}H_{22}N_2O_6$
Formula weight	410.42
Temperature	130(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	C2
Unit cell dimensions	a = 43.90(2) Å α = 90°
	b = 7.172(3) Å β = 96.00(4)°
	c = 6.176(3) Å γ = 90°
Volume, Z	1934(2) $Å^3$, 4
Density (calculated)	1.410 Mg/m^3
Absorption coefficient	0.861 mm^{-1}
F(000)	864
Crystal size	0.20 x 0.14 x 0.02 mm
Crystal color	colorless
Theta range for data collection	2.02 to 56.13°
Scan type	θ–2θ
Limiting indices	-46<=h<=46, 0<=k<=7, 0<=l<=6
Reflections collected	1394
Independent reflections	1394 [R(int) = 0.0000]
Absorption correction	XABS2
Max. and min. transmission	0.99 and 0.91
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1394 / 1 / 283
Goodness-of-fit on F^2	1.060
Final R indices [I>2σ(I)]	R1 = 0.0485, wR2 = 0.1250
R indices (all data)	R1 = 0.0536, wR2 = 0.1311
Absolute structure parameter	-0.3(5)
Extinction coefficient	none
Largest diff. peak and hole	0.356 and -0.315 e^- / $Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **ZASPDKP**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
O(1)	4685(1)	3209(6)	3414(5)	30(1)
O(2)	4136(1)	5478(5)	1485(5)	30(1)
O(3)	3974(1)	2494(6)	1632(5)	30(1)
O(4)	326(1)	3898(6)	8889(5)	30(1)
O(5)	847(1)	1583(5)	3290(6)	31(1)
O(6)	1039(1)	4475(5)	3035(5)	28(1)
N(1)	5141(1)	3540(7)	2078(6)	23(1)
N(2)	132(1)	3608(7)	3109(6)	25(1)
C(1)	4839(1)	3546(8)	1870(7)	21(1)
C(2)	4671(1)	4070(8)	-316(8)	22(1)
C(3)	4364(1)	3084(9)	-607(7)	26(1)
C(4)	4153(1)	3883(8)	960(7)	24(1)
C(5)	3757(1)	3042(9)	3158(7)	28(1)
C(6)	3439(1)	3214(8)	2028(7)	30(1)
C(7)	3193(1)	2549(8)	3046(8)	30(1)
C(8)	2897(1)	2730(9)	2096(8)	36(2)
C(9)	2839(1)	3603(9)	69(8)	35(1)
C(10)	3082(1)	4252(8)	-958(8)	32(1)

C(11)	3378(1)	4077(8)	-4(8)	29(1)
C(12)	171(1)	3616(8)	7099(7)	22(1)
C(13)	329(1)	3144(9)	5121(7)	26(1)
C(14)	636(1)	4088(9)	5208(7)	25(1)
C(15)	845(1)	3212(9)	3714(8)	26(1)
C(16)	1263(1)	3797(9)	1621(7)	29(1)
C(17)	1573(1)	3618(8)	2862(7)	26(1)
C(18)	1829(1)	4303(8)	1976(8)	33(1)
C(19)	2119(1)	4117(9)	3054(8)	33(1)
C(20)	2157(1)	3218(10)	5051(8)	37(1)
C(21)	1905(1)	2532(8)	5979(8)	34(1)
C(22)	1616(1)	2731(8)	4898(8)	31(1)

Table 3. Selected hydrogen bond lengths [Å] and angles [deg] for **ZASPDKP**.

Bond lengths	
N(1)-H(1N)	0.877
H(1N)--O(1)	1.972(54)
N(1)-H(1N)--O(1)	2.819(5)
N(2)-H(2N)	0.863
H(2N)--O(4)	1.993(53)
N(2)-H(2N)--O(4)	2.832(5)
Bond angles	
N(1)-H(1N)-O(1)	161.99(5.34)
N(2)-H(2N)-O(4)	163.84(4.88)

Table 4. Bond lengths [Å] and angles [deg] for **ZASPDKP**.

Bond lengths	
O(1)-C(1)	1.250(5)
O(2)-C(4)	1.193(7)
O(3)-C(4)	1.361(6)
O(3)-C(5)	1.463(6)
O(4)-C(12)	1.252(5)
O(5)-C(15)	1.198(7)
O(6)-C(15)	1.341(6)
O(6)-C(16)	1.463(6)
N(1)-C(1)	1.320(6)
N(2)-C(13)	1.476(6)
C(1)-C(2)	1.516(7)
C(2)-C(3)	1.517(7)
C(3)-C(4)	1.519(7)
C(5)-C(6)	1.497(7)
C(6)-C(7)	1.389(7)
C(6)-C(11)	1.400(7)
C(7)-C(8)	1.377(7)
C(8)-C(9)	1.399(8)
C(9)-C(10)	1.376(7)
C(10)-C(11)	1.376(7)
C(12)-C(13)	1.506(7)
C(13)-C(14)	1.502(8)
C(14)-C(15)	1.507(7)
C(16)-C(17)	1.497(7)
C(17)-C(18)	1.388(7)
C(17)-C(22)	1.404(7)
C(18)-C(19)	1.382(7)

C(19)-C(20)	1.386(8)
C(20)-C(21)	1.387(8)
C(21)-C(22)	1.380(7)
Bond angles	
C(4)-O(3)-C(5)	115.9(4)
C(15)-O(6)-C(16)	116.7(5)
O(1)-C(1)-N(1)	123.0(4)
O(1)-C(1)-C(2)	118.4(4)
N(1)-C(1)-C(2)	118.5(4)
C(1)-C(2)-C(3)	109.5(4)
C(2)-C(3)-C(4)	110.0(5)
O(2)-C(4)-O(3)	124.3(5)
O(2)-C(4)-C(3)	126.5(5)
O(3)-C(4)-C(3)	109.2(5)
O(3)-C(5)-C(6)	111.1(4)
C(7)-C(6)-C(11)	118.2(5)
C(7)-C(6)-C(5)	119.3(5)
C(11)-C(6)-C(5)	122.4(4)
C(8)-C(7)-C(6)	121.3(5)
C(7)-C(8)-C(9)	119.8(5)
C(10)-C(9)-C(8)	119.2(5)
C(9)-C(10)-C(11)	120.9(5)
C(10)-C(11)-C(6)	120.5(5)
O(4)-C(12)-C(13)	119.9(4)
N(2)-C(13)-C(14)	111.8(4)
N(2)-C(13)-C(12)	110.7(4)
C(14)-C(13)-C(12)	110.9(4)
C(13)-C(14)-C(15)	113.1(5)
O(5)-C(15)-O(6)	124.9(5)
O(5)-C(15)-C(14)	124.0(5)
O(6)-C(15)-C(14)	111.0(5)
O(6)-C(16)-C(17)	110.7(4)
C(18)-C(17)-C(22)	118.5(5)
C(18)-C(17)-C(16)	119.8(4)
C(22)-C(17)-C(16)	121.7(4)
C(19)-C(18)-C(17)	121.3(5)
C(18)-C(19)-C(20)	119.4(5)
C(19)-C(20)-C(21)	120.5(5)
C(22)-C(21)-C(20)	119.7(5)
C(21)-C(22)-C(17)	120.6(5)

Table 5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **ZASPDKP**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U11 + ... + 2hka^*b^*U12]$

atom	U11	U22	U33	U23	U13	U12
O(1)	29(2)	36(2)	23(2)	-1(2)	-1(1)	-2(2)
O(2)	36(2)	26(3)	27(2)	-2(2)	3(2)	2(2)
O(3)	29(2)	29(2)	32(2)	0(2)	6(1)	1(2)
O(4)	28(2)	39(2)	22(2)	1(2)	2(1)	-2(2)
O(5)	36(2)	27(3)	31(2)	-2(2)	5(2)	0(2)
O(6)	27(2)	27(2)	29(2)	-5(2)	4(1)	-2(2)
N(1)	26(2)	27(3)	16(2)	3(2)	1(2)	-1(2)
N(2)	27(2)	33(3)	15(2)	4(2)	5(2)	-2(2)
C(1)	29(3)	17(3)	17(2)	-5(2)	2(2)	-2(2)
C(2)	32(3)	19(3)	16(2)	0(2)	4(2)	2(2)

C(3)	26(3)	32(3)	20(2)	-3(2)	-2(2)	-1(2)
C(4)	24(3)	22(3)	24(2)	-6(3)	-5(2)	1(3)
C(5)	28(3)	31(3)	25(2)	-3(3)	3(2)	0(2)
C(6)	30(3)	28(3)	31(3)	-5(3)	5(2)	3(3)
C(7)	33(3)	26(3)	32(3)	0(3)	6(2)	2(3)
C(8)	27(3)	40(4)	41(3)	0(3)	8(2)	-1(3)
C(9)	29(3)	33(4)	43(3)	-7(3)	-1(2)	1(3)
C(10)	39(3)	24(3)	32(3)	-2(3)	1(2)	-2(3)
C(11)	35(3)	20(3)	32(3)	6(2)	8(2)	-2(2)
C(12)	35(3)	15(3)	15(2)	2(2)	2(2)	-1(2)
C(13)	34(3)	28(3)	16(2)	4(2)	-3(2)	4(3)
C(14)	28(3)	28(3)	19(2)	-4(2)	0(2)	3(2)
C(15)	23(3)	31(4)	23(2)	-1(3)	-3(2)	1(3)
C(16)	30(3)	31(3)	29(2)	1(3)	11(2)	6(3)
C(17)	24(3)	22(3)	31(3)	-3(3)	7(2)	1(2)
C(18)	33(3)	31(4)	35(3)	-4(3)	6(2)	1(3)
C(19)	26(3)	32(4)	42(3)	2(3)	9(2)	-1(3)
C(20)	28(3)	36(4)	44(3)	-2(3)	-3(2)	8(3)
C(21)	41(3)	31(3)	28(3)	-2(3)	-1(2)	5(3)
C(22)	31(3)	29(4)	33(3)	-1(3)	5(2)	-1(3)

Table 6. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **ZASPDKP**.

atom	x	y	z	U(eq)
H(1N)	5224(12)	3256(91)	3392(87)	28
H(2N)	224(11)	3786(93)	1955(83)	30
H(2)	4662(11)	5462(92)	-362(79)	27
H(3A)	4394(1)	1733(9)	-329(7)	31
H(3B)	4270(1)	3245(9)	-2123(7)	31
H(5A)	3820(1)	4251(9)	3834(7)	34
H(5B)	3758(1)	2100(9)	4330(7)	34
H(7)	3231(1)	1958(8)	4424(8)	36
H(8)	2732(1)	2262(9)	2815(8)	43
H(9)	2635(1)	3747(9)	-590(8)	43
H(10)	3044(1)	4827(8)	-2345(8)	39
H(11)	3543(1)	4547(8)	-729(8)	35
H(13)	347(12)	1797(95)	5079(83)	31
H(14A)	735(1)	4041(9)	6720(7)	30
H(14B)	604(1)	5416(9)	4806(7)	30
H(16A)	1274(1)	4675(9)	393(7)	35
H(16B)	1197(1)	2569(9)	1011(7)	35
H(18)	1804(1)	4910(8)	602(8)	40
H(19)	2292(1)	4602(9)	2433(8)	40
H(20)	2356(1)	3071(10)	5789(8)	44
H(21)	1932(1)	1926(8)	7354(8)	41
H(22)	1443(1)	2264(8)	5538(8)	37

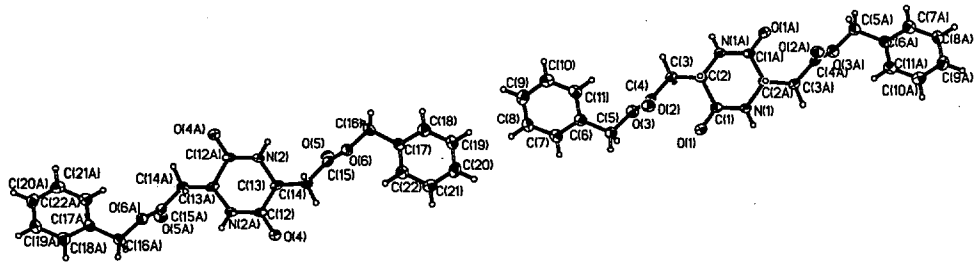

Figure 1. 50% probability displacement ellipsoids of ZASPDKP.

Table 1. Crystal data and structure refinement for **ASPDKP + PPY**.

