Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information for

Three modes of reactivity for anhydrous TEMPO-H: Reactions of a good hydrogen atom donor with low valent carbon centres

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Table 1. Crystal data and structure refinement for anhydrous TEMPO-H.

Identification code	ng033	
Empirical formula	C9 H19 N O	
Formula weight	157.25	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	trigonal	
Space group	*R*-3	
Unit cell dimensions	*a* = 18.7761(16) Å	α= 90°
	b = 18.7761(16) Å	β= 90°
	c = 43.329(4) Å	γ = 120°
Volume	13229(2) $Å^3$	
Z	54	
Density (calculated)	1.066 Mg/m^3	
Absorption coefficient	0.068 mm^{-1}	
F(000)	4752	
Crystal size	.3112 x .2925 x .2716 mm^3	
Theta range for data collection	2.17 to 25.00°	
Index ranges	-22<=h<=22, -21<=k<=21, -51<=l<=38	
Reflections collected	21413	
Independent reflections	5195 [R(int) = 0.0471]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7459 and 0.6486	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5195 / 0 / 322	
Goodness-of-fit on F^2	1.096	
Final R indices [I>2sigma(I)]	R1 = 0.0420, wR2 = 0.0861	
R indices (all data)	R1 = 0.0781, wR2 = 0.0993	
Largest diff. peak and hole	0.200 and -0.199 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for anhydrous TEMPO-H. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4387(1)	8877(1)	518(1)	21(1)
C(2)	4432(1)	8083(1)	514(1)	24(1)
C(3)	4882(1)	8002(1)	792(1)	26(1)
C(4)	4459(1)	8043(1)	1085(1)	25(1)
C(5)	4409(1)	8832(1)	1112(1)	21(1)
C(6)	5231(1)	9632(1)	444(1)	26(1)
C(7)	3774(1)	8818(1)	271(1)	30(1)
C(8)	5257(1)	9575(1)	1191(1)	27(1)
C(9)	3813(1)	8724(1)	1373(1)	31(1)
C(10)	1362(1)	9237(1)	560(1)	23(1)
C(11)	476(1)	9067(1)	593(1)	26(1)
C(12)	39(1)	8573(1)	879(1)	28(1)
C(13)	540(1)	9014(1)	1163(1)	27(1)
C(14)	1427(1)	9174(1)	1151(1)	24(1)
C(15)	1789(1)	9881(1)	308(1)	33(1)
C(16)	1379(1)	8456(1)	465(1)	32(1)
C(17)	1449(1)	8374(1)	1196(1)	31(1)
C(18)	1915(1)	9756(1)	1413(1)	33(1)
C(19)	4438(1)	1976(1)	539(1)	27(1)
C(20)	3770(1)	2218(1)	547(1)	34(1)
C(21)	3830(1)	2719(1)	831(1)	40(1)
C(22)	3786(1)	2241(1)	1122(1)	35(1)
C(23)	4455(1)	1999(1)	1131(1)	27(1)
C(24)	5289(1)	2725(1)	470(1)	37(1)
C(25)	4240(1)	1338(1)	286(1)	34(1)
C(26)	5311(1)	2753(1)	1191(1)	37(1)
C(27)	4270(1)	1380(1)	1391(1)	38(1)
N(1)	4021(1)	8895(1)	821(1)	19(1)
N(2)	1783(1)	9628(1)	856(1)	22(1)
N(3)	4371(1)	1547(1)	837(1)	22(1)
O(1)	4010(1)	9661(1)	836(1)	26(1)

O(2)	2627(1)	9781(1)	835(1)	27(1)
O(3)	5027(1)	1344(1)	837(1)	26(1)

Table 3. Bond lengths [Å] and angles [°] for anhydrous TEMPO-H.

C(1)-N(1)	1.4884(19)
C(1)-C(7)	1.534(2)
C(1)-C(2)	1.536(2)
C(1)-C(6)	1.542(2)
C(2)-C(3)	1.520(2)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-C(4)	1.520(2)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.535(2)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-N(1)	1.4932(19)
C(5)-C(9)	1.529(2)
C(5)-C(8)	1.541(2)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-N(2)	1.4935(19)
C(10)-C(15)	1.528(2)
C(10)-C(11)	1.536(2)
C(10)-C(16)	1.538(2)
C(11)-C(12)	1.521(2)
C(11)-H(11A)	0.9900

C(11)-H(11B)	0.9900
C(12)-C(13)	1.519(2)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.538(2)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-N(2)	1.4957(19)
C(14)-C(18)	1.525(2)
C(14)-C(17)	1.536(2)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-N(3)	1.494(2)
C(19)-C(25)	1.526(2)
C(19)-C(20)	1.534(2)
C(19)-C(24)	1.541(2)
C(20)-C(21)	1.517(2)
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.525(3)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(23)	1.536(2)
C(22)-H(22A)	0.9900
C(22)-H(22B)	0.9900
C(23)-N(3)	1.494(2)

C(23)-C(27)	1.530(2)
C(23)-C(26)	1.542(2)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
N(1)-O(1)	1.4503(16)
N(2)-O(2)	1.4653(16)
N(3)-O(3)	1.4602(15)
O(1)-H(1)	0.89(2)
O(2)-H(2)	0.89(2)
O(3)-H(3)	0.94(2)

N(1)-C(1)-C(7)	106.14(12)
N(1)-C(1)-C(2)	106.37(12)
C(7)-C(1)-C(2)	109.04(13)
N(1)-C(1)-C(6)	115.89(13)
C(7)-C(1)-C(6)	108.06(13)
C(2)-C(1)-C(6)	111.08(13)
C(3)-C(2)-C(1)	112.98(13)
C(3)-C(2)-H(2A)	109.0
C(1)-C(2)-H(2A)	109.0
C(3)-C(2)-H(2B)	109.0
C(1)-C(2)-H(2B)	109.0
H(2A)-C(2)-H(2B)	107.8
C(2)-C(3)-C(4)	109.08(13)
C(2)-C(3)-H(3A)	109.9
C(4)-C(3)-H(3A)	109.9

C(2)-C(3)-H(3B)	109.9
C(4)-C(3)-H(3B)	109.9
H(3A)-C(3)-H(3B)	108.3
C(3)-C(4)-C(5)	113.53(13)
C(3)-C(4)-H(4A)	108.9
C(5)-C(4)-H(4A)	108.9
C(3)-C(4)-H(4B)	108.9
C(5)-C(4)-H(4B)	108.9
H(4A)-C(4)-H(4B)	107.7
N(1)-C(5)-C(9)	106.39(12)
N(1)-C(5)-C(4)	106.12(12)
C(9)-C(5)-C(4)	108.83(13)
N(1)-C(5)-C(8)	116.02(13)
C(9)-C(5)-C(8)	108.30(13)
C(4)-C(5)-C(8)	110.92(13)
C(1)-C(6)-H(6A)	109.5
C(1)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(1)-C(7)-H(7A)	109.5
C(1)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(1)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(5)-C(9)-H(9A)	109.5
C(5)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5

C(5)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
N(2)-C(10)-C(15)	106.69(13)
N(2)-C(10)-C(11)	105.96(12)
C(15)-C(10)-C(11)	108.33(13)
N(2)-C(10)-C(16)	116.16(13)
C(15)-C(10)-C(16)	108.15(13)
C(11)-C(10)-C(16)	111.24(13)
C(12)-C(11)-C(10)	113.58(13)
C(12)-C(11)-H(11A)	108.9
C(10)-C(11)-H(11A)	108.9
C(12)-C(11)-H(11B)	108.9
C(10)-C(11)-H(11B)	108.9
H(11A)-C(11)-H(11B)	107.7
C(13)-C(12)-C(11)	109.27(13)
C(13)-C(12)-H(12A)	109.8
C(11)-C(12)-H(12A)	109.8
C(13)-C(12)-H(12B)	109.8
C(11)-C(12)-H(12B)	109.8
H(12A)-C(12)-H(12B)	108.3
C(12)-C(13)-C(14)	113.19(13)
C(12)-C(13)-H(13A)	108.9
C(14)-C(13)-H(13A)	108.9
C(12)-C(13)-H(13B)	108.9
C(14)-C(13)-H(13B)	108.9
H(13A)-C(13)-H(13B)	107.8
N(2)-C(14)-C(18)	106.86(13)
N(2)-C(14)-C(17)	116.30(13)
C(18)-C(14)-C(17)	107.80(13)
N(2)-C(14)-C(13)	105.77(12)
C(18)-C(14)-C(13)	108.61(13)
C(17)-C(14)-C(13)	111.22(13)
C(10)-C(15)-H(15A)	109.5
C(10)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5

C(10)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(10)-C(16)-H(16A)	109.5
C(10)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(10)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(14)-C(17)-H(17A)	109.5
C(14)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(14)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(14)-C(18)-H(18A)	109.5
C(14)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(14)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
N(3)-C(19)-C(25)	106.04(13)
N(3)-C(19)-C(20)	106.14(13)
C(25)-C(19)-C(20)	109.59(14)
N(3)-C(19)-C(24)	115.48(14)
C(25)-C(19)-C(24)	108.14(14)
C(20)-C(19)-C(24)	111.24(13)
C(21)-C(20)-C(19)	112.65(14)
C(21)-C(20)-H(20A)	109.1
C(19)-C(20)-H(20A)	109.1
C(21)-C(20)-H(20B)	109.1
C(19)-C(20)-H(20B)	109.1
H(20A)-C(20)-H(20B)	107.8
C(20)-C(21)-C(22)	109.80(14)
C(20)-C(21)-H(21A)	109.7
C(22)-C(21)-H(21A)	109.7

C(20)-C(21)-H(21B)	109.7
C(22)-C(21)-H(21B)	109.7
H(21A)-C(21)-H(21B)	108.2
C(21)-C(22)-C(23)	112.54(14)
C(21)-C(22)-H(22A)	109.1
C(23)-C(22)-H(22A)	109.1
C(21)-C(22)-H(22B)	109.1
C(23)-C(22)-H(22B)	109.1
H(22A)-C(22)-H(22B)	107.8
N(3)-C(23)-C(27)	106.05(13)
N(3)-C(23)-C(22)	106.04(13)
C(27)-C(23)-C(22)	109.55(14)
N(3)-C(23)-C(26)	115.50(13)
C(27)-C(23)-C(26)	108.10(14)
C(22)-C(23)-C(26)	111.38(14)
C(19)-C(24)-H(24A)	109.5
C(19)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(19)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(19)-C(25)-H(25A)	109.5
C(19)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(19)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
C(23)-C(26)-H(26A)	109.5
C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(23)-C(27)-H(27A)	109.5
C(23)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5

C(23)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
O(1)-N(1)-C(1)	107.44(11)
O(1)-N(1)-C(5)	106.68(11)
C(1)-N(1)-C(5)	119.71(12)
O(2)-N(2)-C(10)	107.16(11)
O(2)-N(2)-C(14)	107.36(11)
C(10)-N(2)-C(14)	118.52(12)
O(3)-N(3)-C(19)	106.67(11)
O(3)-N(3)-C(23)	106.52(11)
C(19)-N(3)-C(23)	118.29(12)
N(1)-O(1)-H(1)	105.8(12)
N(2)-O(2)-H(2)	106.0(13)
N(3)-O(3)-H(3)	103.4(12)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for anhydrous TEMPO-H. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	22(1)	20(1)	20(1)	1(1)	2(1)	9(1)
C(2)	24(1)	20(1)	25(1)	-2(1)	5(1)	9(1)
C(3)	24(1)	20(1)	35(1)	-1(1)	1(1)	12(1)
C(4)	26(1)	23(1)	28(1)	2(1)	-4(1)	12(1)
C(5)	24(1)	20(1)	18(1)	0(1)	-1(1)	10(1)
C(6)	27(1)	24(1)	26(1)	3(1)	6(1)	11(1)
C(7)	31(1)	30(1)	24(1)	3(1)	-3(1)	11(1)
C(8)	28(1)	26(1)	26(1)	-4(1)	-5(1)	12(1)
C(9)	32(1)	33(1)	24(1)	0(1)	3(1)	14(1)
C(10)	23(1)	27(1)	21(1)	-3(1)	-2(1)	13(1)
C(11)	23(1)	26(1)	29(1)	-2(1)	-5(1)	13(1)
C(12)	22(1)	24(1)	38(1)	1(1)	1(1)	12(1)
C(13)	29(1)	26(1)	28(1)	5(1)	8(1)	15(1)
C(14)	26(1)	25(1)	22(1)	1(1)	1(1)	14(1)
C(15)	30(1)	40(1)	24(1)	3(1)	-1(1)	15(1)
C(16)	34(1)	35(1)	33(1)	-8(1)	-2(1)	20(1)
C(17)	34(1)	29(1)	33(1)	4(1)	-3(1)	17(1)
C(18)	38(1)	33(1)	24(1)	0(1)	-2(1)	14(1)
C(19)	23(1)	25(1)	33(1)	9(1)	3(1)	13(1)
C(20)	24(1)	28(1)	50(1)	12(1)	1(1)	13(1)
C(21)	21(1)	23(1)	77(2)	1(1)	2(1)	13(1)
C(22)	20(1)	29(1)	52(1)	-17(1)	0(1)	9(1)
C(23)	22(1)	26(1)	31(1)	-9(1)	-1(1)	10(1)
C(24)	26(1)	33(1)	50(1)	17(1)	7(1)	14(1)
C(25)	32(1)	45(1)	25(1)	4(1)	1(1)	19(1)
C(26)	24(1)	33(1)	51(1)	-16(1)	-5(1)	12(1)
C(27)	35(1)	45(1)	26(1)	-7(1)	-2(1)	14(1)
N(1)	23(1)	15(1)	23(1)	0(1)	1(1)	12(1)
N(2)	17(1)	26(1)	24(1)	0(1)	0(1)	12(1)
N(3)	20(1)	21(1)	27(1)	0(1)	-1(1)	13(1)
O(1)	24(1)	19(1)	41(1)	-1(1)	1(1)	13(1)

