A chiral spiroborate anion from diphenyl-L-tartramide

$[B\{L\text{-}Tar(NHPh)_2\}_2]^-$ applied to some challenging resolutions

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Supplementary Material

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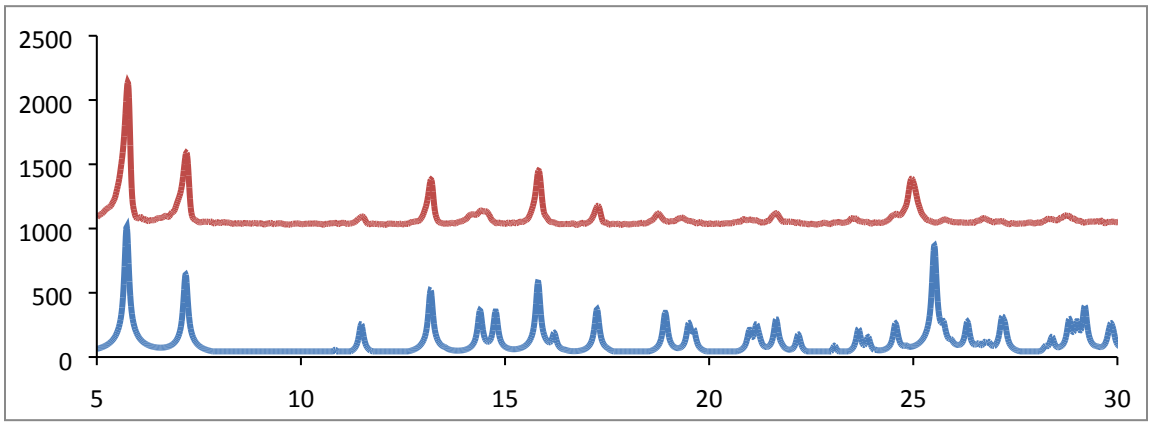
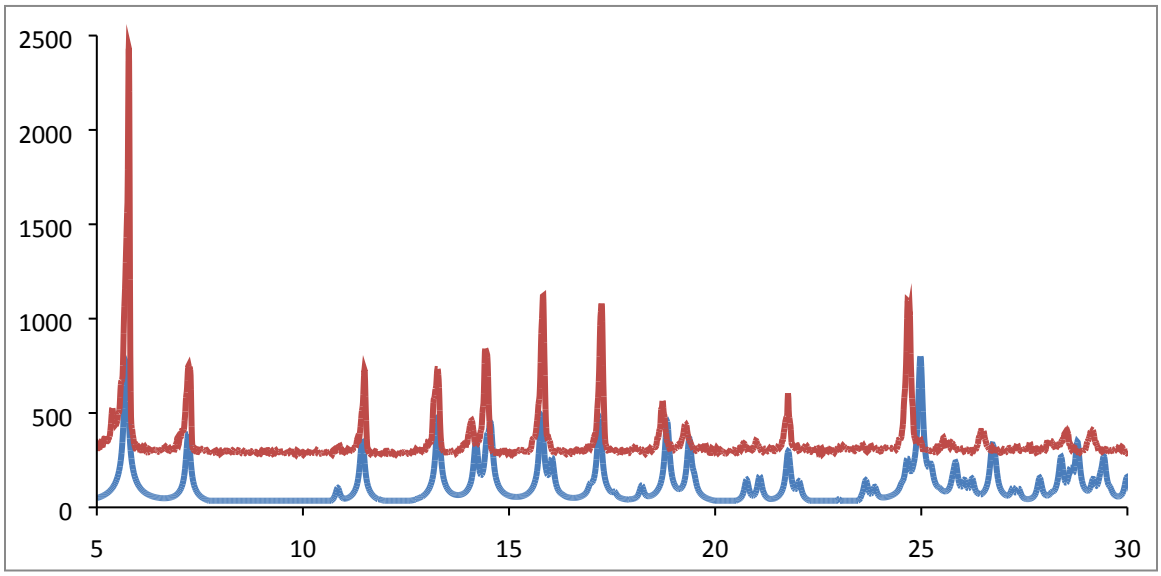
Powder XRD Data

Phase purity of the bis(diphenyltartramido)borate salts described products described is shown by powder X-ray diffraction patterns (PANalytical, Xpert Pro) 2θ range 5-50°, step size 0.02°. The top pattern is experimental, lower pattern is that simulated from a single XRD of the sample.

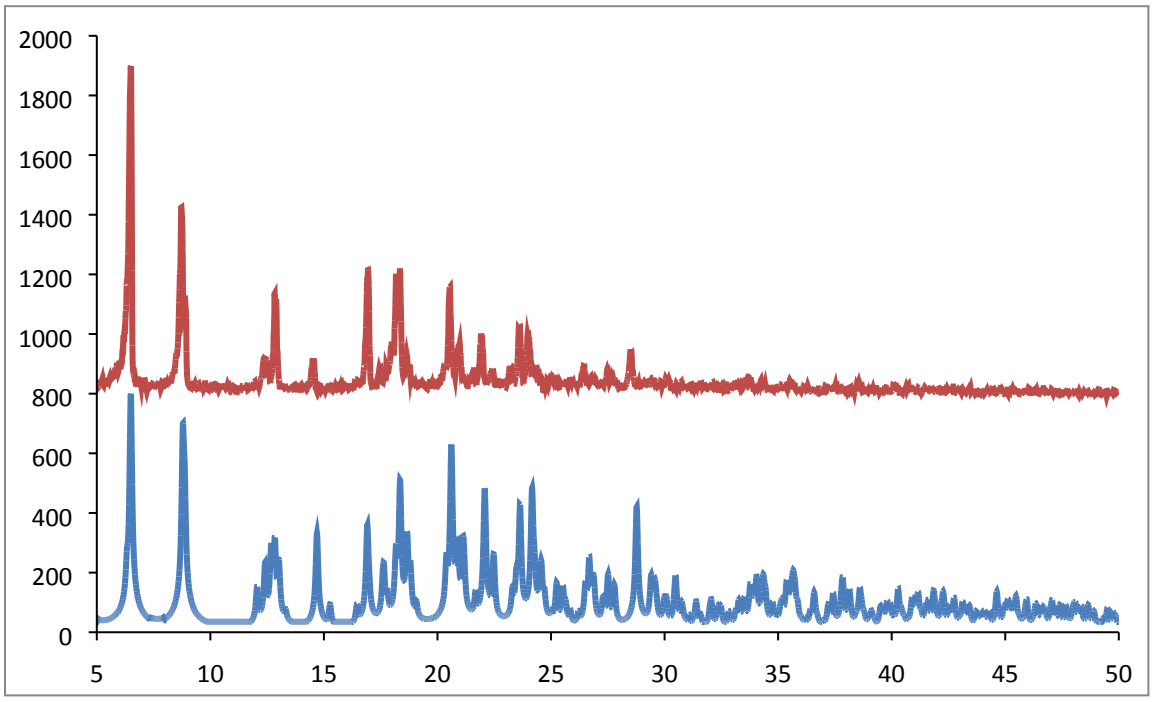
K [B{Tar(NHPh)$_2$}$_2$] (2) gem81



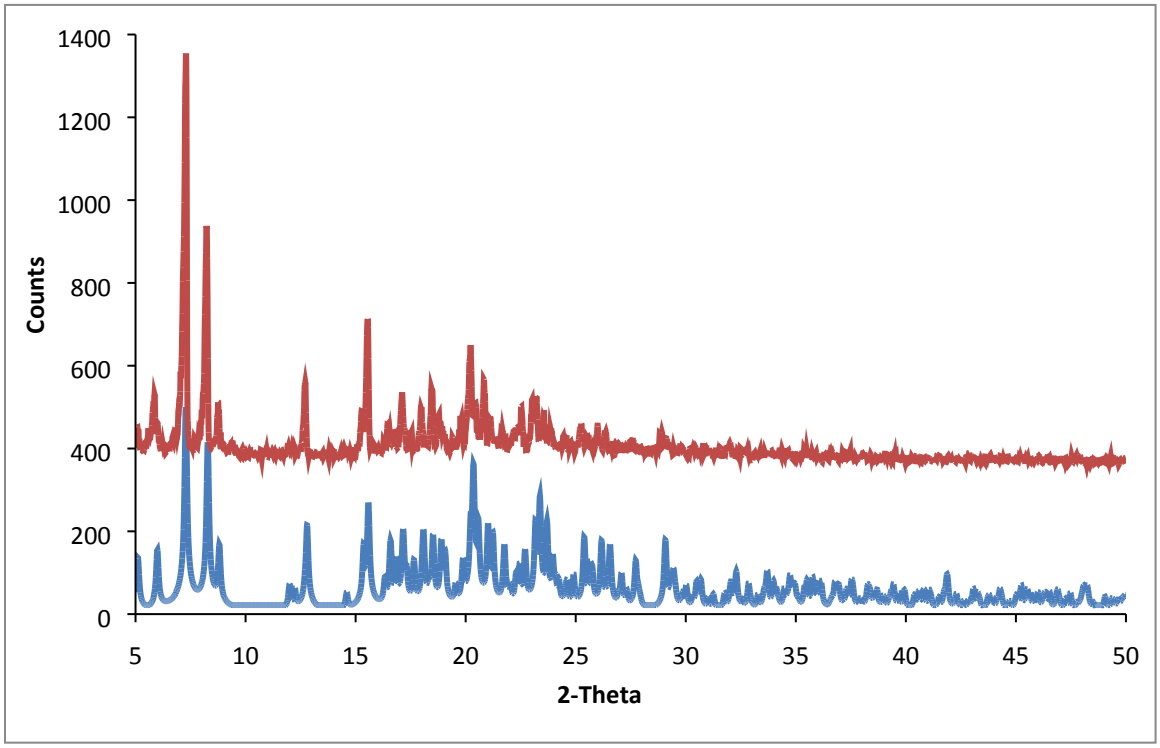
[NH4] [B{Tar(NHPh)$_2$}$_2$] (3) gem 57



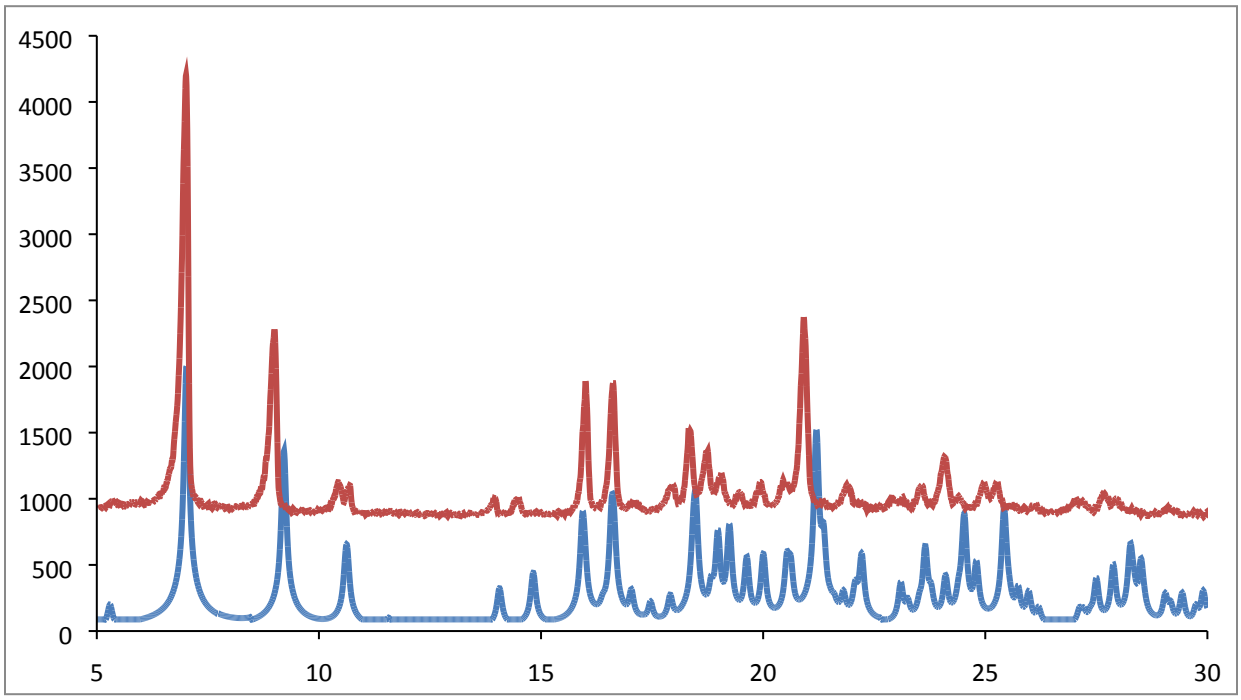
Na [B{Tar(NHPh)$_2$}$_2$] 2MeOH (4) gem84



[NH$_3$CHMeEt] [B{Tar(NHPh)$_2$}$_2$] (5) gem71a

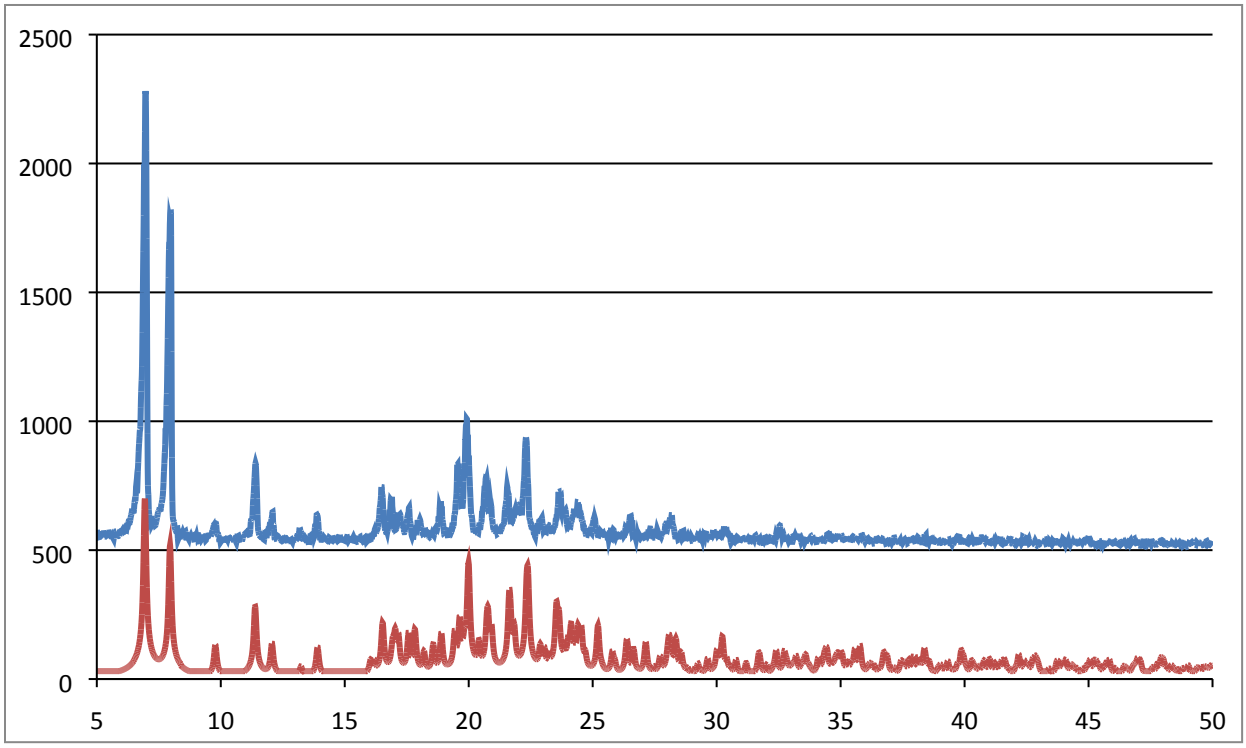


[R/(S)-$NH_3CHMePr$] [$B\{Tar(NHPh)_2\}_2$] (6) lawr 435

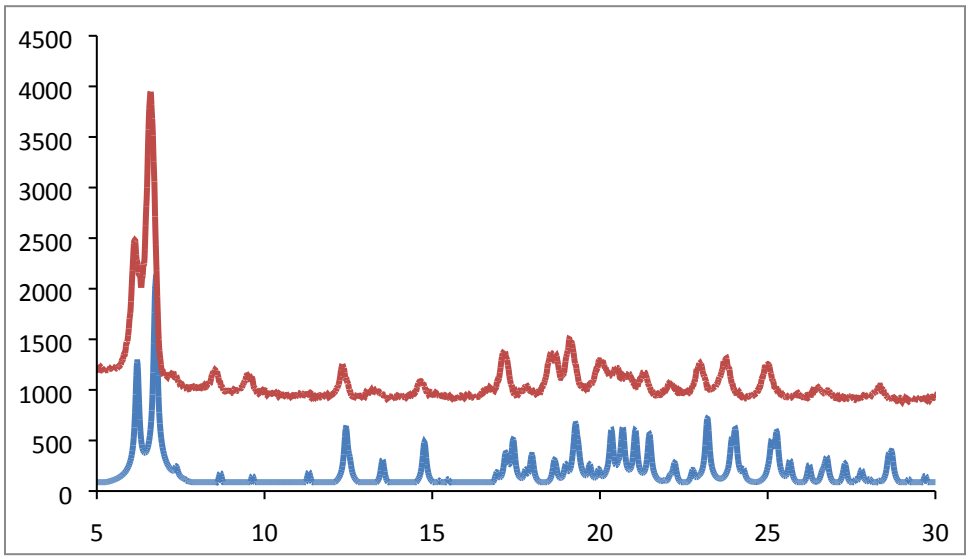


Note peaks around 11° are for [002] and [021] diffraction maxima, which are split at RT.