Identification code	ASPDKP + PPY
Empirical formula	C30H28N4O6
Formula weight	540.56
Temperature	130(2) K
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	P1
Unit cell dimensions	a = 6.2561(12) Å _ = 111.14(2)°
	b = 14.645(4) Å _ = 94.60(2)(2)°
	c = 15.660(3) Å __= 95.27(2)°
Volume, Z	1322.6(5) Å3, 2
Density (calculated)	1.357 Mg/m3
Absorption coefficient	0.791 mm-1
F(000)	568
Crystal size	0.12 x 0.08 x 0.02 mm
Crystal color	colorless
Theta range for data collection	3.05 to 56.05 °
Scan type	θ–2θ
Limiting indices	0<=h<=6, -15<=k<=15, -16<=l<=16
Reflections collected	3465
Independent reflections	3465 [R(int) = 0.0000]
Absorption correction	XABS2
Max. and min. transmission	0.99 and 0.95
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3465 / 3 / 746
Goodness-of-fit on F^2	1.177
Final R indices [I>2σ(I)]	R1 = 0.0568, wR^2 = 0.1310
R indices (all data)	R1 = 0.0781, wR^2 = 0.1474
Absolute structure parameter	0.3(4)
Extinction coefficient	0.0004(4)
Largest diff. peak and hole	0.860 and -0.838 e^- / $Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **ASPDKP + PPY**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

atom	x	y	z	U(eq)
N(1)	21239(10)	14338(5)	9764(5)	25(2)
N(2)	25111(10)	14936(5)	9325(5)	24(2)
N(7)	24944(10)	11948(5)	7532(5)	24(2)
N(8)	29008(9)	12526(5)	7230(5)	25(2)
O(1)	19717(8)	15544(4)	9472(4)	33(2)
O(2)	26722(8)	13778(4)	9684(5)	41(2)
O(3)	21862(10)	13114(5)	11797(5)	45(2)
O(4)	19876(9)	12661(5)	10423(4)	40(2)
O(5)	26253(9)	16085(4)	8168(4)	36(2)
O(6)	25439(9)	17619(4)	8803(4)	37(2)
O(7)	23558(8)	13139(4)	7159(4)	29(1)
O(8)	30465(9)	11457(4)	7758(4)	37(2)
O(9)	23849(9)	10030(4)	8158(4)	34(2)
O(10)	24340(10)	11052(5)	9626(4)	49(2)
O(11)	29333(9)	13671(5)	5716(4)	38(2)
O(12)	30678(8)	15047(4)	6902(4)	31(1)
C(1)	21269(12)	15059(6)	9447(5)	23(2)
C(2)	23222(12)	15296(6)	9027(5)	21(2)

C(3)	25085(12)	14154(6)	9574(6)	29(2)
C(4)	22973(12)	13724(6)	9755(6)	27(2)
C(5)	23374(13)	13599(7)	10675(7)	35(2)
C(6)	21517(14)	13087(6)	10944(7)	32(2)
C(7)	23609(12)	16391(6)	9203(6)	26(2)
C(8)	25256(12)	16683(7)	8669(6)	27(2)
C(53)	25097(12)	12679(6)	7229(5)	23(2)
C(54)	27241(12)	12926(6)	6898(6)	23(2)
C(55)	28861(12)	11815(6)	7562(6)	23(2)
C(56)	26679(11)	11387(6)	7684(6)	19(2)
C(57)	26755(12)	11372(6)	8660(6)	27(2)
C(58)	24835(13)	10754(7)	8778(6)	30(2)
C(59)	27769(12)	14029(6)	7121(6)	25(2)
C(60)	29363(13)	14215(6)	6497(6)	25(2)
N(3)	28157(11)	17995(5)	7755(5)	32(2)
N(4)	33419(11)	15234(5)	5741(5)	32(2)
N(5)	11344(12)	9911(6)	10010(5)	44(2)
N(6)	18533(12)	12410(6)	12363(5)	39(2)
C(9)	27859(13)	18644(6)	7359(6)	32(2)
C(10)	29213(14)	18834(7)	6762(6)	36(2)
C(11)	31034(12)	18342(6)	6585(6)	27(2)
C(12)	31324(13)	17670(6)	6992(6)	29(2)
C(14)	32523(12)	18536(6)	5952(6)	26(2)
C(15)	32880(14)	19457(7)	5890(6)	33(2)
C(16)	34253(15)	19640(7)	5314(6)	42(2)
C(17)	35266(15)	18863(8)	4757(7)	42(3)
C(18)	34940(14)	17954(7)	4800(6)	39(2)
C(19)	33569(14)	17787(7)	5400(6)	38(2)
C(20)	35510(13)	15647(6)	5982(6)	29(2)
C(21)	36811(13)	15707(6)	5331(6)	28(2)
C(22)	36046(12)	15334(6)	4405(6)	26(2)
C(23)	33897(13)	14906(6)	4164(6)	31(2)
C(24)	32681(14)	14854(6)	4852(6)	32(2)
C(25)	37399(12)	15418(6)	3688(6)	28(2)
C(26)	39016(13)	16203(7)	3901(6)	35(2)
C(27)	40000(18)	16278(8)	3236(7)	57(3)
C(28)	39984(14)	15552(7)	2359(6)	40(2)
C(29)	38376(13)	14773(7)	2145(6)	38(2)
C(30)	37109(12)	14689(6)	2807(6)	30(2)
C(31)	9515(15)	10211(7)	10333(7)	45(3)
C(32)	8258(13)	9711(7)	10724(7)	39(2)
C(33)	8724(13)	8844(6)	10796(6)	28(2)
C(34)	10626(16)	8523(7)	10443(8)	50(3)
C(35)	11833(16)	9069(8)	10055(8)	55(3)
C(36)	7425(13)	8301(7)	11239(6)	31(2)
C(37)	5901(16)	8720(8)	11792(7)	47(3)
C(38)	4648(17)	8222(10)	12219(8)	61(3)
C(39)	4948(17)	7281(9)	12100(7)	58(3)
C(40)	6451(18)	6823(8)	11554(7)	51(3)
C(41)	7649(15)	7332(7)	11130(7)	39(2)
C(43)	14927(14)	11651(7)	12247(6)	36(2)
C(44)	15155(14)	11789(6)	13186(6)	33(2)
C(45)	17138(16)	12266(6)	13698(7)	42(2)
C(46)	18727(16)	12547(7)	13258(7)	40(2)

C(47)	13389(15)	11438(7)	13621(7)	38(2)
C(48)	12013(15)	10569(8)	13130(7)	47(3)
C(49)	10449(16)	10233(8)	13553(7)	50(3)
C(50)	10189(16)	10750(9)	14453(8)	57(3)
C(51)	11532(15)	11621(8)	14949(7)	45(3)
C(52)	13118(16)	11969(7)	14540(6)	43(3)

Table 3. Selected hydrogen bond lengths [Å] and angles [deg] for **ASPDKP + PPY**.

Bond lengths	
N(1)-H(1N)	0.912
H(1N)--O(2)	1.997(76)
N(1)-H(1N)--O(2)	2.848(7)
N(2)-H(2N)	0.716
H(2N)--O(1)	2.242(78)
N(2)-H(2N)--O(1)	2.902(7)
N(7)-H(7N)	0.908
H(7N)--O(8)	2.024(79)
N(7)-H(7N)--O(8)	2.911(7)
N(8)-H(8N)	1.095
H(8N)--O(7)	1.845(73)
N(8)-H(8N)--O(7)	2.927(7)
O(3)-H(3O)	1.111
H(3)--N(6)	1.517
O(3)-H(3O)--N(6)	2.599
O(6)-H(6O)	1.064
H(6O)--N(3)	1.552
O(6)-H(6O)--N(3)	2.612
Bond angles	
N(1)-H(1N)-O(2)	154.69(6.59)
N(2)-H(2N)-O(1)	145.57(7.70)
N(7)-H(7N)-O(8)	165.24(6.51)
N(8)-H(8N)-O(7)	168.91(5.80)
O(3)-H(3O)-N(6)	162.9
O(6)-H(6O)-N(3)	162.9

Table 4. Bond lengths [Å] and angles [deg] for **ASPDKP + PPY**.

Bond lengths	
N(1)-C(1)	1.318(10)
N(1)-C(4)	1.469(10)
N(2)-C(3)	1.336(11)
N(2)-C(2)	1.447(10)
N(7)-C(53)	1.316(10)
N(7)-C(56)	1.474(9)
N(8)-C(55)	1.321(10)
N(8)-C(54)	1.442(10)
O(1)-C(1)	1.249(9)
O(2)-C(3)	1.235(9)
O(3)-C(6)	1.322(10)
O(4)-C(6)	1.220(10)
O(5)-C(8)	1.207(9)
O(6)-C(8)	1.303(10)
O(7)-C(53)	1.244(9)
O(8)-C(55)	1.241(9)
O(9)-C(58)	1.221(10)

O(10)-C(58)	1.312(10)
O(11)-C(60)	1.193(10)
O(12)-C(60)	1.319(10)
C(1)-C(2)	1.504(11)
C(2)-C(7)	1.517(11)
C(3)-C(4)	1.503(11)
C(4)-C(5)	1.520(12)
C(5)-C(6)	1.496(12)
C(7)-C(8)	1.503(11)
C(53)-C(54)	1.536(10)
C(54)-C(59)	1.522(11)
C(55)-C(56)	1.505(10)
C(56)-C(57)	1.533(11)
C(57)-C(58)	1.501(11)
C(59)-C(60)	1.524(11)
N(3)-C(9)	1.327(11)
N(3)-C(13)	1.357(10)
N(4)-C(24)	1.323(11)
N(4)-C(20)	1.352(11)
N(5)-C(35)	1.322(13)
N(5)-C(31)	1.336(12)
N(6)-C(46)	1.336(11)
N(6)-C(42)	1.345(12)
C(9)-C(10)	1.393(12)
C(10)-C(11)	1.397(11)
C(11)-C(12)	1.368(12)
C(11)-C(14)	1.495(11)
C(12)-C(13)	1.373(12)
C(14)-C(19)	1.385(12)
C(14)-C(15)	1.385(12)
C(15)-C(16)	1.372(13)
C(16)-C(17)	1.400(13)
C(17)-C(18)	1.355(13)
C(18)-C(19)	1.391(12)
C(20)-C(21)	1.377(11)
C(21)-C(22)	1.378(11)
C(22)-C(23)	1.391(11)
C(22)-C(25)	1.491(11)
C(23)-C(24)	1.388(12)
C(25)-C(26)	1.382(12)
C(25)-C(30)	1.392(11)
C(26)-C(27)	1.284(13)
C(27)-C(28)	1.399(13)
C(28)-C(29)	1.373(13)
C(29)-C(30)	1.386(12)
C(31)-C(32)	1.350(13)
C(32)-C(33)	1.370(12)
C(33)-C(34)	1.401(12)
C(33)-C(36)	1.464(12)
C(34)-C(35)	1.375(14)
C(36)-C(37)	1.376(12)
C(36)-C(41)	1.389(12)
C(37)-C(38)	1.388(14)
C(38)-C(39)	1.36(2)

C(39)-C(40)	1.38(2)
C(40)-C(41)	1.376(14)
C(42)-C(43)	1.363(13)
C(43)-C(44)	1.404(12)
C(44)-C(45)	1.395(13)
C(44)-C(47)	1.489(13)
C(45)-C(46)	1.368(13)
C(47)-C(48)	1.392(13)
C(47)-C(52)	1.401(13)
C(48)-C(49)	1.375(14)
C(49)-C(50)	1.370(14)
C(50)-C(51)	1.38(2)
C(51)-C(52)	1.378(14)
Bond angles	
C(1)-N(1)-C(4)	126.0(7)
C(3)-N(2)-C(2)	125.4(7)
C(53)-N(7)-C(56)	127.5(7)
C(55)-N(8)-C(54)	126.8(7)
O(1)-C(1)-N(1)	122.3(7)
O(1)-C(1)-C(2)	118.8(7)
N(1)-C(1)-C(2)	118.9(7)
N(2)-C(2)-C(1)	111.8(7)
N(2)-C(2)-C(7)	112.6(6)
C(1)-C(2)-C(7)	110.9(6)
O(2)-C(3)-N(2)	123.3(7)
O(2)-C(3)-C(4)	118.1(8)
N(2)-C(3)-C(4)	118.6(7)
N(1)-C(4)-C(3)	112.8(7)
N(1)-C(4)-C(5)	110.9(7)
C(3)-C(4)-C(5)	107.2(7)
C(6)-C(5)-C(4)	116.0(7)
O(4)-C(6)-O(3)	123.2(8)
O(4)-C(6)-C(5)	123.6(9)
O(3)-C(6)-C(5)	113.1(8)
C(8)-C(7)-C(2)	115.4(7)
O(5)-C(8)-O(6)	125.5(8)
O(5)-C(8)-C(7)	121.5(8)
O(6)-C(8)-C(7)	113.1(7)
O(7)-C(53)-N(7)	123.0(7)
O(7)-C(53)-C(54)	119.1(7)
N(7)-C(53)-C(54)	117.8(7)
N(8)-C(54)-C(59)	111.9(7)
N(8)-C(54)-C(53)	112.5(6)
C(59)-C(54)-C(53)	111.8(6)
O(8)-C(55)-N(8)	122.4(7)
O(8)-C(55)-C(56)	117.7(7)
N(8)-C(55)-C(56)	119.9(7)
N(7)-C(56)-C(55)	112.3(7)
N(7)-C(56)-C(57)	109.7(6)
C(55)-C(56)-C(57)	109.1(6)
C(58)-C(57)-C(56)	112.9(7)
O(9)-C(58)-O(10)	122.6(8)
O(9)-C(58)-C(57)	123.9(7)
O(10)-C(58)-C(57)	113.4(8)