O(2)	18(1)	28(1)	38(1)	-1(1)	-1(1)	13(1)
O(3)	23(1)	23(1)	38(1)	-1(1)	0(1)	15(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for anhydrous TEMPO-H.

	x	y	z	U(eq)
H(2A)	3867	7605	509	29
H(2B)	4717	8070	323	29
H(3A)	5462	8453	791	31
H(3B)	4875	7472	783	31
H(4A)	4761	8004	1265	31
H(4B)	3895	7563	1091	31
H(6A)	5215	10136	488	40
H(6B)	5359	9623	225	40
H(6C)	5655	9617	571	40
H(7A)	3226	8359	320	46
H(7B)	3948	8727	69	46
H(7C)	3757	9332	267	46
H(8A)	5673	9583	1052	41
H(8B)	5399	9531	1405	41
H(8C)	5238	10084	1165	41
H(9A)	3801	9236	1400	47
H(9B)	3996	8590	1565	47
H(9C)	3261	8277	1321	47
H(11A)	485	9598	599	31
H(11B)	159	8764	408	31
H(12A)	-515	8512	894	34
H(12B)	-26	8017	866	34
H(13A)	263	8680	1348	32
H(13B)	555	9547	1185	32
H(15A)	1840	10404	374	49
H(15B)	1463	9696	117	49
H(15C)	2337	9958	269	49
H(16A)	1932	8540	497	48
H(16B)	1230	8338	247	48
H(16C)	984	7992	591	48

H(17A)	1023	7938	1069	47
H(17B)	1350	8211	1414	47
H(17C)	1990	8462	1135	47
H(18A)	2464	9815	1423	50
H(18B)	1628	9533	1609	50
H(18C)	1968	10295	1377	50
H(20A)	3818	2542	360	40
H(20B)	3223	1713	544	40
H(21A)	3374	2840	831	48
H(21B)	4356	3248	827	48
H(22A)	3239	1737	1132	42
H(22B)	3844	2581	1305	42
H(24A)	5357	3201	588	55
H(24B)	5333	2851	249	55
H(24C)	5719	2601	529	55
H(25A)	4699	1232	264	51
H(25B)	4155	1546	90	51
H(25C)	3740	826	341	51
H(26A)	5737	2627	1128	56
H(26B)	5371	2889	1411	56
H(26C)	5370	3223	1071	56
H(27A)	3763	866	1343	56
H(27B)	4200	1606	1585	56
H(27C)	4726	1271	1411	56
H(1)	3479(12)	9519(12)	835(4)	54(6)
H(2)	2951(13)	10324(13)	842(5)	69(8)
H(3)	4741(13)	768(14)	837(5)	68(7)

Table 6. Hydrogen bonds for anhydrous TEMPO-H [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(2)	0.89(2)	1.89(2)	2.7172(16)	152.1(17)
O(2)-H(2)...N(3)#1	0.89(2)	2.50(2)	3.2953(17)	149.0(18)
O(3)-H(3)...O(1)#2	0.94(2)	1.83(2)	2.7562(16)	169.2(19)

Symmetry transformations used to generate equivalent atoms:

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

Table 1. Crystal data and structure refinement for $[CHNC_6H_2(CH_3)_3]_2C\cdots HO(NC_5H_6(CH_3)_4)$.

Identification code	ng029	
Empirical formula	$C_{30}\ H_{43}\ N_3\ O$	
Formula weight	461.67	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 10.989(2) Å	α= 90°
	b = 15.262(3) Å	β= 94.250(3)°
	c = 16.648(4) Å	γ = 90°
Volume	2784.5(10) $Å^3$	
Z	4	
Density (calculated)	1.101 Mg/m^3	
Absorption coefficient	0.067 mm^{-1}	
F(000)	1008	
Crystal size	0.232 x 0.189 x 0.177 mm^3	
Theta range for data collection	1.81 to 28.77°	
Index ranges	-14<=h<=13, -20<=k<=20, -20<=l<=22	
Reflections collected	22240	
Independent reflections	6707 [R(int) = 0.0392]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7458 and 0.6662	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6707 / 0 / 311	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.1140	
R indices (all data)	R1 = 0.0695, wR2 = 0.1271	
Largest diff. peak and hole	0.273 and -0.247 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $[CHNC_6H_2(CH_3)_3]_2C\cdots HO(NC_5H_6(CH_3)_4)$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	260(1)	6481(1)	1065(1)	25(1)
N(2)	-167(1)	7837(1)	998(1)	25(1)
N(3)	4883(1)	2364(1)	1290(1)	23(1)
O(1)	3904(1)	2420(1)	1821(1)	28(1)
C(1)	167(1)	7199(1)	1544(1)	23(1)
C(2)	-13(2)	6666(1)	254(1)	34(1)
C(3)	-284(2)	7522(1)	212(1)	33(1)
C(4)	511(1)	5614(1)	1383(1)	23(1)
C(5)	1692(1)	5397(1)	1677(1)	24(1)
C(6)	1887(1)	4563(1)	2002(1)	25(1)
C(7)	948(1)	3958(1)	2040(1)	24(1)
C(8)	-217(1)	4204(1)	1745(1)	26(1)
C(9)	-463(1)	5027(1)	1412(1)	26(1)
C(10)	2726(1)	6043(1)	1676(1)	38(1)
C(11)	1203(1)	3060(1)	2389(1)	32(1)
C(12)	-1736(1)	5276(1)	1105(1)	42(1)
C(13)	-453(1)	8721(1)	1225(1)	24(1)
C(14)	-1555(1)	8872(1)	1565(1)	24(1)
C(15)	-1824(1)	9729(1)	1778(1)	26(1)
C(16)	-1021(1)	10418(1)	1678(1)	30(1)
C(17)	72(1)	10235(1)	1346(1)	31(1)
C(18)	377(1)	9393(1)	1107(1)	28(1)
C(19)	-2408(1)	8134(1)	1738(1)	29(1)
C(20)	-1317(2)	11335(1)	1945(1)	43(1)
C(21)	1575(1)	9222(1)	748(1)	39(1)
C(22)	4719(1)	1529(1)	831(1)	27(1)
C(23)	5704(2)	1499(1)	227(1)	34(1)
C(24)	5708(2)	2312(1)	-303(1)	36(1)
C(25)	5871(1)	3120(1)	231(1)	32(1)
C(26)	4897(1)	3203(1)	834(1)	25(1)

C(27)	3444(2)	1384(1)	411(1)	36(1)
C(28)	4959(2)	788(1)	1447(1)	34(1)
C(29)	3666(1)	3484(1)	411(1)	34(1)
C(30)	5299(1)	3910(1)	1448(1)	32(1)

Table 3. Bond lengths [Å] and angles [°] for $[CHNC_6H_2(CH_3)_3]_2C\cdots HO(NC_5H_6(CH_3)_4)$.

N(1)-C(1)	1.3629(17)
N(1)-C(2)	1.3905(18)
N(1)-C(4)	1.4446(16)
N(2)-C(1)	1.3648(16)
N(2)-C(3)	1.3913(18)
N(2)-C(13)	1.4422(17)
N(3)-O(1)	1.4448(14)
N(3)-C(26)	1.4895(17)
N(3)-C(22)	1.4898(17)
O(1)-H(1)	0.96(2)
C(2)-C(3)	1.340(2)
C(2)-H(2)	0.9500
C(3)-H(3)	0.9500
C(4)-C(5)	1.3923(19)
C(4)-C(9)	1.3987(19)
C(5)-C(6)	1.3926(18)
C(5)-C(10)	1.5048(19)
C(6)-C(7)	1.3908(19)
C(6)-H(6)	0.9500
C(7)-C(8)	1.389(2)
C(7)-C(11)	1.5060(18)
C(8)-C(9)	1.3919(19)
C(8)-H(8)	0.9500
C(9)-C(12)	1.503(2)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(11)-H(11D)	0.9800
C(11)-H(11E)	0.9800
C(11)-H(11F)	0.9800
C(12)-H(12A)	0.9800

C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(14)	1.3926(19)
C(13)-C(18)	1.3963(19)
C(14)-C(15)	1.3925(19)
C(14)-C(19)	1.5068(19)
C(15)-C(16)	1.390(2)
C(15)-H(15)	0.9500
C(16)-C(17)	1.388(2)
C(16)-C(20)	1.512(2)
C(17)-C(18)	1.392(2)
C(17)-H(17)	0.9500
C(18)-C(21)	1.509(2)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-C(23)	1.532(2)
C(22)-C(27)	1.534(2)
C(22)-C(28)	1.5351(19)
C(23)-C(24)	1.523(2)
C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900
C(24)-C(25)	1.523(2)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.524(2)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(30)	1.5293(19)
C(26)-C(29)	1.5388(19)

C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800

C(1)-N(1)-C(2)	112.64(11)
C(1)-N(1)-C(4)	122.89(11)
C(2)-N(1)-C(4)	124.27(11)
C(1)-N(2)-C(3)	112.43(11)
C(1)-N(2)-C(13)	123.10(11)
C(3)-N(2)-C(13)	124.31(11)
O(1)-N(3)-C(26)	107.30(10)
O(1)-N(3)-C(22)	107.30(10)
C(26)-N(3)-C(22)	118.62(10)
N(3)-O(1)-H(1)	103.3(12)
N(1)-C(1)-N(2)	102.23(11)
C(3)-C(2)-N(1)	106.27(12)
C(3)-C(2)-H(2)	126.9
N(1)-C(2)-H(2)	126.9
C(2)-C(3)-N(2)	106.43(12)
C(2)-C(3)-H(3)	126.8
N(2)-C(3)-H(3)	126.8
C(5)-C(4)-C(9)	122.08(12)
C(5)-C(4)-N(1)	119.65(12)
C(9)-C(4)-N(1)	118.22(12)
C(4)-C(5)-C(6)	117.80(12)
C(4)-C(5)-C(10)	121.85(12)
C(6)-C(5)-C(10)	120.32(12)

C(7)-C(6)-C(5)	122.11(12)
C(7)-C(6)-H(6)	118.9
C(5)-C(6)-H(6)	118.9
C(8)-C(7)-C(6)	118.16(12)
C(8)-C(7)-C(11)	121.53(12)
C(6)-C(7)-C(11)	120.30(12)
C(7)-C(8)-C(9)	122.10(13)
C(7)-C(8)-H(8)	119.0
C(9)-C(8)-H(8)	119.0
C(8)-C(9)-C(4)	117.75(12)
C(8)-C(9)-C(12)	120.76(13)
C(4)-C(9)-C(12)	121.49(13)
C(5)-C(10)-H(10A)	109.5
C(5)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(5)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(7)-C(11)-H(11A)	109.5
C(7)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(7)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(7)-C(11)-H(11D)	109.5
H(11A)-C(11)-H(11D)	141.1
H(11B)-C(11)-H(11D)	56.3
H(11C)-C(11)-H(11D)	56.3
C(7)-C(11)-H(11E)	109.5
H(11A)-C(11)-H(11E)	56.3
H(11B)-C(11)-H(11E)	141.1
H(11C)-C(11)-H(11E)	56.3
H(11D)-C(11)-H(11E)	109.5
C(7)-C(11)-H(11F)	109.5
H(11A)-C(11)-H(11F)	56.3
H(11B)-C(11)-H(11F)	56.3

H(11C)-C(11)-H(11F)	141.1
H(11D)-C(11)-H(11F)	109.5
H(11E)-C(11)-H(11F)	109.5
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(14)-C(13)-C(18)	122.14(12)
C(14)-C(13)-N(2)	118.31(12)
C(18)-C(13)-N(2)	119.55(12)
C(15)-C(14)-C(13)	117.80(12)
C(15)-C(14)-C(19)	120.37(13)
C(13)-C(14)-C(19)	121.76(12)
C(16)-C(15)-C(14)	122.04(13)
C(16)-C(15)-H(15)	119.0
C(14)-C(15)-H(15)	119.0
C(17)-C(16)-C(15)	118.14(13)
C(17)-C(16)-C(20)	121.04(13)
C(15)-C(16)-C(20)	120.80(14)
C(16)-C(17)-C(18)	122.20(13)
C(16)-C(17)-H(17)	118.9
C(18)-C(17)-H(17)	118.9
C(17)-C(18)-C(13)	117.67(13)
C(17)-C(18)-C(21)	120.56(13)
C(13)-C(18)-C(21)	121.77(13)
C(14)-C(19)-H(19A)	109.5
C(14)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(14)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(16)-C(20)-H(20A)	109.5
C(16)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5

C(16)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(18)-C(21)-H(21A)	109.5
C(18)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(18)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(3)-C(22)-C(23)	107.26(11)
N(3)-C(22)-C(27)	115.37(12)
C(23)-C(22)-C(27)	111.23(12)
N(3)-C(22)-C(28)	106.20(11)
C(23)-C(22)-C(28)	108.76(12)
C(27)-C(22)-C(28)	107.76(12)
C(24)-C(23)-C(22)	112.89(13)
C(24)-C(23)-H(23A)	109.0
C(22)-C(23)-H(23A)	109.0
C(24)-C(23)-H(23B)	109.0
C(22)-C(23)-H(23B)	109.0
H(23A)-C(23)-H(23B)	107.8
C(23)-C(24)-C(25)	109.04(12)
C(23)-C(24)-H(24A)	109.9
C(25)-C(24)-H(24A)	109.9
C(23)-C(24)-H(24B)	109.9
C(25)-C(24)-H(24B)	109.9
H(24A)-C(24)-H(24B)	108.3
C(24)-C(25)-C(26)	113.17(12)
C(24)-C(25)-H(25A)	108.9
C(26)-C(25)-H(25A)	108.9
C(24)-C(25)-H(25B)	108.9
C(26)-C(25)-H(25B)	108.9
H(25A)-C(25)-H(25B)	107.8
N(3)-C(26)-C(25)	107.39(11)
N(3)-C(26)-C(30)	106.21(11)
C(25)-C(26)-C(30)	108.42(12)