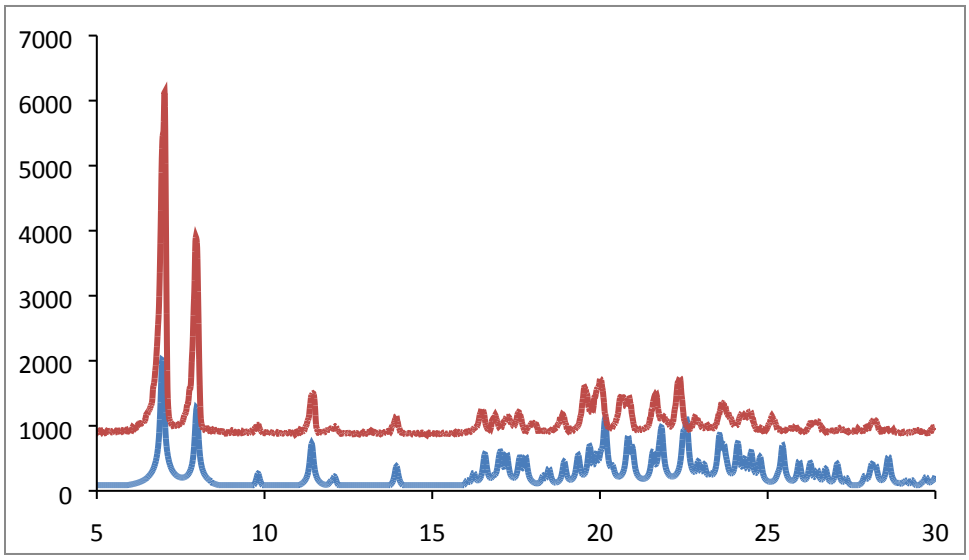
[$NH_3CHMePh$][$B\{Tar(NHPh)_2\}_2$] MeOH (7) gem64a



[S-NH_3CHEtPh][B{Tar$(NHPh)_2\}_2$] MeOH (8)

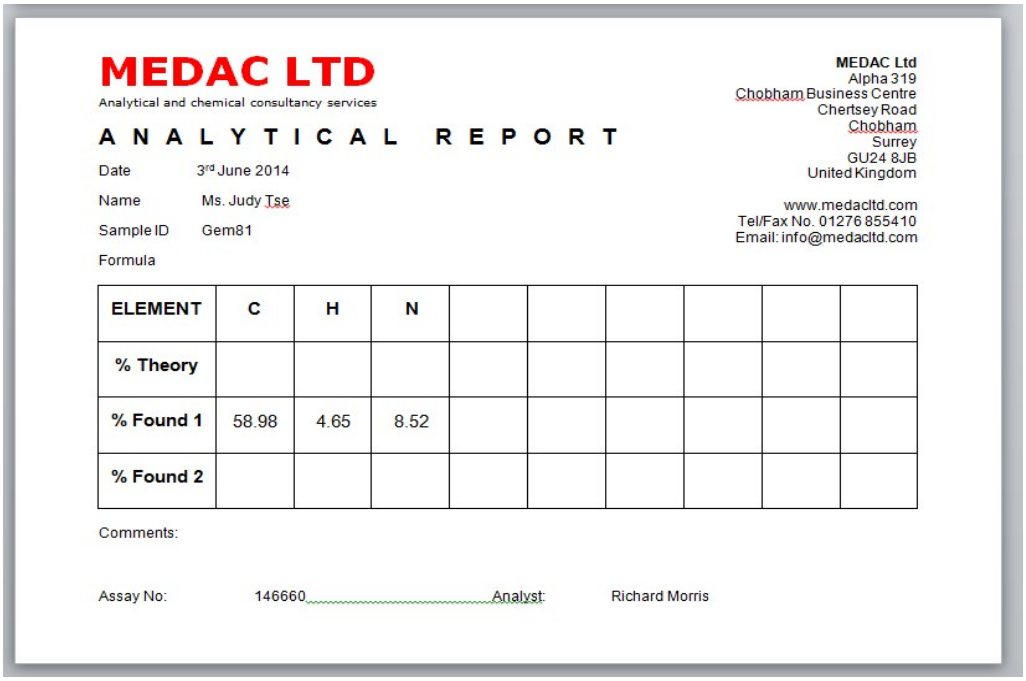


[S-NH_3CH(CH_2OH)Ph][B{Tar$(NHPh)_2\}_2$] MeOH (9)



Elemental Combustion (CHN) Analysis
Analyses listed in the manuscript obtained from Medac Ltd, Surrey, U.K.

K [B{Tar(NHPh)$_2$}$_2$] (2) (gem81)



MEDAC LTD
Analytical and chemical consultancy services

A N A L Y T I C A L R E P O R T

Date 3rd June 2014
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Formula

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Tel/Fax No. 01276 855410
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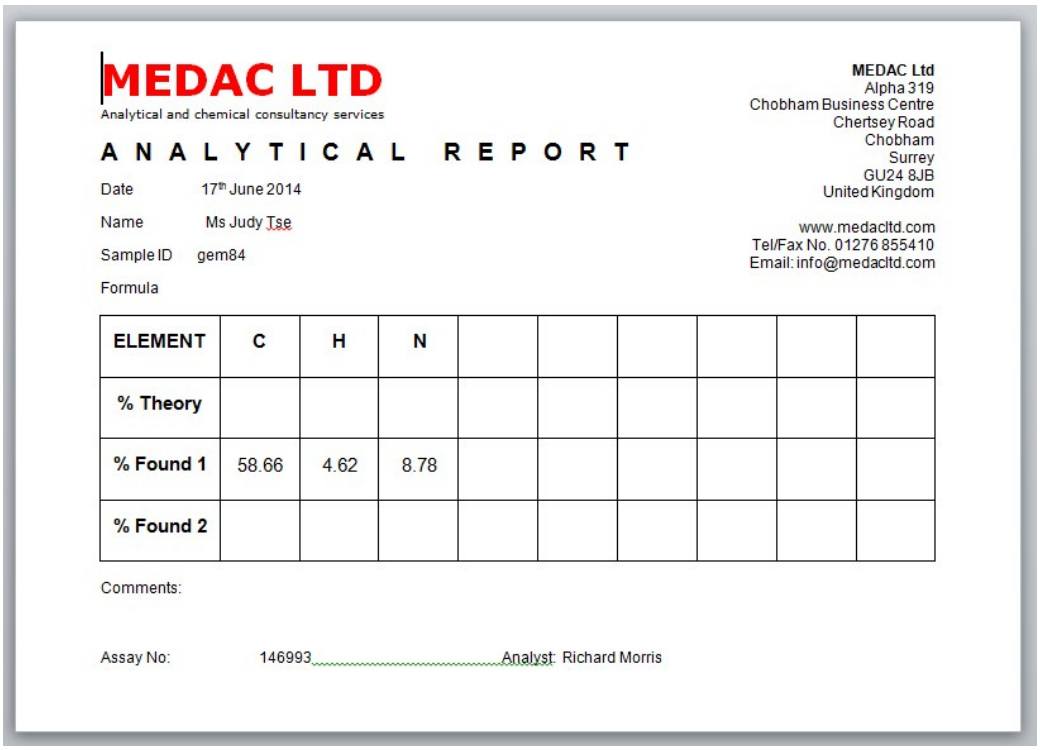
ELEMENT	C	H	N						
% Theory									
% Found 1	58.98	4.65	8.52						
% Found 2									

Comments:

Assay No: 146660 Analyst: Richard Morris

Na [B{Tar(NHPh)$_2$}$_2$] .2MeOH (4)



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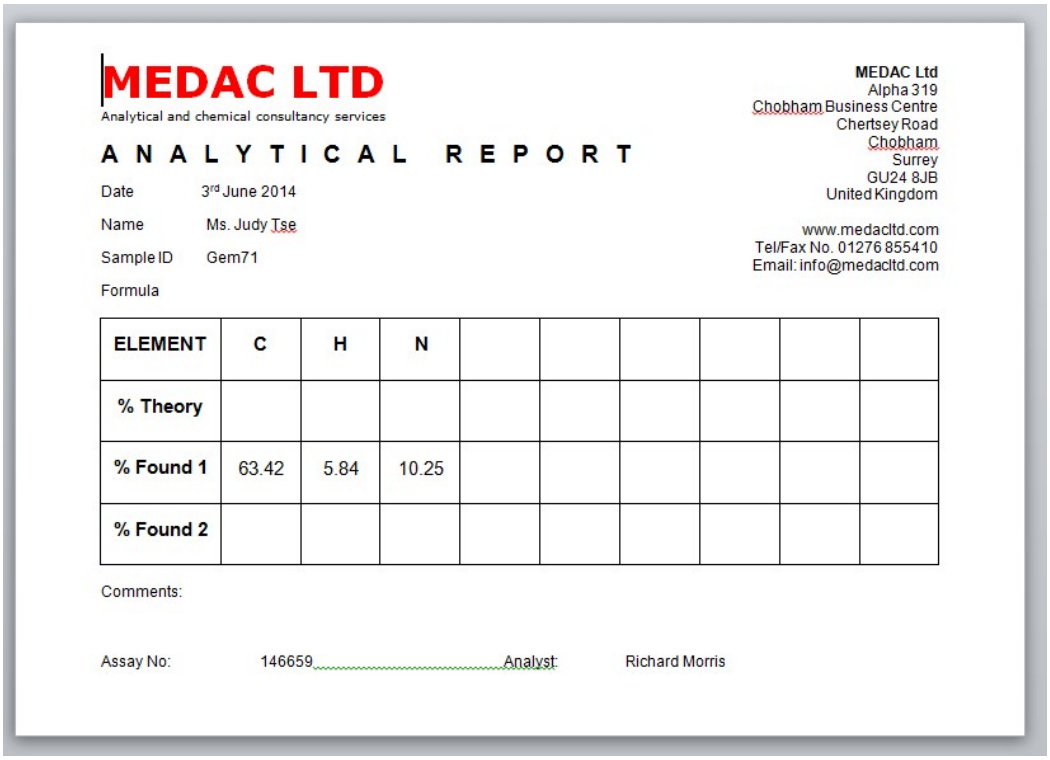
ELEMENT	C	H	N						
% Theory									
% Found 1	58.66	4.62	8.78						
% Found 2									

Comments:

Assay No: 146993 Analyst: Richard Morris

[$NH_3CHMeEt$] [$B\{Tar(NHPh)_2\}_2$] (5) gem71a



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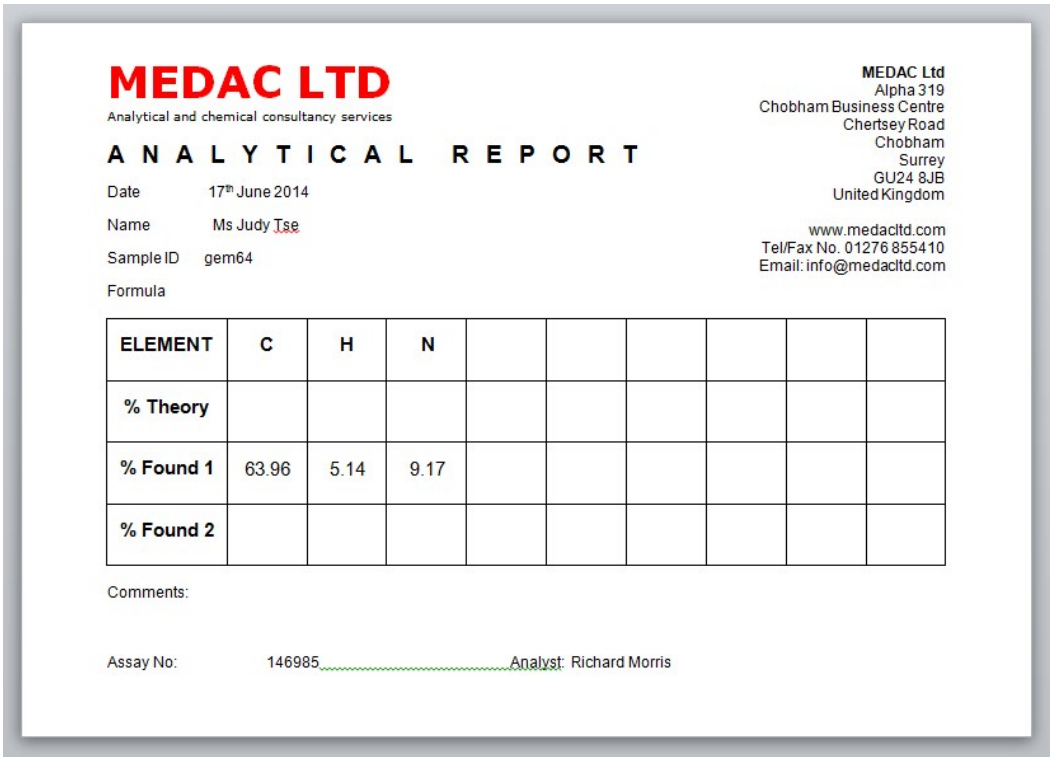
ELEMENT	C	H	N						
% Theory									
% Found 1	63.42	5.84	10.25						
% Found 2									

Comments:

Assay No: 146659 Analyst: Richard Morris

[$NH_3CHMePh$] [$B\{Tar(NHPh)_2\}_2$] MeOH (7) gem64a



MEDAC LTD

Analytical and chemical consultancy services

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Date 17th June 2014

Name Ms Judy Tse

Sample ID gem64

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ELEMENT	C	H	N						
% Theory									
% Found 1	63.96	5.14	9.17						
% Found 2									

Comments:

Assay No: 146985 Analyst: Richard Morris

Single Crystal Structure Determinations for 2-9

Compound 2 K[B{Tar(NHPh)$_2$}$_2$]

Table 2.1 Crystal data and structure refinement for **2** K[B{Tar(NHPh)$_2$}$_2$]

Identification code	gem81a
Empirical formula	$C_{32}H_{28}BKN_4O_8$
Formula weight	646.49
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	C2
a/Å	30.9006(5)
b/Å	13.4265(2)
c/Å	6.99592(11)
α/°	90
β/°	94.2992(14)
γ/°	90
Volume/Å^3	2894.34(8)
Z	4
ρ_{calc}g/cm^3	1.484
μ/mm^{-1}	2.137
F(000)	1344.0
Crystal size/mm^3	0.05 × 0.03 × 0.02
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	10.846 to 135.998
Index ranges	-37 ≤ h ≤ 36, -15 ≤ k ≤ 16, -7 ≤ l ≤ 8
Reflections collected	10784
Independent reflections	4836 [R_{int} = 0.0202, R_{sigma} = 0.0246]
Data/restraints/parameters	4836/1/417
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0336, wR_2 = 0.0873
Final R indexes [all data]	R_1 = 0.0348, wR_2 = 0.0884
Largest diff. peak/hole / e Å^{-3}	0.95/-0.20
Flack parameter	0.015(4)

Table 2.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **2** K[B{Tar(NHPh)$_2$}$_2$].

U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*Z*	U(eq)
B1	5000	2735(4)	5000	14.9(10)
C1	4022.2(9)	1374(2)	4320(4)	14.8(6)
K1	5000	3293.8(6)	10000	14.5(2)
N1	4271.2(8)	567(2)	4661(4)	14.8(5)
O1	3627.0(7)	1431.3(18)	4411(3)	20.6(5)
B2	5000	5770(4)	10000	12.2(10)
C2	4278.5(9)	2305(2)	3848(4)	14.4(6)
K2	5000	5233.0(6)	5000	15.1(2)
O2	4723.4(6)	2115.5(16)	3657(3)	16.0(5)
C3	4267.5(9)	3061(2)	5552(4)	13.2(6)
O3	4698.3(6)	3360.5(16)	5973(3)	14.1(4)
C4	3971.4(10)	3953(2)	5026(4)	13.3(6)
N4	3546.7(8)	3690(2)	4844(4)	17.9(6)
O4	4114.4(7)	4797.2(18)	4832(3)	16.1(5)
C11	4025.1(9)	7098(2)	10455(4)	14.1(6)
N11	4252.3(8)	7949(2)	10566(4)	14.7(5)
O11	3634.8(7)	7008.4(18)	9974(3)	19.9(5)
C12	4297.0(9)	6178(2)	10956(4)	14.2(6)
O12	4746.3(6)	6378.5(17)	11280(3)	16.4(4)
C13	4254.1(9)	5439(2)	9219(4)	12.4(6)
O13	4679.9(6)	5145.8(16)	8927(3)	13.5(4)
C14	3971.7(9)	4538(2)	9607(4)	12.7(6)
N14	3546.1(8)	4777(2)	9603(4)	16.6(6)
O14	4123.6(7)	3699.9(18)	9874(3)	17.0(5)
C21	4153.0(10)	-435(3)	4940(4)	15.1(6)
C22	4475.0(11)	-1071(3)	5736(4)	18.2(7)
C23	4391.7(11)	-2083(3)	5890(5)	21.6(7)
C24	3988.7(12)	-2459(3)	5298(5)	23.7(7)
C25	3667.3(11)	-1817(3)	4512(5)	22.5(7)
C26	3743.9(10)	-806(3)	4331(4)	17.9(7)
C31	3175.6(10)	4316(3)	4605(5)	17.5(7)
C32	2773.8(10)	3833(3)	4415(5)	19.9(7)
C33	2395.1(10)	4391(3)	4280(5)	23.1(7)
C34	2407.7(11)	5419(3)	4359(5)	25.5(8)
C35	2808.4(12)	5889(3)	4499(7)	33.5(9)
C36	3192.6(11)	5339(3)	4612(6)	31.9(9)
C41	4120.0(11)	8930(3)	10103(4)	15.9(7)
C42	3701.8(10)	9172(3)	9353(5)	18.2(7)
C43	3604.5(11)	10160(3)	8923(5)	23.2(7)
C44	3914.0(12)	10900(3)	9189(5)	24.6(7)
C45	4328.2(13)	10654(3)	9932(5)	25.2(8)

C46	4429.6(11)	9677(3)	10398(5)	19.2(7)
C51	3180.1(10)	4152(3)	9651(4)	17.5(7)
C52	2774.0(11)	4593(3)	9284(5)	22.8(7)
C53	2401.6(11)	4017(3)	9238(5)	28.1(9)
C54	2426.5(12)	3002(3)	9553(6)	31.8(9)
C55	2829.6(12)	2562(3)	9953(6)	30.8(9)
C56	3208.4(11)	3131(3)	10003(6)	24.8(8)