C(60)-C(59)-C(54)	110.3(6)
O(11)-C(60)-O(12)	124.8(8)
O(11)-C(60)-C(59)	122.2(7)
O(12)-C(60)-C(59)	112.9(7)
C(9)-N(3)-C(13)	116.8(7)
C(24)-N(4)-C(20)	117.8(7)
C(35)-N(5)-C(31)	116.6(8)
C(46)-N(6)-C(42)	116.1(8)
N(3)-C(9)-C(10)	123.8(8)
C(9)-C(10)-C(11)	118.8(9)
C(12)-C(11)-C(10)	117.0(8)
C(12)-C(11)-C(14)	123.0(7)
C(10)-C(11)-C(14)	120.0(8)
C(11)-C(12)-C(13)	121.1(8)
N(3)-C(13)-C(12)	122.4(8)
C(19)-C(14)-C(15)	118.2(8)
C(19)-C(14)-C(11)	120.3(8)
C(15)-C(14)-C(11)	121.5(7)
C(16)-C(15)-C(14)	121.8(8)
C(15)-C(16)-C(17)	118.6(9)
C(18)-C(17)-C(16)	120.9(9)
C(17)-C(18)-C(19)	119.7(9)
C(14)-C(19)-C(18)	120.9(9)
N(4)-C(20)-C(21)	121.4(8)
C(22)-C(21)-C(20)	121.3(8)
C(21)-C(22)-C(23)	116.8(8)
C(21)-C(22)-C(25)	122.4(7)
C(23)-C(22)-C(25)	120.7(8)
C(24)-C(23)-C(22)	119.1(8)
N(4)-C(24)-C(23)	123.6(8)
C(26)-C(25)-C(30)	119.1(8)
C(26)-C(25)-C(22)	120.3(8)
C(30)-C(25)-C(22)	120.6(8)
C(25)-C(26)-C(27)	117.2(9)
C(28)-C(27)-C(26)	127.3(10)
C(29)-C(28)-C(27)	113.9(9)
C(28)-C(29)-C(30)	120.6(9)
C(29)-C(30)-C(25)	120.1(8)
N(5)-C(31)-C(32)	122.4(10)
C(31)-C(32)-C(33)	122.7(8)
C(32)-C(33)-C(34)	114.6(8)
C(32)-C(33)-C(36)	123.9(8)
C(34)-C(33)-C(36)	121.4(8)
C(35)-C(34)-C(33)	119.6(9)
N(5)-C(35)-C(34)	123.9(9)
C(37)-C(36)-C(41)	115.6(8)
C(37)-C(36)-C(33)	122.1(8)
C(41)-C(36)-C(33)	122.3(7)
C(36)-C(37)-C(38)	123.2(10)
C(39)-C(38)-C(37)	118.8(10)
C(38)-C(39)-C(40)	120.5(10)
C(41)-C(40)-C(39)	119.2(10)
C(40)-C(41)-C(36)	122.6(9)
N(6)-C(42)-C(43)	123.4(9)

C(42)-C(43)-C(44)	120.0(9)
C(45)-C(44)-C(43)	116.7(9)
C(45)-C(44)-C(47)	121.1(8)
C(43)-C(44)-C(47)	122.2(8)
C(46)-C(45)-C(44)	118.8(9)
N(6)-C(46)-C(45)	125.0(9)
C(48)-C(47)-C(52)	119.0(10)
C(48)-C(47)-C(44)	120.8(8)
C(52)-C(47)-C(44)	120.3(9)
C(49)-C(48)-C(47)	120.1(9)
C(50)-C(49)-C(48)	121.0(10)
C(49)-C(50)-C(51)	119.6(10)
C(52)-C(51)-C(50)	120.4(9)
C(51)-C(52)-C(47)	120.0(10)

Table 5. Anisotropic displacement parameters ($Å^2$ x 10^3) for **ASPDKP + PPY**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U11 + ... + 2hka^*b^*U12]$

atom	U11	U22	U33	U23	U13	U12
N(1)	36(1)	47(1)	48(1)	-1(1)	24(1)	-9(1)
N(1)	4(3)	33(4)	41(4)	18(4)	6(3)	5(3)
N(2)	0(3)	33(4)	42(4)	17(4)	3(3)	4(3)
N(7)	7(3)	31(4)	35(4)	14(3)	5(3)	5(3)
N(8)	0(3)	38(4)	42(4)	19(4)	7(3)	6(3)
O(1)	12(3)	42(4)	51(4)	20(3)	14(3)	12(3)
O(2)	10(3)	32(4)	84(5)	20(3)	11(3)	13(3)
O(3)	31(4)	57(5)	52(5)	28(4)	-2(3)	4(3)
O(4)	23(4)	46(4)	45(4)	15(3)	-2(3)	-7(3)
O(5)	32(3)	39(4)	45(4)	21(3)	22(3)	16(3)
O(6)	25(3)	37(4)	55(4)	20(3)	19(3)	10(3)
O(7)	7(3)	34(3)	48(4)	17(3)	7(3)	7(2)
O(8)	18(3)	43(4)	65(4)	34(3)	13(3)	14(3)
O(9)	21(3)	38(4)	36(4)	9(3)	6(3)	-4(3)
O(10)	39(4)	62(5)	37(4)	13(4)	15(3)	-16(3)
O(11)	34(4)	45(4)	27(4)	5(3)	8(3)	0(3)
O(12)	20(3)	31(3)	41(4)	12(3)	6(3)	1(3)
C(1)	9(4)	35(5)	24(5)	9(4)	3(3)	6(4)
C(2)	13(4)	27(5)	22(5)	4(4)	10(3)	11(3)
C(3)	8(4)	37(5)	36(5)	6(4)	4(4)	3(4)
C(4)	8(4)	30(5)	39(5)	7(4)	7(4)	0(3)
C(5)	15(4)	39(5)	51(6)	18(5)	3(4)	5(4)
C(6)	28(5)	32(5)	46(6)	24(5)	4(5)	12(4)
C(7)	15(4)	34(5)	28(5)	7(4)	5(4)	5(4)
C(8)	15(4)	33(6)	36(5)	14(4)	9(4)	7(4)
C(53)	9(4)	27(5)	29(5)	8(4)	-3(3)	1(4)
C(54)	13(4)	31(5)	33(5)	16(4)	12(4)	7(4)
C(55)	8(4)	26(5)	38(5)	14(4)	5(4)	6(4)
C(56)	2(4)	26(4)	34(5)	13(4)	9(3)	10(3)
C(57)	16(4)	32(5)	35(5)	13(4)	7(4)	4(4)
C(58)	16(5)	50(6)	30(5)	20(5)	9(4)	13(4)
C(59)	12(4)	30(5)	33(5)	12(4)	5(4)	5(4)
C(60)	24(5)	18(5)	35(5)	12(4)	4(4)	8(4)
N(3)	24(4)	37(4)	35(4)	13(4)	9(3)	4(3)
N(4)	28(4)	30(4)	37(5)	9(4)	13(4)	6(3)
N(5)	33(5)	52(6)	40(5)	14(4)	7(4)	-12(4)

N(6)	31(5)	41(5)	46(5)	20(4)	0(4)	1(4)
C(9)	13(4)	35(5)	50(6)	17(5)	5(4)	4(4)
C(10)	34(5)	35(5)	39(6)	13(4)	9(4)	10(4)
C(11)	18(4)	29(5)	27(5)	1(4)	3(4)	0(4)
C(12)	24(5)	27(5)	42(6)	15(4)	11(4)	11(4)
C(13)	30(5)	32(5)	39(6)	14(4)	7(4)	12(4)
C(14)	16(4)	27(5)	34(5)	8(4)	8(4)	4(4)
C(15)	33(5)	38(6)	36(5)	20(4)	9(4)	10(4)
C(16)	45(6)	33(6)	44(6)	11(5)	3(5)	-1(5)
C(17)	32(5)	56(7)	49(6)	30(6)	15(5)	3(5)
C(18)	36(5)	39(6)	40(6)	12(5)	12(5)	10(4)
C(19)	31(5)	39(6)	41(6)	13(5)	1(4)	4(4)
C(20)	29(5)	33(5)	29(5)	16(4)	5(4)	4(4)
C(21)	15(4)	30(5)	35(5)	7(4)	7(4)	2(4)
C(22)	19(5)	32(5)	31(5)	14(4)	4(4)	9(4)
C(23)	25(5)	29(5)	35(5)	10(4)	2(4)	2(4)
C(24)	27(5)	27(5)	39(6)	10(4)	4(4)	-4(4)
C(25)	15(4)	42(6)	29(5)	14(4)	3(4)	4(4)
C(26)	16(5)	59(7)	29(5)	15(5)	5(4)	4(4)
C(27)	71(8)	51(7)	43(7)	14(6)	10(6)	-7(6)
C(28)	23(5)	61(7)	35(6)	15(5)	11(4)	1(5)
C(29)	29(5)	54(6)	23(5)	6(4)	6(4)	8(5)
C(30)	13(4)	44(6)	34(5)	13(5)	0(4)	11(4)
C(31)	39(6)	47(6)	48(6)	16(5)	14(5)	6(5)
C(32)	13(5)	51(6)	64(7)	28(5)	17(4)	13(4)
C(33)	24(5)	26(5)	24(5)	-1(4)	2(4)	1(4)
C(34)	46(6)	40(6)	72(8)	21(6)	28(6)	20(5)
C(35)	36(6)	57(7)	71(8)	15(6)	33(6)	16(5)
C(36)	16(4)	40(6)	35(5)	12(4)	6(4)	2(4)
C(37)	58(7)	42(6)	55(7)	26(5)	27(6)	24(5)
C(38)	46(7)	82(9)	77(8)	48(7)	31(6)	20(6)
C(39)	54(7)	76(9)	52(7)	39(7)	10(6)	-11(6)
C(40)	64(7)	38(6)	47(7)	14(5)	3(6)	2(5)
C(41)	37(6)	38(6)	44(6)	15(5)	8(5)	16(5)
C(42)	43(6)	32(5)	36(5)	8(4)	1(5)	18(5)
C(43)	26(5)	41(6)	36(6)	7(5)	1(4)	14(4)
C(44)	33(5)	30(5)	32(5)	5(4)	3(4)	13(4)
C(45)	51(7)	34(6)	35(6)	9(5)	-2(5)	5(5)
C(46)	48(6)	34(6)	41(6)	17(5)	-2(5)	7(5)
C(47)	31(5)	43(6)	38(6)	10(5)	1(4)	16(5)
C(48)	32(6)	53(7)	42(6)	2(5)	5(5)	9(5)
C(49)	36(6)	45(6)	56(7)	3(6)	6(5)	7(5)
C(51)	40(6)	60(7)	36(6)	15(5)	6(5)	22(5)
C(52)	46(6)	41(6)	35(6)	4(5)	-3(5)	18(5)

Table 6. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **ASPDKP + PPY**.

atom	x	y	z	U(eq)
H(1N)	19948(137)	14107(60)	9881(55)	30
H(2N)	26117(142)	15221(65)	9276(60)	29
H(7N)	23628(140)	11721(58)	7667(55)	28
H(8N)	30675(135)	12817(59)	7267(53)	30
H(3O)	20335(179)	12745(79)	11921(69)	67
H(6O)	26630(160)	17785(70)	8415(67)	56

H(10O)	23129(179)	10593(80)	9716(74)	73
H(12O)	32099(145)	15164(64)	6387(62)	47
H(2)	22895(12)	14939(6)	8344(5)	25
H(4)	22525(12)	13058(6)	9261(6)	33
H(5A)	24620(13)	13225(7)	10656(7)	42
H(5B)	23791(13)	14262(7)	11163(7)	42
H(7A)	22218(12)	16604(6)	9053(6)	32
H(7B)	24080(12)	16754(6)	9869(6)	32
H(54)	27039(12)	12599(6)	6210(6)	28
H(56)	26347(11)	10692(6)	7229(6)	23
H(57A)	28090(12)	11111(6)	8799(6)	33
H(57B)	26824(12)	12056(6)	9109(6)	33
H(59A)	26425(12)	14310(6)	7034(6)	30
H(59B)	28403(12)	14361(6)	7774(6)	30
H(9)	26652(13)	18999(6)	7490(6)	38
H(10)	28904(14)	19291(7)	6480(6)	43
H(12)	32518(13)	17304(6)	6872(6)	35
H(13)	30192(13)	17054(6)	7853(6)	40
H(15)	32155(14)	19975(7)	6257(6)	40
H(16)	34511(15)	20280(7)	5292(6)	50
H(17)	36195(15)	18975(8)	4344(7)	51
H(18)	35644(14)	17434(7)	4422(6)	46
H(19)	33348(14)	17150(7)	5431(6)	45
H(20)	36093(13)	15899(6)	6614(6)	35
H(21)	38265(13)	16013(6)	5524(6)	34
H(23)	33271(13)	14654(6)	3538(6)	37
H(24)	31241(14)	14528(6)	4676(6)	39
H(26)	39384(13)	16667(7)	4515(6)	42
H(27)	40833(18)	16896(8)	3352(7)	68
H(28)	40994(14)	15595(7)	1949(6)	48
H(29)	38130(13)	14286(7)	1538(6)	45
H(30)	36041(12)	14133(6)	2658(6)	36
H(31)	9083(15)	10798(7)	10287(7)	54
H(32)	6998(13)	9972(7)	10958(7)	47
H(34)	11079(16)	7932(7)	10471(8)	60
H(35)	13094(16)	8827(8)	9805(8)	66
H(37)	5696(16)	9383(8)	11885(7)	56
H(38)	3598(17)	8536(10)	12589(8)	73
H(39)	4114(17)	6935(9)	12395(7)	69
H(40)	6659(18)	6163(8)	11471(7)	61
H(41)	8669(15)	7008(7)	10748(7)	47
H(42)	16408(15)	11864(7)	11238(7)	45
H(43)	13600(14)	11339(7)	11870(6)	43
H(45)	17380(16)	12392(6)	14339(7)	50
H(46)	20070(16)	12865(7)	13617(7)	48
H(48)	12155(15)	10209(8)	12501(7)	56
H(49)	9534(16)	9633(8)	13216(7)	60
H(50)	9095(16)	10512(9)	14736(8)	68
H(51)	11359(15)	11979(8)	15574(7)	54
H(52)	14026(16)	12570(7)	14882(6)	52

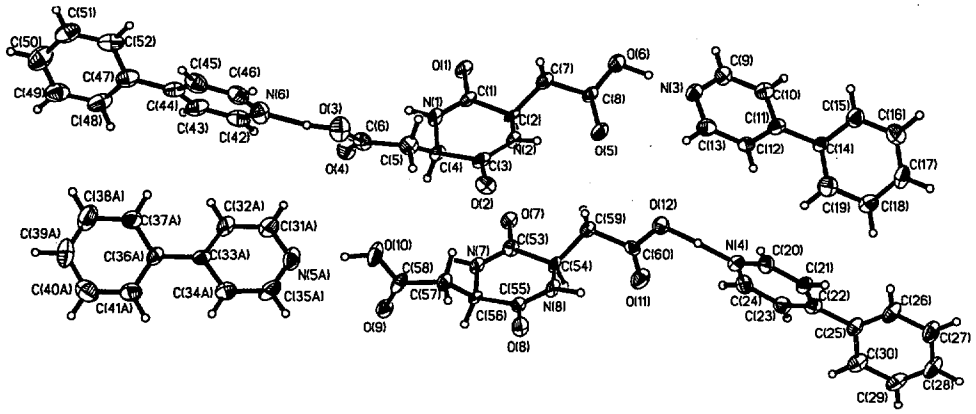

Figure 1. 50% probability displacement ellipsoids of **ASPDKP + PPY**.