N(3)-C(26)-C(29)	115.53(11)
C(25)-C(26)-C(29)	111.04(12)
C(30)-C(26)-C(29)	107.97(11)
C(22)-C(27)-H(27A)	109.5
C(22)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(22)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(22)-C(28)-H(28A)	109.5
C(22)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(22)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(26)-C(29)-H(29A)	109.5
C(26)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(26)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(26)-C(30)-H(30A)	109.5
C(26)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(26)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $[CHNC_6H_2(CH_3)_3]_2C\cdots HO(NC_5H_6(CH_3)_4)$.
The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	36(1)	22(1)	17(1)	1(1)	5(1)	5(1)
N(2)	33(1)	22(1)	19(1)	2(1)	4(1)	4(1)
N(3)	22(1)	29(1)	18(1)	0(1)	5(1)	1(1)
O(1)	23(1)	43(1)	20(1)	0(1)	5(1)	3(1)
C(1)	29(1)	21(1)	21(1)	2(1)	4(1)	2(1)
C(2)	55(1)	31(1)	17(1)	0(1)	4(1)	9(1)
C(3)	52(1)	31(1)	17(1)	4(1)	4(1)	9(1)
C(4)	34(1)	19(1)	17(1)	-1(1)	6(1)	4(1)
C(5)	28(1)	23(1)	23(1)	-1(1)	8(1)	0(1)
C(6)	26(1)	23(1)	27(1)	0(1)	6(1)	3(1)
C(7)	33(1)	20(1)	20(1)	-1(1)	7(1)	1(1)
C(8)	31(1)	25(1)	24(1)	-3(1)	4(1)	-5(1)
C(9)	31(1)	26(1)	21(1)	-3(1)	1(1)	1(1)
C(10)	32(1)	27(1)	56(1)	7(1)	10(1)	-3(1)
C(11)	38(1)	23(1)	34(1)	4(1)	6(1)	1(1)
C(12)	34(1)	40(1)	49(1)	6(1)	-8(1)	1(1)
C(13)	30(1)	21(1)	20(1)	3(1)	0(1)	4(1)
C(14)	28(1)	23(1)	20(1)	2(1)	-2(1)	0(1)
C(15)	27(1)	27(1)	26(1)	-1(1)	0(1)	3(1)
C(16)	35(1)	23(1)	31(1)	0(1)	-3(1)	1(1)
C(17)	32(1)	24(1)	36(1)	6(1)	0(1)	-4(1)
C(18)	29(1)	27(1)	28(1)	7(1)	2(1)	1(1)
C(19)	33(1)	27(1)	28(1)	-3(1)	4(1)	-4(1)
C(20)	48(1)	25(1)	55(1)	-6(1)	1(1)	1(1)
C(21)	34(1)	40(1)	46(1)	7(1)	10(1)	1(1)
C(22)	33(1)	28(1)	22(1)	0(1)	6(1)	-2(1)
C(23)	45(1)	32(1)	27(1)	-3(1)	14(1)	0(1)
C(24)	47(1)	38(1)	25(1)	1(1)	15(1)	-3(1)
C(25)	39(1)	31(1)	28(1)	4(1)	8(1)	-4(1)
C(26)	27(1)	28(1)	20(1)	1(1)	0(1)	0(1)
C(27)	44(1)	37(1)	27(1)	1(1)	-2(1)	-12(1)

C(28)	43(1)	30(1)	29(1)	4(1)	8(1)	0(1)
C(29)	37(1)	34(1)	29(1)	2(1)	-6(1)	4(1)
C(30)	35(1)	31(1)	29(1)	-3(1)	-2(1)	0(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[CHNC_6H_2(CH_3)_3]_2C\cdots HO(NC_5H_6(CH_3)_4)$.

	x	y	z	U(eq)
H(1)	4311(18)	2336(13)	2344(13)	58(6)
H(2)	-8	6266	-183	41
H(3)	-512	7849	-261	40
H(6)	2688	4403	2203	30
H(8)	-867	3797	1770	32
H(10A)	2690	6444	2133	57
H(10B)	2657	6379	1173	57
H(10C)	3505	5728	1720	57
H(11A)	2072	3011	2563	47
H(11B)	986	2615	1979	47
H(11C)	716	2971	2852	47
H(11D)	444	2720	2366	47
H(11E)	1530	3116	2951	47
H(11F)	1800	2760	2077	47
H(12A)	-1783	5310	516	62
H(12B)	-1944	5847	1327	62
H(12C)	-2311	4833	1272	62
H(15)	-2580	9846	1999	32
H(17)	631	10699	1278	37
H(19A)	-2124	7850	2246	44
H(19B)	-2424	7705	1300	44
H(19C)	-3231	8368	1782	44
H(20A)	-882	11455	2469	65
H(20B)	-2198	11386	1993	65
H(20C)	-1064	11758	1548	65
H(21A)	1819	8611	848	59
H(21B)	2202	9613	997	59
H(21C)	1483	9330	166	59
H(23A)	6513	1439	525	41
H(23B)	5572	976	-120	41

H(24A)	4930	2352	-640	43
H(24B)	6383	2275	-664	43
H(25A)	5847	3649	-114	39
H(25B)	6684	3095	529	39
H(27A)	2825	1501	792	54
H(27B)	3370	777	222	54
H(27C)	3324	1783	-50	54
H(28A)	5716	909	1777	51
H(28B)	5037	231	1163	51
H(28C)	4278	752	1794	51
H(29A)	3484	3121	-68	50
H(29B)	3710	4101	251	50
H(29C)	3021	3411	782	50
H(30A)	4698	3956	1852	48
H(30B)	5361	4474	1172	48
H(30C)	6096	3754	1713	48

Table 6. Torsion angles [°] for $[CHNC_6H_2(CH_3)_3]_2C\cdots HO(NC_5H_6(CH_3)_4)$.

C(2)-N(1)-C(1)-N(2)	-0.32(16)
C(4)-N(1)-C(1)-N(2)	-175.34(12)
C(3)-N(2)-C(1)-N(1)	0.42(15)
C(13)-N(2)-C(1)-N(1)	176.03(12)
C(1)-N(1)-C(2)-C(3)	0.10(18)
C(4)-N(1)-C(2)-C(3)	175.04(13)
N(1)-C(2)-C(3)-N(2)	0.16(18)
C(1)-N(2)-C(3)-C(2)	-0.38(18)
C(13)-N(2)-C(3)-C(2)	-175.92(13)
C(1)-N(1)-C(4)-C(5)	-76.04(17)
C(2)-N(1)-C(4)-C(5)	109.52(16)
C(1)-N(1)-C(4)-C(9)	101.39(15)
C(2)-N(1)-C(4)-C(9)	-73.05(18)
C(9)-C(4)-C(5)-C(6)	0.60(19)
N(1)-C(4)-C(5)-C(6)	177.94(12)
C(9)-C(4)-C(5)-C(10)	-177.37(13)
N(1)-C(4)-C(5)-C(10)	0.0(2)
C(4)-C(5)-C(6)-C(7)	-0.3(2)
C(10)-C(5)-C(6)-C(7)	177.72(13)
C(5)-C(6)-C(7)-C(8)	-0.2(2)
C(5)-C(6)-C(7)-C(11)	179.40(13)
C(6)-C(7)-C(8)-C(9)	0.3(2)
C(11)-C(7)-C(8)-C(9)	-179.24(13)
C(7)-C(8)-C(9)-C(4)	0.0(2)
C(7)-C(8)-C(9)-C(12)	-179.40(14)
C(5)-C(4)-C(9)-C(8)	-0.5(2)
N(1)-C(4)-C(9)-C(8)	-177.83(12)
C(5)-C(4)-C(9)-C(12)	178.92(14)
N(1)-C(4)-C(9)-C(12)	1.55(19)
C(1)-N(2)-C(13)-C(14)	-73.29(17)
C(3)-N(2)-C(13)-C(14)	101.79(16)
C(1)-N(2)-C(13)-C(18)	106.18(15)
C(3)-N(2)-C(13)-C(18)	-78.74(18)
C(18)-C(13)-C(14)-C(15)	0.85(19)

N(2)-C(13)-C(14)-C(15)	-179.68(11)
C(18)-C(13)-C(14)-C(19)	-176.06(12)
N(2)-C(13)-C(14)-C(19)	3.40(18)
C(13)-C(14)-C(15)-C(16)	-1.4(2)
C(19)-C(14)-C(15)-C(16)	175.55(13)
C(14)-C(15)-C(16)-C(17)	0.7(2)
C(14)-C(15)-C(16)-C(20)	-177.60(13)
C(15)-C(16)-C(17)-C(18)	0.5(2)
C(20)-C(16)-C(17)-C(18)	178.87(14)
C(16)-C(17)-C(18)-C(13)	-1.0(2)
C(16)-C(17)-C(18)-C(21)	180.00(14)
C(14)-C(13)-C(18)-C(17)	0.3(2)
N(2)-C(13)-C(18)-C(17)	-179.13(12)
C(14)-C(13)-C(18)-C(21)	179.27(13)
N(2)-C(13)-C(18)-C(21)	-0.2(2)
O(1)-N(3)-C(22)-C(23)	176.18(10)
C(26)-N(3)-C(22)-C(23)	54.52(15)
O(1)-N(3)-C(22)-C(27)	51.64(14)
C(26)-N(3)-C(22)-C(27)	-70.02(15)
O(1)-N(3)-C(22)-C(28)	-67.65(12)
C(26)-N(3)-C(22)-C(28)	170.69(11)
N(3)-C(22)-C(23)-C(24)	-53.71(16)
C(27)-C(22)-C(23)-C(24)	73.31(16)
C(28)-C(22)-C(23)-C(24)	-168.17(13)
C(22)-C(23)-C(24)-C(25)	56.86(17)
C(23)-C(24)-C(25)-C(26)	-56.92(17)
O(1)-N(3)-C(26)-C(25)	-176.14(10)
C(22)-N(3)-C(26)-C(25)	-54.48(14)
O(1)-N(3)-C(26)-C(30)	68.02(12)
C(22)-N(3)-C(26)-C(30)	-170.32(11)
O(1)-N(3)-C(26)-C(29)	-51.64(14)
C(22)-N(3)-C(26)-C(29)	70.02(15)
C(24)-C(25)-C(26)-N(3)	53.61(15)
C(24)-C(25)-C(26)-C(30)	167.98(12)
C(24)-C(25)-C(26)-C(29)	-73.57(16)

Table 7. Hydrogen bonds for $[CHNC_6H_2(CH_3)_3]_2C\cdots HO(NC_5H_6(CH_3)_4)$ [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...C(1)#1	0.96(2)	1.91(2)	2.8543(17)	169.6(18)
O(1)-H(1)...N(1)#1	0.96(2)	2.96(2)	3.8469(17)	155.0(15)
O(1)-H(1)...N(2)#1	0.96(2)	2.95(2)	3.8424(16)	155.6(15)

Symmetry transformations used to generate equivalent atoms:

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

Table 8. Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane) for $[CHNC_6H_2(CH_3)_3]_2C\cdots HO(NC_5H_6(CH_3)_4)$.

10.6857 (0.0030) x + 3.2280 (0.0112) y - 2.8417 (0.0130) z = 2.0657 (0.0082)

* 0.0012 (0.0009) N1
* 0.0022 (0.0009) N2
* -0.0021 (0.0008) C1
* 0.0002 (0.0010) C2
* -0.0015 (0.0010) C3
0.5972 (0.0032) O1_$2
0.2843 (0.0200) H1_$2

Rms deviation of fitted atoms = 0.0016

Table 1. Crystal data and structure refinement for $Ph_3PC(H)C(=O)O(NC_5H_6(CH_3)_4)$.

Identification code	mm001	
Empirical formula	$C_{29}\ H_{34}\ N\ O_2\ P_1$	
Formula weight	459.54	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.9030(13) Å	α= 90°
	b = 12.1631(13) Å	β= 93.6420(10)°
	c = 18.100(2) Å	γ = 90°
Volume	2615.1(5) $Å^3$	
Z	4	
Density (calculated)	1.167 Mg/m^3	
Absorption coefficient	0.130 mm^{-1}	
F(000)	984	
Crystal size	0.4021 x 0.3726 x 0.2189 mm^3	
Theta range for data collection	2.02 to 28.69°	
Index ranges	-15<=h<=16, -16<=k<=16, -22<=l<=23	
Reflections collected	20480	
Independent reflections	6326 [R(int) = 0.0492]	
Completeness to theta = 28.69°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7457 and 0.6680	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6326 / 0 / 302	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0419, wR2 = 0.1017	
R indices (all data)	R1 = 0.0591, wR2 = 0.1133	
Largest diff. peak and hole	0.448 and -0.286 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $Ph_3PC(H)C(=O)O(NC_5H_6(CH_3)_4)$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	7610(1)	2170(1)	859(1)	15(1)
N(1)	3989(1)	2995(1)	1005(1)	17(1)
O(1)	4603(1)	2523(1)	1651(1)	17(1)
O(2)	6250(1)	2049(1)	2158(1)	19(1)
C(1)	8145(1)	804(1)	1055(1)	18(1)
C(2)	7498(1)	68(1)	1437(1)	22(1)
C(3)	7943(1)	-939(1)	1664(1)	25(1)
C(4)	9027(1)	-1225(1)	1500(1)	25(1)
C(5)	9660(1)	-515(1)	1092(1)	26(1)
C(6)	9225(1)	500(1)	870(1)	23(1)
C(7)	8022(1)	2507(1)	-58(1)	16(1)
C(8)	7385(1)	2110(1)	-676(1)	22(1)
C(9)	7701(1)	2356(1)	-1384(1)	26(1)
C(10)	8646(1)	2996(1)	-1483(1)	24(1)
C(11)	9281(1)	3384(1)	-874(1)	21(1)
C(12)	8977(1)	3140(1)	-162(1)	19(1)
C(13)	8412(1)	3076(1)	1484(1)	20(1)
C(14)	9260(1)	2720(2)	1984(1)	31(1)
C(15)	9857(1)	3489(2)	2428(1)	41(1)
C(16)	9605(2)	4595(2)	2368(1)	39(1)
C(17)	8744(2)	4951(2)	1883(1)	32(1)
C(18)	8148(1)	4198(1)	1443(1)	25(1)
C(19)	6189(1)	2357(1)	872(1)	17(1)
C(20)	5739(1)	2304(1)	1570(1)	16(1)
C(21)	3730(1)	4156(1)	1206(1)	19(1)
C(22)	3007(1)	4633(1)	553(1)	25(1)
C(23)	1967(1)	3945(2)	351(1)	30(1)
C(24)	2328(1)	2783(2)	164(1)	29(1)
C(25)	3043(1)	2224(1)	797(1)	23(1)
C(26)	4851(1)	4779(1)	1269(1)	24(1)

C(27)	3159(1)	4316(1)	1939(1)	24(1)
C(28)	3565(2)	1182(1)	496(1)	31(1)
C(29)	2305(1)	1891(2)	1429(1)	29(1)

Table 3. Bond lengths [Å] and angles [°] for $Ph_3PC(H)C(=O)O(NC_5H_6(CH_3)_4)$.