Table 2.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **2** K[B{Tar(NHPh)$_2$}$_2$].
The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
B1	15(2)	12(3)	18(2)	0	-1.2(19)	0
C1	12.3(14)	16.3(15)	15.5(14)	-4.1(12)	-0.2(11)	-2.7(12)
K1	11.9(4)	12.8(5)	18.6(4)	0	0.9(3)	0
N1	11.0(12)	13.8(13)	19.9(13)	0.2(10)	2.7(10)	-3.3(10)
O1	14.0(11)	18.9(12)	29.2(12)	0.5(10)	3.7(9)	-1.1(9)
B2	6(2)	13(3)	17(2)	0	0.4(17)	0
C2	10.2(13)	14.4(15)	18.8(15)	-1.8(12)	1.8(10)	-1.0(11)
K2	11.8(4)	14.8(5)	18.6(4)	0	1.1(3)	0
O2	10.9(10)	16.4(11)	21.1(11)	-6.2(9)	3.8(8)	-2.0(8)
C3	9.1(13)	14.0(15)	16.6(14)	-0.1(12)	0.5(11)	-0.1(11)
O3	9.1(10)	14.8(10)	18.1(11)	-2.8(8)	-0.9(8)	0.6(8)
C4	11.6(14)	15.0(17)	13.6(13)	-1.5(11)	2.5(11)	2.2(12)
N4	11.5(13)	12.0(13)	30.0(15)	0.9(11)	0.7(10)	-1.2(11)
O4	10.9(11)	16.2(12)	21.3(12)	-0.7(9)	1.2(9)	-2.0(9)
C11	14.4(14)	14.2(15)	14.0(14)	-0.1(11)	3.6(11)	1.5(11)
N11	11.0(11)	15.4(13)	17.6(13)	1.4(10)	-0.3(9)	1.4(10)
O11	10.1(10)	18.1(12)	31.1(13)	-2.0(10)	-0.4(9)	2.8(9)
C12	10.1(13)	14.3(16)	18.0(14)	-2.3(12)	-0.2(11)	-0.8(11)
O12	10.4(10)	18.3(11)	20.0(11)	-5.1(9)	-2.1(8)	1.3(8)
C13	9.9(13)	12.2(15)	15.1(14)	-1.8(11)	0.7(10)	-1.2(11)
O13	6.9(9)	15.0(11)	19.0(10)	-3.2(8)	3.1(8)	-1.4(8)
C14	11.0(14)	15.9(16)	11.3(13)	-4.3(11)	2.0(10)	-0.9(12)
N14	11.5(13)	13.8(14)	24.5(14)	-1.5(11)	1.6(10)	-0.6(11)
O14	14.4(12)	14.2(12)	22.5(11)	0.8(9)	2.3(9)	0.6(9)
C21	18.5(16)	14.0(16)	13.4(14)	-1.9(12)	5.1(12)	-1.2(12)
C22	19.2(15)	21.0(18)	14.6(14)	-1.5(12)	2.4(12)	1.4(13)
C23	28.5(17)	19.6(17)	17.3(16)	0.6(13)	4.4(13)	2.7(14)
C24	36(2)	13.9(16)	21.6(17)	-2.4(13)	6.7(15)	-2.5(14)
C25	26.4(17)	23.1(19)	18.1(15)	-3.6(13)	2.1(13)	-8.1(14)
C26	18.9(15)	20.6(18)	14.0(14)	-0.3(12)	0.6(11)	-3.3(13)
C31	11.2(15)	21.7(18)	19.8(16)	0.5(13)	1.7(11)	0.5(13)
C32	13.4(16)	22.0(18)	24.5(16)	-0.7(13)	3.5(12)	-2.9(14)
C33	9.9(15)	34(2)	25.3(17)	-1.6(15)	1.7(12)	-2.5(14)

C34	14.7(16)	30(2)	31.2(18)	-3.3(15)	-1.5(13)	7.8(14)
C35	19.4(18)	23(2)	57(3)	-0.7(17)	-3.0(17)	3.5(15)
C36	14.8(17)	23(2)	57(2)	-1.1(18)	-3.9(16)	-0.3(15)
C41	18.4(16)	16.4(17)	13.0(14)	-0.7(12)	3.0(12)	3.3(12)
C42	17.6(15)	20.6(18)	16.7(14)	2.7(13)	3.8(11)	2.1(13)
C43	26.5(17)	22.5(18)	21.4(16)	3.9(14)	6.3(13)	12.0(14)
C44	41(2)	14.0(16)	20.1(17)	0.6(13)	8.7(15)	4.2(14)
C45	39(2)	19.6(18)	16.9(16)	-0.6(13)	4.9(14)	-6.9(15)
C46	21.7(16)	19.9(17)	15.9(15)	-3.1(13)	1.2(12)	-3.0(13)
C51	11.9(15)	22.3(18)	18.7(15)	-3.4(13)	4.4(11)	-2.1(13)
C52	15.9(16)	30(2)	22.3(17)	2.3(14)	0.4(13)	0.8(15)
C53	13.5(16)	48(3)	23.2(17)	-0.2(16)	1.4(13)	-6.6(16)
C54	17.7(17)	47(3)	32(2)	-13.5(18)	9.0(14)	-14.8(17)
C55	22.7(19)	25(2)	47(2)	-12.9(17)	12.0(16)	-9.7(16)
C56	15.8(16)	20.0(19)	39(2)	-7.9(15)	7.9(14)	-3.7(14)

Table 2.4 Bond Lengths for **2** K[B{Tar(NHPh)$_2$}$_2$].

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
B1	K1^1	3.5776(11)	C3	C4	1.535(4)
B1	K1	3.5776(11)	C4	N4	1.356(4)
B1	K2	3.354(5)	C4	O4	1.228(4)
B1	O2	1.478(4)	N4	C31	1.421(4)
B1	O2^2	1.478(4)	C11	N11	1.340(4)
B1	O3^2	1.461(4)	C11	O11	1.234(4)
B1	O3	1.461(4)	C11	C12	1.520(4)
C1	N1	1.340(4)	N11	C41	1.410(4)
C1	O1	1.230(4)	C12	O12	1.416(3)
C1	C2	1.529(4)	C12	C13	1.566(4)
K1	B1^3	3.5776(11)	O12	K2^3	3.074(2)
K1	B2	3.324(5)	C13	O13	1.403(3)
K1	K2^3	4.3606(7)	C13	C14	1.528(4)
K1	O2^2	3.179(2)	C14	N14	1.354(4)
K1	O2^3	3.179(2)	C14	O14	1.228(4)
K1	O3	2.902(2)	N14	C51	1.411(4)
K1	O3^4	2.902(2)	C21	C22	1.395(5)
K1	O13	2.759(2)	C21	C26	1.395(4)
K1	O13^4	2.759(2)	C22	C23	1.389(5)
K1	O14^4	2.757(2)	C23	C24	1.378(5)
K1	O14	2.757(2)	C24	C25	1.396(5)
N1	C21	1.411(4)	C25	C26	1.386(5)
B2	K2	3.5715(11)	C31	C32	1.398(4)
B2	K2^3	3.5715(11)	C31	C36	1.375(6)
B2	O12^4	1.480(3)	C32	C33	1.387(5)

B2	O12	1.480(3)	C33	C34	1.382(6)
B2	O13[4]	1.460(3)	C34	C35	1.387(5)
B2	O13	1.460(3)	C35	C36	1.395(5)
C2	O2	1.415(3)	C41	C42	1.396(4)
C2	C3	1.567(4)	C41	C46	1.391(5)
K2	B2[1]	3.5715(11)	C42	C43	1.388(5)
K2	O3	2.784(2)	C43	C44	1.382(5)
K2	O3[2]	2.783(2)	C44	C45	1.385(5)
K2	O4[2]	2.792(2)	C45	C46	1.382(5)
K2	O4	2.792(2)	C51	C52	1.394(5)
K2	O12[4]	3.074(2)	C51	C56	1.395(5)
K2	O12[1]	3.074(2)	C52	C53	1.385(5)
K2	O13	2.992(2)	C53	C54	1.382(7)
K2	O13[2]	2.992(2)	C54	C55	1.388(6)
O2	K1[1]	3.179(2)	C55	C56	1.396(5)
C3	O3	1.400(3)			

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

Table 2.5 Bond Angles for **2** K[B{Tar(NHPh)$_2$}$_2$].

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
K1[1]	B1	K1	155.77(17)	O3	K2	B2	85.31(9)
K2	B1	K1	77.89(8)	O3[2]	K2	B2	116.51(9)
K2	B1	K1[1]	77.89(8)	O3[2]	K2	O3	50.84(9)
O2[2]	B1	K1	62.53(10)	O3[2]	K2	O4	98.37(7)
O2[2]	B1	K1[1]	134.22(13)	O3	K2	O4[2]	98.38(7)
O2	B1	K1	134.22(13)	O3[2]	K2	O4[2]	58.39(7)
O2	B1	K1[1]	62.53(10)	O3	K2	O4	58.39(7)
O2	B1	K2	124.22(19)	O3[2]	K2	O12[1]	108.29(6)
O2[2]	B1	K2	124.23(19)	O3	K2	O12[4]	108.29(6)
O2[2]	B1	O2	111.6(4)	O3[2]	K2	O12[4]	126.17(6)
O3	B1	K1[1]	112.43(17)	O3	K2	O12[1]	126.17(6)
O3[2]	B1	K1[1]	51.46(8)	O3[2]	K2	O13	109.21(6)
O3	B1	K1	51.46(8)	O3[2]	K2	O13[2]	66.44(6)
O3[2]	B1	K1	112.43(17)	O3	K2	O13	66.44(6)
O3	B1	K2	54.88(19)	O3	K2	O13[2]	109.21(6)
O3[2]	B1	K2	54.88(19)	O4	K2	B1	77.90(5)
O3[2]	B1	O2	112.72(11)	O4[2]	K2	B1	77.90(5)
O3	B1	O2	105.13(11)	O4	K2	K1	81.35(5)
O3	B1	O2[2]	112.72(11)	O4[2]	K2	K1	84.27(5)
O3[2]	B1	O2[2]	105.13(11)	O4[2]	K2	B2	94.19(5)
O3[2]	B1	O3	109.8(4)	O4	K2	B2[1]	94.19(5)
N1	C1	C2	113.6(2)	O4[2]	K2	B2[1]	90.66(5)
O1	C1	N1	126.9(3)	O4	K2	B2	90.66(5)

O1	C1	C2	119.5(3)	O4	K2	O4^{2}	155.81(10)
B1^{3}	K1	B1	155.77(17)	O4	K2	O12^{1}	83.24(6)
B1^{3}	K1	K2^{3}	48.78(8)	O4^{2}	K2	O12^{1}	109.11(6)
B1	K1	K2^{3}	155.45(9)	O4	K2	O12^{4}	109.11(6)
B2	K1	B1	102.11(8)	O4^{2}	K2	O12^{4}	83.24(6)
B2	K1	B1^{3}	102.11(8)	O4^{2}	K2	O13	110.11(6)
B2	K1	K2^{3}	53.339(12)	O4	K2	O13^{2}	110.11(6)
O2^{2}	K1	B1^{3}	134.59(9)	O4^{2}	K2	O13^{2}	68.89(6)
O2^{2}	K1	B1	24.36(7)	O4	K2	O13	68.89(6)
O2^{3}	K1	B1	134.59(9)	O12^{1}	K2	B1	120.03(4)
O2^{3}	K1	B1^{3}	24.36(7)	O12^{4}	K2	B1	120.03(4)
O2^{2}	K1	B2	119.85(4)	O12^{1}	K2	K1	164.29(4)
O2^{3}	K1	B2	119.85(4)	O12^{4}	K2	K1	68.59(4)
O2^{3}	K1	K2^{3}	68.62(4)	O12^{1}	K2	B2	135.20(9)
O2^{2}	K1	K2^{3}	163.51(4)	O12^{4}	K2	B2	24.28(7)
O2^{2}	K1	O2^{3}	120.30(8)	O12^{4}	K2	B2^{1}	135.20(9)
O3^{4}	K1	B1	158.78(6)	O12^{1}	K2	B2^{1}	24.28(7)
O3	K1	B1	23.19(6)	O12^{4}	K2	O12^{1}	119.95(9)
O3^{4}	K1	B1^{3}	23.19(6)	O13	K2	B1	87.76(4)
O3	K1	B1^{3}	158.78(6)	O13^{2}	K2	B1	87.76(4)
O3^{4}	K1	B2	88.23(5)	O13^{2}	K2	K1	137.16(5)
O3	K1	B2	88.23(5)	O13	K2	K1	38.74(4)
O3	K1	K2^{3}	137.82(5)	O13	K2	B2^{1}	158.71(5)
O3^{4}	K1	K2^{3}	38.93(4)	O13^{2}	K2	B2^{1}	23.66(6)
O3^{4}	K1	O2^{2}	135.27(6)	O13	K2	B2	23.66(6)
O3	K1	O2^{2}	47.18(5)	O13^{2}	K2	B2	158.71(5)
O3^{4}	K1	O2^{3}	47.18(5)	O13	K2	O12^{1}	135.75(6)
O3	K1	O2^{3}	135.27(6)	O13^{2}	K2	O12^{1}	47.38(5)
O3^{4}	K1	O3	176.46(9)	O13	K2	O12^{4}	47.37(5)
O13	K1	B1	87.11(9)	O13^{2}	K2	O12^{4}	135.75(6)
O13^{4}	K1	B1	115.39(9)	O13	K2	O13^{2}	175.52(9)
O13^{4}	K1	B1^{3}	87.11(9)	B1	O2	K1^{1}	93.11(14)
O13	K1	B1^{3}	115.39(9)	C2	O2	B1	111.0(2)
O13	K1	B2	25.69(4)	C2	O2	K1^{1}	107.97(16)
O13^{4}	K1	B2	25.69(4)	O3	C3	C2	105.8(2)
O13^{4}	K1	K2^{3}	42.72(4)	O3	C3	C4	111.5(2)
O13	K1	K2^{3}	70.03(4)	C4	C3	C2	111.7(2)
O13	K1	O2^{3}	123.70(6)	B1	O3	K1	105.35(10)
O13	K1	O2^{2}	110.01(6)	B1	O3	K2	99.7(2)
O13^{4}	K1	O2^{2}	123.70(6)	K2	O3	K1	100.14(7)
O13^{4}	K1	O2^{3}	110.01(6)	C3	O3	B1	111.5(2)
O13^{4}	K1	O3^{4}	68.01(6)	C3	O3	K1	115.24(16)
O13^{4}	K1	O3	108.59(7)	C3	O3	K2	122.58(17)
O13	K1	O3^{4}	108.59(7)	N4	C4	C3	112.0(3)
O13	K1	O3	68.01(6)	O4	C4	C3	122.2(3)
O13	K1	O13^{4}	51.37(8)	O4	C4	N4	125.7(3)

O14	K1	B1	94.72(5)	C4	N4	C31	128.6(3)
O14^{4}	K1	B1	90.04(5)	C4	O4	K2	123.3(2)
O14^{4}	K1	B1^{3}	94.72(5)	N11	C11	C12	113.7(2)
O14	K1	B1^{3}	90.04(5)	O11	C11	N11	126.6(3)
O14	K1	B2	78.60(5)	O11	C11	C12	119.7(3)
O14^{4}	K1	B2	78.60(5)	C11	N11	C41	129.9(3)
O14^{4}	K1	K2^{3}	85.15(5)	C11	C12	C13	108.8(2)
O14	K1	K2^{3}	81.28(5)	O12	C12	C11	113.6(2)
O14	K1	O2^{2}	113.29(6)	O12	C12	C13	105.6(2)
O14	K1	O2^{3}	78.55(6)	B2	O12	K2^{3}	97.06(15)
O14^{4}	K1	O2^{3}	113.29(6)	C12	O12	B2	110.8(2)
O14^{4}	K1	O2^{2}	78.55(6)	C12	O12	K2^{3}	103.01(17)
O14	K1	O3^{4}	105.55(6)	O13	C13	C12	105.4(2)
O14^{4}	K1	O3	105.56(6)	O13	C13	C14	111.0(2)
O14^{4}	K1	O3^{4}	73.72(6)	C14	C13	C12	112.4(2)
O14	K1	O3	73.72(6)	K1	O13	K2	98.54(6)
O14^{4}	K1	O13	99.31(7)	B2	O13	K1	99.33(19)
O14	K1	O13	58.80(6)	B2	O13	K2	101.04(10)
O14^{4}	K1	O13^{4}	58.79(6)	C13	O13	K1	122.30(17)
O14	K1	O13^{4}	99.31(7)	C13	O13	B2	111.8(2)
O14^{4}	K1	O14	157.19(10)	C13	O13	K2	120.07(16)
C1	N1	C21	130.1(3)	N14	C14	C13	112.3(3)
K1	B2	K2^{3}	78.36(8)	O14	C14	C13	122.4(3)
K1	B2	K2	78.36(8)	O14	C14	N14	125.3(3)
K2	B2	K2^{3}	156.71(16)	C14	N14	C51	129.7(3)
O12^{4}	B2	K1	123.52(19)	C14	O14	K1	123.3(2)
O12	B2	K1	123.52(19)	C22	C21	N1	117.0(3)
O12^{4}	B2	K2	58.66(10)	C22	C21	C26	120.4(3)
O12	B2	K2	137.99(14)	C26	C21	N1	122.4(3)
O12	B2	K2^{3}	58.66(10)	C23	C22	C21	119.9(3)
O12^{4}	B2	K2^{3}	137.99(14)	C24	C23	C22	120.2(3)
O12^{4}	B2	O12	113.0(4)	C23	C24	C25	119.5(3)
O13	B2	K1	54.98(18)	C26	C25	C24	121.3(3)
O13^{4}	B2	K1	54.99(18)	C25	C26	C21	118.6(3)
O13^{4}	B2	K2^{3}	55.30(8)	C32	C31	N4	116.1(3)
O13	B2	K2	55.30(8)	C36	C31	N4	124.0(3)
O13^{4}	B2	K2	109.74(16)	C36	C31	C32	119.8(3)
O13	B2	K2^{3}	109.74(16)	C33	C32	C31	119.6(3)
O13^{4}	B2	O12	112.04(12)	C34	C33	C32	121.1(3)
O13	B2	O12^{4}	112.04(12)	C33	C34	C35	118.6(3)
O13^{4}	B2	O12^{4}	104.99(11)	C34	C35	C36	121.0(4)
O13	B2	O12	104.99(11)	C31	C36	C35	119.8(4)
O13	B2	O13^{4}	110.0(4)	C42	C41	N11	123.2(3)
C1	C2	C3	108.9(2)	C46	C41	N11	117.1(3)
O2	C2	C1	113.3(2)	C46	C41	C42	119.7(3)
O2	C2	C3	105.4(2)	C43	C42	C41	118.9(3)

B1	K2	K1	53.339(12)	C44	C43	C42	121.4(3)
B1	K2	B2[1]	101.64(8)	C43	C44	C45	119.3(3)
B1	K2	B2	101.64(8)	C46	C45	C44	120.1(3)
B2	K2	K1	48.31(8)	C45	C46	C41	120.6(3)
B2[1]	K2	K1	154.98(8)	C52	C51	N14	117.1(3)
B2[1]	K2	B2	156.71(16)	C52	C51	C56	119.6(3)
O3	K2	B1	25.42(4)	C56	C51	N14	123.3(3)
O3[2]	K2	B1	25.42(4)	C53	C52	C51	120.2(4)
O3	K2	K1	40.93(4)	C54	C53	C52	120.7(4)
O3[2]	K2	K1	71.15(4)	C53	C54	C55	119.4(4)
O3[2]	K2	B2[1]	85.31(9)	C54	C55	C56	120.7(4)
O3	K2	B2[1]	116.51(9)	C51	C56	C55	119.4(3)

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

Table 2.6 Hydrogen Bonds for **2** K[B{Tar(NHPh)$_2$}$_2$].

D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
N1	H1	O2	0.88	2.15	2.630(3)	113.9
N4	H4	O1	0.88	2.24	3.060(4)	155.7
N11	H11	O12	0.88	2.14	2.628(3)	114.5
N14	H14	O11	0.88	2.19	3.018(4)	155.5

Table 2.7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **2** K[B{Tar(NHPh)$_2$}$_2$].