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

Identification code	ASPDKP
Empirical formula	$C_8H_{10}N_2O_6$
Formula weight	230.18
Temperature	130(2) K
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	P1
Unit cell dimensions	a = 4.9845(10) Å α = 82.50(3)°
	b = 5.0390(10) Å β = 88.47(3)°
	c = 18.853(4) Å γ = 75.33(3)°
Volume, Z	454.2(2) $Å^3$, 2
Density (calculated)	1.683 Mg/m^3
Absorption coefficient	1.275 mm^{-1}
F(000)	240
Crystal size	0.18 x 0.06 x 0.04 mm
Crystal color	colorless
Theta range for data collection	2.36 to 57.14°
Scan type	θ–2θ
Limiting indices	-5<=h<=4,, -5<=k<=0, -20<=l<=19
Reflections collected	1240
Independent reflections	1215 [R(int) = 0.0000]
Absorption correction	XABS2
Max. and min. transmission	0.96 and 0.93
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1215 / 3 / 369
Goodness-of-fit on F^2	1.083
Final R indices [I>2σ(I)]	R1 = 0.0344, wR2 = 0.0852
R indices (all data)	R1 = 0.0346, wR2 = 0.0856
Absolute structure parameter	0.1(2)
Extinction coefficient	none
Largest diff. peak and hole	0.296 and -0.317 e^- / $Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **ASPDKP**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

atom	x	y	z	U(eq)
N(1)	7157(6)	15227(6)	8527(2)	12(1)
O(1)	12099(5)	8855(5)	8930(1)	14(1)
C(1)	11180(7)	11227(8)	8643(2)	11(1)
N(2)	11942(6)	12161(7)	8001(2)	13(1)
O(2)	10949(6)	11056(6)	10459(1)	24(1)
C(2)	9045(7)	13323(7)	9036(2)	12(1)
O(3)	8993(6)	7601(5)	10322(2)	19(1)
C(3)	7458(7)	11790(8)	9571(2)	14(1)
N(3)	6971(7)	9075(6)	3721(2)	12(1)
O(4)	6381(5)	18028(5)	7488(1)	14(1)
C(4)	9333(7)	10094(7)	10160(2)	16(1)
N(4)	3643(6)	14007(6)	3196(2)	12(1)
O(5)	10232(5)	14605(5)	5754(1)	16(1)
C(5)	7928(8)	16190(7)	7884(2)	11(1)
O(6)	8391(5)	12539(5)	6695(1)	16(1)
C(7)	11464(8)	15379(8)	6891(2)	13(1)
O(7)	1315(5)	14353(5)	4249(1)	15(1)
C(8)	9826(7)	14050(7)	6441(2)	12(1)

O(8)	7150(5)	11995(5)	5038(1)	16(1)
O(9)	5472(6)	9750(5)	5974(1)	16(1)
C(9)	2952(8)	12996(8)	3845(2)	14(1)
O(10)	9872(5)	9261(5)	2776(1)	16(1)
C(10)	4249(8)	9917(8)	4037(2)	12(1)
O(11)	2523(6)	15010(6)	1377(2)	24(1)
C(11)	4224(8)	9026(8)	4832(2)	13(1)
O(12)	4591(6)	18426(5)	1462(1)	18(1)
C(12)	5775(7)	10409(7)	5284(2)	12(1)
C(13)	7619(8)	10086(7)	3070(2)	11(1)
C(14)	5320(8)	12331(8)	2688(2)	13(1)
C(15)	6513(8)	14140(8)	2132(2)	16(1)
C(16)	4328(8)	15905(8)	1624(2)	15(1)

Table 3. Selected hydrogen bond lengths [Å] and angles [deg] for **ASPDKP**.

Bond lengths	
N(1)-H(1N)	0.926(54)
H(1N)--O(1)	1.98(5)
N(1)-H(1N)--O(1)	2.864(4)
N(2)-H(2N)	0.874(52)
H(2N)--O(4)	1.92(5)
N(2)-H(2N)--O(4)	2.871(4)
N(3)-H(3N)	0.917(57)
H(3N)--O(7)	1.97(6)
N(3)-H(3N)--O(7)	2.868(4)
N(4)-H(4N)	0.949(48)
H(4N)--O(10)	1.93(5)
N(4)-H(4N)--O(10)	2.860(4)
O(3)-H(3O)	0.896(61)
H(3O)--O(11)	1.78(6)
O(3)-H(3O)--O(11)	2.665(4)
O(5)-H(5O)	0.972(77)
H(5O)--O(8)	1.77(8)
O(5)-H(5O)--O(8)	2.740(4)
O(9)-H(9O)	0.847(54)
H(9O)--O(6)	1.91(5)
O(9)-H(9O)--O(6)	2.753(4)
O(12)-H(12O)	0.890(68)
H(12O)--O(2)	1.78(6)
O(12)-H(12O)--O(2)	2.633(4)
Bond angles	
N(1)-H(1N)-O(1)	162.61(4.00)
N(2)-H(2N)-O(4)	162.53(3.51)
N(3)-H(3N)-O(7)	167.21(4.50)
N(4)-H(4N)-O(10)	166.23(3.74)
O(3)-H(3O)-O(11)	176.09(4.86)
O(5)-H(5O)-O(8)	174.73(6.42)
O(9)-H(9O)-O(6)	174.24(4.14)
O(12)-H(12O)-O(2)	161.18(5.27)

Table 4. Bond lengths [Å] and angles [deg] for **ASPDKP**.

Bond lengths	
N(1)-C(5)	1.329(5)
N(1)-C(2)	1.442(5)

O(1)-C(1)	1.225(5)
C(1)-N(2)	1.322(5)
C(1)-C(2)	1.546(5)
N(2)-C(6)	1.456(5)
O(2)-C(4)	1.223(5)
C(2)-C(3)	1.518(5)
O(3)-C(4)	1.306(5)
C(3)-C(4)	1.496(5)
N(3)-C(13)	1.330(5)
N(3)-C(10)	1.452(5)
O(4)-C(5)	1.224(4)
N(4)-C(9)	1.335(5)
N(4)-C(14)	1.463(5)
O(5)-C(8)	1.311(5)
C(5)-C(6)	1.522(6)
O(6)-C(8)	1.217(5)
C(6)-C(7)	1.509(5)
C(7)-C(8)	1.515(5)
O(7)-C(9)	1.238(5)
O(8)-C(12)	1.219(5)
O(9)-C(12)	1.315(5)
C(9)-C(10)	1.521(5)
O(10)-C(13)	1.238(5)
C(10)-C(11)	1.509(6)
O(11)-C(16)	1.230(5)
C(11)-C(12)	1.507(6)
O(12)-C(16)	1.306(5)
C(13)-C(14)	1.512(6)
C(14)-C(15)	1.508(5)
C(15)-C(16)	1.496(6)

Bonds angles	
C(5)-N(1)-C(2)	123.3(3)
O(1)-C(1)-N(2)	123.4(3)
O(1)-C(1)-C(2)	120.2(3)
N(2)-C(1)-C(2)	116.4(3)
C(1)-N(2)-C(6)	122.5(3)
N(1)-C(2)-C(3)	110.2(3)
N(1)-C(2)-C(1)	110.0(3)
C(3)-C(2)-C(1)	109.7(3)
C(4)-C(3)-C(2)	110.8(3)
C(13)-N(3)-C(10)	123.8(3)
O(2)-C(4)-O(3)	125.1(3)
O(2)-C(4)-C(3)	121.3(3)
O(3)-C(4)-C(3)	113.6(3)
C(9)-N(4)-C(14)	124.3(3)
O(4)-C(5)-N(1)	122.6(3)
O(4)-C(5)-C(6)	121.1(3)
N(1)-C(5)-C(6)	116.1(3)
N(2)-C(6)-C(7)	111.5(3)
N(2)-C(6)-C(5)	111.0(3)
C(7)-C(6)-C(5)	113.6(3)
C(6)-C(7)-C(8)	115.9(3)
O(6)-C(8)-O(5)	124.0(3)
O(6)-C(8)-C(7)	123.4(3)

O(5)-C(8)-C(7)	112.5(3)
O(7)-C(9)-N(4)	124.4(3)
O(7)-C(9)-C(10)	122.0(3)
N(4)-C(9)-C(10)	113.5(3)
N(3)-C(10)-C(11)	113.3(3)
C(11)-C(10)-C(9)	112.1(3)
C(12)-C(11)-C(10)	115.5(3)
O(8)-C(12)-O(9)	123.2(4)
O(8)-C(12)-C(11)	123.8(3)
O(9)-C(12)-C(11)	113.0(3)
O(10)-C(13)-N(3)	124.4(4)
O(10)-C(13)-C(14)	121.0(3)
N(3)-C(13)-C(14)	114.6(3)
N(4)-C(14)-C(15)	110.1(3)
N(4)-C(14)-C(13)	110.9(3)
C(15)-C(14)-C(13)	110.3(3)
C(16)-C(15)-C(14)	111.6(3)
O(11)-C(16)-O(12)	124.4(4)
O(11)-C(16)-C(15)	122.4(3)
O(12)-C(16)-C(15)	113.2(3)

Table 5. Anisotropic displacement parameters ($Å^2$ x 10^3) for **ASPDKP**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U11 + ... + 2hka^*b^*U12]$

atom	U11	U22	U33	U23	U13	U12
N(1)	10(2)	8(2)	11(2)	5(1)	1(1)	5(1)
O(1)	15(1)	6(2)	15(1)	5(1)	1(1)	5(1)
C(1)	8(2)	9(2)	15(2)	1(2)	0(2)	0(2)
N(2)	9(2)	8(2)	16(2)	2(1)	1(1)	6(1)
O(2)	37(2)	11(1)	21(2)	7(1)	-12(1)	-4(1)
C(2)	13(2)	5(2)	13(2)	7(2)	-1(2)	2(2)
O(3)	24(1)	11(1)	17(1)	9(1)	-1(1)	-2(1)
C(3)	10(2)	10(2)	16(2)	4(2)	0(2)	5(2)
N(3)	15(2)	4(2)	14(2)	5(1)	-4(1)	2(1)
O(4)	13(1)	8(1)	13(1)	9(1)	-4(1)	4(1)
C(4)	19(2)	9(2)	17(2)	-2(2)	6(2)	3(2)
N(4)	17(2)	6(2)	9(2)	5(1)	1(1)	2(1)
O(5)	1(1)	14(2)	12(2)	3(1)	1(1)	-5(1)
C(5)	16(2)	5(2)	11(2)	1(2)	-2(2)	-4(2)
O(6)	17(1)	12(1)	18(1)	3(1)	0(1)	-6(1)
C(6)	13(2)	5(2)	16(2)	4(2)	-3(2)	-2(2)
C(7)	11(2)	6(2)	20(2)	2(2)	0(2)	-1(2)
O(7)	14(1)	11(1)	15(1)	1(1)	3(1)	3(1)
C(8)	10(2)	6(2)	17(2)	3(2)	0(2)	4(2)
O(8)	17(1)	14(1)	17(1)	3(1)	-2(1)	-5(1)
O(9)	22(2)	13(2)	13(2)	5(1)	-1(1)	-5(1)
C(9)	14(2)	12(2)	16(2)	5(2)	-5(2)	-6(2)
O(10)	13(1)	9(1)	19(2)	2(1)	2(1)	4(1)
C(10)	15(2)	7(2)	12(2)	2(2)	-2(2)	-2(2)
O(11)	28(2)	13(1)	29(2)	10(1)	-10(1)	-4(1)
C(11)	14(2)	4(2)	17(2)	6(2)	-4(2)	1(2)
O(12)	24(1)	6(1)	20(1)	7(1)	-7(1)	1(1)
C(12)	9(2)	5(2)	17(2)	5(2)	0(2)	4(2)
C(13)	14(2)	4(2)	15(2)	3(2)	-3(2)	-3(2)
C(14)	17(2)	8(2)	14(2)	3(2)	-3(2)	-4(2)