P(1)-C(19)	1.7075(14)
P(1)-C(1)	1.8065(15)
P(1)-C(7)	1.8085(14)
P(1)-C(13)	1.8086(15)
N(1)-O(1)	1.4562(15)
N(1)-C(21)	1.4950(19)
N(1)-C(25)	1.4955(19)
O(1)-C(20)	1.3944(16)
O(2)-C(20)	1.2315(17)
C(1)-C(2)	1.392(2)
C(1)-C(6)	1.3983(19)
C(2)-C(3)	1.387(2)
C(2)-H(2)	0.9300
C(3)-C(4)	1.387(2)
C(3)-H(3)	0.9300
C(4)-C(5)	1.389(2)
C(4)-H(4)	0.9300
C(5)-C(6)	1.388(2)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(12)	1.395(2)
C(7)-C(8)	1.397(2)
C(8)-C(9)	1.391(2)
C(8)-H(8)	0.9300
C(9)-C(10)	1.388(2)
C(9)-H(9)	0.9300
C(10)-C(11)	1.380(2)
C(10)-H(10)	0.9300
C(11)-C(12)	1.3936(19)
C(11)-H(11)	0.9300
C(12)-H(12)	0.9300
C(13)-C(14)	1.381(2)
C(13)-C(18)	1.401(2)
C(14)-C(15)	1.398(3)

C(14)-H(14)	0.9300
C(15)-C(16)	1.381(3)
C(15)-H(15)	0.9300
C(16)-C(17)	1.375(3)
C(16)-H(16)	0.9300
C(17)-C(18)	1.381(2)
C(17)-H(17)	0.9300
C(18)-H(18)	0.9300
C(19)-C(20)	1.4046(19)
C(19)-H(19)	0.966(18)
C(21)-C(22)	1.531(2)
C(21)-C(26)	1.532(2)
C(21)-C(27)	1.5416(19)
C(22)-C(23)	1.519(2)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-C(24)	1.521(2)
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(24)-C(25)	1.541(2)
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(25)-C(28)	1.528(2)
C(25)-C(29)	1.540(2)
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(27)-H(27A)	0.9600
C(27)-H(27B)	0.9600
C(27)-H(27C)	0.9600
C(28)-H(28A)	0.9600
C(28)-H(28B)	0.9600
C(28)-H(28C)	0.9600
C(29)-H(29A)	0.9600
C(29)-H(29B)	0.9600
C(29)-H(29C)	0.9600

C(19)-P(1)-C(1)	117.21(7)
C(19)-P(1)-C(7)	108.03(7)
C(1)-P(1)-C(7)	106.02(6)
C(19)-P(1)-C(13)	113.19(7)
C(1)-P(1)-C(13)	105.79(7)
C(7)-P(1)-C(13)	105.83(7)
O(1)-N(1)-C(21)	106.17(10)
O(1)-N(1)-C(25)	106.65(10)
C(21)-N(1)-C(25)	119.32(11)
C(20)-O(1)-N(1)	115.58(9)
C(2)-C(1)-C(6)	119.63(13)
C(2)-C(1)-P(1)	119.30(10)
C(6)-C(1)-P(1)	120.94(11)
C(3)-C(2)-C(1)	120.17(13)
C(3)-C(2)-H(2)	119.9
C(1)-C(2)-H(2)	119.9
C(2)-C(3)-C(4)	120.03(14)
C(2)-C(3)-H(3)	120.0
C(4)-C(3)-H(3)	120.0
C(3)-C(4)-C(5)	120.11(14)
C(3)-C(4)-H(4)	119.9
C(5)-C(4)-H(4)	119.9
C(6)-C(5)-C(4)	120.11(14)
C(6)-C(5)-H(5)	119.9
C(4)-C(5)-H(5)	119.9
C(5)-C(6)-C(1)	119.85(14)
C(5)-C(6)-H(6)	120.1
C(1)-C(6)-H(6)	120.1
C(12)-C(7)-C(8)	119.31(12)
C(12)-C(7)-P(1)	121.30(11)
C(8)-C(7)-P(1)	119.38(11)
C(9)-C(8)-C(7)	119.85(14)
C(9)-C(8)-H(8)	120.1
C(7)-C(8)-H(8)	120.1
C(10)-C(9)-C(8)	120.55(15)

C(10)-C(9)-H(9)	119.7
C(8)-C(9)-H(9)	119.7
C(11)-C(10)-C(9)	119.75(13)
C(11)-C(10)-H(10)	120.1
C(9)-C(10)-H(10)	120.1
C(10)-C(11)-C(12)	120.34(14)
C(10)-C(11)-H(11)	119.8
C(12)-C(11)-H(11)	119.8
C(11)-C(12)-C(7)	120.20(14)
C(11)-C(12)-H(12)	119.9
C(7)-C(12)-H(12)	119.9
C(14)-C(13)-C(18)	119.48(15)
C(14)-C(13)-P(1)	123.64(12)
C(18)-C(13)-P(1)	116.87(12)
C(13)-C(14)-C(15)	119.39(17)
C(13)-C(14)-H(14)	120.3
C(15)-C(14)-H(14)	120.3
C(16)-C(15)-C(14)	120.42(18)
C(16)-C(15)-H(15)	119.8
C(14)-C(15)-H(15)	119.8
C(17)-C(16)-C(15)	120.42(17)
C(17)-C(16)-H(16)	119.8
C(15)-C(16)-H(16)	119.8
C(16)-C(17)-C(18)	119.61(17)
C(16)-C(17)-H(17)	120.2
C(18)-C(17)-H(17)	120.2
C(17)-C(18)-C(13)	120.65(16)
C(17)-C(18)-H(18)	119.7
C(13)-C(18)-H(18)	119.7
C(20)-C(19)-P(1)	116.19(11)
C(20)-C(19)-H(19)	123.8(11)
P(1)-C(19)-H(19)	119.5(10)
O(2)-C(20)-O(1)	112.77(11)
O(2)-C(20)-C(19)	126.32(13)
O(1)-C(20)-C(19)	120.89(13)
N(1)-C(21)-C(22)	106.53(12)

N(1)-C(21)-C(26)	107.05(11)
C(22)-C(21)-C(26)	108.38(12)
N(1)-C(21)-C(27)	115.91(12)
C(22)-C(21)-C(27)	111.04(12)
C(26)-C(21)-C(27)	107.64(13)
C(23)-C(22)-C(21)	112.78(13)
C(23)-C(22)-H(22A)	109.0
C(21)-C(22)-H(22A)	109.0
C(23)-C(22)-H(22B)	109.0
C(21)-C(22)-H(22B)	109.0
H(22A)-C(22)-H(22B)	107.8
C(22)-C(23)-C(24)	109.16(13)
C(22)-C(23)-H(23A)	109.8
C(24)-C(23)-H(23A)	109.8
C(22)-C(23)-H(23B)	109.8
C(24)-C(23)-H(23B)	109.8
H(23A)-C(23)-H(23B)	108.3
C(23)-C(24)-C(25)	113.24(13)
C(23)-C(24)-H(24A)	108.9
C(25)-C(24)-H(24A)	108.9
C(23)-C(24)-H(24B)	108.9
C(25)-C(24)-H(24B)	108.9
H(24A)-C(24)-H(24B)	107.7
N(1)-C(25)-C(28)	107.05(12)
N(1)-C(25)-C(29)	115.75(12)
C(28)-C(25)-C(29)	108.08(13)
N(1)-C(25)-C(24)	106.41(12)
C(28)-C(25)-C(24)	108.55(13)
C(29)-C(25)-C(24)	110.76(13)
C(21)-C(26)-H(26A)	109.5
C(21)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(21)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(21)-C(27)-H(27A)	109.5

C(21)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(21)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(25)-C(28)-H(28A)	109.5
C(25)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(25)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(25)-C(29)-H(29A)	109.5
C(25)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(25)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $Ph_3PC(H)C(=O)O(NC_5H_6(CH_3)_4)$.

The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	14(1)	16(1)	15(1)	0(1)	3(1)	2(1)
N(1)	14(1)	21(1)	16(1)	3(1)	-1(1)	2(1)
O(1)	13(1)	21(1)	15(1)	3(1)	2(1)	3(1)
O(2)	19(1)	21(1)	18(1)	1(1)	0(1)	4(1)
C(1)	19(1)	17(1)	17(1)	1(1)	4(1)	4(1)
C(2)	23(1)	20(1)	24(1)	1(1)	10(1)	4(1)
C(3)	31(1)	21(1)	25(1)	4(1)	13(1)	4(1)
C(4)	33(1)	20(1)	24(1)	3(1)	7(1)	10(1)
C(5)	23(1)	27(1)	29(1)	4(1)	8(1)	10(1)
C(6)	21(1)	22(1)	25(1)	4(1)	7(1)	4(1)
C(7)	15(1)	17(1)	16(1)	1(1)	4(1)	5(1)
C(8)	16(1)	27(1)	22(1)	-3(1)	3(1)	0(1)
C(9)	21(1)	40(1)	18(1)	-4(1)	0(1)	2(1)
C(10)	23(1)	32(1)	18(1)	5(1)	6(1)	8(1)
C(11)	18(1)	23(1)	23(1)	3(1)	6(1)	1(1)
C(12)	17(1)	21(1)	18(1)	0(1)	2(1)	2(1)
C(13)	17(1)	24(1)	18(1)	-3(1)	6(1)	-2(1)
C(14)	19(1)	43(1)	30(1)	-10(1)	0(1)	7(1)
C(15)	17(1)	70(1)	36(1)	-20(1)	-2(1)	4(1)
C(16)	25(1)	55(1)	38(1)	-25(1)	16(1)	-18(1)
C(17)	41(1)	30(1)	28(1)	-8(1)	18(1)	-14(1)
C(18)	32(1)	24(1)	20(1)	-1(1)	8(1)	-4(1)
C(19)	14(1)	21(1)	17(1)	1(1)	2(1)	2(1)
C(20)	15(1)	13(1)	21(1)	-1(1)	2(1)	2(1)
C(21)	17(1)	20(1)	21(1)	4(1)	4(1)	4(1)
C(22)	22(1)	28(1)	26(1)	8(1)	3(1)	7(1)
C(23)	22(1)	41(1)	28(1)	9(1)	-4(1)	5(1)
C(24)	23(1)	40(1)	24(1)	0(1)	-4(1)	-2(1)
C(25)	18(1)	27(1)	22(1)	0(1)	-1(1)	-2(1)
C(26)	23(1)	19(1)	32(1)	2(1)	5(1)	0(1)
C(27)	23(1)	27(1)	24(1)	-1(1)	7(1)	5(1)

C(28)	29(1)	28(1)	36(1)	-8(1)	-1(1)	-4(1)
C(29)	21(1)	34(1)	32(1)	4(1)	3(1)	-7(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for $Ph_3PC(H)C(=O)O(NC_5H_6(CH_3)_4)$.

	x	y	z	U(eq)
H(2)	6766	252	1540	26
H(3)	7514	-1424	1927	30
H(4)	9331	-1893	1663	30
H(5)	10376	-720	967	31
H(6)	9650	977	599	27
H(8)	6751	1681	-614	26
H(9)	7275	2091	-1795	32
H(10)	8850	3162	-1958	29
H(11)	9916	3811	-940	25
H(12)	9412	3400	246	22
H(14)	9431	1976	2025	37
H(15)	10428	3255	2766	49
H(16)	10020	5103	2657	46
H(17)	8565	5695	1853	39
H(18)	7566	4438	1115	30
H(19)	5765(15)	2583(15)	425(10)	28(5)
H(22A)	2775	5371	677	30
H(22B)	3458	4683	126	30
H(23A)	1546	4267	-71	36
H(23B)	1485	3927	763	36
H(24A)	2758	2807	-273	35
H(24B)	1661	2342	47	35
H(26A)	5297	4521	1695	37
H(26B)	4709	5551	1321	37
H(26C)	5249	4654	832	37
H(27A)	2391	4072	1879	37
H(27B)	3177	5080	2072	37
H(27C)	3552	3895	2322	37
H(28A)	4033	1372	102	47
H(28B)	2978	695	310	47

H(28C)	4011	823	885	47
H(29A)	2778	1665	1851	43
H(29B)	1822	1293	1268	43
H(29C)	1854	2506	1561	43

Table 6. Torsion angles [°] for $Ph_3PC(H)C(=O)O(NC_5H_6(CH_3)_4)$.