Atom	***x***	***y***	***z***	**U(eq)**
H1	4552	679	4720	18
H2	4145	2617	2646	17
H3	4161	2713	6690	16
H4	3494	3047	4878	21
H11	4526	7885	10992	18
H12	4190	5849	12113	17
H13	4127	5798	8056	15
H14	3489	5419	9564	20
H22	4751	-812	6172	22
H23	4613	-2518	6405	26
H24	3930	-3149	5425	28
H25	3391	-2079	4093	27
H26	3522	-374	3804	21
H32	2760	3126	4378	24
H33	2123	4061	4131	28
H34	2147	5796	4319	31

H35	2822	6596	4519	40
H36	3465	5671	4692	38
H42	3487	8668	9141	22
H43	3319	10331	8435	28
H44	3843	11571	8865	30
H45	4543	11158	10122	30
H46	4713	9514	10924	23
H52	2753	5290	9065	27
H53	2126	4323	8986	34
H54	2170	2609	9497	38
H55	2848	1867	10195	37
H56	3483	2824	10274	30

Compound 3 $[NH_4][B\{Tar(NHPh)_2\}_2]$

Table 3.1 Crystal data and structure refinement for **3** $[NH_4][B\{Tar(NHPh)_2\}_2]$.

Identification code	gem57d_twin1_hklf5
Empirical formula	$C_{32}H_{32}BN_5O_8$
Formula weight	625.43
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	C2
a/Å	30.9663(9)
b/Å	13.3119(4)
c/Å	7.0955(3)
α/°	90
β/°	93.965(3)
γ/°	90
Volume/Å^3	2917.92(17)
Z	4
ρ_{calc}g/cm^3	1.424
μ/mm^{-1}	0.855
F(000)	1312.0
Crystal size/mm^3	0.1 × 0.05 × 0.03
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.23 to 151.47
Index ranges	$-38 \leq h \leq 38$, $-16 \leq k \leq 16$, $-8 \leq l \leq 8$
Reflections collected	8914
Independent reflections	8914 [R_{int} = ?, R_{sigma} = 0.0400]
Data/restraints/parameters	8914/1/422
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R_1 = 0.0425, wR_2 = 0.1147
Final R indexes [all data]	R_1 = 0.0485, wR_2 = 0.1170
Largest diff. peak/hole / e Å^{-3}	0.23/-0.23
Flack parameter	0.09(16)

Table 3.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **3** $[NH_4][B\{Tar(NHPh)_2\}_2]$.
U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O11	3636.5(9)	1295(2)	4231(5)	22.7(6)
O12	4736.3(8)	2011(2)	3632(4)	16.9(6)
O13	4685.9(8)	3274(2)	5891(4)	16.1(6)
O14	4092.3(9)	4686(2)	4952(4)	19.7(6)
N11	4282.5(11)	440(3)	4587(5)	18.1(7)
N14	3537.9(11)	3540(3)	4767(6)	22.1(8)
C11	4033.2(12)	1245(3)	4201(6)	17.7(8)
C12	4289.3(12)	2198(3)	3778(6)	15.9(8)
C13	4262.7(12)	2929(3)	5472(6)	16.1(8)
C14	3958.2(13)	3816(3)	5025(6)	17.1(8)
C31	4161.2(13)	-573(3)	4906(6)	17.8(8)
C32	4477.9(13)	-1206(3)	5733(6)	20.2(8)
C33	4394.2(14)	-2224(3)	5937(6)	23.5(9)
C34	3993.9(15)	-2607(3)	5315(7)	25.5(10)
C35	3677.7(14)	-1972(3)	4520(6)	24.1(9)
C36	3756.3(14)	-952(3)	4300(6)	20.3(9)
C41	3164.5(13)	4157(3)	4571(6)	21.6(9)
C42	3176.1(15)	5199(4)	4604(9)	34.7(13)
C43	2791.0(16)	5736(4)	4516(10)	38.2(13)
C44	2397.1(15)	5256(4)	4377(7)	27.8(11)
C45	2385.8(14)	4220(4)	4296(7)	28.9(11)
C46	2767.7(14)	3663(4)	4396(7)	23.8(9)
B1	5000	2647(5)	5000	16.5(13)
O21	5900.1(9)	3568(2)	286(5)	19.2(6)
O22	5325.8(8)	4997(2)	1002(4)	16.3(6)
O23	5247.8(8)	6253(2)	-1288(4)	16.8(6)
O24	6358.2(9)	6894(2)	-127(5)	22.4(6)
N2	5000	3018(4)	0	17.9(10)
N21	6460.8(11)	4688(3)	366(6)	21.2(8)
N24	5742.5(10)	7843(3)	-591(5)	17.4(7)
C21	6041.6(13)	4423(3)	420(6)	17.9(8)
C22	5746.5(12)	5326(3)	733(6)	16.1(8)
C23	5696.7(11)	6050(3)	-1002(6)	16.2(8)
C24	5969.3(12)	6983(3)	-536(6)	17.3(8)
C51	6830.2(13)	4057(3)	347(6)	21.9(9)
C52	6808.0(14)	3028(4)	29(8)	27.3(10)
C53	7188.4(16)	2466(4)	119(9)	34.0(12)
C54	7585.4(15)	2913(4)	497(8)	33.3(12)
C55	7604.1(15)	3949(5)	785(7)	29.9(11)
C56	7230.8(14)	4514(4)	712(7)	25.3(10)
C61	5879.3(14)	8825(3)	-96(6)	19.0(8)
C62	5573.7(14)	9585(3)	-365(7)	23.3(9)

C63	5678.0(16)	10570(3)	153(7)	29.3(10)
C64	6090.5(16)	10797(4)	901(7)	28.1(10)
C65	6394.7(15)	10047(4)	1129(7)	27.3(10)
C66	6295.8(14)	9050(3)	653(6)	20.6(9)
B2	5000	5624(5)	0	15.9(13)
N1	5000	5283(4)	5000	17.3(10)

Table 3.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **3** $[NH_4][B\{Tar(NHPh)_2\}_2]$. Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O11	15.8(13)	20.2(15)	32.4(17)	0.9(13)	3.0(11)	-1.1(12)
O12	15.0(12)	15.4(13)	20.6(15)	-2.7(12)	2.5(11)	-1.3(10)
O13	15.4(12)	14.3(13)	18.4(14)	-2.5(11)	-0.9(11)	-1.0(10)
O14	18.7(14)	14.9(14)	25.5(16)	0.0(12)	1.0(11)	1.1(12)
N11	15.9(15)	14.3(17)	24.2(18)	0.9(14)	1.8(13)	-3.7(13)
N14	16.2(17)	13.7(18)	36(2)	-0.6(15)	0.6(14)	0.3(14)
C11	17.9(18)	15.7(19)	19(2)	-2.1(16)	0.7(14)	-0.8(16)
C12	14.3(17)	14(2)	19.8(19)	0.7(15)	1.4(14)	-2.0(13)
C13	12.2(17)	18(2)	18(2)	0.5(16)	1.7(14)	-1.7(15)
C14	14.6(18)	17(2)	20(2)	-0.1(16)	3.4(14)	0.7(15)
C31	21(2)	13(2)	20(2)	-0.8(16)	6.1(15)	-1.6(15)
C32	18.8(19)	21(2)	22(2)	-0.4(17)	3.4(15)	-0.6(15)
C33	30(2)	21(2)	20(2)	4.0(18)	3.7(17)	3.1(17)
C34	36(2)	14(2)	26(2)	-1.9(17)	7.6(19)	-4.3(17)
C35	26(2)	22(2)	25(2)	-4.7(18)	4.6(17)	-8.0(17)
C36	22(2)	19(2)	19.9(19)	-2.0(17)	1.4(16)	1.4(16)
C41	15(2)	23(3)	27(2)	0.8(18)	0.6(16)	2.0(16)
C42	19(2)	24(3)	60(4)	-2(2)	0(2)	0.3(18)
C43	25(2)	24(2)	65(4)	-4(2)	-5(2)	6(2)
C44	19(2)	31(3)	33(3)	-3(2)	-1.7(18)	6.7(17)
C45	17(2)	36(3)	35(3)	-2(2)	4.6(18)	-1.3(19)
C46	20(2)	21(2)	30(2)	0.0(18)	3.2(17)	-2.7(17)
B1	18(3)	10(3)	21(3)	0	0(2)	0
O21	16.5(14)	15.3(15)	26.1(16)	-1.4(12)	3.1(11)	-2.0(11)
O22	13.1(12)	14.8(13)	21.3(15)	3.7(11)	3.6(11)	-0.2(10)
O23	14.4(12)	16.3(13)	19.6(14)	2.8(12)	0.8(10)	-0.7(11)
O24	16.6(14)	15.3(15)	35.0(18)	1.3(13)	1.0(12)	-3.1(11)
N2	19(2)	15(3)	20(3)	0	0.1(18)	0
N21	15.4(17)	16.9(18)	32(2)	2.6(16)	3.3(13)	-0.9(14)
N24	13.7(15)	15.4(17)	22.8(18)	1.3(14)	-0.7(13)	-1.7(13)
C21	17.6(19)	20(2)	16.6(19)	1.9(16)	1.7(14)	1.0(16)
C22	14.4(17)	17(2)	16.8(19)	-0.3(16)	0.3(14)	-1.3(14)
C23	13.1(17)	17(2)	18.3(19)	3.3(16)	1.6(14)	0.5(14)
C24	17.4(18)	16.7(19)	18.4(19)	-0.5(17)	4.5(14)	-2.8(15)

C51	16(2)	25(2)	26(2)	7.5(18)	5.1(16)	3.6(16)
C52	19(2)	22(2)	41(3)	8(2)	6.3(18)	2.2(17)
C53	28(2)	25(3)	50(3)	8(2)	15(2)	9(2)
C54	23(2)	43(3)	34(3)	12(2)	8.4(19)	16(2)
C55	16(2)	50(3)	25(2)	2(2)	2.4(16)	1.5(19)
C56	20(2)	30(3)	26(2)	1.9(19)	3.6(16)	0.5(19)
C61	24(2)	15(2)	18.8(19)	-0.6(16)	3.0(16)	-2.7(16)
C62	23.9(19)	20(2)	26(2)	3.1(18)	2.2(17)	2.6(17)
C63	41(3)	22(2)	25(2)	2.8(19)	4(2)	6.6(19)
C64	43(3)	18(2)	25(3)	-2.4(18)	10(2)	-4.5(18)
C65	29(2)	25(2)	28(2)	-2.7(19)	4.5(19)	-9.1(18)
C66	20(2)	16(2)	25(2)	-1.3(17)	3.5(16)	-3.1(15)
B2	14(3)	15(3)	19(3)	0	4(2)	0
N1	17(2)	14(3)	21(3)	0	1.1(19)	0

Table 3.4 Bond Lengths for **3** $[NH_4][B\{Tar(NHPh)_2\}_2]$.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O11	C11	1.232(5)	O21	C21	1.221(5)
O12	C12	1.417(4)	O22	C22	1.400(5)
O12	B1	1.489(4)	O22	B2	1.456(5)
O13	C13	1.401(4)	O23	C23	1.417(4)
O13	B1	1.459(5)	O23	B2	1.490(5)
O14	C14	1.232(5)	O24	C24	1.225(5)
N11	C11	1.338(5)	N21	C21	1.348(5)
N11	C31	1.422(5)	N21	C51	1.420(5)
N14	C14	1.353(5)	N24	C24	1.343(5)
N14	C41	1.417(5)	N24	C61	1.411(5)
C11	C12	1.536(5)	C21	C22	1.535(6)
C12	C13	1.553(6)	C22	C23	1.563(5)
C13	C14	1.531(5)	C23	C24	1.525(5)
C31	C32	1.392(6)	C51	C52	1.389(7)
C31	C36	1.392(6)	C51	C56	1.389(6)
C32	C33	1.389(6)	C52	C53	1.393(6)
C33	C34	1.384(7)	C53	C54	1.375(8)
C34	C35	1.384(7)	C54	C55	1.395(8)
C35	C36	1.390(6)	C55	C56	1.376(7)
C41	C42	1.388(7)	C61	C62	1.389(6)
C41	C46	1.391(6)	C61	C66	1.393(6)
C42	C43	1.388(7)	C62	C63	1.393(7)
C43	C44	1.374(7)	C63	C64	1.383(7)
C44	C45	1.380(7)	C64	C65	1.375(7)
C45	C46	1.393(6)	C65	C66	1.398(6)
B1	$O12^1$	1.489(4)	B2	$O22^2$	1.456(5)
B1	$O13^1$	1.459(5)	B2	$O23^2$	1.490(5)

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

Table 3.5 Bond Angles for **3** $[NH_4][B\{Tar(NHPh)_2\}_2]$.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C12	O12	B1	110.3(3)	C22	O22	B2	112.0(3)
C13	O13	B1	111.2(3)	C23	O23	B2	110.3(3)
C11	N11	C31	129.6(3)	C21	N21	C51	128.6(4)
C14	N14	C41	128.8(4)	C24	N24	C61	129.4(3)
O11	C11	N11	127.0(4)	O21	C21	N21	125.6(4)
O11	C11	C12	119.2(4)	O21	C21	C22	121.8(4)
N11	C11	C12	113.7(3)	N21	C21	C22	112.6(4)
O12	C12	C11	112.9(3)	O22	C22	C21	110.2(3)
O12	C12	C13	105.7(3)	O22	C22	C23	105.0(3)
C11	C12	C13	108.1(3)	C21	C22	C23	113.4(3)
O13	C13	C12	105.7(3)	O23	C23	C22	105.8(3)
O13	C13	C14	110.1(3)	O23	C23	C24	113.5(3)
C14	C13	C12	112.8(3)	C24	C23	C22	108.0(3)
O14	C14	N14	125.0(4)	O24	C24	N24	126.4(4)
O14	C14	C13	122.0(4)	O24	C24	C23	119.5(4)
N14	C14	C13	113.0(4)	N24	C24	C23	114.1(3)
C32	C31	N11	117.1(4)	C52	C51	N21	123.6(4)
C36	C31	N11	122.5(4)	C56	C51	N21	116.7(4)
C36	C31	C32	120.2(4)	C56	C51	C52	119.7(4)
C33	C32	C31	120.3(4)	C51	C52	C53	119.3(4)
C34	C33	C32	119.7(4)	C54	C53	C52	121.2(5)
C33	C34	C35	119.9(4)	C53	C54	C55	118.9(4)
C34	C35	C36	121.2(4)	C56	C55	C54	120.5(5)
C35	C36	C31	118.7(4)	C55	C56	C51	120.3(5)
C42	C41	N14	123.9(4)	C62	C61	N24	116.8(4)
C42	C41	C46	119.7(4)	C62	C61	C66	120.0(4)
C46	C41	N14	116.4(4)	C66	C61	N24	123.2(4)
C43	C42	C41	119.5(5)	C61	C62	C63	120.4(4)
C44	C43	C42	121.3(5)	C64	C63	C62	119.9(4)
C43	C44	C45	119.1(5)	C65	C64	C63	119.6(4)
C44	C45	C46	120.7(4)	C64	C65	C66	121.6(4)
C41	C46	C45	119.6(4)	C61	C66	C65	118.5(4)
O12[1]	B1	O12	110.6(5)	O22[2]	B2	O22	110.1(5)
O13[1]	B1	O12[1]	104.85(14)	O22[2]	B2	O23[2]	104.62(14)
O13[1]	B1	O12	113.27(15)	O22	B2	O23[2]	113.00(16)
O13	B1	O12	104.85(14)	O22[2]	B2	O23	113.00(16)
O13	B1	O12[1]	113.27(15)	O22	B2	O23	104.62(14)
O13[1]	B1	O13	110.2(5)	O23[2]	B2	O23	111.7(5)

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

Table 3.6 Hydrogen Bonds for **3** $[NH_4][B\{Tar(NHPh)_2\}_2]$.

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N11	H11	O12	0.88	2.15	2.634(4)	114.0
N14	H14	O11	0.88	2.20	3.031(5)	156.9
N2	H2A	O21[1]	0.80	2.22	2.875(3)	139.5
N2	H2A	O22[1]	0.80	2.20	2.893(6)	145.6
N2	H2B	O12[1]	0.89	2.21	3.065(4)	160.3
N2	H2B	O13[2]	0.89	2.47	3.028(3)	121.0
N21	H21	O24	0.88	2.15	2.972(5)	156.0
N24	H24	O23	0.88	2.16	2.640(4)	113.9
N1	H1A	O13[3]	0.78	2.28	2.929(5)	141.2
N1	H1A	O14[3]	0.78	2.25	2.919(3)	143.7
N1	H1B	O22	0.96	2.46	3.099(3)	123.3
N1	H1B	O23[1]	0.96	2.05	2.985(4)	162.3

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

Table 3.7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **3** $[NH_4][B\{Tar(NHPh)_2\}_2]$.

Atom	*x*	*y*	*z*	U(eq)
H11	4563	554	4653	22
H14	3490	2889	4715	27
H12	4163	2521	2593	19
H13	4163	2552	6582	19
H32	4752	-942	6159	24
H33	4611	-2656	6500	28
H34	3936	-3304	5435	31
H35	3402	-2238	4118	29
H36	3538	-522	3747	24
H42	3446	5543	4685	42
H43	2800	6449	4553	46
H44	2136	5632	4337	33
H45	2115	3884	4171	35
H46	2757	2951	4345	29
H2A	4815	3435	-181	430(140)
H2B	5013	2655	-1050	120(40)
H21	6512	5338	338	25
H24	5468	7787	-996	21
H22	5862	5708	1871	19

H23	5801	5711	-2143	19
H52	6536	2711	-247	33
H53	7173	1761	-85	41
H54	7843	2523	561	40
H55	7877	4268	1033	36
H56	7247	5219	912	30
H62	5292	9433	-906	28
H63	5466	11084	-7	35
H64	6163	11468	1255	34
H65	6679	10210	1623	33
H66	6508	8538	835	25
H1A	5186	4922	4741	39(17)
H1B	4984	5628	3803	50(20)

Compound 4 Na [B{Tar(NHPh)$_2$}$_2$] 2MeOH

Table 4.1 Crystal data and structure refinement for **4** Na [B{Tar(NHPh)$_2$}$_2$] 2MeOH.