C(15)	15(2)	12(2)	15(2)	8(2)	-1(2)	0(2)
C(16)	20(2)	11(2)	11(2)	2(2)	4(2)	-2(2)

Table 6. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **ASPDKP.**

atom	x	y	z	U(eq)
H(1N)	5463(108)	16074(103)	8713(23)	16(11)
H(2N)	13371(102)	11203(93)	7787(22)	8(10)
H(2)	9914(99)	14401(101)	9290(26)	21(12)
H(3O)	10114(117)	6728(111)	10689(30)	32(14)
H(3A)	6566(109)	10562(111)	9356(29)	32(13)
H(3B)	6118(102)	13121(109)	9780(26)	23(12)
H(3N)	8191(110)	7541(112)	3949(28)	26(13)
H(4N)	2639(94)	15829(97)	3017(23)	13(11)
H(5O)	9242(153)	13610(147)	5491(36)	60(19)
H(6)	11903(79)	16266(76)	7899(20)	6(9)
H(7A)	13466(87)	14590(78)	6797(19)	3(9)
H(7B)	11136(98)	17345(111)	6721(26)	22(11)
H(9O)	6338(102)	10702(99)	6173(26)	20(12)
H(10)	3270(82)	8912(83)	3845(20)	0(8)
H(11A)	2185(93)	9413(82)	5003(21)	10(9)
H(11B)	4864(113)	7230(118)	4950(29)	32(14)
H(12O)	3558(126)	19603(129)	1121(34)	40(15)
H(14)	4184(87)	11501(83)	2479(20)	3(9)
H(15A)	7362(79)	15373(82)	2374(20)	5(9)
H(15B)	7915(107)	12969(101)	1822(26)	28(12)

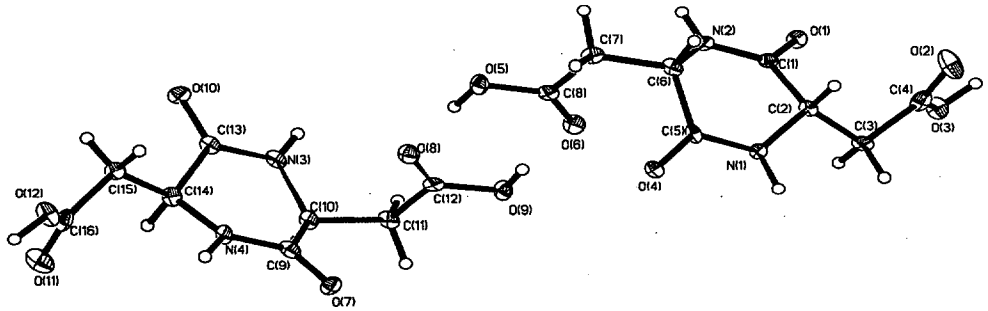

Figure 1. 50% probability displacement ellipsoids of **ASPDKP.**

Table 1. Crystal data and structure refinement for **ASPDKP + BPY**

Identification code	ASPDKP + BPY
Empirical formula	$C_{18}H_{18}N_4O_6$
Formula weight	386.36
Temperature	130(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 5.5440(6) Å α = 90 °
	b = 27.073(3) Å β = 99.814(8) °
	c = 6.0450(6) Å γ = 90 °
Volume, Z	894.0(2) $Å^3$, 2
Density (calculated)	1.435 Mg/m^3
Absorption coefficient	0.927 mm^{-1}
F(000)	404
Crystal size	0.04 x 0.08 x 0.10 mm
Crystal color	colorless
Theta range for data collection	3.26 to 56.45 °
Scan type	θ–2θ
Limiting indices	-5<=h<=5, 0<=k<=28, 0<=l<=6
Reflections collected	1196
Independent reflections	1196[R(int) = 0.0000]
Absorption correction	XABS2
Max. and min. transmission	0.97 and 0.94
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1196 / 1 / 263
Goodness-of-fit on F^2	1.097
Final R indices [I>2σ(I)]	R1 = 0.0338, wR2 = 0.0926
R indices (all data)	R1 = 0.0350, wR2 = 0.0939
Absolute structure parameter	0.1(3)
Extinction coefficient	none
Largest diff. peak and hole	0.505 and -0.175 $e^- / Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **ASPDKP + BPY**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

atom	x	y	z	U(eq)
N(1)	3280(6)	3819(1)	11789(6)	17(1)
N(2)	3328(6)	3437(1)	7622(5)	20(1)
O(1)	3395(5)	4200(1)	6112(4)	22(1)
O(2)	8696(5)	4665(1)	8036(4)	24(1)
O(3)	5783(5)	5162(1)	8932(5)	25(1)
O(4)	3056(5)	3061(1)	13266(4)	26(1)
O(5)	8389(5)	2548(1)	7064(4)	23(1)
O(6)	4931(5)	2154(1)	7441(4)	25(1)
C(1)	3487(7)	3923(1)	7768(6)	17(1)
C(2)	3843(7)	4161(1)	10091(6)	16(1)
C(3)	6445(7)	4370(1)	10736(6)	20(1)
C(4)	6926(7)	4779(1)	9145(6)	18(1)
C(5)	3317(7)	3328(1)	11674(6)	17(1)
C(6)	3679(7)	3093(1)	9489(6)	17(1)
C(7)	6192(7)	2847(1)	9818(6)	21(1)
C(8)	6436(7)	2480(1)	7961(6)	18(1)
N(3)	9429(6)	5313(1)	15026(5)	21(1)
N(4)	11165(6)	6916(1)	6108(5)	19(1)

C(9)	11260(7)	5242(1)	13870(6)	22(1)
C(10)	11665(7)	5545(1)	12133(6)	20(1)
C(11)	10145(7)	5954(1)	11535(6)	15(1)
C(12)	8279(7)	6031(1)	12784(6)	18(1)
C(13)	7994(7)	5706(1)	14484(6)	19(1)
C(14)	10524(7)	6288(1)	9666(6)	15(1)
C(15)	12419(7)	6216(1)	8444(6)	20(1)
C(16)	12686(7)	6535(1)	6727(6)	19(1)
C(17)	9334(7)	6983(1)	7273(6)	20(1)
C(18)	8973(7)	6688(1)	9040(6)	18(1)

Table 3. Selected hydrogen bond lengths [Å] and angles [deg] for **ASPDKP + BPY**.

Bond lengths	
N(1)-H(1N)	0.864
H(1N)--O(1)	1.938(49)
N(1)-H(1N)--O(1)	2.800(4)
N(2)-H(2N)	0.847
H(2N)--O(4)	1.958(50)
N(2)-H(2N)--O(4)	2.803(4)
O(2)-H(2O)	1.066
H(2O)--N(3)	1.557(52)
O(2)-H(2O)--N(3)	2.610(4)
O(5)-H(5O)	0.840
H(5O)--N(4)	1.777(6)
O(5)-H(5O)--N(4)	2.611(4)
Bond angles	
N(1)-H(1N)-O(1)	175.90(4.09)
N(2)-H(2N)-O(4)	176.11(4.15)
O(2)-H(2O)-N(3)	160.25(4.22)
O(5)-H(5O)-N(4)	171.75(3.11)

Table 4. Bond lengths [Å] and angles [deg] for **ASPDKP + BPY**.

Bond lengths	
N(1)-C(5)	1.331(5)
N(1)-C(2)	1.454(5)
N(2)-C(1)	1.321(5)
N(2)-C(6)	1.451(5)
O(1)-C(1)	1.244(5)
O(2)-C(4)	1.316(5)
O(3)-C(4)	1.211(5)
O(4)-C(5)	1.232(5)
O(5)-C(8)	1.304(5)
O(6)-C(8)	1.219(5)
C(1)-C(2)	1.526(5)
C(2)-C(3)	1.538(6)
C(3)-C(4)	1.518(5)
C(5)-C(6)	1.511(5)
C(6)-C(7)	1.526(6)
C(7)-C(8)	1.522(5)
N(3)-C(13)	1.335(5)
N(3)-C(9)	1.341(5)
N(4)-C(17)	1.343(5)
N(4)-C(16)	1.345(5)
C(9)-C(10)	1.381(5)

C(10)-C(11)	1.401(5)
C(11)-C(12)	1.396(5)
C(11)-C(14)	1.490(5)
C(12)-C(13)	1.382(5)
C(14)-C(18)	1.393(5)
C(14)-C(15)	1.397(5)
C(15)-C(16)	1.378(5)
C(17)-C(18)	1.376(5)

Bond angles	
C(5)-N(1)-C(2)	126.2(3)
C(1)-N(2)-C(6)	126.1(3)
O(1)-C(1)-N(2)	123.5(3)
O(1)-C(1)-C(2)	117.9(3)
N(2)-C(1)-C(2)	118.5(3)
N(1)-C(2)-C(1)	111.9(3)
N(1)-C(2)-C(3)	111.2(3)
C(1)-C(2)-C(3)	110.9(3)
C(4)-C(3)-C(2)	111.5(3)
O(3)-C(4)-O(2)	124.7(3)
O(3)-C(4)-C(3)	123.1(3)
O(2)-C(4)-C(3)	112.2(3)
O(4)-C(5)-N(1)	122.7(3)
O(4)-C(5)-C(6)	119.1(3)
N(1)-C(5)-C(6)	118.2(3)
N(2)-C(6)-C(5)	112.9(3)
N(2)-C(6)-C(7)	112.3(3)
C(5)-C(6)-C(7)	108.9(3)
C(8)-C(7)-C(6)	112.5(3)
O(6)-C(8)-O(5)	125.0(3)
O(6)-C(8)-C(7)	121.4(3)
O(5)-C(8)-C(7)	113.6(3)
C(13)-N(3)-C(9)	117.3(3)
C(17)-N(4)-C(16)	116.8(3)
N(3)-C(9)-C(10)	123.1(3)
C(9)-C(10)-C(11)	119.9(3)
C(12)-C(11)-C(10)	116.5(3)
C(12)-C(11)-C(14)	122.2(3)
C(10)-C(11)-C(14)	121.3(3)
C(13)-C(12)-C(11)	119.8(3)
N(3)-C(13)-C(12)	123.4(3)
C(18)-C(14)-C(15)	116.7(3)
C(18)-C(14)-C(11)	121.1(3)
C(15)-C(14)-C(11)	122.1(3)
C(16)-C(15)-C(14)	119.9(4)
N(4)-C(16)-C(15)	123.2(3)
N(4)-C(17)-C(18)	123.5(3)
C(17)-C(18)-C(14)	119.9(3)

Table 5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **ASPDKP + BPY**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U11 + ... + 2hka^*b^*U12]$

atom	U11	U22	U33	U23	U13	U12
N(1)	36(1)	47(1)	48(1)	-1(1)	24(1)	-9(1)
N(1)	32(2)	8(2)	12(2)	-2(1)	10(1)	0(1)
N(2)	42(2)	10(2)	8(2)	-2(1)	6(1)	1(1)

O(1)	48(2)	10(1)	10(1)	2(1)	9(1)	2(1)
O(2)	30(2)	20(2)	26(2)	9(1)	14(1)	5(1)
O(3)	34(2)	11(1)	31(2)	-1(1)	13(1)	2(1)
O(4)	52(2)	13(1)	13(1)	-1(1)	11(1)	-7(1)
O(5)	31(2)	18(2)	22(1)	-11(1)	10(1)	-6(1)
O(6)	36(2)	15(1)	27(1)	-8(1)	13(1)	-7(1)
C(1)	27(2)	9(2)	17(2)	1(2)	11(2)	-1(2)
C(2)	28(2)	9(2)	11(2)	4(2)	7(1)	0(2)
C(3)	29(2)	14(2)	17(2)	-1(2)	7(2)	0(2)
C(4)	23(2)	14(2)	19(2)	-1(2)	4(2)	-1(2)
C(5)	25(2)	10(2)	16(2)	-2(2)	6(1)	-2(2)
C(6)	30(2)	8(2)	14(2)	-1(2)	6(2)	-4(2)
C(7)	32(2)	15(2)	15(2)	-4(2)	1(2)	2(2)
C(8)	28(2)	10(2)	15(2)	3(2)	3(2)	3(2)
N(3)	29(2)	14(2)	20(2)	2(1)	5(1)	0(1)
N(4)	26(2)	10(2)	20(2)	0(1)	5(1)	1(1)
C(9)	32(2)	11(2)	24(2)	5(2)	8(2)	6(2)
C(10)	27(2)	13(2)	19(2)	3(2)	7(2)	2(2)
C(11)	22(2)	10(2)	13(2)	-5(2)	0(2)	-4(2)
C(12)	21(2)	13(2)	20(2)	-1(2)	5(2)	2(2)
C(13)	25(2)	19(2)	13(2)	-1(2)	6(1)	0(2)
C(14)	22(2)	7(2)	15(2)	-1(2)	1(2)	-2(2)
C(15)	27(2)	13(2)	19(2)	0(2)	2(2)	1(2)
C(16)	24(2)	16(2)	19(2)	0(2)	7(2)	0(2)
C(17)	29(2)	8(2)	22(2)	1(2)	5(2)	3(2)
C(18)	24(2)	11(2)	20(2)	-4(2)	7(2)	1(2)

Table 6. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for **ASPDKP + BPY**.