C(21)-N(1)-O(1)-C(20)	-110.41(12)
C(25)-N(1)-O(1)-C(20)	121.35(12)
C(19)-P(1)-C(1)-C(2)	-21.06(15)
C(7)-P(1)-C(1)-C(2)	-141.70(12)
C(13)-P(1)-C(1)-C(2)	106.21(13)
C(19)-P(1)-C(1)-C(6)	163.02(12)
C(7)-P(1)-C(1)-C(6)	42.37(14)
C(13)-P(1)-C(1)-C(6)	-69.72(13)
C(6)-C(1)-C(2)-C(3)	3.1(2)
P(1)-C(1)-C(2)-C(3)	-172.84(12)
C(1)-C(2)-C(3)-C(4)	-1.2(2)
C(2)-C(3)-C(4)-C(5)	-1.6(3)
C(3)-C(4)-C(5)-C(6)	2.3(3)
C(4)-C(5)-C(6)-C(1)	-0.4(2)
C(2)-C(1)-C(6)-C(5)	-2.4(2)
P(1)-C(1)-C(6)-C(5)	173.55(13)
C(19)-P(1)-C(7)-C(12)	135.87(12)
C(1)-P(1)-C(7)-C(12)	-97.71(12)
C(13)-P(1)-C(7)-C(12)	14.35(13)
C(19)-P(1)-C(7)-C(8)	-45.36(13)
C(1)-P(1)-C(7)-C(8)	81.06(13)
C(13)-P(1)-C(7)-C(8)	-166.88(11)
C(12)-C(7)-C(8)-C(9)	-0.6(2)
P(1)-C(7)-C(8)-C(9)	-179.44(12)
C(7)-C(8)-C(9)-C(10)	0.0(2)
C(8)-C(9)-C(10)-C(11)	0.4(2)
C(9)-C(10)-C(11)-C(12)	-0.2(2)
C(10)-C(11)-C(12)-C(7)	-0.5(2)
C(8)-C(7)-C(12)-C(11)	0.9(2)
P(1)-C(7)-C(12)-C(11)	179.64(11)
C(19)-P(1)-C(13)-C(14)	130.50(13)
C(1)-P(1)-C(13)-C(14)	0.86(14)
C(7)-P(1)-C(13)-C(14)	-111.37(13)
C(19)-P(1)-C(13)-C(18)	-50.10(13)

C(1)-P(1)-C(13)-C(18)	-179.75(11)
C(7)-P(1)-C(13)-C(18)	68.03(12)
C(18)-C(13)-C(14)-C(15)	-1.5(2)
P(1)-C(13)-C(14)-C(15)	177.93(12)
C(13)-C(14)-C(15)-C(16)	-0.1(3)
C(14)-C(15)-C(16)-C(17)	1.6(3)
C(15)-C(16)-C(17)-C(18)	-1.6(2)
C(16)-C(17)-C(18)-C(13)	0.0(2)
C(14)-C(13)-C(18)-C(17)	1.5(2)
P(1)-C(13)-C(18)-C(17)	-177.91(11)
C(1)-P(1)-C(19)-C(20)	70.16(13)
C(7)-P(1)-C(19)-C(20)	-170.26(11)
C(13)-P(1)-C(19)-C(20)	-53.42(13)
N(1)-O(1)-C(20)-O(2)	170.70(11)
N(1)-O(1)-C(20)-C(19)	-10.72(18)
P(1)-C(19)-C(20)-O(2)	-6.3(2)
P(1)-C(19)-C(20)-O(1)	175.35(10)
O(1)-N(1)-C(21)-C(22)	-175.75(10)
C(25)-N(1)-C(21)-C(22)	-55.42(15)
O(1)-N(1)-C(21)-C(26)	68.45(12)
C(25)-N(1)-C(21)-C(26)	-171.22(12)
O(1)-N(1)-C(21)-C(27)	-51.65(15)
C(25)-N(1)-C(21)-C(27)	68.68(17)
N(1)-C(21)-C(22)-C(23)	54.63(16)
C(26)-C(21)-C(22)-C(23)	169.53(13)
C(27)-C(21)-C(22)-C(23)	-72.43(17)
C(21)-C(22)-C(23)-C(24)	-58.12(17)
C(22)-C(23)-C(24)-C(25)	57.32(17)
O(1)-N(1)-C(25)-C(28)	-69.59(14)
C(21)-N(1)-C(25)-C(28)	170.33(12)
O(1)-N(1)-C(25)-C(29)	50.97(16)
C(21)-N(1)-C(25)-C(29)	-69.12(17)
O(1)-N(1)-C(25)-C(24)	174.49(10)
C(21)-N(1)-C(25)-C(24)	54.40(16)
C(23)-C(24)-C(25)-N(1)	-52.95(16)
C(23)-C(24)-C(25)-C(28)	-167.85(13)

C(23)-C(24)-C(25)-C(29)	73.64(17)

Table 7. Intramolecular Distances (X..X in Å) for $Ph_3PC(H)C(=O)O(NC_5H_6(CH_3)_4)$.

2.9408 (0.0010) P1 - O2

Table 8. Least-squares planes (x,y,z in crystal coordinates) and deviations from them (* indicates atom used to define plane) for $Ph_3PC(H)C(=O)O(NC_5H_6(CH_3)_4)$.

2.7248 (0.0031) x + 11.5249 (0.0022) y + 3.7674 (0.0089) z = 4.8363 (0.0022)

* 0.0612 (0.0006) P1
* -0.1046 (0.0010) C19
* -0.0264 (0.0012) C20
* -0.0523 (0.0009) O1
* 0.0408 (0.0006) O2
* 0.0814 (0.0006) N1
-0.1285 (0.0183) H19

Rms deviation of fitted atoms = 0.0663

Table 1. Crystal data and structure refinement for $[CH_2N\ i\text{-}Pr_2C_6H_3]_2CH\cdots OC_6H_2CH_3(C(CH_3)_3)_2$.

Identification code	NG035	
Empirical formula	$C_{42}\ H_{62}\ N_2\ O$	
Formula weight	610.94	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 10.2181(7) Å	α= 90°
	b = 19.3153(14) Å	β= 90°
	c = 19.5555(14) Å	γ = 90°
Volume	3859.6(5) $Å^3$	
Z	4	
Density (calculated)	1.051 Mg/m^3	
Absorption coefficient	0.061 mm^{-1}	
F(000)	1344	
Crystal size	0.298 x 0.213 x 0.201 mm^3	
Theta range for data collection	2.11 to 26.50°	
Index ranges	-12<=h<=12, -24<=k<=24, -24<=l<=24	
Reflections collected	42693	
Independent reflections	4462 [R(int) = 0.1297]	
Completeness to theta = 26.50°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9877 and 0.9819	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4462 / 393 / 549	
Goodness-of-fit on F^2	0.956	
Final R indices [I>2sigma(I)]	R1 = 0.0438, wR2 = 0.0945	
R indices (all data)	R1 = 0.0675, wR2 = 0.1026	
Extinction coefficient	0.0080(12)	
Largest diff. peak and hole	0.204 and -0.158 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[CH_2N\ i\text{-}Pr_2C_6H_3]_2CH\cdots OC_6H_2CH_3(C(CH_3)_3)_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
N(1)	4469(2)	1728(1)	2333(1)	27(1)
N(2)	2921(2)	1374(1)	3018(1)	24(1)
O(1)	4744(2)	4872(1)	2421(1)	34(1)
C(1)	3990(3)	1204(1)	2677(1)	23(1)
C(2)	3714(3)	2367(1)	2466(2)	33(1)
C(3)	2526(3)	2088(1)	2844(2)	32(1)
C(4A)	5646(12)	1758(15)	1895(6)	35(1)
C(5A)	5537(8)	1716(7)	1173(5)	38(1)
C(6A)	6721(8)	1783(4)	812(4)	37(2)
C(7A)	7915(7)	1857(4)	1136(4)	39(2)
C(8A)	8012(9)	1871(4)	1844(3)	38(2)
C(9A)	6849(12)	1813(8)	2229(4)	36(1)
C(4B)	5527(12)	1716(15)	1880(6)	35(1)
C(5B)	5177(8)	1642(6)	1201(5)	37(2)
C(6B)	6147(7)	1683(4)	697(4)	39(2)
C(7B)	7411(8)	1823(4)	901(4)	39(2)
C(8B)	7727(9)	1912(5)	1586(4)	38(1)
C(9B)	6780(12)	1878(8)	2109(4)	37(1)
C(10)	4010(5)	1536(2)	898(2)	69(1)
C(11A)	3860(12)	2196(5)	413(6)	69(3)
C(12A)	4204(12)	900(6)	471(5)	74(3)
C(11B)	3268(12)	1947(5)	333(6)	67(3)
C(12B)	3694(12)	739(5)	699(5)	59(3)
C(13)	7052(3)	1915(2)	2927(2)	53(1)
C(14A)	8173(9)	1490(7)	3097(8)	60(3)
C(15A)	7286(11)	2726(5)	2973(5)	58(3)
C(14B)	7824(11)	1253(6)	3258(8)	70(4)
C(15B)	7708(12)	2552(5)	3256(5)	61(3)
C(16)	1998(3)	899(1)	3325(1)	28(1)
C(17)	1668(3)	999(1)	4014(1)	31(1)

C(18)	712(3)	571(2)	4290(2)	41(1)
C(19)	111(3)	68(2)	3902(2)	49(1)
C(20)	458(3)	-18(2)	3232(2)	48(1)
C(21)	1408(3)	389(2)	2922(2)	36(1)
C(22)	2267(3)	1555(2)	4459(2)	40(1)
C(23)	2825(4)	1261(2)	5126(2)	55(1)
C(24)	1272(4)	2120(2)	4623(2)	55(1)
C(25)	1724(4)	282(2)	2170(2)	47(1)
C(26A)	443(10)	511(7)	1794(6)	72(4)
C(27A)	1961(17)	-491(6)	2066(8)	56(3)
C(26B)	1002(11)	756(6)	1677(6)	59(3)
C(27B)	1707(18)	-453(6)	1895(8)	58(3)
C(28)	3823(3)	4448(1)	2229(1)	27(1)
C(29)	2927(3)	4149(1)	2712(1)	25(1)
C(30)	1902(3)	3741(1)	2482(2)	28(1)
C(31)	1716(3)	3574(1)	1796(2)	28(1)
C(32)	2625(3)	3825(2)	1340(2)	33(1)
C(33)	3675(3)	4246(2)	1527(1)	36(1)
C(34)	3128(3)	4286(1)	3484(1)	32(1)
C(35)	2110(4)	3915(2)	3931(2)	51(1)
C(36)	3018(4)	5059(2)	3646(2)	49(1)
C(37)	4479(3)	4025(2)	3693(2)	45(1)
C(38)	574(3)	3139(2)	1565(2)	39(1)
C(39A)	4537(5)	4577(3)	996(2)	37(1)
C(40A)	5986(5)	4404(3)	1154(3)	48(2)
C(41A)	4327(6)	5375(3)	964(3)	48(2)
C(42A)	4214(5)	4315(3)	281(2)	60(2)
C(39B)	4972(5)	4268(3)	995(2)	45(2)
C(40B)	6155(5)	4007(3)	1311(2)	53(3)
C(41B)	4946(15)	5058(6)	832(7)	51(3)
C(42B)	4701(13)	3934(7)	284(5)	41(3)

Table 3. Bond lengths [Å] and angles [°] for[CH_2N *i*-$Pr_2C_6H_3]_2CH\cdots OC_6H_2CH_3(C(CH_3)_3)_2$.

N(1)-C(1)	1.309(3)
N(1)-C(4B)	1.399(9)
N(1)-C(2)	1.478(3)
N(1)-C(4A)	1.478(9)
N(2)-C(1)	1.321(3)
N(2)-C(16)	1.446(3)
N(2)-C(3)	1.477(3)
O(1)-C(28)	1.303(3)
C(1)-H(1)	1.00(3)
C(2)-C(3)	1.519(4)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4A)-C(9A)	1.397(11)
C(4A)-C(5A)	1.417(11)
C(5A)-C(6A)	1.407(9)
C(5A)-C(10)	1.688(9)
C(6A)-C(7A)	1.382(9)
C(6A)-H(6A)	0.9500
C(7A)-C(8A)	1.388(8)
C(7A)-H(7A)	0.9500
C(8A)-C(9A)	1.411(10)
C(8A)-H(8A)	0.9500
C(9A)-C(13)	1.395(9)
C(4B)-C(5B)	1.383(11)
C(4B)-C(9B)	1.392(11)
C(5B)-C(10)	1.347(9)
C(5B)-C(6B)	1.400(9)
C(6B)-C(7B)	1.378(9)
C(6B)-H(6B)	0.9500
C(7B)-C(8B)	1.389(9)
C(7B)-H(7B)	0.9500
C(8B)-C(9B)	1.409(10)

C(8B)-H(8B)	0.9500
C(9B)-C(13)	1.626(9)
C(10)-C(12A)	1.499(10)
C(10)-C(11B)	1.557(10)
C(10)-C(11A)	1.597(10)
C(10)-C(12B)	1.620(10)
C(10)-H(10)	1.0000
C(11A)-H(11A)	0.9800
C(11A)-H(11B)	0.9800
C(11A)-H(11C)	0.9800
C(12A)-H(12A)	0.9800
C(12A)-H(12B)	0.9800
C(12A)-H(12C)	0.9800
C(11B)-H(11D)	0.9800
C(11B)-H(11E)	0.9800
C(11B)-H(11F)	0.9800
C(12B)-H(12D)	0.9800
C(12B)-H(12E)	0.9800
C(12B)-H(12F)	0.9800
C(13)-C(14A)	1.448(11)
C(13)-C(15B)	1.542(9)
C(13)-C(15A)	1.586(10)
C(13)-C(14B)	1.636(11)
C(13)-H(13)	1.0000
C(14A)-H(14A)	0.9800
C(14A)-H(14B)	0.9800
C(14A)-H(14C)	0.9800
C(15A)-H(15A)	0.9800
C(15A)-H(15B)	0.9800
C(15A)-H(15C)	0.9800
C(14B)-H(14D)	0.9800
C(14B)-H(14E)	0.9800
C(14B)-H(14F)	0.9800
C(15B)-H(15D)	0.9800
C(15B)-H(15E)	0.9800
C(15B)-H(15F)	0.9800