Identification code	gem84cult
Empirical formula	$C_{34}H_{36}BN_4NaO_{10}$
Formula weight	694.47
Temperature/K	99.97(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	7.61035(16)
b/Å	15.1976(3)
c/Å	29.4158(5)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3402.21(11)
Z	4
ρ_{calc}g/cm^3	1.356
μ/mm^{-1}	0.940
F(000)	1456.0
Crystal size/mm^3	0.2 × 0.05 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	12.012 to 135.996
Index ranges	$-7 \leq h \leq 9$, $-11 \leq k \leq 18$, $-35 \leq l \leq 34$
Reflections collected	9737
Independent reflections	6079 [R_{int} = 0.0308, R_{sigma} = 0.0401]
Data/restraints/parameters	6079/0/477
Goodness-of-fit on F^2	1.017
Final R indexes [I>=2σ (I)]	R_1 = 0.0328, wR_2 = 0.0784
Final R indexes [all data]	R_1 = 0.0368, wR_2 = 0.0803
Largest diff. peak/hole / e Å^{-3}	0.17/-0.17
Flack parameter	-0.04(5)

Table 4.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **4** Na [B{Tar(NHPh)$_2$}$_2$] 2MeOH.
U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	***x***	***y***	***z***	**U(eq)**
Na1	1307.5(13)	8005.4(6)	5148.5(3)	23.6(2)
O1	1721(3)	7865.7(11)	5967.3(6)	27.1(4)
O1S	3006(2)	9346.6(12)	5101.2(7)	29.9(4)
O2	3331(2)	6806.0(10)	5358.8(5)	20.0(3)
O3	2310(2)	5354.2(10)	5343.7(5)	20.9(3)
O4	3262(3)	5169.6(12)	6519.4(6)	31.4(4)
O11	2780(3)	7850.8(11)	4449.1(5)	26.4(4)
O12	1235(2)	6380.8(11)	4770.0(5)	20.2(3)
O13	4121(2)	5890.2(11)	4716.4(5)	20.5(3)
O14	2280(3)	4642.3(11)	3798.4(6)	31.9(4)
N2	2531(3)	6973.8(15)	6564.3(7)	26.0(4)
N4	2664(3)	4131.0(14)	5983.6(7)	23.5(4)
N11	1964(3)	7509.2(13)	3721.8(6)	20.6(4)
N14	3369(3)	4276.2(13)	4499.2(7)	21.4(4)
C1	2430(3)	7204.1(15)	6120.3(8)	21.0(5)
C1S	2963(4)	9927.1(17)	5478.5(10)	31.9(6)
C2	3285(3)	6512.6(15)	5812.0(7)	20.2(5)
C3	2171(3)	5655.2(16)	5795.8(7)	20.6(5)
C4	2782(3)	4961.8(16)	6135.7(8)	22.2(5)
C11	2204(3)	7334.1(15)	4167.3(7)	20.2(5)
C12	1705(3)	6392.7(15)	4307.0(7)	20.2(5)
C13	3366(3)	5801.7(15)	4281.5(7)	21.0(5)
C14	2924(3)	4840.6(16)	4166.6(8)	22.3(5)
C21	1701(4)	7351.2(19)	6948.5(9)	30.3(6)
C22	796(4)	8135(2)	6938.9(10)	35.6(7)
C23	-23(4)	8432(2)	7336.3(11)	45.6(8)
C24	91(4)	7952(3)	7735.9(11)	52.1(10)
C25	1024(5)	7170(3)	7744.2(10)	48.6(9)
C26	1817(4)	6865(2)	7350.1(9)	37.7(7)
C31	3049(3)	3344.0(16)	6221.9(8)	24.1(5)
C32	2327(4)	2569.2(18)	6054.3(8)	29.5(6)
C33	2720(5)	1773.8(18)	6260.0(9)	37.8(7)
C34	3826(5)	1747(2)	6634.0(10)	42.0(8)
C35	4520(4)	2521(2)	6805.8(9)	36.5(7)
C36	4138(4)	3328.5(19)	6603.9(9)	29.3(6)
C41	2321(3)	8307.8(16)	3492.1(8)	20.7(5)
C42	2776(3)	9084.6(16)	3715.9(8)	22.8(5)
C43	3097(4)	9839.4(17)	3457.6(9)	27.5(5)
C44	2957(4)	9828.2(18)	2991.5(9)	33.0(6)
C45	2502(4)	9053.1(18)	2773.3(9)	32.1(6)
C46	2180(4)	8296.9(17)	3020.9(8)	26.8(5)
C51	3316(3)	3342.7(15)	4505.6(8)	22.0(5)

C52	2566(4)	2840.0(17)	4161.5(8)	26.7(5)
C53	2590(4)	1925.5(17)	4200.7(9)	29.8(6)
C54	3334(4)	1512.4(17)	4572.6(9)	31.1(6)
C55	4063(4)	2021.7(17)	4915.5(9)	27.6(5)
C56	4058(3)	2931.0(16)	4884.4(8)	24.3(5)
B1	2749(4)	6101.8(17)	5050.2(9)	18.8(5)
O2S	1103(4)	5953.2(14)	3233.4(7)	44.8(6)
C2S	149(5)	5720(2)	2843.1(10)	43.0(8)

Table 4.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **4** Na [B{Tar(NHPh)$_2$}$_2$] 2MeOH. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Na1	28.5(5)	19.8(5)	22.5(4)	-0.8(4)	0.4(4)	4.4(4)
O1	33.7(10)	21.5(9)	26.2(8)	-2.7(7)	-2.2(7)	4.1(8)
O1S	22.9(9)	24.8(9)	42.1(10)	-4.5(8)	0.9(8)	3.6(8)
O2	25.9(9)	16.6(8)	17.5(7)	0.5(6)	-0.9(6)	-2.9(7)
O3	27.5(9)	16.9(8)	18.3(7)	0.2(6)	-2.8(7)	-2.3(7)
O4	48.7(12)	25.0(9)	20.6(8)	1.5(7)	-6.7(8)	-1.7(9)
O11	39.0(10)	20.0(8)	20.0(7)	-1.1(6)	-0.5(7)	-3.6(8)
O12	20.0(8)	21.1(8)	19.5(7)	1.7(6)	-0.2(6)	1.8(6)
O13	22.1(8)	19.1(8)	20.1(8)	-1.3(6)	-1.1(7)	1.1(7)
O14	48.8(12)	21.7(9)	25.1(8)	-3.2(7)	-10.2(9)	2.9(8)
N2	31.9(12)	26.9(11)	19.1(9)	-2.6(8)	-0.4(9)	2.3(10)
N4	29.1(11)	22.2(10)	19.1(9)	3.5(8)	-3.8(9)	-1.8(9)
N11	25.1(11)	16.8(9)	20.0(9)	-0.4(8)	-0.8(8)	-0.5(8)
N14	25.8(10)	17.1(10)	21.4(9)	-1.7(8)	-3.0(8)	1.5(8)
C1	18.0(11)	21.0(11)	24.0(11)	-2.6(9)	-0.9(9)	-2.6(10)
C1S	27.3(14)	22.9(12)	45.4(15)	-3.8(11)	1.1(11)	1.2(11)
C2	22.3(12)	19.3(11)	18.9(11)	0.7(8)	-0.9(9)	-0.1(9)
C3	21.7(11)	21.1(11)	19.0(10)	0.2(9)	-1.8(9)	-1.1(9)
C4	21.6(12)	23.4(12)	21.7(11)	3.4(9)	1.2(9)	-3.2(10)
C11	21.5(11)	18.5(12)	20.4(10)	-0.2(9)	0.9(9)	1.5(9)
C12	23.6(12)	19.2(11)	17.7(10)	0.0(8)	-3.1(9)	-1.2(10)
C13	26.4(12)	18.7(11)	18.0(10)	-1.5(9)	-1.7(9)	-0.7(10)
C14	26.7(13)	19.9(12)	20.3(11)	-0.9(9)	0.2(10)	1.7(10)
C21	27.8(14)	39.2(16)	23.8(12)	-10.9(11)	1.0(10)	-9.0(12)
C22	29.9(14)	42.1(17)	34.9(14)	-17.4(12)	-2.3(12)	-1.5(13)
C23	32.9(16)	58(2)	45.9(17)	-32.3(16)	-1.5(13)	-3.0(15)
C24	36.2(17)	84(3)	35.5(16)	-31.0(18)	8.9(13)	-20.4(18)
C25	46.4(19)	72(2)	27.2(14)	-9.9(15)	4.3(13)	-20.9(18)
C26	40.5(17)	49.5(18)	23.1(13)	-6.2(12)	-0.2(12)	-12.7(14)
C31	27.3(13)	22.7(12)	22.2(11)	3.9(9)	4.3(10)	3.1(10)
C32	37.0(15)	24.1(12)	27.3(12)	2.6(9)	3.7(11)	1.8(11)
C33	57.9(19)	20.8(13)	34.8(14)	1.2(10)	11.8(14)	4.8(13)

C34	63(2)	30.7(15)	32.4(15)	12.1(11)	16.4(14)	18.5(15)
C35	42.7(16)	42.6(17)	24.2(12)	9.9(12)	6.3(11)	16.6(13)
C36	31.2(14)	32.8(14)	24.1(12)	3.9(10)	2.6(10)	5.4(12)
C41	17.6(11)	19.8(11)	24.8(11)	2.7(9)	2.2(9)	4.7(9)
C42	24.4(12)	20.3(11)	23.8(11)	0.4(9)	1.0(10)	0.7(10)
C43	27.8(14)	19.6(12)	35.0(13)	0.8(10)	1.3(11)	-0.6(10)
C44	35.7(16)	26.1(13)	37.2(14)	11.4(11)	3.1(12)	1.1(12)
C45	41.2(15)	31.3(14)	23.9(12)	6.8(10)	0.9(12)	2.9(12)
C46	31.3(14)	23.1(12)	26.1(12)	0.2(9)	-0.5(10)	4.9(11)
C51	22.4(12)	16.9(11)	26.7(12)	-1.1(9)	0.7(10)	1.6(10)
C52	27.8(13)	22.2(12)	30.2(12)	-2.4(10)	-4.6(11)	4.2(10)
C53	31.1(14)	22.4(12)	36.0(13)	-6.1(10)	-3.3(12)	0.3(11)
C54	34.4(14)	18.4(12)	40.3(14)	2.2(11)	0.3(12)	1.8(11)
C55	28.5(13)	23.8(13)	30.5(12)	4.9(10)	0.7(10)	3.4(10)
C56	25.3(12)	22.5(12)	25.0(11)	-0.7(10)	-0.3(10)	-1.4(10)
B1	20.1(13)	15.6(12)	20.8(12)	1.0(9)	-0.8(10)	0.0(10)
O2S	78.6(18)	24.7(10)	31.0(10)	-1.2(8)	-24.3(11)	-2.8(11)
C2S	62(2)	32.9(16)	33.8(15)	-1.8(12)	-17.6(15)	-4.5(15)

Table 4.4 Bond Lengths for **4** Na [B{Tar(NHPh)$_2$}$_2$] 2MeOH.

Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
Na1	Na1^1	4.1955(8)	N14	C51	1.419(3)
Na1	Na1^2	4.1955(8)	C1	C2	1.533(3)
Na1	O1	2.4382(19)	C2	C3	1.555(3)
Na1	O1S	2.418(2)	C3	C4	1.525(3)
Na1	O2	2.4649(19)	C11	C12	1.536(3)
Na1	O2^1	2.728(2)	C12	C13	1.553(3)
Na1	O11	2.3545(19)	C13	C14	1.537(3)
Na1	O12	2.7090(19)	C21	C22	1.376(4)
Na1	O13^1	2.3965(19)	C21	C26	1.396(4)
Na1	B1	3.108(3)	C22	C23	1.399(4)
Na1	B1^1	3.085(3)	C23	C24	1.386(5)
O1	C1	1.227(3)	C24	C25	1.384(6)
O1S	C1S	1.418(3)	C25	C26	1.387(4)
O2	Na1^2	2.728(2)	C31	C32	1.390(4)
O2	C2	1.406(3)	C31	C36	1.397(4)
O2	B1	1.471(3)	C32	C33	1.384(4)
O3	C3	1.411(3)	C33	C34	1.386(5)
O3	B1	1.466(3)	C34	C35	1.385(5)
O4	C4	1.228(3)	C35	C36	1.394(4)
O11	C11	1.223(3)	C41	C42	1.395(4)
O12	C12	1.408(3)	C41	C46	1.390(3)
O12	B1	1.479(3)	C42	C43	1.398(3)
O13	Na1^2	2.3966(19)	C43	C44	1.375(4)

O13	C13	1.409(3)	C44	C45	1.385(4)
O13	B1	1.469(3)	C45	C46	1.383(4)
O14	C14	1.227(3)	C51	C52	1.391(3)
N2	C1	1.354(3)	C51	C56	1.397(3)
N2	C21	1.416(3)	C52	C53	1.395(4)
N4	C4	1.342(3)	C53	C54	1.383(4)
N4	C31	1.417(3)	C54	C55	1.387(4)
N11	C11	1.350(3)	C55	C56	1.385(3)
N11	C41	1.415(3)	B1	Na1[2]	3.085(3)
N14	C14	1.345(3)	O2S	C2S	1.404(3)

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

Table 4.5 Bond Angles for **4** Na [B{Tar(NHPh)$_2$}$_2$] 2MeOH.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
Na1[1]	Na1	Na1[2]	130.18(5)	C11	N11	C41	127.4(2)
O1	Na1	Na1[1]	106.90(6)	C14	N14	C51	129.8(2)
O1	Na1	Na1[2]	93.26(5)	O1	C1	N2	126.2(2)
O1	Na1	O2	66.87(6)	O1	C1	C2	122.1(2)
O1	Na1	O2[1]	131.04(7)	N2	C1	C2	111.7(2)
O1	Na1	O12	109.23(6)	O2	C2	C1	110.73(19)
O1	Na1	B1[1]	109.79(7)	O2	C2	C3	104.48(17)
O1	Na1	B1	88.02(7)	C1	C2	C3	111.16(19)
O1S	Na1	Na1[1]	141.41(6)	O3	C3	C2	105.06(18)
O1S	Na1	Na1[2]	79.15(5)	O3	C3	C4	111.79(19)
O1S	Na1	O1	93.52(7)	C4	C3	C2	113.13(19)
O1S	Na1	O2	107.69(7)	O4	C4	N4	124.6(2)
O1S	Na1	O2[1]	108.90(7)	O4	C4	C3	121.0(2)
O1S	Na1	O12	139.08(7)	N4	C4	C3	114.3(2)
O1S	Na1	B1[1]	95.03(7)	O11	C11	N11	125.4(2)
O1S	Na1	B1	126.21(8)	O11	C11	C12	120.3(2)
O2[1]	Na1	Na1[1]	34.04(4)	N11	C11	C12	114.21(19)
O2	Na1	Na1[2]	38.28(4)	O12	C12	C11	109.48(18)
O2	Na1	Na1[1]	110.37(6)	O12	C12	C13	104.25(17)
O2[1]	Na1	Na1[2]	132.67(5)	C11	C12	C13	108.9(2)
O2	Na1	O2[1]	137.20(5)	O13	C13	C12	103.47(17)
O2	Na1	O12	56.08(5)	O13	C13	C14	112.33(19)
O2	Na1	B1[1]	157.10(8)	C14	C13	C12	112.5(2)
O2[1]	Na1	B1	109.88(7)	O14	C14	N14	125.9(2)
O2[1]	Na1	B1[1]	28.49(6)	O14	C14	C13	121.0(2)
O2	Na1	B1	27.67(6)	N14	C14	C13	113.0(2)
O11	Na1	Na1[1]	102.31(6)	C22	C21	N2	123.9(3)
O11	Na1	Na1[2]	49.44(5)	C22	C21	C26	120.5(3)
O11	Na1	O1	142.47(8)	C26	C21	N2	115.6(3)

O11	Na1	O1S	77.25(7)	C21	C22	C23	119.0(3)
O11	Na1	O2[1]	85.86(6)	C24	C23	C22	120.7(3)
O11	Na1	O2	81.27(6)	C25	C24	C23	119.9(3)
O11	Na1	O12	63.87(6)	C24	C25	C26	119.7(3)
O11	Na1	O13[1]	123.04(7)	C25	C26	C21	120.2(3)
O11	Na1	B1[1]	107.23(7)	C32	C31	N4	117.3(2)
O11	Na1	B1	69.98(7)	C32	C31	C36	120.4(2)
O12	Na1	Na1[2]	66.37(5)	C36	C31	N4	122.3(2)
O12	Na1	Na1[1]	64.04(5)	C33	C32	C31	120.0(3)
O12	Na1	O2[1]	81.60(5)	C32	C33	C34	120.3(3)
O12	Na1	B1[1]	107.76(7)	C35	C34	C33	119.8(3)
O12	Na1	B1	28.41(6)	C34	C35	C36	120.9(3)
O13[1]	Na1	Na1[1]	70.20(4)	C35	C36	C31	118.8(3)
O13[1]	Na1	Na1[2]	157.02(6)	C42	C41	N11	123.2(2)
O13[1]	Na1	O1	89.24(6)	C46	C41	N11	116.8(2)
O13[1]	Na1	O1S	77.89(6)	C46	C41	C42	120.0(2)
O13[1]	Na1	O2	155.50(6)	C41	C42	C43	118.8(2)
O13[1]	Na1	O2[1]	55.98(5)	C44	C43	C42	121.2(2)
O13[1]	Na1	O12	133.81(7)	C43	C44	C45	119.5(2)
O13[1]	Na1	B1[1]	27.61(6)	C46	C45	C44	120.5(2)
O13[1]	Na1	B1	155.86(8)	C45	C46	C41	120.1(2)
B1	Na1	Na1[1]	87.71(6)	C52	C51	N14	123.4(2)
B1	Na1	Na1[2]	47.12(6)	C52	C51	C56	120.0(2)
B1[1]	Na1	Na1[1]	47.58(5)	C56	C51	N14	116.5(2)
B1[1]	Na1	Na1[2]	156.60(6)	C51	C52	C53	118.8(2)
B1[1]	Na1	B1	134.57(8)	C54	C53	C52	121.6(2)
C1	O1	Na1	119.38(15)	C53	C54	C55	119.1(2)
C1S	O1S	Na1	117.84(16)	C56	C55	C54	120.5(2)
Na1	O2	Na1[2]	107.69(6)	C55	C56	C51	120.1(2)
C2	O2	Na1[2]	124.91(14)	Na1[2]	B1	Na1	85.30(7)
C2	O2	Na1	117.20(14)	O2	B1	Na1	51.07(10)
C2	O2	B1	110.30(17)	O2	B1	Na1[2]	62.16(12)
B1	O2	Na1	101.26(13)	O2	B1	O12	111.69(19)
B1	O2	Na1[2]	89.36(13)	O3	B1	Na1[2]	130.75(16)
C3	O3	B1	108.72(17)	O3	B1	Na1	125.90(15)
C11	O11	Na1	119.05(16)	O3	B1	O2	105.61(18)
C12	O12	Na1	112.37(13)	O3	B1	O12	111.9(2)
C12	O12	B1	110.17(18)	O3	B1	O13	112.71(19)
B1	O12	Na1	90.94(12)	O12	B1	Na1	60.65(11)
C13	O13	Na1[2]	120.04(14)	O12	B1	Na1[2]	116.90(14)
C13	O13	B1	109.75(19)	O13	B1	Na1	121.13(15)
B1	O13	Na1[2]	103.26(13)	O13	B1	Na1[2]	49.13(11)
C1	N2	C21	129.8(2)	O13	B1	O2	111.0(2)
C4	N4	C31	128.0(2)	O13	B1	O12	104.14(18)

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

Table 4.6 Hydrogen Bonds for **4** Na [B{Tar(NHPh)$_2$}$_2$] 2MeOH.