atom	x	y	z	U(eq)
H(1N)	3335(71)	3922(16)	13148(80)	20
H(2N)	3207(76)	3312(17)	6324(80)	23
H(2O)	8985(88)	4963(19)	6960(81)	36
H(5O)	8384(44)	2347(12)	6002(51)	35
H(2)	2672(7)	4443(1)	10020(6)	19
H(3)	6662(7)	4502(1)	12285(6)	24
H(3B)	7650(7)	4102(1)	10705(6)	24
H(6)	2423(7)	2827(1)	9134(6)	20
H(7A)	7466(7)	3105(1)	9861(6)	25
H(7B)	6478(7)	2673(1)	11280(6)	25
H(9)	12330(7)	4970(1)	14264(6)	26
H(10)	12971(7)	5477(1)	11345(6)	23
H(12)	7208(7)	6305(1)	12466(6)	21
H(13)	6710(7)	5765(1)	15310(6)	23
H(15)	13521(7)	5948(1)	8797(6)	24
H(16)	14010(7)	6483(1)	5942(6)	23
H(17)	8229(7)	7249(1)	6855(6)	24
H(18)	7670(7)	6756(1)	9830(6)	22

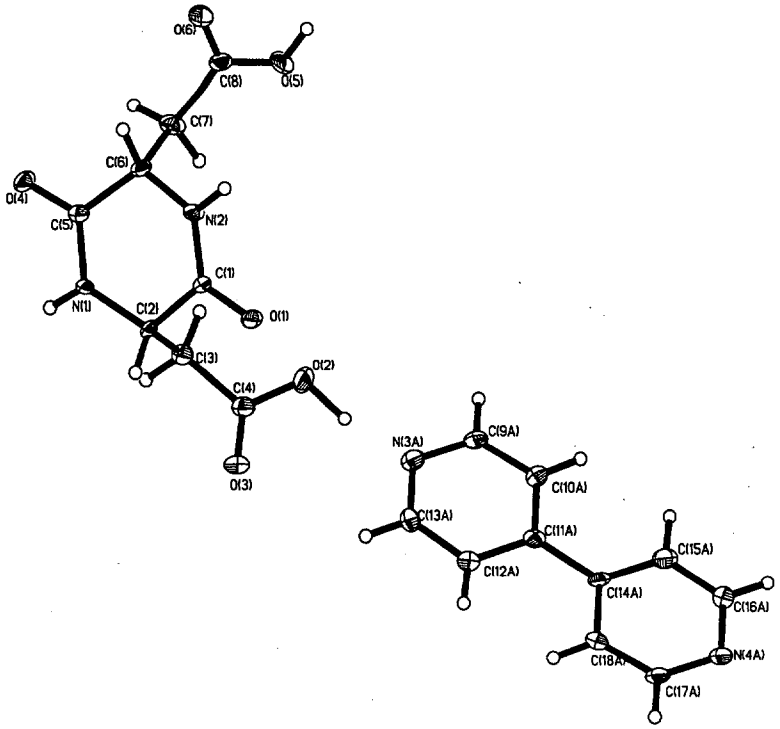

Figure 1. 50% probability displacement ellipsoids of **ASPDKP + BPY**.

Table 1. Crystal data and structure refinement for **ASPDKP + BPETE**.

Identification code	ASPDKP + BPETE
Empirical formula	$C_{20}H_{20}N_4O_6$
Formula weight	412.40
Temperature	130(2) K
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	P1
Unit cell dimensions	a = 6.1779(13) Å α = 82.63(2)°
	b = 6.187(2) Å β = 83.92(2)°
	c = 13.404(3) Å γ = 68.23(2)°
Volume, Z	471.0(2) $Å^3$, 1
Density (calculated)	1.454 Mg/m^3
Absorption coefficient	0.919 mm^{-1}
F(000)	216
Crystal size	0.52 x 0.14 x 0.08 mm
Crystal color	pale yellow
Theta range for data collection	3.33 to 57.10°
Scan type	θ–2θ
Limiting indices	0<=h<=6, -5<=k<=6, -13<=l<=14
Reflections collected	1240
Independent reflections	1240 [R(int) = 0.0000]
Absorption correction	XABS2
Max. and min. transmission	0.94 and 0.89
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1239 / 3 / 288
Goodness-of-fit on F^2	1.042
Final R indices [I>2σ(I)]	R1 = 0.0860, wR2 = 0.2423
R indices (all data)	R1 = 0.0981, wR2 = 0.2761
Absolute structure parameter	-0.2(9)
Extinction coefficient	none
Largest diff. peak and hole	0.612 and -0.432 $e^- / Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **ASPDKP + BPETE**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

atom	x	y	z	U(eq)
N(1)	17445(16)	19420(16)	9501(7)	38(2)
N(2)	16017(15)	15760(13)	10118(6)	35(2)
O(1)	15022(15)	21652(12)	10694(6)	49(2)
O(2)	18709(14)	13452(13)	9010(6)	48(2)
O(3)	23263(13)	19046(13)	8167(6)	43(2)
O(4)	20707(14)	19099(14)	7114(6)	46(2)
O(5)	13098(21)	15584(20)	13042(10)	102(5)
O(6)	11509(23)	16064(23)	11568(10)	103(5)
C(1)	15717(21)	19881(18)	10256(8)	38(3)
C(2)	14608(19)	18004(17)	10534(8)	33(2)
C(3)	17685(17)	15429(17)	9363(8)	34(3)
C(4)	18389(17	17381(16)	8892(8)	30(2)
C(5)	20988(21)	16660(18)	8630(8)	39(3)
C(6)	21599(20)	18415(20)	7900(9)	39(3)
C(7)	14217(21)	17753(19)	11664(8)	41(3)
C(8)	12841(36)	16387(27)	12166(15)	79(5)
N(3)	9905(19)	12829(18)	12909(11)	57(3)
N(4)	4218(18)	2269(18)	16919(7)	46(3)

C(9)	10577(28)	12114(25)	13775(13)	63(4)
C(10)	9810(27)	10661(25)	14462(11)	65(4)
C(11)	8259(26)	9732(21)	14174(10)	54(3)
C(12)	7563(23)	10424(23)	13224(11)	55(4)
C(13)	8447(23)	11919(23)	12605(11)	56(3)
C(14)	7597(28)	8136(29)	14925(13)	71(4)
C(15)	6306(30)	7094(28)	14872(19)	97(7)
C(16)	5577(22)	5460(24)	15639(11)	57(4)
C(17)	6552(21	4624(26)	16541(13)	67(5)
C(18)	5828(20)	3030(22)	17180(9)	48(3)
C(19)	3345(22)	3073(22)	16047(10)	48(3)
C(20)	3937(23)	4620(27)	15403(10)	57(4)

Table 3. Selected hydrogen bond lengths [Å] and angles [deg] for **ASPDKP + BPETE**

Bond lengths	
N(1)-H(1N)	0.721(137)
H(1N)--O(2)	1.93(12)
N(1)-H(1N)--O2	2.857(12)
N(2)-H(2N)	0.880
H(2N)--O(1)	2.15(14)
N(2)-H(2N)--O(1)	2.829(10)
O(3)-H(3A)	0.840
H(3A)--N(3)	1.876(16)
O(3)-H(3A)--N(3)	2.893(23)
O(6)-H(6)	0.840
H(6)--N(4)	2.085(18)
O(6)-H(6)--N(4)	2.633(27)
C(9)-H(9)	0.950
H(9)--O(5)	2.46(2)
C(9)-H(9)--O(5)	3.103(18)
C(19)-H(19)	0.950
H(19)--O(4)	2.91(6)
C(19)-H(19)--O(4)	3.511(15)
Bond angles	
N(1)-H(1N)-O(2)	165.89(63)
N(2)-H(2N)-O(1)	166.97(32)
O(3)-H(3A)-N(3)	162.15(32)
O(6)-H(6)-N(4)	143.29(47)
C(9)-H(9)-O(2)	125.22(53)
C(19)-H(19)-O(4)	116.14(26)

Table 4. Bond lengths [Å] and angles [deg] for **ASPDKP + BPETE.**

Bond lengths	
N(1)-C(1)	1.37(2)
N(1)-C(4)	1.488(14)
N(2)-C(3)	1.343(14)
N(2)-C(2)	1.481(13)
O(1)-C(1)	1.221(13)
O(2)-C(3)	1.278(13)
O(3)-C(6)	1.323(14)
O(4)-C(6)	1.196(14)
O(5)-C(8)	1.22(2)
O(6)-C(8)	1.29(3)
C(1)-C(2)	1.543(13)

C(2)-C(7)	1.51(2)
C(3)-C(4)	1.478(14)
C(4)-C(5)	1.51(2)
C(5)-C(6)	1.49(2)
C(7)-C(8)	1.47(2)
N(3)-C(9)	1.24(2)
N(3)-C(13)	1.34(2)
N(4)-C(19)	1.30(2)
N(4)-C(18)	1.34(2)
C(9)-C(10)	1.38(2)
C(10)-C(11)	1.39(2)
C(11)-C(12)	1.35(2)
C(11)-C(14)	1.45(2)
C(12)-C(13)	1.39(2)
C(14)-C(15)	1.21(2)
C(15)-C(16)	1.50(2)
C(16)-C(17)	1.36(2)
C(16)-C(20)	1.38(2)
C(17)-C(18)	1.39(2)
C(19)-C(20)	1.33(2)
Bond angles	
C(1)-N(1)-C(4)	129.3(9)
C(3)-N(2)-C(2)	126.7(8)
O(1)-C(1)-N(1)	124.2(9)
O(1)-C(1)-C(2)	120.2(10)
N(1)-C(1)-C(2)	115.6(10)
N(2)-C(2)-C(7)	112.9(8)
N(2)-C(2)-C(1)	112.6(9)
C(7)-C(2)-C(1)	107.6(8)
O(2)-C(3)-N(2)	122.4(9)
O(2)-C(3)-C(4)	116.9(10)
N(2)-C(3)-C(4)	120.7(9)
C(3)-C(4)-N(1)	111.3(9)
C(3)-C(4)-C(5)	113.3(8)
N(1)-C(4)-C(5)	113.1(8)
C(6)-C(5)-C(4)	112.8(9)
O(4)-C(6)-O(3)	123.2(10)
O(4)-C(6)-C(5)	121.6(10)
O(3)-C(6)-C(5)	115.2(10)
C(8)-C(7)-C(2)	121.3(12)
O(5)-C(8)-O(6)	126(2)
O(5)-C(8)-C(7)	121(2)
O(6)-C(8)-C(7)	113(2)
C(9)-N(3)-C(13)	115.7(12)
C(19)-N(4)-C(18)	117.8(11)
N(3)-C(9)-C(10)	126.0(13)
C(9)-C(10)-C(11)	119.3(12)
C(12)-C(11)-C(10)	115.7(12)
C(12)-C(11)-C(14)	128.0(14)
C(10)-C(11)-C(14)	116.3(13)
C(11)-C(12)-C(13)	119.5(12)
N(3)-C(13)-C(12)	123.5(13)
C(15)-C(14)-C(11)	130(2)
CC(17)-C(16)-C(20)	117.1(13)

C(17)-C(16)-C(15)	124(2)
C(20)-C(16)-C(15)	119(2)
C(16)-C(17)-C(18)	119.4(13)
N(4)-C(18)-C(17)	121.3(11)
N(4)-C(19)-C(20)	124.1(12)
C(19)-C(20)-C(16)	120.3(12)

Table 5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **ASPDKP + BPETE**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U11 + ... + 2hka^*b^*U12]$

atom			U11	U22	U33	U23	U13	U12
N(1)	52(6)	32(5)	43(5)		2(4)		2(5)	-34(5)
N(2)	49(5)	26(5)	41(5)		-7(4)		-2(5)	-26(4)
O(1)	83(6)	25(4)	52(5)		-23(4)		26(4)	-37(4)
O(2)	59(5)	42(5)	54(5)		-4(4)		-9(4)	-31(4)
O(3)	41(4)	49(5)	52(5)		2(4)		-9(4)	-32(4)
O(4)	50(5)	59(5)	35(5)		11(4)		-11(4)	-29(4)
O(5)	92(9)	70(7)	108(10)		42(7)		30(7)	-15(6)
O(6)	15(10)	109(10)	122(10)		-77(8)		79(8)	-84(8)
C(1)	64(8)	34(7)	31(6)		2(5)		-7(6)	-36(6)
C(2)	51(6)	24(5)	40(6)		-14(4)		2(5)	-30(5)
C(3)	36(6)	22(6)	44(6)		-1(5)		-7(5)	-12(4)
C(4)	41(6)	21(5)	41(6)		-8(4)		-7(5)	-22(4)
C(5)	56(7)	33(6)	38(6)		-2(4)		-2(5)	-29(5)
C(6)	43(6)	40(7)	44(7)		-4(5)		-5(5)	-24(5)
C(7)	45(6)	38(6)	37(6)		10(5)		3(5)	-18(5)
C(8)	106(14)	44(9)	89(13)		-25(9)		34(11)	-33(9)
N(3)	47(6)	38(6)	96(9)		-15(6)		13(6)	-29(5)
N(4)	50(6)	49(6)	43(6)		-6(5)		-3(5)	-22(5)
C(9)	62(8)	51(9)	87(12)		-23(8)		1(8)	-30(7)
C(10)	77(9)	68(9)	53(8)		-12(7)		-36(7)	-19(8)
C(11)	73(9)	33(7)	55(8)		-11(6)		5(7)	-20(6)
C(12)	48(7)	47(7)	81(10)		-13(7)		-1(7)	-30(6)
C(13)	53(8)	53(8)	59(8)		-7(6)		-1(6)	-17(6)
C(14)	61(9)	73(11)	80(11)		3(9)		-7(8)	-27(9)
C(15)	60(10)	46(10)	169(20)		-14(10)		20(12)	-8(8)
C(16)	40(7)	57(8)	59(8)		7(7)		-4(6)	-4(6)
C(17)	29(6)	63(9)	115(14)		-32(9)		3(8)	-19(6)
C(18)	40(6)	59(8)	42(7)		-6(6)		-21(6)	-9(6)
C(19)	49(7)	54(8)	46(7)		-8(6)		-21(6)	-19(6)
C(20)	47(7)	79(10)	49(8)		-7(7)		-7(6)	-26(7)