C(16)-C(21)	1.398(4)
C(16)-C(17)	1.402(4)
C(17)-C(18)	1.388(4)
C(17)-C(22)	1.512(4)
C(18)-C(19)	1.378(5)
C(18)-H(18)	0.9500
C(19)-C(20)	1.366(5)
C(19)-H(19)	0.9500
C(20)-C(21)	1.389(4)
C(20)-H(20)	0.9500
C(21)-C(25)	1.519(4)
C(22)-C(24)	1.524(4)
C(22)-C(23)	1.534(4)
C(22)-H(22)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(27B)	1.519(12)
C(25)-C(26B)	1.521(10)
C(25)-C(27A)	1.527(12)
C(25)-C(26A)	1.565(10)
C(25)-H(25)	1.0000
C(26A)-H(26A)	0.9800
C(26A)-H(26B)	0.9800
C(26A)-H(26C)	0.9800
C(27A)-H(27A)	0.9800
C(27A)-H(27B)	0.9800
C(27A)-H(27C)	0.9800
C(26B)-H(26D)	0.9800
C(26B)-H(26E)	0.9800
C(26B)-H(26F)	0.9800
C(27B)-H(27D)	0.9800
C(27B)-H(27E)	0.9800

C(27B)-H(27F)	0.9800
C(28)-C(33)	1.435(4)
C(28)-C(29)	1.437(4)
C(29)-C(30)	1.384(4)
C(29)-C(34)	1.547(4)
C(30)-C(31)	1.394(4)
C(30)-H(30)	0.9500
C(31)-C(32)	1.377(4)
C(31)-C(38)	1.507(4)
C(32)-C(33)	1.395(4)
C(32)-H(32)	0.9500
C(33)-C(39A)	1.503(5)
C(33)-C(39B)	1.685(5)
C(34)-C(37)	1.525(4)
C(34)-C(36)	1.531(4)
C(34)-C(35)	1.535(4)
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39A)-C(42A)	1.524(6)
C(39A)-C(40A)	1.549(6)
C(39A)-C(41A)	1.558(7)
C(40A)-H(40A)	0.9800
C(40A)-H(40B)	0.9800
C(40A)-H(40C)	0.9800
C(41A)-H(41A)	0.9800
C(41A)-H(41B)	0.9800

C(41A)-H(41C)	0.9800
C(42A)-H(42A)	0.9800
C(42A)-H(42B)	0.9800
C(42A)-H(42C)	0.9800
C(39B)-C(40B)	1.4486
C(39B)-C(42B)	1.557(11)
C(39B)-C(41B)	1.559(12)
C(40B)-H(40D)	0.9800
C(40B)-H(40E)	0.9800
C(40B)-H(40F)	0.9800
C(41B)-H(41D)	0.9800
C(41B)-H(41E)	0.9800
C(41B)-H(41F)	0.9800
C(42B)-H(42D)	0.9800
C(42B)-H(42E)	0.9800
C(42B)-H(42F)	0.9800

C(1)-N(1)-C(4B)	126.9(12)
C(1)-N(1)-C(2)	111.1(2)
C(4B)-N(1)-C(2)	122.0(12)
C(1)-N(1)-C(4A)	129.2(12)
C(2)-N(1)-C(4A)	119.6(12)
C(1)-N(2)-C(16)	126.2(2)
C(1)-N(2)-C(3)	109.9(2)
C(16)-N(2)-C(3)	120.7(2)
N(1)-C(1)-N(2)	112.1(2)
N(1)-C(1)-H(1)	121.3(15)
N(2)-C(1)-H(1)	126.6(15)
N(1)-C(2)-C(3)	101.9(2)
N(1)-C(2)-H(2A)	111.4
C(3)-C(2)-H(2A)	111.4
N(1)-C(2)-H(2B)	111.4
C(3)-C(2)-H(2B)	111.4
H(2A)-C(2)-H(2B)	109.3
N(2)-C(3)-C(2)	103.0(2)
N(2)-C(3)-H(3A)	111.2

C(2)-C(3)-H(3A)	111.2
N(2)-C(3)-H(3B)	111.2
C(2)-C(3)-H(3B)	111.2
H(3A)-C(3)-H(3B)	109.1
C(9A)-C(4A)-C(5A)	122.6(7)
C(9A)-C(4A)-N(1)	116.6(9)
C(5A)-C(4A)-N(1)	120.8(9)
C(6A)-C(5A)-C(4A)	115.3(7)
C(6A)-C(5A)-C(10)	130.9(7)
C(4A)-C(5A)-C(10)	113.7(7)
C(7A)-C(6A)-C(5A)	122.6(6)
C(7A)-C(6A)-H(6A)	118.7
C(5A)-C(6A)-H(6A)	118.7
C(6A)-C(7A)-C(8A)	121.5(6)
C(6A)-C(7A)-H(7A)	119.3
C(8A)-C(7A)-H(7A)	119.3
C(7A)-C(8A)-C(9A)	118.1(7)
C(7A)-C(8A)-H(8A)	121.0
C(9A)-C(8A)-H(8A)	121.0
C(13)-C(9A)-C(4A)	126.8(9)
C(13)-C(9A)-C(8A)	112.7(8)
C(4A)-C(9A)-C(8A)	119.8(7)
C(5B)-C(4B)-C(9B)	124.8(7)
C(5B)-C(4B)-N(1)	114.2(9)
C(9B)-C(4B)-N(1)	120.2(10)
C(10)-C(5B)-C(4B)	131.8(7)
C(10)-C(5B)-C(6B)	109.1(7)
C(4B)-C(5B)-C(6B)	119.1(7)
C(7B)-C(6B)-C(5B)	118.2(7)
C(7B)-C(6B)-H(6B)	120.9
C(5B)-C(6B)-H(6B)	120.9
C(6B)-C(7B)-C(8B)	121.4(7)
C(6B)-C(7B)-H(7B)	119.3
C(8B)-C(7B)-H(7B)	119.3
C(7B)-C(8B)-C(9B)	122.3(7)
C(7B)-C(8B)-H(8B)	118.9

C(9B)-C(8B)-H(8B)	118.9
C(4B)-C(9B)-C(8B)	114.1(7)
C(4B)-C(9B)-C(13)	118.9(9)
C(8B)-C(9B)-C(13)	126.5(8)
C(5B)-C(10)-C(12A)	104.6(8)
C(5B)-C(10)-C(11B)	131.6(7)
C(12A)-C(10)-C(11B)	95.0(7)
C(5B)-C(10)-C(11A)	102.9(7)
C(12A)-C(10)-C(11A)	109.6(6)
C(5B)-C(10)-C(12B)	115.3(8)
C(11B)-C(10)-C(12B)	102.6(6)
C(11A)-C(10)-C(12B)	126.6(6)
C(12A)-C(10)-C(5A)	103.0(7)
C(11B)-C(10)-C(5A)	124.8(6)
C(11A)-C(10)-C(5A)	96.5(6)
C(12B)-C(10)-C(5A)	117.2(7)
C(5B)-C(10)-H(10)	107.9
C(12A)-C(10)-H(10)	115.2
C(11B)-C(10)-H(10)	102.4
C(11A)-C(10)-H(10)	115.2
C(12B)-C(10)-H(10)	87.6
C(5A)-C(10)-H(10)	115.2
C(10)-C(11A)-H(11A)	109.5
C(10)-C(11A)-H(11B)	109.5
H(11A)-C(11A)-H(11B)	109.5
C(10)-C(11A)-H(11C)	109.5
H(11A)-C(11A)-H(11C)	109.5
H(11B)-C(11A)-H(11C)	109.5
C(10)-C(12A)-H(12A)	109.5
C(10)-C(12A)-H(12B)	109.5
H(12A)-C(12A)-H(12B)	109.5
C(10)-C(12A)-H(12C)	109.5
H(12A)-C(12A)-H(12C)	109.5
H(12B)-C(12A)-H(12C)	109.5
C(10)-C(11B)-H(11D)	109.5
C(10)-C(11B)-H(11E)	109.5

H(11D)-C(11B)-H(11E)	109.5
C(10)-C(11B)-H(11F)	109.5
H(11D)-C(11B)-H(11F)	109.5
H(11E)-C(11B)-H(11F)	109.5
C(10)-C(12B)-H(12D)	109.5
C(10)-C(12B)-H(12E)	109.5
H(12D)-C(12B)-H(12E)	109.5
C(10)-C(12B)-H(12F)	109.5
H(12D)-C(12B)-H(12F)	109.5
H(12E)-C(12B)-H(12F)	109.5
C(9A)-C(13)-C(14A)	105.1(9)
C(9A)-C(13)-C(15B)	125.8(7)
C(14A)-C(13)-C(15B)	90.7(7)
C(9A)-C(13)-C(15A)	102.6(7)
C(14A)-C(13)-C(15A)	115.3(7)
C(14A)-C(13)-C(9B)	109.6(9)
C(15B)-C(13)-C(9B)	121.3(7)
C(15A)-C(13)-C(9B)	97.2(7)
C(9A)-C(13)-C(14B)	110.3(9)
C(15B)-C(13)-C(14B)	104.4(7)
C(15A)-C(13)-C(14B)	132.5(7)
C(9B)-C(13)-C(14B)	115.9(8)
C(9A)-C(13)-H(13)	111.1
C(14A)-C(13)-H(13)	111.1
C(15B)-C(13)-H(13)	110.3
C(15A)-C(13)-H(13)	111.1
C(9B)-C(13)-H(13)	111.8
C(14B)-C(13)-H(13)	88.0
C(13)-C(14A)-H(14A)	109.5
C(13)-C(14A)-H(14B)	109.5
H(14A)-C(14A)-H(14B)	109.5
C(13)-C(14A)-H(14C)	109.5
H(14A)-C(14A)-H(14C)	109.5
H(14B)-C(14A)-H(14C)	109.5
C(13)-C(15A)-H(15A)	109.5
C(13)-C(15A)-H(15B)	109.5

H(15A)-C(15A)-H(15B)	109.5
C(13)-C(15A)-H(15C)	109.5
H(15A)-C(15A)-H(15C)	109.5
H(15B)-C(15A)-H(15C)	109.5
C(13)-C(14B)-H(14D)	109.5
C(13)-C(14B)-H(14E)	109.5
H(14D)-C(14B)-H(14E)	109.5
C(13)-C(14B)-H(14F)	109.5
H(14D)-C(14B)-H(14F)	109.5
H(14E)-C(14B)-H(14F)	109.5
C(13)-C(15B)-H(15D)	109.5
C(13)-C(15B)-H(15E)	109.5
H(15D)-C(15B)-H(15E)	109.5
C(13)-C(15B)-H(15F)	109.5
H(15D)-C(15B)-H(15F)	109.5
H(15E)-C(15B)-H(15F)	109.5
C(21)-C(16)-C(17)	122.3(3)
C(21)-C(16)-N(2)	119.6(2)
C(17)-C(16)-N(2)	117.9(2)
C(18)-C(17)-C(16)	117.4(3)
C(18)-C(17)-C(22)	119.0(3)
C(16)-C(17)-C(22)	123.6(3)
C(19)-C(18)-C(17)	121.3(3)
C(19)-C(18)-H(18)	119.3
C(17)-C(18)-H(18)	119.3
C(20)-C(19)-C(18)	119.8(3)
C(20)-C(19)-H(19)	120.1
C(18)-C(19)-H(19)	120.1
C(19)-C(20)-C(21)	122.1(3)
C(19)-C(20)-H(20)	118.9
C(21)-C(20)-H(20)	118.9
C(20)-C(21)-C(16)	117.0(3)
C(20)-C(21)-C(25)	119.6(3)
C(16)-C(21)-C(25)	123.3(3)
C(17)-C(22)-C(24)	111.1(3)
C(17)-C(22)-C(23)	112.1(3)

C(24)-C(22)-C(23)	109.5(3)
C(17)-C(22)-H(22)	108.0
C(24)-C(22)-H(22)	108.0
C(23)-C(22)-H(22)	108.0
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(27B)-C(25)-C(21)	117.9(7)
C(27B)-C(25)-C(26B)	109.4(8)
C(21)-C(25)-C(26B)	115.4(6)
C(21)-C(25)-C(27A)	107.2(7)
C(26B)-C(25)-C(27A)	125.5(8)
C(27B)-C(25)-C(26A)	95.0(8)
C(21)-C(25)-C(26A)	103.8(5)
C(27A)-C(25)-C(26A)	110.2(8)
C(27B)-C(25)-H(25)	114.7
C(21)-C(25)-H(25)	111.7
C(26B)-C(25)-H(25)	82.7
C(27A)-C(25)-H(25)	111.7
C(26A)-C(25)-H(25)	111.7
C(25)-C(26A)-H(26A)	109.5
C(25)-C(26A)-H(26B)	109.5
H(26A)-C(26A)-H(26B)	109.5
C(25)-C(26A)-H(26C)	109.5
H(26A)-C(26A)-H(26C)	109.5
H(26B)-C(26A)-H(26C)	109.5
C(25)-C(27A)-H(27A)	109.5

C(25)-C(27A)-H(27B)	109.5
H(27A)-C(27A)-H(27B)	109.5
C(25)-C(27A)-H(27C)	109.5
H(27A)-C(27A)-H(27C)	109.5
H(27B)-C(27A)-H(27C)	109.5
C(25)-C(26B)-H(26D)	109.5
C(25)-C(26B)-H(26E)	109.5
H(26D)-C(26B)-H(26E)	109.5
C(25)-C(26B)-H(26F)	109.5
H(26D)-C(26B)-H(26F)	109.5
H(26E)-C(26B)-H(26F)	109.5
C(25)-C(27B)-H(27D)	109.5
C(25)-C(27B)-H(27E)	109.5
H(27D)-C(27B)-H(27E)	109.5
C(25)-C(27B)-H(27F)	109.5
H(27D)-C(27B)-H(27F)	109.5
H(27E)-C(27B)-H(27F)	109.5
O(1)-C(28)-C(33)	121.4(3)
O(1)-C(28)-C(29)	121.6(2)
C(33)-C(28)-C(29)	116.9(2)
C(30)-C(29)-C(28)	119.8(2)
C(30)-C(29)-C(34)	121.0(2)
C(28)-C(29)-C(34)	119.2(2)
C(29)-C(30)-C(31)	123.2(3)
C(29)-C(30)-H(30)	118.4
C(31)-C(30)-H(30)	118.4
C(32)-C(31)-C(30)	116.8(3)
C(32)-C(31)-C(38)	121.6(3)
C(30)-C(31)-C(38)	121.6(3)
C(31)-C(32)-C(33)	123.7(3)
C(31)-C(32)-H(32)	118.2
C(33)-C(32)-H(32)	118.2
C(32)-C(33)-C(28)	119.3(3)
C(32)-C(33)-C(39A)	121.2(3)
C(28)-C(33)-C(39A)	118.9(3)
C(32)-C(33)-C(39B)	117.2(3)