D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
O1S	H1S	O12[1]	0.85(4)	1.89(4)	2.721(3)	166(3)
N2	H2	O4	0.86(3)	1.99(3)	2.801(3)	157(3)
N4	H4	O3	0.85(3)	2.20(3)	2.659(3)	114(2)
N11	H11	O2S	0.89(3)	1.96(3)	2.844(3)	172(3)
N14	H14	O3	0.92(3)	2.37(3)	3.083(2)	134(3)
N14	H14	O13	0.92(3)	2.02(3)	2.599(3)	120(2)
O2S	H2S	O14	0.84(5)	1.91(5)	2.745(3)	170(4)

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

Table 4.8 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **4** Na [B{Tar(NHPh)$_2$}$_2$] 2MeOH.

Atom	*x*	*y*	*z*	U(eq)
H1S	4030(50)	9120(20)	5095(11)	38(9)
H2	2990(40)	6460(20)	6600(9)	24(7)
H4	2350(40)	4089(19)	5707(10)	28(8)
H11	1630(40)	7050(20)	3555(10)	33(8)
H14	3750(40)	4579(19)	4753(10)	25(7)
H1SA	2742	9591	5757	48
H1SB	2024	10360	5435	48
H1SC	4094	10232	5504	48
H2A	4502	6379	5920	24
H3	916	5805	5860	25
H12	738	6156	4112	24
H13	4191	6042	4048	25
H22	729	8469	6667	43
H23	-663	8968	7332	55
H24	-470	8159	8004	62
H25	1120	6844	8019	58
H26	2441	6324	7353	45
H32	1565	2585	5799	35
H33	2230	1244	6144	45
H34	4107	1200	6772	50
H35	5266	2502	7065	44
H36	4610	3859	6724	35
H42	2866	9100	4038	27
H43	3418	10370	3607	33
H44	3170	10348	2821	40
H45	2411	9041	2451	39
H46	1862	7769	2869	32
H52	2046	3115	3904	32
H53	2083	1578	3966	36
H54	3346	889	4593	37
H55	4570	1745	5174	33
H56	4559	3275	5121	29
H2S	1420(60)	5510(30)	3383(14)	68(13)
H2SA	-952	5435	2933	65
H2SB	846	5312	2658	65
H2SC	-112	6249	2665	65

Compound 5 [R/(S)-$NH_3CHMeEt$] [$B\{Tar(NHPh)_2\}_2$]

Table 5.1 Crystal data and structure refinement for **5** [R/(S)-$NH_3CHMeEt$] [$B\{Tar(NHPh)_2\}_2$].

Identification code	gem71a
Empirical formula	$C_{36}H_{40}BN_5O_8$
Formula weight	681.54
Temperature/K	100.01(10)
Crystal system	orthorhombic
Space group	$P2_12_12_1$
a/Å	5.49285(12)
b/Å	21.2422(5)
c/Å	29.4393(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3434.97(13)
Z	4
ρ_{calc}g/cm^3	1.318
μ/mm^{-1}	0.769
F(000)	1440.0
Crystal size/mm^3	0.5 × 0.01 × 0.01
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.324 to 135.998
Index ranges	$-6 \le h \le 4$, $-23 \le k \le 25$, $-29 \le l \le 35$
Reflections collected	9855
Independent reflections	6178 [R_{int} = 0.0305, R_{sigma} = 0.0571]
Data/restraints/parameters	6178/30/506
Goodness-of-fit on F^2	1.006
Final R indexes [I>=2σ (I)]	R_1 = 0.0404, wR_2 = 0.0865
Final R indexes [all data]	R_1 = 0.0535, wR_2 = 0.0906
Largest diff. peak/hole / e Å^{-3}	0.22/-0.20
Flack parameter	0.05(14)

Table 5.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **5** [R/(S)-$NH_3CHMeEt$] [B{Tar$(NHPh)_2$}$_2$].
U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	7626(4)	6560.7(11)	6951.7(7)	23.8(5)
O2	6337(4)	5643.9(11)	6365.6(7)	20.5(5)
O3	2147(4)	5580.0(12)	6273.3(7)	25.1(5)
O4	1827(4)	5074.8(12)	7430.1(7)	26.9(5)
O11	7951(4)	6197.7(11)	4977.5(7)	25.9(5)
O12	4657(4)	5977.4(10)	5651.7(7)	20.8(5)
O13	4686(5)	4900.7(10)	5811.1(7)	25.5(5)
O14	2071(5)	4637.2(12)	4714.8(7)	31.7(6)
N1	5666(5)	6066.9(14)	7539.8(9)	24.2(6)
N4	76(5)	4683.2(13)	6780.2(9)	22.1(6)
N11	5722(5)	5610.9(14)	4472.2(9)	24.7(6)
N14	1392(5)	4197.6(13)	5416.2(9)	23.0(6)
C1	6339(5)	6137.2(15)	7101.2(10)	19.3(6)
C2	5373(6)	5607.4(15)	6804.1(10)	19.1(6)
C3	2545(6)	5627.9(16)	6743.2(10)	20.9(7)
C4	1423(6)	5097.3(15)	7017.8(10)	20.5(6)
C11	6206(6)	5868.7(15)	4883.6(10)	20.7(7)
C12	4300(6)	5673.6(14)	5233.7(9)	18.3(6)
C13	4594(6)	4957.2(15)	5334.5(10)	21.7(6)
C14	2543(6)	4580.7(15)	5122.2(10)	23.5(7)
C21	6390(6)	6414.3(16)	7927.5(10)	24.7(7)
C22	8339(6)	6826.9(17)	7926.8(11)	28.0(8)
C23	8991(7)	7128.6(17)	8331.1(12)	32.2(8)
C24	7719(8)	7014.5(18)	8727.7(12)	35.5(9)
C25	5776(8)	6604.6(18)	8724.8(11)	34.9(9)
C26	5090(7)	6304.1(17)	8326.0(11)	29.2(8)
C31	-1200(6)	4156.7(15)	6951.4(11)	22.8(7)
C32	-432(7)	3832.1(17)	7335.6(11)	31.1(8)
C33	-1759(8)	3315.3(19)	7484.7(14)	40.8(10)
C34	-3817(8)	3120.1(18)	7259.3(14)	41.2(10)
C35	-4565(7)	3441.7(17)	6872.6(13)	37.7(9)
C36	-3268(6)	3958.3(17)	6719.3(12)	30.3(8)
C41	7136(6)	5611.5(16)	4067.3(10)	23.1(7)
C42	9271(7)	5942.8(17)	4020.5(11)	29.2(8)
C43	10502(7)	5922.9(19)	3605.5(11)	34.2(8)
C44	9585(8)	5579.5(19)	3244.6(12)	38.0(9)
C45	7441(7)	5251.4(18)	3296.2(11)	34.9(9)
C46	6216(6)	5260.8(17)	3706.4(10)	27.7(7)
C51	-519(6)	3771.6(15)	5345.7(11)	23.5(7)
C52	-1900(6)	3757.4(16)	4947.5(11)	25.8(7)
C53	-3875(6)	3350.8(17)	4922.1(13)	30.9(8)
C54	-4453(7)	2950.6(18)	5277.6(13)	35.1(8)

C55	-3030(7)	2959.6(18)	5668.9(13)	38.6(9)
C56	-1092(6)	3370.0(16)	5702.2(12)	29.0(8)
B1	4485(7)	5522.7(18)	6025.2(12)	23.1(8)
N62	9225(5)	6569.2(13)	5958.2(9)	24.9(6)
C61	12297(14)	7256(4)	6312(3)	33.7(16)
C61A	8010(30)	7569(7)	5539(6)	39(4)
C62	10665(14)	7153(3)	5896(3)	27.6(15)
C62A	9980(30)	7237(8)	5796(6)	36(3)
C63	8901(11)	7698(3)	5834.4(19)	31.7(12)
C63A	10910(20)	7615(6)	6182(4)	43(3)
C64	7306(15)	7627(4)	5423(3)	39.6(19)
C64A	12860(30)	7328(9)	6451(6)	47(4)

Table 5.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **5** [R/(S)-$NH_3CHMeEt$] [$B\{Tar(NHPh)_2\}_2$]. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	24.8(12)	25.8(12)	20.9(11)	-1.6(9)	3.4(9)	-2.9(10)
O2	17.7(11)	29.8(12)	14.0(10)	-1.5(9)	2.8(8)	-2.0(10)
O3	21.4(11)	37.7(14)	16.2(10)	5.9(10)	-1.7(9)	-2.3(11)
O4	29.0(12)	33.2(13)	18.4(11)	4.2(10)	-0.3(10)	-9.4(11)
O11	28.1(12)	28.5(12)	21.1(11)	-2.1(9)	2.2(10)	-5.8(11)
O12	27.4(11)	20.6(11)	14.4(10)	-0.3(8)	1.4(9)	-0.9(10)
O13	38.9(13)	21.1(11)	16.4(10)	2.3(9)	-5.3(10)	-2.6(10)
O14	43.2(15)	33.2(13)	18.8(11)	1.5(10)	-3.3(11)	-10.6(12)
N1	25.4(15)	29.3(16)	17.8(13)	-2.7(11)	1.9(11)	-5.9(13)
N4	19.7(13)	27.3(14)	19.3(13)	4.0(11)	-1.2(11)	-1.2(11)
N11	25.9(15)	31.5(16)	16.7(13)	-1.0(11)	2.2(11)	-6.2(13)
N14	28.6(15)	22.1(14)	18.4(13)	1.1(11)	-2.7(12)	-2.9(12)
C1	16.2(15)	23.4(16)	18.4(15)	0.7(13)	-0.7(12)	3.2(13)
C2	20.9(15)	21.7(15)	14.6(14)	0.2(12)	2.6(12)	-0.8(13)
C3	22.3(15)	23.0(17)	17.5(15)	1.0(13)	-0.6(13)	1.2(14)
C4	15.1(14)	24.7(16)	21.8(15)	1.8(13)	2.7(12)	0.8(13)
C11	20.6(16)	23.1(16)	18.3(15)	3.7(13)	-2.2(13)	2.1(13)
C12	18.5(15)	20.8(15)	15.4(14)	-0.7(12)	0.1(12)	-1.5(13)
C13	26.4(16)	20.6(15)	18.0(14)	0.4(12)	-0.5(13)	0.6(14)
C14	28.4(17)	19.8(16)	22.2(16)	-2.9(13)	2.8(14)	0.2(14)
C21	28.4(17)	26.1(17)	19.5(15)	-1.9(13)	-2.2(14)	5.8(14)
C22	27.7(18)	32.9(19)	23.3(17)	-4.5(14)	-1.3(15)	5.4(15)
C23	32(2)	32.0(19)	32.3(19)	-8.4(15)	-7.5(16)	4.0(16)
C24	48(2)	35(2)	23.2(17)	-8.7(16)	-9.4(17)	13.0(19)
C25	52(2)	35(2)	17.5(16)	-3.2(15)	3.4(16)	11.6(19)
C26	32.5(19)	31.5(19)	23.5(16)	-2.1(14)	3.2(15)	3.2(16)
C31	19.2(16)	22.0(16)	27.2(16)	-3.0(13)	5.2(13)	2.2(13)

C32	32.9(19)	28.9(18)	31.3(18)	4.8(15)	-2.4(16)	-3.7(16)
C33	51(2)	30(2)	41(2)	9.1(17)	2.1(19)	-6.0(19)
C34	42(2)	26.0(19)	56(2)	-1.1(18)	10(2)	-9.5(18)
C35	31.0(19)	28.7(19)	53(2)	-9.9(18)	-1.3(18)	-6.2(17)
C36	28.6(18)	26.9(19)	35.4(19)	-4.8(15)	-1.0(15)	2.3(15)
C41	26.0(17)	25.7(17)	17.6(15)	2.8(13)	0.3(13)	5.6(14)
C42	30.0(18)	33.7(19)	24.0(17)	-1.0(14)	1.5(15)	0.8(16)
C43	30.8(19)	41(2)	30.7(18)	4.0(16)	10.2(15)	1.6(18)
C44	47(2)	44(2)	23.0(17)	-2.1(16)	9.2(17)	11(2)
C45	42(2)	42(2)	21.0(17)	-6.0(15)	0.6(16)	8.3(18)
C46	28.8(18)	31.3(18)	22.9(16)	-2.7(14)	-0.2(14)	0.4(15)
C51	21.9(16)	19.1(15)	29.4(17)	-6.8(13)	3.4(14)	1.1(14)
C52	26.5(17)	23.4(16)	27.4(17)	-6.5(14)	1.0(14)	2.3(14)
C53	22.0(17)	32.9(19)	37.7(19)	-15.1(16)	-0.6(15)	5.3(15)
C54	20.8(17)	30.5(19)	54(2)	-12.0(17)	3.2(17)	-3.4(16)
C55	42(2)	29(2)	45(2)	1.2(17)	9.2(19)	-7.6(17)
C56	30.2(19)	25.4(18)	31.4(18)	0.7(15)	1.7(15)	-1.0(15)
B1	24.3(18)	23.9(19)	21.3(18)	2.6(15)	-1.5(15)	-3.7(16)
N62	28.7(15)	23.3(14)	22.7(14)	0.5(11)	-2.4(12)	-4.0(12)
C61	30(3)	23(3)	48(3)	1(2)	0(3)	-1(2)
C61A	43(7)	19(6)	56(7)	5(5)	-6(5)	-7(5)
C62	25(3)	20(3)	38(3)	4(2)	8(2)	-1(2)
C62A	36(7)	23(5)	49(6)	10(4)	1(5)	-8(4)
C63	31(3)	24(2)	40(3)	2(2)	3(2)	2(2)
C63A	43(6)	31(5)	55(6)	3(4)	-4(5)	-8(4)
C64	40(4)	35(4)	43(3)	-5(3)	-3(3)	12(3)
C64A	43(7)	44(8)	53(7)	11(5)	-2(6)	-9(6)

Table 5.4 Bond Lengths for **5** [R/(S)-$NH_3CHMeEt$] [$B\{Tar(NHPh)_2\}_2$].

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.226(4)	C23	C24	1.382(5)
O2	C2	1.398(3)	C24	C25	1.377(6)
O2	B1	1.451(4)	C25	C26	1.389(5)
O3	C3	1.404(4)	C31	C32	1.390(5)
O3	B1	1.483(4)	C31	C36	1.391(5)
O4	C4	1.235(4)	C32	C33	1.389(5)
O11	C11	1.218(4)	C33	C34	1.375(6)
O12	C12	1.403(3)	C34	C35	1.390(6)
O12	B1	1.467(4)	C35	C36	1.384(5)
O13	C13	1.409(3)	C41	C42	1.375(5)
O13	B1	1.468(4)	C41	C46	1.393(5)
O14	C14	1.233(4)	C42	C43	1.397(5)
N1	C1	1.351(4)	C43	C44	1.384(5)
N1	C21	1.416(4)	C44	C45	1.377(6)
N4	C4	1.346(4)	C45	C46	1.383(5)
N4	C31	1.413(4)	C51	C52	1.396(5)
N11	C11	1.356(4)	C51	C56	1.389(5)
N11	C41	1.423(4)	C52	C53	1.389(5)
N14	C14	1.346(4)	C53	C54	1.385(5)
N14	C51	1.402(4)	C54	C55	1.392(5)
C1	C2	1.521(4)	C55	C56	1.379(5)
C2	C3	1.564(4)	N62	C62	1.482(8)
C3	C4	1.518(4)	N62	C62A	1.553(17)
C11	C12	1.526(4)	C61	C62	1.533(10)
C12	C13	1.559(4)	C61A	C62A	1.50(2)
C13	C14	1.517(5)	C62	C63	1.520(8)
C21	C22	1.384(5)	C62A	C63A	1.48(2)
C21	C26	1.393(5)	C63	C64	1.501(9)
C22	C23	1.398(5)	C63A	C64A	1.47(2)

Table 5.5 Bond Angles for **5** [R/(S)-$NH_3CHMeEt$] [B{Tar$(NHPh)_2$}$_2$].

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	O2	B1	111.2(2)	C25	C26	C21	119.7(4)
C3	O3	B1	110.9(2)	C32	C31	N4	122.2(3)
C12	O12	B1	110.2(2)	C32	C31	C36	119.8(3)
C13	O13	B1	110.4(2)	C36	C31	N4	118.0(3)
C1	N1	C21	129.5(3)	C33	C32	C31	119.4(4)
C4	N4	C31	127.2(3)	C34	C33	C32	121.2(4)
C11	N11	C41	129.9(3)	C33	C34	C35	119.3(4)
C14	N14	C51	130.3(3)	C36	C35	C34	120.3(4)
O1	C1	N1	125.6(3)	C35	C36	C31	120.0(3)
O1	C1	C2	122.5(3)	C42	C41	N11	123.4(3)
N1	C1	C2	111.9(3)	C42	C41	C46	120.5(3)
O2	C2	C1	111.0(3)	C46	C41	N11	116.1(3)
O2	C2	C3	105.6(2)	C41	C42	C43	119.0(3)
C1	C2	C3	113.1(3)	C44	C43	C42	120.7(4)
O3	C3	C2	105.4(2)	C45	C44	C43	119.6(3)
O3	C3	C4	114.1(3)	C44	C45	C46	120.4(3)
C4	C3	C2	108.7(3)	C45	C46	C41	119.8(3)
O4	C4	N4	125.8(3)	C52	C51	N14	123.1(3)
O4	C4	C3	118.6(3)	C56	C51	N14	117.0(3)
N4	C4	C3	115.6(3)	C56	C51	C52	119.9(3)
O11	C11	N11	126.1(3)	C53	C52	C51	118.9(3)
O11	C11	C12	122.8(3)	C54	C53	C52	121.3(4)
N11	C11	C12	111.1(3)	C53	C54	C55	119.2(3)
O12	C12	C11	111.8(3)	C56	C55	C54	120.1(4)
O12	C12	C13	105.5(2)	C55	C56	C51	120.6(4)
C11	C12	C13	108.8(2)	O2	B1	O3	104.6(2)
O13	C13	C12	106.1(2)	O2	B1	O12	110.8(3)
O13	C13	C14	113.1(3)	O2	B1	O13	113.8(3)
C14	C13	C12	111.1(3)	O12	B1	O3	111.8(3)
O14	C14	N14	125.9(3)	O12	B1	O13	105.4(2)
O14	C14	C13	120.4(3)	O13	B1	O3	110.5(3)
N14	C14	C13	113.7(3)	N62	C62	C61	109.5(6)
C22	C21	N1	123.1(3)	N62	C62	C63	108.2(5)
C22	C21	C26	120.3(3)	C63	C62	C61	111.1(6)
C26	C21	N1	116.6(3)	C61A	C62A	N62	113.2(13)
C21	C22	C23	119.2(3)	C63A	C62A	N62	110.5(12)
C24	C23	C22	120.6(4)	C63A	C62A	C61A	112.5(16)
C25	C24	C23	119.8(3)	C64	C63	C62	113.2(5)
C24	C25	C26	120.4(3)	C64A	C63A	C62A	116.2(13)

Table 5.6 Hydrogen Bonds for **5** [R/(S)-$NH_3CHMeEt$] [B{Tar$(NHPh)_2$}$_2$].