Table 6. Hydrogen atom coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for **ASPDKP + BPETE.**

atom	x	y	z	U(eq)
H(1N)	17983(237)	20287(235)	9408(97)	46
H(2N)	15731(15)	14517(13)	10395(6)	42
H(3A)	23835(178)	19631(239)	7656(18)	65
H(6)	11013(361)	15020(317)	11839(82)	155
H(2)	13047(19)	18602(17)	10241(8)	40
H(4)	17622(17)	17909(16)	8238(8)	37
H(5A)	21799(21)	16436(18)	9255(8)	47
H(5B)	21556(21)	15143(18)	8336(8)	47
H(7A)	15777(21)	17075(19)	11943(8)	49
H(7B)	13473(21)	19352(19)	11879(8)	49

H(9)	11724(28)	12619(25)	13981(13)	76
H(10)	10332(27)	10294(25)	15126(11)	78
H(12)	6476(23)	9890(23)	12982(11)	66
H(13)	7999(23)	12320(23)	11929(11)	67
H(14)	8282(28)	7873(29)	15553(13)	86
H(15)	5642(30)	7353(28)	14240(19)	116
H(17)	7714(21)	5126(26)	16732(13)	80
H(18)	6488(20)	2469(22)	17814(9)	58
H(19)	2217(22)	2524(22)	15857(10)	58
H(20)	3224(23)	5146(27)	14779(10)	69

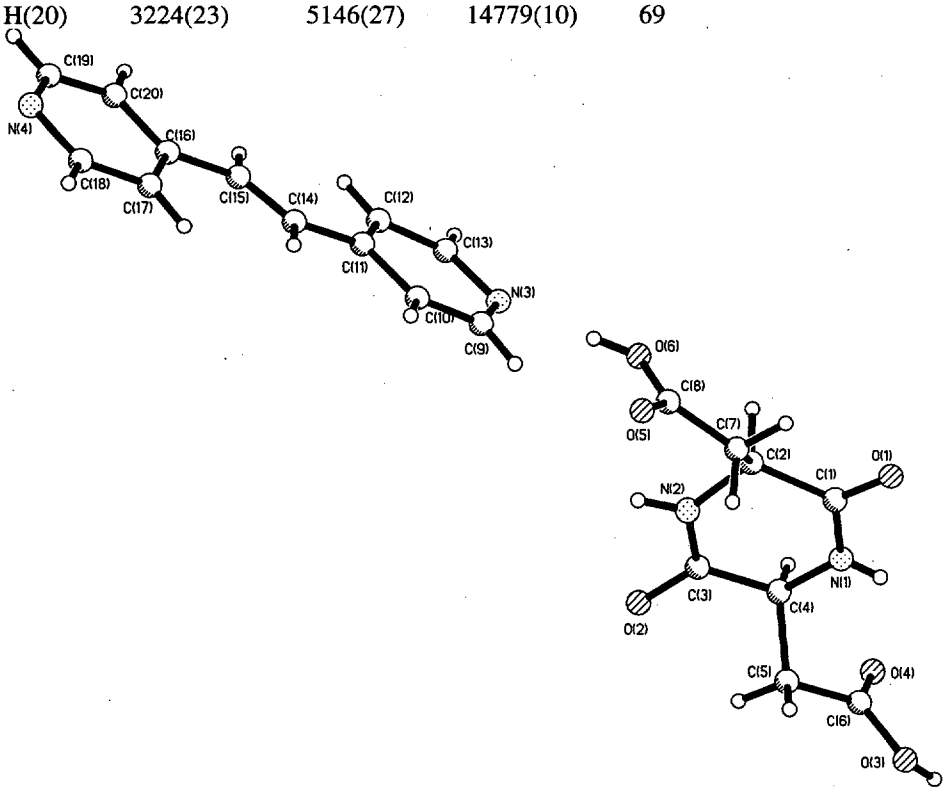

Figure 1. 50% probability displacement ellipsoids of **ASPDKP + BPETE.**

Table 1. Crystal data and structure refinement for **ASPDKP + BPACE.**

Identification code	ASPDKP + BPACE
Empirical formula	$C_{26}H_{22}N_4O_{10}$
Formula weight	550.48
Temperature	130(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	C2
Unit cell dimensions	a = 28.616(5) Å α = 9 ° b = 14.284(2) Å β = 90.762(14)° c = 6.0426(11) Å γ = 90°
Volume, Z	2469.7(7) $Å^3$, 4
Density (calculated)	1.480 Mg/m^3
Absorption coefficient	0.985 mm^{-1}
F(000)	1144
Crystal size	0.60 x 0.04 x 0.02 mm
Crystal color	colorless
Theta range for data collection	3.09 to 56.44°
Scan type	ω–2θ
Limiting indices	-30<=h<=30, -3<=k<=15, 0<=l<=6
Reflections collected	1727
Independent reflections	1727 [R(int) = 0.0000]
Absorption correction	none
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1727 / 1 / 373
Goodness-of-fit on F^2	1.194
Final R indices [I>2σ(I)]	R1 = 0.0505, wR2 = 0.1239
R indices (all data)	R1 = 0.0513, wR2 = 0.1253
Absolute structure parameter	0.2(3)
Extinction coefficient	none
Largest diff. peak and hole	0.364and -0.490 e^- / $Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **ASPDKP + BPACE.** U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

atom	x	y	z	U(eq)
N(1)	7143(4)	5533(2)	5673(4)	42(1)
N(1)	182(1)	6776(3)	-2911(5)	23(1)
O(1)	-530(1)	6634(2)	-1417(4)	28(1)
C(1)	-275(1)	6748(3)	-3033(6)	22(1)
O(2)	1540(1)	5853(2)	-1948(5)	35(1)
C(2)	513(1)	6892(3)	-4720(6)	22(1)
N(2)	4821(1)	4554(3)	7907(5)	24(1)
O(3)	1300(1)	7336(2)	-2030(5)	32(1)
C(3)	925(1)	6220(3)	-4423(6)	22(1)
N(3)	2871(1)	3973(3)	3506(5)	26(1)
C(4)	1269(1)	6542(3)	-2661(6)	21(1)
O(4)	5538(1)	4489(3)	6434(4)	34(1)
N(4)	2221(1)	6348(3)	905(6)	28(1)
O(5)	3639(1)	5114(2)	7176(5)	37(1)
C(5)	5283(1)	4556(3)	8040(6)	24(1)
O(6)	3577(1)	3587(2)	6433(4)	32(1)
C(6)	4487(1)	4686(3)	9684(6)	23(1)
C(7)	4078(1)	4021(3)	9401(6)	23(1)
O(7)	1452(1)	3583(2)	-1417(4)	30(1)

C(8)	3746(1)	4313(3)	7558(6)	21(1)
O(8)	1187(1)	4306(2)	1640(4)	26(1)
C(9)	2804(1)	3615(3)	1477(6)	25(1)
O(9)	3490(1)	7263(2)	6389(4)	31(1)
C(10)	2369(1)	3609(3)	432(6)	22(1)
O(10)	3855(1)	6646(2)	3433(4)	27(1)
C(11)	1989(1)	3963(3)	1525(6)	22(1)
C(12)	2052(1)	4336(3)	3628(6)	28(1)
C(13)	2498(2)	4326(3)	4517(6)	30(1)
C(14)	1518(1)	3927(3)	387(6)	23(1)
C(15)	719(1)	4294(4)	687(7)	32(1)
C(16)	397(1)	4289(3)	2519(7)	29(1)
C(17)	144(1)	4277(3)	4094(7)	27(1)
C(18)	2210(1)	6742(3)	2912(7)	28(1)
C(19)	2615(1)	6906(3)	4181(6)	24(1)
C(20)	3040(1)	6669(3)	3309(6)	20(1)
C(21)	3059(1)	6258(3)	1221(6)	25(1)
C(22)	2637(1)	6112(3)	107(6)	26(1)
C(23)	3483(1)	6888(3)	4597(6)	24(1)
C(24)	4300(1)	6906(4)	4376(7)	36(1)
C(25)	4622(2)	6956(3)	2551(8)	34(1)
C(26)	4865(1)	6986(3)	928(8)	32(1)

Table 3. Selected hydrogen bond lengths [Å] and angles [deg] for **ASPDKP + BPACE.**

Bond lengths	
N(1)-H(1N)	0.874
H(1N)--O(1)	1.923(43)
N(1)-H(1N)--O(1)	2.789(3)
N(2)-H(2N)	0.876
H(2N)--O(4)	1.927(45)
N(2)-H(2N)--O(4)	2.803(3)
O(2)-H(2O)	0.968
H(2O)--N(4)	1.743
O(2)-H(2O)--N(4)	2.677
O(6)-H(6O)	0.971
H(6O)--N(3)	1.833
O(6)-H(6O)--N(3)	2.783
Bond angles	
N(1)-H(1N)-O(1)	173.53(4.05)
N(2)-H(2N)-O(4)	176.65(4.53)
O(2)-H(2O)-N(4)	162.2
O(6)-H(6O)-N(3)	151.3

Table 4. Bond lengths [Å] and angles [deg] for **ASPDKP + BPACE.**

Bond lengths	
N(1)-C(1)	1.311(5)
N(1)-C(2)	1.465(5)
O(1)-C(1)	1.237(4)
O(2)-C(4)	1.323(5)
C(2)-C(3)	1.528(6)
N(2)-C(5)	1.324(5)
N(2)-C(6)	1.460(5)
O(3)-C(4)	1.200(5)
C(3)-C(4)	1.512(5)

N(3)-C(9)	1.340(5)
N(3)-C(13)	1.335(6)
O(4)-C(5)	1.225(4)
N(4)-C(18)	1.338(6)
N(4)-C(22)	1.335(6)
O(5)-C(8)	1.206(6)
C(6)-C(8)	1.327(5)
C(6)-C(7)	1.515(6)
C(7)-C(8)	1.512(5)
O(7)-C(14)	1.209(5)
O(8)-C(14)	1.336(5)
O(8)-C(15)	1.450(5)
C(9)-C(10)	1.389(6)
O(9)-C(23)	1.208(5)
C(10)-C(11)	1.376(5)
O(10)-C(23)	1.329(5)
O(10)-C(24)	1.437(5)
C(11)-C(12)	1.387(5)
C(11)-C(14)	1.505(5)
C(12)-C(13)	1.379(6)
C(15)-C(16)	1.449(6)
C(16)-C(17)	1.204(6)
C(18)-C(19)	1.401(6)
C(19)-C(20)	1.375(6)
C(20)-C(21)	1.393(6)
C(20)-C(23)	1.512(5)
C(21)-C(22)	1.389(6)
C(24)-C(25)	1.447(6)
C(25)-C(26)	1.211(6)

Bond angles	
C(1)-N(1)-C(2)	128.1(3)
O(1)-C(1)-N(1)	123.9(3)
N(1)-C(2)-C(3)	110.2(3)
C(5)-N(2)-C(6)	128.2(3)
C(4)-C(3)-C(2)	112.6(3)
C(9)-N(3)-C(13)	117.2(3)
O(3)-C(4)-O(2)	124.0(4)
O(3)-C(4)-C(3)	123.8(4)
O(2)-C(4)-C(3)	112.2(4)
C(18)-N(4)-C(22)	117.7(3)
O(4)-C(5)-N(2)	123.8(4)
N(2)-C(6)-C(7)	110.4(3)
C(8)-C(7)-C(6)	112.8(4)
O(5)-C(8)-O(6)	123.6(4)
O(5)-C(8)-C(7)	123.9(4)
O(6)-C(8)-C(7)	112.5(4)
C(14)-O(8)-C(15)	115.4(3)
N(3)-C(9)-C(10)	122.3(4)
C(11)-C(10)-C(9)	119.3(3)
C(23)-O(10)-C(24)	115.8(3)
C(10)-C(11)-C(12)	119.1(4)
C(10)-C(11)-C(14)	118.4(3)
C(12)-C(11)-C(14)	122.4(3)
C(11)-C(12)-C(13)	117.5(4)

N(3)-C(13)-C(12)	124.5(4)
O(7)-C(14)-O(8)	124.9(3)
O(7)-C(14)-C(11)	123.6(3)
O(8)-C(14)-C(11)	111.4(3)
C(16)-C(15)-O(8)	106.8(3)
C(17)-C(16)-C(15)	177.5(4)
N(4)-C(18)-C(19)	122.5(4)
C(20)-C(19)-C(18)	118.6(4)
C(21)-C(20)-C(19)	119.7(4)
C(21)-C(20)-C(23)	120.8(3)
C(19)-C(20)-C(23)	119.5(3)
C(20)-C(21)-C(22)	117.3(4)
N(4)-C(22)-C(21)	124.1(4)
O(9)-C(23)-O(10)	125.9(3)
O(9)-C(23)-C(20)	123.8(3)
O(10)-C(23)-C(20)	110.3(3)
O(10)-C(24)-C(25)	106.2(3)
C(26)-C(25)-C(24)	175.5(4)