C(28)-C(33)-C(39B)	120.1(3)
C(37)-C(34)-C(36)	109.5(3)
C(37)-C(34)-C(35)	107.9(3)
C(36)-C(34)-C(35)	106.7(2)
C(37)-C(34)-C(29)	109.0(2)
C(36)-C(34)-C(29)	111.0(2)
C(35)-C(34)-C(29)	112.7(2)
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(34)-C(37)-H(37A)	109.5
C(34)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(34)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(31)-C(38)-H(38A)	109.5
C(31)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(31)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(33)-C(39A)-C(42A)	111.4(3)
C(33)-C(39A)-C(40A)	109.3(4)
C(42A)-C(39A)-C(40A)	108.5(4)
C(33)-C(39A)-C(41A)	111.5(4)
C(42A)-C(39A)-C(41A)	105.2(4)

C(40A)-C(39A)-C(41A)	110.7(4)
C(39A)-C(40A)-H(40A)	109.5
C(39A)-C(40A)-H(40B)	109.5
H(40A)-C(40A)-H(40B)	109.5
C(39A)-C(40A)-H(40C)	109.5
H(40A)-C(40A)-H(40C)	109.5
H(40B)-C(40A)-H(40C)	109.5
C(39A)-C(41A)-H(41A)	109.5
C(39A)-C(41A)-H(41B)	109.5
H(41A)-C(41A)-H(41B)	109.5
C(39A)-C(41A)-H(41C)	109.5
H(41A)-C(41A)-H(41C)	109.5
H(41B)-C(41A)-H(41C)	109.5
C(39A)-C(42A)-H(42A)	109.5
C(39A)-C(42A)-H(42B)	109.5
H(42A)-C(42A)-H(42B)	109.5
C(39A)-C(42A)-H(42C)	109.5
H(42A)-C(42A)-H(42C)	109.5
H(42B)-C(42A)-H(42C)	109.5
C(40B)-C(39B)-C(42B)	112.6(4)
C(40B)-C(39B)-C(41B)	116.3(6)
C(42B)-C(39B)-C(41B)	102.8(7)
C(40B)-C(39B)-C(33)	112.6(2)
C(42B)-C(39B)-C(33)	113.6(6)
C(41B)-C(39B)-C(33)	97.9(6)
C(39B)-C(40B)-H(40D)	109.5
C(39B)-C(40B)-H(40E)	109.5
H(40D)-C(40B)-H(40E)	109.5
C(39B)-C(40B)-H(40F)	109.5
H(40D)-C(40B)-H(40F)	109.5
H(40E)-C(40B)-H(40F)	109.5
C(39B)-C(41B)-H(41D)	109.5
C(39B)-C(41B)-H(41E)	109.5
H(41D)-C(41B)-H(41E)	109.5
C(39B)-C(41B)-H(41F)	109.5
H(41D)-C(41B)-H(41F)	109.5

H(41E)-C(41B)-H(41F)	109.5
C(39B)-C(42B)-H(42D)	109.5
C(39B)-C(42B)-H(42E)	109.5
H(42D)-C(42B)-H(42E)	109.5
C(39B)-C(42B)-H(42F)	109.5
H(42D)-C(42B)-H(42F)	109.5
H(42E)-C(42B)-H(42F)	109.5

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for $[CH_2N\ i\text{-}Pr_2C_6H_3]_2CH\cdots OC_6H_2CH_3(C(CH_3)_3)_2$.
The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	42(1)	18(1)	21(1)	1(1)	8(1)	3(1)
N(2)	31(1)	21(1)	20(1)	1(1)	2(1)	3(1)
O(1)	35(1)	33(1)	33(1)	-1(1)	-6(1)	-11(1)
C(1)	35(2)	21(1)	14(1)	-1(1)	-2(1)	2(1)
C(2)	46(2)	20(1)	32(2)	-1(1)	10(2)	7(1)
C(3)	41(2)	22(1)	32(2)	3(1)	9(1)	7(1)
C(4A)	58(3)	16(3)	30(2)	4(2)	27(2)	5(3)
C(5A)	63(3)	20(2)	30(2)	8(2)	27(3)	7(3)
C(6A)	58(4)	22(2)	32(3)	3(2)	25(3)	-1(3)
C(7A)	55(3)	25(2)	35(3)	2(3)	26(3)	-5(3)
C(8A)	57(3)	20(2)	37(3)	2(3)	25(3)	-3(2)
C(9A)	50(2)	16(2)	40(3)	4(2)	28(2)	-2(2)
C(4B)	59(3)	16(3)	31(2)	3(2)	25(2)	4(2)
C(5B)	62(3)	18(3)	30(2)	7(2)	31(3)	10(3)
C(6B)	59(4)	26(3)	33(3)	6(2)	29(3)	5(3)
C(7B)	57(4)	25(2)	34(3)	5(2)	26(3)	2(3)
C(8B)	54(3)	23(2)	36(3)	4(3)	25(3)	-1(2)
C(9B)	55(3)	16(3)	40(3)	3(2)	30(3)	-2(2)
C(10)	137(4)	49(2)	22(2)	0(2)	-3(2)	50(2)
C(11A)	113(9)	69(7)	26(4)	10(5)	-4(6)	46(6)
C(12A)	107(9)	75(7)	40(6)	-19(5)	-30(5)	49(6)
C(11B)	107(9)	54(6)	39(5)	9(5)	-3(6)	27(5)
C(12B)	92(7)	52(5)	34(6)	-20(4)	-2(5)	32(5)
C(13)	35(2)	50(2)	72(3)	-27(2)	16(2)	-13(2)
C(14A)	18(4)	96(10)	66(8)	-23(6)	10(4)	-13(5)
C(15A)	59(7)	69(7)	46(6)	-33(5)	19(5)	-31(5)
C(14B)	47(8)	89(10)	74(9)	-21(6)	-7(7)	4(6)
C(15B)	63(7)	68(7)	53(7)	-26(5)	-3(5)	-30(6)
C(16)	29(2)	25(2)	28(2)	6(1)	-3(1)	0(1)
C(17)	29(2)	33(2)	30(2)	6(1)	2(1)	1(1)
C(18)	38(2)	44(2)	40(2)	15(2)	4(2)	0(2)

C(19)	44(2)	43(2)	61(2)	19(2)	-7(2)	-14(2)
C(20)	49(2)	35(2)	60(2)	9(2)	-24(2)	-12(2)
C(21)	42(2)	26(2)	40(2)	6(1)	-14(2)	-2(2)
C(22)	47(2)	45(2)	27(2)	-2(1)	14(2)	-10(2)
C(23)	61(2)	80(3)	25(2)	-8(2)	7(2)	-1(2)
C(24)	73(3)	45(2)	47(2)	0(2)	32(2)	-5(2)
C(25)	64(2)	38(2)	39(2)	-7(1)	-20(2)	-3(2)
C(26A)	84(9)	103(11)	30(6)	-5(6)	-23(6)	36(7)
C(27A)	57(6)	55(5)	55(7)	-21(4)	-14(5)	7(4)
C(26B)	76(8)	66(7)	36(5)	4(4)	-10(5)	2(6)
C(27B)	71(6)	48(4)	56(6)	-13(4)	-17(5)	6(4)
C(28)	29(2)	24(1)	30(2)	3(1)	-7(1)	-1(1)
C(29)	30(2)	16(1)	29(2)	0(1)	-3(1)	3(1)
C(30)	28(2)	21(1)	35(2)	2(1)	5(1)	1(1)
C(31)	27(2)	22(1)	37(2)	1(1)	-6(1)	0(1)
C(32)	35(2)	36(2)	27(2)	2(1)	-10(1)	-7(1)
C(33)	37(2)	44(2)	26(2)	4(1)	-8(1)	-12(2)
C(34)	44(2)	22(1)	30(2)	-5(1)	3(1)	-5(1)
C(35)	80(3)	41(2)	32(2)	-7(2)	13(2)	-22(2)
C(36)	67(2)	28(2)	52(2)	-12(2)	17(2)	-6(2)
C(37)	64(2)	42(2)	28(2)	-6(1)	-16(2)	3(2)
C(38)	38(2)	35(2)	45(2)	-2(1)	-6(2)	-5(2)
C(39A)	40(2)	49(3)	22(2)	-4(2)	3(2)	-19(2)
C(40A)	46(3)	54(3)	44(3)	-18(2)	13(2)	-25(3)
C(41A)	52(3)	55(3)	36(3)	15(2)	1(2)	-22(3)
C(42A)	62(4)	84(4)	33(3)	-7(3)	10(3)	-30(3)
C(39B)	51(4)	56(4)	27(3)	-6(4)	6(4)	-20(4)
C(40B)	44(6)	74(7)	41(6)	-7(6)	22(5)	-32(6)
C(41B)	66(6)	58(6)	30(5)	0(5)	-8(5)	-20(5)
C(42B)	42(5)	60(6)	22(4)	-9(5)	14(4)	-12(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[CH_2N\ i\text{-}Pr_2C_6H_3]_2CH\cdots OC_6H_2CH_3(C(CH_3)_3)_2$.

	x	y	z	U(eq)
H(1)	4430(20)	742(14)	2671(13)	28
H(2A)	3459	2598	2034	39
H(2B)	4215	2695	2753	39
H(3A)	2344	2362	3261	38
H(3B)	1741	2091	2547	38
H(6A)	6699	1778	326	45
H(7A)	8687	1899	868	46
H(8A)	8837	1917	2063	45
H(6B)	5940	1617	228	47
H(7B)	8080	1859	566	46
H(8B)	8613	1998	1707	45
H(10)	3334	1494	1266	83
H(11A)	3010	2179	181	104
H(11B)	4562	2194	71	104
H(11C)	3917	2619	688	104
H(12A)	3371	767	260	111
H(12B)	4519	521	761	111
H(12C)	4850	995	113	111
H(11D)	2413	1733	252	100
H(11E)	3780	1940	-90	100
H(11F)	3146	2427	483	100
H(12D)	2801	706	519	89
H(12E)	3774	447	1107	89
H(12F)	4315	581	351	89
H(13)	6265	1774	3198	63
H(14A)	8353	1525	3588	90
H(14B)	8937	1651	2838	90
H(14C)	7988	1007	2978	90
H(15A)	6479	2970	2849	87
H(15B)	7988	2859	2658	87

H(15C)	7535	2850	3442	87
H(14D)	7949	1329	3749	105
H(14E)	8679	1203	3036	105
H(14F)	7308	832	3186	105
H(15D)	7768	2485	3751	92
H(15E)	7185	2966	3159	92
H(15F)	8589	2611	3065	92
H(18)	467	627	4755	49
H(19)	-542	-220	4099	59
H(20)	36	-367	2971	58
H(22)	3002	1772	4198	48
H(23A)	2105	1124	5428	83
H(23B)	3359	1614	5353	83
H(23C)	3368	856	5024	83
H(24A)	1684	2473	4911	82
H(24B)	528	1916	4867	82
H(24C)	965	2332	4197	82
H(25)	2495	565	2024	56
H(26A)	560	458	1299	108
H(26B)	257	997	1901	108
H(26C)	-288	222	1947	108
H(27A)	2162	-580	1584	84
H(27B)	1174	-749	2196	84
H(27C)	2698	-640	2350	84
H(26D)	1011	1231	1855	89
H(26E)	95	599	1628	89
H(26F)	1435	745	1230	89
H(27D)	1914	-447	1406	87
H(27E)	836	-654	1963	87
H(27F)	2359	-731	2138	87
H(30)	1296	3568	2809	34
H(32)	2532	3705	871	39
H(35A)	2280	4018	4413	76
H(35B)	2168	3415	3855	76
H(35C)	1232	4077	3808	76
H(36A)	2150	5227	3511	74

H(36B)	3691	5314	3392	74
H(36C)	3142	5132	4138	74
H(37A)	5147	4251	3412	67
H(37B)	4523	3522	3626	67
H(37C)	4633	4133	4176	67
H(38A)	897	2733	1316	59
H(38B)	11	3414	1264	59
H(38C)	71	2987	1965	59
H(40A)	6551	4625	813	72
H(40B)	6112	3901	1139	72
H(40C)	6212	4576	1610	72
H(41A)	3465	5475	768	72
H(41B)	5008	5585	679	72
H(41C)	4375	5569	1427	72
H(42A)	4772	4550	-54	90
H(42B)	3294	4411	178	90
H(42C)	4369	3814	259	90
H(40D)	6297	4243	1748	80
H(40E)	6902	4092	1008	80
H(40F)	6066	3508	1390	80
H(41D)	4710	5316	1246	77
H(41E)	4300	5149	473	77
H(41F)	5814	5206	675	77
H(42D)	3873	4111	102	62
H(42E)	4647	3430	334	62
H(42F)	5414	4051	-31	62

Table 6. Torsion angles [°] for$[CH_2N\ i\text{-}Pr_2C_6H_3]_2CH\cdots OC_6H_2CH_3(C(CH_3)_3)_2$.