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°

N1	H1	O4	0.88(4)	2.16(4)	2.999(4)	160(3)
N4	H4	O2[1]	0.89(3)	2.60(4)	3.142(3)	120(3)
N4	H4	O3	0.89(3)	2.20(4)	2.674(4)	113(3)
N11	H11	O14	0.87(4)	2.17(4)	2.968(4)	153(3)
N14	H14	O13	0.92(4)	2.06(4)	2.618(4)	118(3)
N62	H62A	O11	0.91	2.21	3.074(3)	158.8
N62	H62C	O3[2]	0.91	1.90	2.802(4)	172.3
N62	H62D	O12	0.91	2.13	2.948(3)	149.4
N62	H62E	O1	0.91	2.16	3.054(3)	169.0

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

Table 5.7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **5** [R/(S)-$NH_3CHMeEt$] [B{Tar$(NHPh)_2$}$_2$].

Atom	***x***	***y***	***z***	**U(eq)**
H1	4540(70)	5777(16)	7582(11)	17(9)
H4	-260(70)	4814(17)	6499(12)	26
H11	4390(70)	5385(17)	4465(11)	21(9)
H14	2100(70)	4214(17)	5698(12)	28
H2	5840	5194	6942	23
H3	1908	6041	6855	25
H12	2627	5762	5116	22
H13	6177	4810	5205	26
H22	9223	6904	7655	34
H23	10321	7415	8333	39
H24	8183	7218	9002	43
H25	4901	6527	8997	42
H26	3740	6025	8325	35
H32	986	3962	7495	37
H33	-1235	3093	7747	49
H34	-4719	2769	7367	49
H35	-5973	3306	6713	45
H36	-3791	4178	6456	36
H42	9901	6182	4267	35
H43	11986	6148	3571	41
H44	10429	5570	2963	46
H45	6801	5017	3049	42
H46	4750	5029	3742	33
H52	-1495	4021	4698	31
H53	-4850	3347	4656	37
H54	-5805	2673	5255	42
H55	-3394	2683	5913	46
H56	-140	3378	5972	35
H62A	8442	6474	5695	30

H62B	8111	6628	6183	30
H62C	10238	6247	6035	30
H62D	8108	6406	5763	30
H62E	8566	6595	6241	30
H62F	10561	6316	5966	30
H61A	11284	7292	6585	50
H61B	13241	7644	6272	50
H61C	13410	6898	6345	50
H61D	7331	7285	5308	59
H61E	8682	7943	5390	59
H61F	6714	7696	5749	59
H62	11702	7112	5619	33
H62G	11367	7180	5580	43
H63A	7859	7730	6108	38
H63B	9839	8094	5808	38
H63C	11506	8021	6062	52
H63D	9526	7708	6387	52
H64A	8322	7607	5150	59
H64B	6207	7990	5402	59
H64C	6347	7240	5450	59
H64D	14021	7121	6248	70
H64E	12159	7016	6659	70
H64F	13693	7655	6627	70

Compound 6 [R/(S)-$NH_3CHMePr$] [$B\{Tar(NHPh)_2\}_2$]

Table 6.1 Crystal data and structure refinement for **6** [R/(S)-$NH_3CHMePr$] [$B\{Tar(NHPh)_2\}_2$].

Identification code	lawr435CuLT
Empirical formula	$C_{37}H_{42}BN_5O_8$
Formula weight	695.56
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	5.56240(9)
b/Å	19.1848(3)
c/Å	16.7363(3)
α/°	90
β/°	95.1248(15)
γ/°	90
Volume/Å^3	1778.85(5)
Z	2
ρ_{calc}g/cm^3	1.299
μ/mm^{-1}	0.752
F(000)	736.0
Crystal size/mm^3	0.8 × 0.05 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.22 to 134.994
Index ranges	$-6 \le h \le 6$, $-22 \le k \le 22$, $-16 \le l \le 20$
Reflections collected	10205
Independent reflections	6296 [R_{int} = 0.0245, R_{sigma} = 0.0417]
Data/restraints/parameters	6296/7/569
Goodness-of-fit on F^2	1.011
Final R indexes [I>=2σ (I)]	R_1 = 0.0300, wR_2 = 0.0702
Final R indexes [all data]	R_1 = 0.0322, wR_2 = 0.0714
Largest diff. peak/hole / e Å^{-3}	0.15/-0.18
Flack parameter	0.10(8)

Table 6.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **6** [R/(S)-$NH_3CHMePr$][B{Tar$(NHPh)_2$}$_2$].
U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	9382(3)	844.2(9)	-77.3(10)	24.8(3)
O2	8576(3)	1331.6(8)	1404.5(9)	19.3(3)
O3	4470(3)	1261.9(8)	1566.1(9)	20.4(3)
O4	3716(3)	2651.2(9)	136.9(10)	29.7(4)
O11	11337(3)	-111.7(9)	3081.7(10)	27.3(4)
O12	7313(3)	476.7(8)	2326.6(9)	19.1(3)
O13	7125(3)	1645.0(8)	2704.8(9)	22.8(3)
O14	6380(3)	1102.0(9)	4707.5(10)	27.3(4)
N1	7094(4)	1725.0(11)	-684.2(12)	25.0(4)
N4	2281(3)	2498.3(10)	1370.1(12)	20.2(4)
N11	9988(3)	67.1(11)	4317.9(12)	21.9(4)
N14	4511(3)	1937.7(10)	3885.6(12)	21.2(4)
C1	8101(4)	1362.7(12)	-45.4(13)	19.5(4)
C2	7408(3)	1668.8(12)	742.9(12)	18.3(4)
C3	4636(4)	1584.2(12)	825.5(13)	19.5(4)
C4	3474(4)	2303.5(12)	741.3(14)	21.8(4)
C11	9825(4)	102.9(11)	3509.9(13)	19.7(4)
C12	7533(4)	481.2(11)	3166.1(13)	18.2(4)
C13	7751(4)	1269.5(11)	3412.4(13)	19.2(4)
C14	6134(4)	1429.3(11)	4075.6(13)	20.1(4)
C21	7158(4)	1568.8(13)	-1512.9(13)	28.2(5)
C22	8729(9)	1104(3)	-1834(2)	29(2)
C23	8675(14)	1022(4)	-2661(3)	32(3)
C24	7049(15)	1403(4)	-3165.9(15)	35(3)
C25	5477(13)	1868(4)	-2844.3(18)	53(2)
C26	5532(8)	1951(2)	-2018(2)	41.7(18)
C22A	9231(15)	1289(4)	-1776(4)	26.0(17)
C23A	9280(30)	1131(6)	-2573(6)	40(3)
C24A	7250(20)	1196(8)	-3109(5)	40(2)
C25A	5240(13)	1432(6)	-2821(4)	55(2)
C26A	5150(13)	1587(6)	-2022(5)	56(3)
C31	1040(4)	3131.4(12)	1463.3(13)	20.2(4)
C32	1746(4)	3750.5(13)	1118.5(15)	27.4(5)
C33	488(5)	4361.8(13)	1245.7(16)	32.5(5)
C34	-1455(5)	4359.8(13)	1708.6(16)	31.8(5)
C35	-2137(4)	3741.2(13)	2058.4(15)	27.4(5)
C36	-900(4)	3128.6(12)	1938.5(14)	21.7(4)
C41	11945(4)	-169.0(11)	4846.0(14)	20.7(4)
C42	13786(4)	-585.6(12)	4599.7(14)	23.2(4)
C43	15644(4)	-795.3(13)	5163.3(16)	29.2(5)
C44	15676(4)	-596.0(14)	5958.0(16)	30.6(5)
C45	13819(5)	-185.2(14)	6197.8(15)	29.4(5)

C46	11947(4)	26.4(12)	5645.1(15)	25.9(5)
C51	2766(4)	2224.0(12)	4349.4(14)	22.2(4)
C52	1241(4)	2732.6(12)	3993.5(16)	27.0(5)
C53	-564(4)	3018.4(12)	4407.6(18)	32.1(6)
C54	-874(5)	2804.5(15)	5166(2)	39.8(7)
C55	529(12)	2262(4)	5466(4)	24.6(13)
C55A	1040(30)	2412(9)	5687(9)	42(4)
C56	2422(18)	1971(6)	5068(6)	26.9(18)
C56A	2610(50)	2088(12)	5237(13)	40(6)
B1	6883(4)	1176.9(12)	2006.0(14)	18.5(5)
N2	11406(3)	100.8(10)	1385.3(12)	24.0(4)
C61	14293(5)	-457.9(15)	571.1(17)	36.4(6)
C62	12814(11)	-565(2)	1272(4)	25.5(12)
C62A	11768(18)	-589(3)	949(5)	23.5(19)
C63	11032(10)	-1149(2)	1091(4)	37.6(16)
C63A	11967(15)	-1159(3)	1582(5)	31(2)
C64	9506(6)	-1354.5(16)	1814(2)	47.2(8)
C65	8130(20)	-1941(6)	1798(9)	61(3)
C65B	9690(20)	-1841(6)	2595(7)	41(2)
C65C	10760(30)	-1771(5)	2395(7)	43(2)

Table 6.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **6** [R/(S)-$NH_3CHMePr$] [$B\{Tar(NHPh)_2\}_2$]. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	25.7(8)	27.6(8)	21.0(8)	-3.7(6)	1.6(6)	4.7(6)
O2	17.0(7)	24.3(7)	16.3(7)	2.7(6)	-0.5(5)	0.9(5)
O3	17.5(7)	22.8(7)	21.1(7)	3.6(6)	1.8(6)	1.3(6)
O4	35.3(9)	33.8(9)	20.6(8)	7.8(7)	5.9(7)	11.0(7)
O11	27.3(8)	34.3(9)	20.6(8)	3.6(7)	4.1(6)	9.5(7)
O12	24.2(7)	17.6(7)	15.1(7)	-1.2(6)	-1.0(5)	0.7(5)
O13	36.1(8)	15.9(7)	16.2(7)	1.5(6)	0.8(6)	-0.7(6)
O14	38.3(9)	25.7(8)	18.0(8)	3.3(6)	3.2(7)	10.2(7)
N1	30.9(10)	28.5(11)	15.3(9)	-1.7(8)	0.7(7)	5.0(8)
N4	20.3(8)	20.2(9)	19.9(9)	3.6(8)	1.1(7)	-0.1(7)
N11	18.7(8)	26.9(10)	20.0(9)	3.2(8)	2.1(7)	6.1(7)
N14	26.7(9)	20.6(9)	15.6(9)	2.1(7)	-1.8(7)	1.1(7)
C1	17.3(9)	22.4(10)	18.6(10)	-2.3(8)	-0.4(7)	-2.4(8)
C2	18.6(9)	21.3(10)	14.3(10)	0.4(8)	-1.9(7)	0.1(8)
C3	18.2(9)	23.2(10)	16.6(10)	-0.1(8)	-0.6(7)	1.6(8)
C4	18.4(9)	25.2(11)	21.3(11)	1.7(9)	-1.6(8)	1.1(8)
C11	20.7(10)	16.5(10)	21.5(11)	3.8(8)	0.1(8)	-0.6(8)
C12	21.6(9)	17.5(10)	15.0(10)	-1.2(8)	-0.3(8)	-0.5(8)
C13	23.4(10)	16.1(10)	17.6(10)	0.9(8)	-1.5(8)	0.1(8)

C14	25.2(10)	18.1(10)	16.4(10)	-2.9(8)	-1.8(8)	-1.3(8)
C21	30.9(12)	36.1(13)	17.8(11)	-3.8(10)	2.9(9)	-6.9(10)
C22	50(4)	10(4)	26(4)	-2(2)	3(3)	5(3)
C23	52(5)	30(5)	15(4)	-8(3)	4(4)	2(4)
C24	38(4)	49(8)	16(4)	-6(3)	-3(3)	-4(4)
C25	63(5)	70(5)	23(3)	-8(4)	-11(3)	40(5)
C26	40(4)	58(5)	25(3)	-18(3)	-10(3)	21(3)
C22A	55(4)	8(3)	15(3)	-2(2)	5(2)	0(3)
C23A	70(6)	25(4)	26(4)	-2(3)	8(4)	7(5)
C24A	60(6)	40(6)	22(4)	-12(3)	13(4)	-14(4)
C25A	34(3)	107(7)	24(3)	-15(4)	-6(2)	-7(4)
C26A	27(3)	110(8)	32(3)	-35(5)	3(2)	-10(4)
C31	19.7(9)	22.3(10)	17.8(10)	0.7(8)	-3.1(8)	0.5(8)
C32	31.4(12)	26.9(12)	24.4(12)	3.3(9)	5.4(9)	-0.1(9)
C33	45.9(14)	21.2(12)	30.7(13)	6.3(10)	5.0(11)	2.9(10)
C34	39.8(13)	24.7(12)	31.0(13)	-2.2(10)	3.1(10)	8.7(10)
C35	27.5(11)	30.3(12)	24.6(12)	-5.4(10)	4.1(9)	0.8(10)
C36	22.7(10)	22.7(11)	19.6(10)	-1.0(8)	0.8(8)	-3.3(8)
C41	20.3(10)	21.1(10)	20.2(11)	6.2(8)	-0.7(8)	-1.9(8)
C42	22.4(10)	24.3(11)	23.0(11)	6.4(9)	3.2(8)	0.2(8)
C43	21.5(10)	33.3(13)	33.1(13)	11.3(10)	3.1(9)	3.7(9)
C44	24.1(11)	35.6(13)	30.6(13)	12.4(11)	-5.7(9)	-1.7(9)
C45	34.7(12)	30.1(12)	22.2(12)	4.9(9)	-4.5(9)	-3.4(10)
C46	28.6(11)	25.3(11)	23.5(11)	3.8(9)	0.9(9)	1.3(9)
C51	19.9(10)	19.7(10)	26.1(11)	1.3(9)	-2.5(8)	-2.2(8)
C52	31.5(11)	20.5(10)	27.1(12)	-4.1(9)	-8.5(9)	0.9(9)
C53	25.2(11)	21.4(12)	47.6(16)	-6.1(10)	-8.9(11)	1.3(9)
C54	28.6(12)	32.4(14)	60.7(19)	6.5(13)	17.3(12)	7.6(10)
C55	29(2)	27(3)	18(3)	-2(2)	4(2)	1.7(18)
C55A	64(10)	42(8)	23(7)	2(5)	22(6)	21(7)
C56	28.2(19)	31(3)	22(4)	-1(3)	6(2)	7.4(18)
C56A	72(11)	36(9)	16(7)	13(7)	24(7)	28(8)
B1	19.7(11)	18.0(11)	17.5(11)	1.0(9)	0.7(9)	0.3(8)
N2	28.5(9)	18.5(9)	26.4(10)	0.8(8)	10.8(8)	0.8(8)
C61	41.4(14)	37.2(14)	32.4(13)	-1.3(11)	14.1(11)	11.2(11)
C62	25(2)	23(2)	28(3)	0.1(18)	-1(2)	10.3(17)
C62A	29(4)	23(4)	19(4)	-2(3)	2(3)	4(3)
C63	41(3)	24(2)	48(4)	-5(2)	6(3)	3.0(18)
C63A	47(4)	19(3)	26(5)	-2(3)	6(4)	9(3)
C64	47.9(17)	30.9(15)	64(2)	10.9(14)	10.1(15)	-2.5(12)
C65	54(6)	47(6)	81(9)	-14(6)	3(6)	-6(5)
C65B	58(7)	35(5)	31(5)	3(4)	5(5)	-5(5)
C65C	72(8)	18(4)	37(6)	2(4)	-2(5)	7(5)

Table 6.4 Bond Lengths for **6** [R/(S)-$NH_3CHMePr$][B{Tar$(NHPh)_2$}$_2$].

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.228(3)	C23A	C24A	1.386(15)
O2	C2	1.392(3)	C24A	C25A	1.334(13)
O2	B1	1.469(3)	C25A	C26A	1.374(10)
O3	C3	1.396(3)	C31	C32	1.392(3)
O3	B1	1.481(3)	C31	C36	1.397(3)
O4	C4	1.229(3)	C32	C33	1.392(4)
O11	C11	1.224(3)	C33	C34	1.385(4)
O12	C12	1.399(3)	C34	C35	1.391(4)
O12	B1	1.458(3)	C35	C36	1.385(3)
O13	C13	1.403(3)	C41	C42	1.390(3)
O13	B1	1.471(3)	C41	C46	1.389(3)
O14	C14	1.227(3)	C42	C43	1.395(3)
N1	C1	1.354(3)	C43	C44	1.382(4)
N1	C21	1.422(3)	C44	C45	1.387(4)
N4	C4	1.346(3)	C45	C46	1.391(3)
N4	C31	1.413(3)	C51	C52	1.391(3)
N11	C11	1.349(3)	C51	C56	1.326(11)
N11	C41	1.414(3)	C51	C56A	1.52(2)
N14	C14	1.348(3)	C52	C53	1.384(4)
N14	C51	1.408(3)	C53	C54	1.360(4)
C1	C2	1.525(3)	C54	C55	1.369(8)
C2	C3	1.569(3)	C54	C55A	1.516(18)
C3	C4	1.525(3)	C55	C56	1.409(8)
C11	C12	1.533(3)	C55A	C56A	1.352(17)
C12	C13	1.569(3)	N2	C62	1.519(4)
C13	C14	1.521(3)	N2	C62A	1.534(7)
C21	C22	1.3900	C61	C62	1.505(5)
C21	C26	1.3900	C61	C62A	1.611(8)
C21	C22A	1.379(8)	C62	C63	1.509(8)
C21	C26A	1.344(8)	C62A	C63A	1.519(12)
C22	C23	1.3900	C63	C64	1.589(6)
C23	C24	1.3900	C63A	C64	1.503(8)
C24	C25	1.3900	C64	C65	1.361(12)
C25	C26	1.3900	C64	C65B	1.602(12)
C22A	C23A	1.371(12)	C64	C65C	1.397(11)

Table 6.5 Bond Angles for **6** [R/(S)-$NH_3CHMePr$][B{Tar$(NHPh)_2$}$_2$].