Table 5. Anisotropic displacement parameters ($Å^2 \times 10^3$) for **ASPDKP + BPACE.** The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U11 + ... + 2hka^*b^*U12]$

atom			U11	U22	U33	U23	U13	U12
N(1)	30(2)	31(2)	9(2)		0(2)		-5(1)	0(2)
O(1)	31(1)	39(2)	13(1)		-2(1)		-2(1)	3(1)
C(1)	32(2)	21(2)	12(2)		-2(2)		-2(2)	3(2)
O(2)	46(2)	22(2)	38(2)		-1(1)		-23(1)	5(1)
C(2)	32(2)	21(2)	13(2)		1(2)		-1(2)	-5(2)
N(2)	32(2)	34(2)	7(2)		-2(2)		-5(2)	-1(2)
O(3)	43(2)	26(2)	27(2)		-6(1)		-13(1)	-1(1)
C(3)	29(2)	24(2)	13(2)		-4(2)		-5(2)	-2(2)
N(3)	40(2)	18(2)	21(2)		2(2)		-10(1)	-5(2)
C(4)	27(2)	22(3)	14(2)		-5(2)		-1(2)	-5(2)
O(4)	33(2)	58(2)	11(1)		2(2)		-2(1)	3(2)
N(4)	41(2)	16(2)	26(2)		6(2)		-11(1)	-4(2)
O(5)	58(2)	28(2)	25(2)		-5(1)		-19(2)	11(2)
C(5)	32(2)	26(2)	15(2)		0(2)		-3(2)	5(2)
O(6)	52(2)	22(2)	23(2)		2(1)		-19(1)	-10(2)
C(6)	31(2)	23(2)	14(2)		0(2)		-4(2)	0(2)
C(7)	31(2)	27(2)	12(2)		3(2)		-5(2)	0(2)
O(7)	38(2)	28(2)	23(2)		-7(1)		-7(1)	2(1)
C(8)	29(2)	25(3)	9(2)		5(2)		-5(1)	3(2)
O(8)	30(1)	26(2)	23(1)		-2(1)		-2(1)	2(1)
C(9)	35(2)	17(2)	22(2)		2(2)		-4(2)	-2(2)
O(9)	49(2)	25(2)	18(2)		-7(1)		-10(1)	3(1)
C(10)	34(2)	13(2)	17(2)		-3(2)		-4(2)	0(2)
O(10)	29(1)	26(2)	26(1)		-6(1)		-7(1)	1(1)
C(11)	34(2)	16(2)	15(2)		0(2)		-4(2)	-3(2)
C(12)	48(2)	20(2)	15(2)		-3(2)		-5(2)	0(2)
C(13)	53(2)	20(2)	18(2)		-2(2)		-12(2)	-6(2)
C(14)	33(2)	17(2)	18(2)		-3(2)		-2(2)	-2(2)
C(15)	31(2)	38(3)	26(2)		-2(2)		-8(2)	2(2)
C(16)	31(2)	19(2)	36(2)		-5(2)		-6(2)	-2(2)
C(17)	29(2)	20(2)	33(2)		-3(2)		-7(2)	0(2)
C(18)	36(2)	17(2)	30(2)		7(2)		-1(2)	-2(2)

C(19)	40(2)	16(2)	15(2)	4(2)	-5(2)	-1(2)
C(20)	37(2)	13(2)	11(2)	1(2)	-8(2)	-1(2)
C(21)	34(2)	20(2)	22(2)	-2(2)	-4(2)	1(2)
C(22)	45(2)	18(2)	14(2)	1(2)	-11(2)	-2(2)
C(23)	37(2)	15(2)	20(2)	3(2)	-9(2)	1(2)
C(24)	36(2)	35(3)	38(3)	-8(2)	-11(2)	-3(2)
C(25)	34(2)	20(2)	49(3)	-6(2)	-17(2)	2(2)
C(26)	31(2)	17(2)	47(3)	2(2)	-11(2)	1(2)

Table 6. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for **ASPDKP + BPACE.**

atom	x	y	z	U(eq)
H(1N)	8518(54)	5862(31)	6061(53)	51
H(1N)	317(15)	6754(39)	-1716(79)	28
H(2O)	1736(17)	6104(46)	-814(96)	53
H(2)	637(1)	7547(3)	-4660(6)	26
H(2N)	4693(15)	4552(37)	6584(83)	29
H(3A)	804(1)	5594(3)	-4019(6)	26
H(3B)	1089(1)	6159(3)	-5848(6)	26
H(6O)	3365(17)	3902(47)	5451(85)	48
H(6)	4365(1)	5341(3)	9590(6)	27
H(7A)	4198(1)	3386(3)	9084(6)	28
H(7B)	3904(1)	3991(3)	10805(6)	28
H(9)	3063(1)	3356(3)	726(6)	30
H(10)	2334(1)	3363(3)	-1022(6)	26
H(12)	1797(1)	4587(3)	4426(6)	34
H(13)	2543(2)	4589(3)	5948(6)	36
H(15A)	667(1)	4854(4)	-249(7)	38
H(15B)	673(1)	3729(4)	-239(7)	38
H(18)	1916(1)	6917(3)	3499(7)	33
H(19)	2596(1)	7175(3)	5615(6)	29
H(21)	3348(1)	6086(3)	584(6)	30
H(22)	2646(1)	5825(3)	-1311(6)	31
H(24A)	4406(1)	6433(4)	5470(7)	44
H(24B)	4278(1)	7521(4)	5126(7)	44

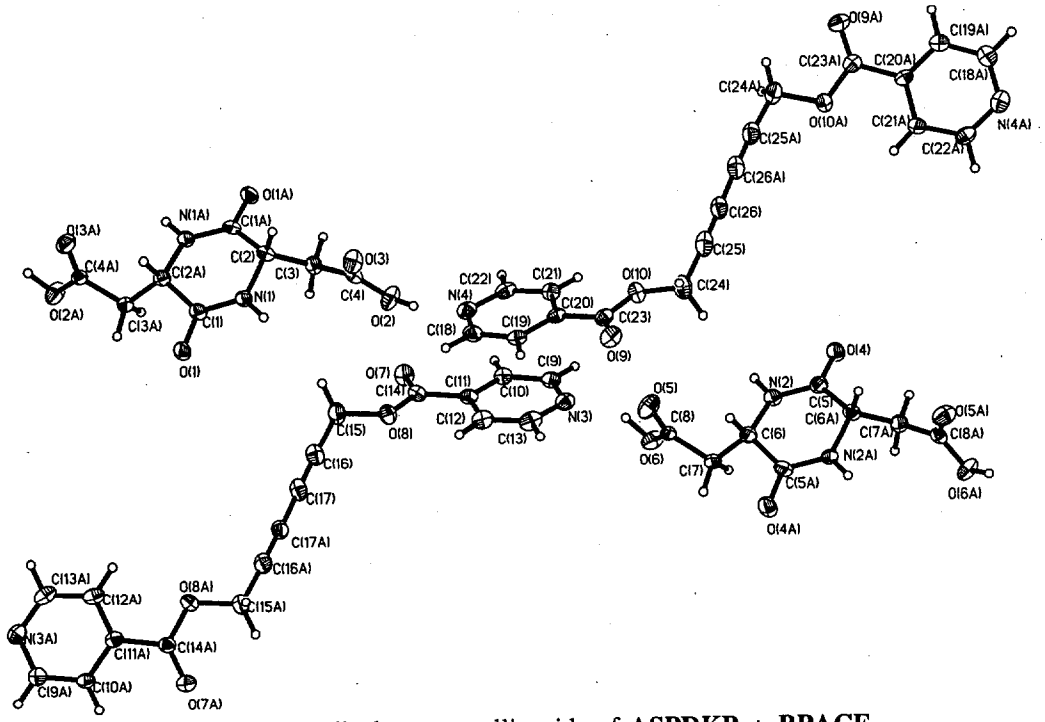

Figure 1. 50% probability displacement ellipsoids of **ASPDKP + BPACE.**

Table 1. Crystal data and structure refinement for **ASPDKP + BPETA.**

Identification code	ASPDKP + BPETA
Empirical formula	$C_{20}H_{22}N_4O_7$
Formula weight	430.42
Temperature	130(2) K
Wavelength	1.54178 Å
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 4.9130(10) Å α = 90°
	b = 10.636(2) Å β = 90°
	c = 37.446(8) Å γ = 90°
Volume, Z	1956.7(7) $Å^3$, 4
Density (calculated)	1.461 Mg/m^3
Absorption coefficient	0.947 mm^{-1}
F(000)	904
Crystal size	0.14 x 0.05 x 0.02 mm
Crystal color	colorless
Theta range for data collection	5.15 to 60.20°
Scan type	θ–2θ
Limiting indices	0<=h<=5, 0<=k<=11, 0<=l<=40
Reflections collected	1558
Independent reflections	1558 [R(int) = 0.0000]
Absorption correction	XABS2
Max. and min. transmission	0.99 and 0.96
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1557 / 0 / 292
Goodness-of-fit on F^2	1.066
Final R indices [I>2σ(I)]	R1 = 0.0582, wR2 = 0.1587
R indices (all data)	R1 = 0.0640, wR2 = 0.1698
Absolute structure parameter	0.3(7)
Extinction coefficient	none
Largest diff. peak and hole	0.275 and -0.389 e^- / $Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **ASPDKP + BPETA.** U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

atom	x	y	z	U(eq)
N(1)	7143(4)	5533(2)	5673(4)	42(1)
N(1)	7319(10)	4357(5)	8507(1)	27(1)
O(1)	8166(8)	6046(4)	8855(1)	30(1)
C(1)	6756(13)	5136(6)	8780(1)	27(1)
N(2)	3309(12)	3556(5)	8943(1)	35(1)
O(2)	7036(11)	5256(7)	9871(1)	73(2)
C(2)	4153(12)	4864(6)	8980(1)	27(1)
O(3)	8119(10)	3877(4)	9443(1)	45(1)
C(3)	4333(12)	5269(6)	9367(1)	28(1)
N(3)	21299(10)	7360(5)	12260(1)	30(1)
O(4)	2750(13)	1789(5)	8618(1)	61(2)
C(4)	6700(14)	4750(7)	9573(2)	38(2)
N(4)	10969(12)	5223(5)	10316(1)	36(1)
O(5)	10021(10)	1919(4)	7701(1)	38(1)
C(5)	3740(15)	2854(6)	8656(1)	37(2)
O(6)	9681(9)	3945(4)	7856(1)	34(1)
C(6)	5489(13)	3406(5)	8366(1)	29(1)
C(7)	7071(14)	2392(6)	8172(1)	35(2)

O(7)	2114(11)	2561(5)	9758(1)	62(2)
C(8)	9056(13)	2836(6)	7894(1)	30(1)
C(9)	20665(13)	6149(6)	12207(1)	29(1)
C(10)	18701(13)	5778(6)	11968(1)	32(2)
C(11)	17338(12)	6671(6)	11766(1)	27(1)
C(12)	18003(14)	7925(6)	11828(1)	32(2)
C(13)	19954(14)	8226(6)	12077(1)	34(2)
C(14)	15330(13)	6290(6)	11484(1)	28(1)
C(15)	16767(13)	6179(6)	11117(1)	30(1)
C(16)	14784(12)	5859(6)	10827(1)	27(1)
C(17)	13829(13)	4621(6)	10792(1)	34(2)
C(18)	11890(16)	4348(6)	10533(2)	37(2)
C(19)	11889(14)	6402(6)	10343(1)	31(2)
C(20)	13804(13)	6733(6)	10594(1)	30(1)

Table 3. Selected hydrogen bond lengths [Å] and angles [deg] for **ASPDKP + BPETA**

Bond lengths	
N(1)-H(1N)	0.890
H(1N)--O(6)	2.088
N(1)-H(1N)--O(6)	2.732
N(2)-H(2N)	0.872
H(2N)--O(3)	2.476
N(2)-H(2N)--O(3)	3.191
N(4)-H(4N)	0.918
H(4N)--O(2)	1.696
N(4)-H(4N--O(2)	2.547
O(5)-H(5O)	1.048
H(5O)--N(3)	1.556
O(5)-H(5O)--N(3)	2.569
Bond angles	
N(1)-H(1N)-O(6)	128.5
N(2)-H(2N)-O(3)	139.7
N(4)-H(4N)-O(2)	152.7
O(5)-H(5O)-N(3)	160.6

Table 4. Bond lengths [Å] and angles [deg] for **ASPDKP + BPETA**

Bond lengths	
N(1)-C(1)	1.343(7)
N(1)-C(6)	1.453(8)
O(1)-C(1)	1.223(7)
C(1)-C(2)	1.510(8)
N(2)-C(5)	1.326(7)
N(2)-C(2)	1.459(8)
O(2)-C(4)	1.252(8)
C(2)-C(3)	1.515(7)
O(3)-C(4)	1.258(8)
C(3)-C(4)	1.500(9)
N(3)-C(13)	1.325(8)
N(3)-C(9)	1.340(8)
O(4)-C(5)	1.242(8)
N(4)-C(18)	1.317(8)
N(4)-C(19)	1.337(8)
O(5)-C(8)	1.304(7)
C(5)-C(6)	1.504(8)