C(4B)-N(1)-C(1)-N(2)	-174.8(7)
C(2)-N(1)-C(1)-N(2)	3.6(3)
C(4A)-N(1)-C(1)-N(2)	179.5(7)
C(16)-N(2)-C(1)-N(1)	165.8(2)
C(3)-N(2)-C(1)-N(1)	6.0(3)
C(1)-N(1)-C(2)-C(3)	-11.0(3)
C(4B)-N(1)-C(2)-C(3)	167.5(6)
C(4A)-N(1)-C(2)-C(3)	172.7(6)
C(1)-N(2)-C(3)-C(2)	-12.4(3)
C(16)-N(2)-C(3)-C(2)	-173.6(2)
N(1)-C(2)-C(3)-N(2)	13.2(3)
C(1)-N(1)-C(4A)-C(9A)	-79(2)
C(4B)-N(1)-C(4A)-C(9A)	-144(27)
C(2)-N(1)-C(4A)-C(9A)	97(2)
C(1)-N(1)-C(4A)-C(5A)	99.9(19)
C(4B)-N(1)-C(4A)-C(5A)	35(23)
C(2)-N(1)-C(4A)-C(5A)	-85(2)
C(9A)-C(4A)-C(5A)-C(6A)	-4(3)
N(1)-C(4A)-C(5A)-C(6A)	177.1(17)
C(9A)-C(4A)-C(5A)-C(10)	172(2)
N(1)-C(4A)-C(5A)-C(10)	-7(2)
C(4A)-C(5A)-C(6A)-C(7A)	2.5(16)
C(10)-C(5A)-C(6A)-C(7A)	-172.5(9)
C(5A)-C(6A)-C(7A)-C(8A)	-0.2(13)
C(6A)-C(7A)-C(8A)-C(9A)	-0.5(12)
C(5A)-C(4A)-C(9A)-C(13)	174.2(14)
N(1)-C(4A)-C(9A)-C(13)	-7(3)
C(5A)-C(4A)-C(9A)-C(8A)	4(3)
N(1)-C(4A)-C(9A)-C(8A)	-177.6(13)
C(7A)-C(8A)-C(9A)-C(13)	-172.9(9)
C(7A)-C(8A)-C(9A)-C(4A)	-1(2)
C(1)-N(1)-C(4B)-C(5B)	95.5(18)
C(2)-N(1)-C(4B)-C(5B)	-82.7(18)

C(4A)-N(1)-C(4B)-C(5B)	-146(27)
C(1)-N(1)-C(4B)-C(9B)	-94(2)
C(2)-N(1)-C(4B)-C(9B)	88(2)
C(4A)-N(1)-C(4B)-C(9B)	24(23)
C(9B)-C(4B)-C(5B)-C(10)	-174.7(19)
N(1)-C(4B)-C(5B)-C(10)	-5(3)
C(9B)-C(4B)-C(5B)-C(6B)	5(3)
N(1)-C(4B)-C(5B)-C(6B)	174.5(15)
C(10)-C(5B)-C(6B)-C(7B)	177.1(8)
C(4B)-C(5B)-C(6B)-C(7B)	-2.5(17)
C(5B)-C(6B)-C(7B)-C(8B)	0.9(12)
C(6B)-C(7B)-C(8B)-C(9B)	-1.2(13)
C(5B)-C(4B)-C(9B)-C(8B)	-5(3)
N(1)-C(4B)-C(9B)-C(8B)	-174.0(16)
C(5B)-C(4B)-C(9B)-C(13)	-177.5(16)
N(1)-C(4B)-C(9B)-C(13)	13(3)
C(7B)-C(8B)-C(9B)-C(4B)	3(2)
C(7B)-C(8B)-C(9B)-C(13)	175.0(10)
C(4B)-C(5B)-C(10)-C(12A)	-125.3(17)
C(6B)-C(5B)-C(10)-C(12A)	55.2(10)
C(4B)-C(5B)-C(10)-C(11B)	124.1(18)
C(6B)-C(5B)-C(10)-C(11B)	-55.5(13)
C(4B)-C(5B)-C(10)-C(11A)	120.1(17)
C(6B)-C(5B)-C(10)-C(11A)	-59.4(9)
C(4B)-C(5B)-C(10)-C(12B)	-98.1(17)
C(6B)-C(5B)-C(10)-C(12B)	82.4(9)
C(4B)-C(5B)-C(10)-C(5A)	156(8)
C(6B)-C(5B)-C(10)-C(5A)	-23(6)
C(6A)-C(5A)-C(10)-C(5B)	154(8)
C(4A)-C(5A)-C(10)-C(5B)	-21(7)
C(6A)-C(5A)-C(10)-C(12A)	50.9(13)
C(4A)-C(5A)-C(10)-C(12A)	-124.2(13)
C(6A)-C(5A)-C(10)-C(11B)	-54.7(14)
C(4A)-C(5A)-C(10)-C(11B)	130.2(14)
C(6A)-C(5A)-C(10)-C(11A)	-61.0(12)
C(4A)-C(5A)-C(10)-C(11A)	123.9(13)

C(6A)-C(5A)-C(10)-C(12B)	76.2(12)
C(4A)-C(5A)-C(10)-C(12B)	-98.9(14)
C(4A)-C(9A)-C(13)-C(14A)	141(2)
C(8A)-C(9A)-C(13)-C(14A)	-47.6(11)
C(4A)-C(9A)-C(13)-C(15B)	-116(2)
C(8A)-C(9A)-C(13)-C(15B)	54.6(13)
C(4A)-C(9A)-C(13)-C(15A)	-98(2)
C(8A)-C(9A)-C(13)-C(15A)	73.3(10)
C(4A)-C(9A)-C(13)-C(9B)	-77(9)
C(8A)-C(9A)-C(13)-C(9B)	94(9)
C(4A)-C(9A)-C(13)-C(14B)	117(2)
C(8A)-C(9A)-C(13)-C(14B)	-71.9(11)
C(4B)-C(9B)-C(13)-C(9A)	89(9)
C(8B)-C(9B)-C(13)-C(9A)	-83(9)
C(4B)-C(9B)-C(13)-C(14A)	128.3(18)
C(8B)-C(9B)-C(13)-C(14A)	-43.3(14)
C(4B)-C(9B)-C(13)-C(15B)	-128.3(18)
C(8B)-C(9B)-C(13)-C(15B)	60.1(14)
C(4B)-C(9B)-C(13)-C(15A)	-111.6(18)
C(8B)-C(9B)-C(13)-C(15A)	76.8(12)
C(4B)-C(9B)-C(13)-C(14B)	103.5(18)
C(8B)-C(9B)-C(13)-C(14B)	-68.2(13)
C(1)-N(2)-C(16)-C(21)	-55.7(4)
C(3)-N(2)-C(16)-C(21)	102.2(3)
C(1)-N(2)-C(16)-C(17)	128.3(3)
C(3)-N(2)-C(16)-C(17)	-73.8(3)
C(21)-C(16)-C(17)-C(18)	-0.4(4)
N(2)-C(16)-C(17)-C(18)	175.5(2)
C(21)-C(16)-C(17)-C(22)	-178.6(3)
N(2)-C(16)-C(17)-C(22)	-2.7(4)
C(16)-C(17)-C(18)-C(19)	0.1(4)
C(22)-C(17)-C(18)-C(19)	178.4(3)
C(17)-C(18)-C(19)-C(20)	0.1(5)
C(18)-C(19)-C(20)-C(21)	0.0(5)
C(19)-C(20)-C(21)-C(16)	-0.3(5)
C(19)-C(20)-C(21)-C(25)	-178.3(3)

C(17)-C(16)-C(21)-C(20)	0.5(4)
N(2)-C(16)-C(21)-C(20)	-175.3(3)
C(17)-C(16)-C(21)-C(25)	178.4(3)
N(2)-C(16)-C(21)-C(25)	2.6(4)
C(18)-C(17)-C(22)-C(24)	-68.4(3)
C(16)-C(17)-C(22)-C(24)	109.7(3)
C(18)-C(17)-C(22)-C(23)	54.4(4)
C(16)-C(17)-C(22)-C(23)	-127.4(3)
C(20)-C(21)-C(25)-C(27B)	-37.0(8)
C(16)-C(21)-C(25)-C(27B)	145.2(8)
C(20)-C(21)-C(25)-C(26B)	94.9(6)
C(16)-C(21)-C(25)-C(26B)	-82.9(6)
C(20)-C(21)-C(25)-C(27A)	-50.2(7)
C(16)-C(21)-C(25)-C(27A)	131.9(7)
C(20)-C(21)-C(25)-C(26A)	66.5(6)
C(16)-C(21)-C(25)-C(26A)	-111.4(6)
O(1)-C(28)-C(29)-C(30)	175.2(2)
C(33)-C(28)-C(29)-C(30)	-6.1(4)
O(1)-C(28)-C(29)-C(34)	-5.1(4)
C(33)-C(28)-C(29)-C(34)	173.6(3)
C(28)-C(29)-C(30)-C(31)	3.1(4)
C(34)-C(29)-C(30)-C(31)	-176.6(3)
C(29)-C(30)-C(31)-C(32)	1.0(4)
C(29)-C(30)-C(31)-C(38)	-178.9(3)
C(30)-C(31)-C(32)-C(33)	-1.9(4)
C(38)-C(31)-C(32)-C(33)	178.0(3)
C(31)-C(32)-C(33)-C(28)	-1.3(4)
C(31)-C(32)-C(33)-C(39A)	-172.3(3)
C(31)-C(32)-C(33)-C(39B)	158.0(4)
O(1)-C(28)-C(33)-C(32)	-176.0(3)
C(29)-C(28)-C(33)-C(32)	5.2(4)
O(1)-C(28)-C(33)-C(39A)	-4.9(5)
C(29)-C(28)-C(33)-C(39A)	176.4(3)
O(1)-C(28)-C(33)-C(39B)	25.3(5)
C(29)-C(28)-C(33)-C(39B)	-153.5(4)
C(30)-C(29)-C(34)-C(37)	120.9(3)

C(28)-C(29)-C(34)-C(37)	-58.9(3)
C(30)-C(29)-C(34)-C(36)	-118.4(3)
C(28)-C(29)-C(34)-C(36)	61.8(3)
C(30)-C(29)-C(34)-C(35)	1.2(4)
C(28)-C(29)-C(34)-C(35)	-178.6(3)
C(32)-C(33)-C(39A)-C(42A)	-7.4(5)
C(28)-C(33)-C(39A)-C(42A)	-178.4(3)
C(39B)-C(33)-C(39A)-C(42A)	81.5(5)
C(32)-C(33)-C(39A)-C(40A)	-127.4(4)
C(28)-C(33)-C(39A)-C(40A)	61.6(5)
C(39B)-C(33)-C(39A)-C(40A)	-38.4(5)
C(32)-C(33)-C(39A)-C(41A)	109.8(4)
C(28)-C(33)-C(39A)-C(41A)	-61.1(5)
C(39B)-C(33)-C(39A)-C(41A)	-161.2(7)
C(32)-C(33)-C(39B)-C(40B)	-117.1(2)
C(28)-C(33)-C(39B)-C(40B)	42.0(3)
C(39A)-C(33)-C(39B)-C(40B)	137.0(5)
C(32)-C(33)-C(39B)-C(42B)	12.4(6)
C(28)-C(33)-C(39B)-C(42B)	171.5(5)
C(39A)-C(33)-C(39B)-C(42B)	-93.4(7)
C(32)-C(33)-C(39B)-C(41B)	120.1(6)
C(28)-C(33)-C(39B)-C(41B)	-80.8(6)
C(39A)-C(33)-C(39B)-C(41B)	14.3(7)

Table 7. Hydrogen bonds for $[CH_2N\ i\text{-}Pr_2C_6H_3]_2CH\cdots OC_6H_2CH_3(C(CH_3)_3)_2$ [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(1)-H(1)...O(1)#1	1.00(3)	1.89(3)	2.886(3)	175(2)

Symmetry transformations used to generate equivalent atoms:

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

Table 8. Least-squares planes (x,y,z in crystal coordinates) and deviations from them for $[CH_2N\ i\text{-}Pr_2C_6H_3]_2CH\cdots OC_6H_2CH_3(C(CH_3)_3)_2$ (* indicates atom used to define plane).

Plane 1

5.2707 (0.0120) x + 4.8658 (0.0269) y + 16.0124 (0.0151) z = 6.9811 (0.0025)

* -0.0490 (0.0016) N1
* 0.0594 (0.0016) N2
* -0.0067 (0.0016) C1
* 0.0764 (0.0017) C2
* -0.0801 (0.0017) C3

Rms deviation of fitted atoms = 0.0604

Plane 2

7.1985 (0.0090) x - 12.6539 (0.0182) y + 5.3380 (0.0232) z = 2.0784 (0.0086)

Angle to plane 1 (with approximate esd) = 65.05 (0.10)

* -0.0026 (0.0020) C16
* 0.0010 (0.0020) C17
* 0.0009 (0.0022) C18
* -0.0011 (0.0023) C19
* -0.0004 (0.0023) C20
* 0.0023 (0.0021) C21

Rms deviation of fitted atoms = 0.0016

Plane 3

- 1.0363 (0.0772) x + 19.2114 (0.0144) y - 0.4101 (0.1065) z = 2.6923 (0.0569)

Angle to plane 1 (with approximate esd) = 79.57 (0.36)

* 0.0218 (0.0154) C4A_a
* -0.0179 (0.0102) C5A_a
* 0.0033 (0.0065) C6A_a

* 0.0079 (0.0071) C7A_a

* -0.0046 (0.0066) C8A_a

* -0.0105 (0.0129) C9A_a

Rms deviation of fitted atoms = 0.0129

Plane 4

- 1.8286 (0.0765) x + 18.9326 (0.0242) y - 1.6597 (0.1147) z = 1.9485 (0.0533)

Angle to plane 1 (with approximate esd) = 85.12 (0.37)

Angle to plane 3 (with approximate esd) = 5.82 (0.30)

* -0.0231 (0.0156) C4B_b

* 0.0147 (0.0103) C5B_b

* -0.0016 (0.0063) C6B_b

* -0.0025 (0.0071) C7B_b

* -0.0054 (0.0068) C8B_b

* 0.0178 (0.0126) C9B_b

Rms deviation of fitted atoms = 0.0136

Plane 5

- 5.8835 (0.0089) x + 15.5973 (0.0121) y - 2.5042 (0.0226) z = 4.0955 (0.0089)

Angle to plane 1 (with approximate esd) = 78.55 (0.10)

* 0.0342 (0.0020) C28

* -0.0256 (0.0018) C29

* -0.0006 (0.0018) C30

* 0.0187 (0.0019) C31

* -0.0094 (0.0020) C32

* -0.0172 (0.0021) C33

0.1061 (0.0037) O1

Rms deviation of fitted atoms = 0.0207