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	O2	B1	110.91(16)	C21	C26A	C25A	120.8(6)
C3	O3	B1	111.18(15)	C32	C31	N4	121.9(2)
C12	O12	B1	111.13(16)	C32	C31	C36	120.0(2)
C13	O13	B1	110.84(16)	C36	C31	N4	118.0(2)

C1	N1	C21	128.1(2)	C33	C32	C31	119.4(2)
C4	N4	C31	127.2(2)	C34	C33	C32	120.8(2)
C11	N11	C41	128.48(19)	C33	C34	C35	119.6(2)
C14	N14	C51	129.2(2)	C36	C35	C34	120.3(2)
O1	C1	N1	125.6(2)	C35	C36	C31	119.9(2)
O1	C1	C2	122.8(2)	C42	C41	N11	123.0(2)
N1	C1	C2	111.52(19)	C46	C41	N11	116.7(2)
O2	C2	C1	111.91(17)	C46	C41	C42	120.2(2)
O2	C2	C3	105.93(17)	C41	C42	C43	119.1(2)
C1	C2	C3	111.27(16)	C44	C43	C42	121.0(2)
O3	C3	C2	105.52(15)	C43	C44	C45	119.3(2)
O3	C3	C4	114.95(18)	C44	C45	C46	120.4(2)
C4	C3	C2	108.06(17)	C41	C46	C45	119.9(2)
O4	C4	N4	126.2(2)	N14	C51	C56A	125.1(9)
O4	C4	C3	119.4(2)	C52	C51	N14	117.5(2)
N4	C4	C3	114.42(19)	C52	C51	C56A	117.0(9)
O11	C11	N11	125.5(2)	C56	C51	N14	121.3(5)
O11	C11	C12	122.1(2)	C56	C51	C52	120.8(5)
N11	C11	C12	112.32(18)	C53	C52	C51	120.4(2)
O12	C12	C11	111.67(17)	C54	C53	C52	120.4(2)
O12	C12	C13	105.51(16)	C53	C54	C55	117.1(4)
C11	C12	C13	108.39(16)	C53	C54	C55A	123.0(6)
O13	C13	C12	105.40(17)	C54	C55	C56	123.6(7)
O13	C13	C14	113.20(18)	C56A	C55A	C54	111.3(14)
C14	C13	C12	110.43(17)	C51	C56	C55	117.3(8)
O14	C14	N14	126.5(2)	C55A	C56A	C51	124.1(17)
O14	C14	C13	119.87(19)	O2	B1	O3	104.18(17)
N14	C14	C13	113.64(19)	O2	B1	O13	113.76(17)
C22	C21	N1	125.7(2)	O12	B1	O2	110.14(17)
C22	C21	C26	120.0	O12	B1	O3	113.31(17)
C26	C21	N1	114.2(2)	O12	B1	O13	105.64(17)
C22A	C21	N1	119.2(4)	O13	B1	O3	110.02(17)
C26A	C21	N1	121.5(4)	C61	C62	N2	107.9(3)
C26A	C21	C22A	118.6(5)	C61	C62	C63	109.9(5)
C21	C22	C23	120.0	C63	C62	N2	108.2(4)
C24	C23	C22	120.0	N2	C62A	C61	102.0(5)
C23	C24	C25	120.0	C63A	C62A	N2	107.1(6)
C26	C25	C24	120.0	C63A	C62A	C61	112.0(7)
C25	C26	C21	120.0	C62	C63	C64	114.7(5)
C23A	C22A	C21	119.1(8)	C64	C63A	C62A	110.4(7)
C22A	C23A	C24A	121.6(8)	C63A	C64	C65B	111.3(6)
C25A	C24A	C23A	117.2(7)	C65	C64	C63	121.9(7)
C24A	C25A	C26A	122.0(7)				

Table 6.6 Hydrogen Bonds for **6** [R/(S)-$NH_3CHMePr$] [$B\{Tar(NHPh)_2\}_2$].

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N1	H1	O4	0.85(4)	2.21(4)	3.006(3)	156(3)
N4	H4	O2[1]	0.85(4)	2.53(3)	3.047(2)	121(3)
N4	H4	O3	0.85(4)	2.23(3)	2.673(2)	112(3)
N11	H11	O14	0.84(4)	2.13(4)	2.938(3)	161(3)
N14	H14	O13	0.83(4)	2.17(3)	2.617(3)	114(3)

[1]-1+X,+Y,+Z

Table 6.7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **6** [R/(S)-$NH_3CHMePr$] [B{Tar$(NHPh)_2$}$_2$].

Atom	*x*	*y*	*z*	U(eq)
H1	6140(60)	2054(19)	-590(20)	34(8)
H4	2040(60)	2173(18)	1700(20)	27(7)
H11	8880(60)	294(17)	4510(20)	29(8)
H14	4570(60)	2127(17)	3440(20)	29(8)
H2	7835	2175	765	22
H3	3912	1274	388	23
H12	6074	268	3375	22
H13	9465	1375	3608	23
H22	9841	843	-1489	34
H23	9749	704	-2881	38
H24	7012	1347	-3731	42
H25	4366	2129	-3189	64
H26	4458	2268	-1798	50
H22A	10606	1206	-1409	31
H23A	10745	973	-2763	48
H24A	7277	1078	-3659	48
H25A	3830	1495	-3178	66
H26A	3652	1708	-1828	67
H32	3075	3756	799	33
H33	968	4785	1012	39
H34	-2316	4778	1787	38
H35	-3458	3739	2381	33
H36	-1371	2707	2179	26
H42	13778	-726	4055	28
H43	16908	-1080	4998	35
H44	16957	-739	6336	37
H45	13827	-47	6743	35
H46	10671	304	5814	31
H52	1441	2885	3463	32
H53	-1595	3366	4160	39
H54	-2014	3022	5475	48
H54A	-2361	2906	5380	48
H55	208	2070	5969	30
H55A	1136	2396	6256	51
H56	3411	1610	5305	32
H56A	3678	1753	5493	48
H2AA	12453	460	1491	29
H2AB	10481	46	1803	29
H2AC	10440	194	930	29
H2BD	12866	302	1523	29
H2BE	10650	18	1836	29
H2BF	10486	392	1056	29
H61A	13222	-345	92	55

H61B	15189	-885	476	55
H61C	15431	-74	689	55
H61D	14033	-144	109	55
H61E	14934	-903	397	55
H61F	15448	-246	977	55
H62	13889	-672	1767	31
H62A	10426	-682	525	28
H63A	11921	-1566	931	45
H63B	9902	-1011	627	45
H63C	12756	-1574	1370	37
H63D	12978	-994	2061	37
H64A	10656	-1384	2300	57
H64B	8420	-957	1897	57
H64C	8610	-1604	1363	57
H64D	8596	-926	1921	57
H65A	6976	-1936	1319	91
H65B	7247	-1959	2279	91
H65C	9169	-2353	1783	91
H65D	10357	-2295	2464	62
H65E	8079	-1904	2777	62
H65F	10748	-1620	3022	62
H65G	11457	-2172	2135	64
H65H	9655	-1935	2777	64
H65I	12061	-1498	2679	64

Compound 7 [R/(S)-$NH_3CHMePh$][$B\{Tar(NHPh)_2\}_2$]

Table 7.1 Crystal data & refinement for **7** [R/(S)-$NH_3CHMePh$] [$B\{Tar(NHPh)_2\}_2$]

Identification code	gem64b
Empirical formula	$C_{41}H_{44}BN_5O_9$
Formula weight	761.62
Temperature/K	99.94(16)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	5.52108(7)
b/Å	15.50732(18)
c/Å	22.1422(3)
α/°	90
β/°	94.8402(12)
γ/°	90
Volume/Å^3	1888.99(4)
Z	2
ρ_{calc}g/cm^3	1.339
μ/mm^{-1}	0.779
F(000)	804.0
Crystal size/mm^3	0.3 × 0.08 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	9.84 to 134.952
Index ranges	$-5 \le h \le 6$, $-18 \le k \le 18$, $-26 \le l \le 19$
Reflections collected	10786
Independent reflections	6743 [R_{int} = 0.0159, R_{sigma} = 0.0261]
Data/restraints/parameters	6743/2/545
Goodness-of-fit on F^2	1.010
Final R indexes [I>=2σ (I)]	R_1 = 0.0281, wR_2 = 0.0711
Final R indexes [all data]	R_1 = 0.0291, wR_2 = 0.0719
Largest diff. peak/hole / e Å^{-3}	0.35/-0.17
Flack parameter	-0.17(6)

Table 7.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **7** [R/(S)-$NH_3CHMePh$] [$B\{Tar(NHPh)_2\}_2$].
U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O1	4553(3)	3769.4(10)	8684.6(8)	30.8(4)
O2	990(3)	2799.1(10)	8113.4(6)	21.8(3)
O3	-161(3)	3225.6(9)	7118.3(6)	20.6(3)
O4	-1604(3)	5313.4(10)	7655.4(7)	29.0(4)
O11	4093(3)	611.4(10)	7954.6(6)	22.3(3)
O12	2718(2)	2029.6(9)	7284.8(6)	17.5(3)
O13	-1325(2)	1797.7(9)	7451.7(6)	19.4(3)
O14	-1513(3)	795.6(11)	5991.2(7)	30.6(4)
N1	2405(3)	5015.2(12)	8514.3(9)	24.2(4)
N4	-3056(3)	4526.2(12)	6827.9(8)	22.7(4)
N11	3964(3)	-195.5(12)	7094.3(9)	22.2(4)
N14	-3484(3)	1957.1(11)	6349.6(8)	18.6(3)
C1	2734(4)	4157.9(14)	8475.5(9)	21.6(4)
C2	613(4)	3696.8(13)	8125.1(9)	19.5(4)
C3	381(4)	3979.8(13)	7449.0(9)	19.6(4)
C4	-1545(4)	4675.7(14)	7324.8(9)	21.0(4)
C11	3471(3)	513.3(13)	7412.5(9)	17.4(4)
C12	2107(3)	1218.4(13)	7038.2(9)	16.8(4)
C13	-721(3)	1153.6(13)	7048.1(9)	18.2(4)
C14	-1946(3)	1284.7(14)	6408.1(10)	19.4(4)
C21	4027(4)	5652.9(15)	8759.9(9)	23.1(4)
C22	6251(4)	5473.6(15)	9079.3(9)	25.0(4)
C23	7678(4)	6151.7(17)	9313.7(11)	30.2(5)
C24	6939(5)	6996.1(19)	9234.8(15)	44.3(7)
C25	4733(5)	7171.4(19)	8912.4(17)	49.4(8)
C26	3282(4)	6504.5(16)	8675.6(13)	34.5(6)
C31	-4947(4)	5050.8(15)	6564.3(10)	24.4(4)
C32	-6023(5)	5706.9(18)	6872.8(12)	35.2(6)
C33	-7960(5)	6161(2)	6580.2(14)	44.9(7)
C34	-8813(5)	5969.0(19)	5994.8(14)	43.8(7)
C35	-7716(5)	5323.7(19)	5687.3(14)	43.1(7)
C36	-5795(4)	4863.5(16)	5968.5(12)	32.4(5)
C41	5415(4)	-915.4(14)	7285.5(10)	24.7(4)
C42	6886(5)	-945.2(17)	7820.5(11)	36.6(6)
C43	8360(8)	-1660(2)	7944.4(13)	61.9(11)
C44	8343(8)	-2344(2)	7549.7(14)	68.0(12)
C45	6862(7)	-2316.2(19)	7020.3(13)	50.0(8)
C46	5389(5)	-1607.7(17)	6885.6(12)	38.2(6)

C51	-4887(4)	2233.9(13)	5818.2(10)	19.2(4)
C52	-6990(4)	2700.0(14)	5891.8(10)	23.1(4)
C53	-8397(4)	2999.8(15)	5382.6(11)	27.7(5)
C54	-7718(4)	2842.4(16)	4806.5(11)	30.5(5)
C55	-5622(4)	2376.1(17)	4739.5(10)	30.0(5)
C56	-4187(4)	2069.8(15)	5241.1(10)	24.5(4)
B1	577(4)	2463.3(16)	7489.9(10)	18.0(4)
N62	6072(3)	2055.9(13)	8514.7(8)	20.8(4)
C62	6539(7)	1787(2)	9163.1(11)	23.0(6)
C63	7831(4)	929.5(15)	9226.3(9)	22.9(4)
C64	7010(4)	335.8(16)	9629.7(10)	27.7(5)
C65	8222(5)	-440.6(16)	9739.3(11)	32.5(5)
C66	10249(4)	-627.4(16)	9442.1(11)	30.0(5)
C67	11072(4)	-45.4(15)	9031.1(10)	26.6(5)
C68	9875(4)	731.7(15)	8924.5(10)	24.4(4)
C61	7969(6)	2488.0(19)	9520.1(14)	41.1(7)
C61A	5540(40)	2255(13)	9597(9)	23(4)
O1S	1779(3)	-461.2(13)	5909.9(8)	40.0(4)
C1S	3153(5)	-244(2)	5424.2(15)	46.7(7)
C0AA	7390(60)	1950(20)	9140(15)	29(9)

Table 7.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **7** [R/(S)-$NH_3CHMePh$] [B{Tar$(NHPh)_2\}_2$]. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O1	29.4(8)	25.2(8)	35.8(9)	-4.9(7)	-8.9(7)	9.0(7)
O2	31.5(7)	16.6(7)	16.7(7)	-1.7(6)	-1.1(6)	6.6(6)
O3	27.2(7)	18.0(7)	15.9(7)	-1.4(6)	-1.2(6)	7.0(6)
O4	36.7(8)	22.1(8)	27.3(8)	-4.4(7)	-1.9(7)	11.6(7)
O11	27.1(7)	21.2(7)	18.3(7)	-0.7(6)	-0.4(6)	5.1(6)
O12	16.4(6)	14.3(7)	21.7(7)	-3.3(5)	0.8(5)	1.0(5)
O13	16.8(6)	22.6(7)	19.0(7)	-1.2(6)	3.3(5)	3.6(6)
O14	30.6(8)	29.8(9)	29.2(8)	-10.8(7)	-9.4(6)	9.5(7)
N1	23.8(9)	22.2(9)	25.5(9)	-4.7(7)	-4.5(7)	6.1(7)
N4	25.9(9)	19.5(9)	22.2(9)	1.0(7)	-0.8(7)	5.4(7)
N11	25.9(9)	17.8(9)	21.4(9)	-3.7(7)	-5.7(7)	5.9(7)
N14	17.6(8)	19.5(9)	18.4(8)	-0.9(7)	0.6(6)	1.1(7)
C1	24.1(10)	23.1(11)	17.3(10)	-2.2(8)	0.8(8)	6.1(9)
C2	22.9(10)	16.7(10)	18.8(10)	-1.2(8)	0.9(8)	5.7(8)
C3	23.2(10)	17.5(10)	18.2(10)	-2.1(8)	1.9(8)	5.2(8)

C4	24.1(10)	19.6(10)	19.5(10)	1.4(8)	2.4(8)	4.1(8)
C11	14.8(8)	17.7(10)	19.7(10)	-0.6(8)	1.1(7)	0.3(8)
C12	14.9(9)	16.5(9)	18.7(10)	-2.3(8)	-0.5(7)	0.3(7)
C13	15.1(9)	17.3(9)	22.1(10)	-1.3(8)	1.0(7)	1.1(7)
C14	13.0(8)	21.0(10)	23.9(10)	-2.9(8)	-0.2(8)	-1.3(8)
C21	23.1(10)	25.5(11)	20.9(10)	-4.6(9)	2.8(8)	0.4(9)
C22	25.9(10)	29.1(12)	19.9(10)	-0.3(9)	0.9(8)	2.7(9)
C23	25.4(11)	37.7(13)	26.9(12)	-1.3(10)	-0.8(9)	-3.6(10)
C24	35.5(13)	32.7(14)	63.4(18)	-9.8(13)	-4.9(13)	-7.9(11)
C25	41.3(15)	26.5(14)	78(2)	-7.0(13)	-11.4(14)	2.3(11)
C26	29.2(12)	26.4(12)	46.5(15)	-3.6(11)	-6.0(11)	2.6(10)
C31	21.7(10)	22.7(10)	28.8(11)	10.0(9)	1.8(8)	1.7(8)
C32	35.2(12)	39.2(14)	32.0(12)	8.3(11)	6.2(10)	17.6(11)
C33	37.2(13)	45.7(16)	53.3(18)	16.0(14)	11.8(13)	21.8(12)
C34	27.9(12)	43.6(16)	58.4(18)	24.5(14)	-4.7(12)	4.2(11)
C35	41.4(14)	37.8(14)	46.1(16)	14.1(13)	-19.2(12)	-4.1(12)
C36	34.1(12)	26.1(13)	35.1(13)	4.8(10)	-8.0(10)	-1.8(10)
C41	28.6(10)	19.1(10)	26.1(11)	-0.3(9)	0.1(9)	6.3(9)
C42	53.0(15)	30.0(13)	25.2(12)	-5.0(10)	-6.3(11)	20.0(12)
C43	100(3)	53.5(19)	27.9(14)	-7.8(13)	-22.9(15)	49.4(19)
C44	118(3)	47.9(19)	33.9(16)	-8.3(14)	-16.3(18)	60(2)
C45	80(2)	32.2(14)	35.3(15)	-10.2(11)	-8.7(14)	25.9(15)
C46	51.3(15)	29.0(13)	31.9(13)	-7.7(11)	-10.8(11)	13.7(11)
C51	17.4(9)	17.5(10)	22.4(10)	2.4(8)	-1.1(8)	-3.8(7)
C52	21.9(9)	21.5(10)	26.0(11)	4.1(8)	2.1(8)	-0.4(8)
C53	21.2(10)	23.6(11)	37.4(13)	7.6(9)	-3.2(9)	0.4(8)
C54	31.6(11)	27.6(12)	30.2(12)	7.9(10)	-9.9(9)	-7.2(10)
C55	35.0(12)	32.9(12)	21.5(11)	2.6(10)	-1.3(9)	-5.1(10)
C56	23.4(10)	26.3(11)	23.5(11)	1.0(9)	0.3(8)	-1.9(9)
B1	18.4(10)	19.5(11)	16.0(11)	0.4(9)	0.0(8)	4.1(9)
N62	20.6(9)	23.0(9)	18.7(9)	0.7(7)	1.4(7)	6.5(8)
C62	24.7(14)	28.1(15)	15.5(13)	-1.8(10)	-2.1(11)	4.7(13)
C63	25.7(10)	25.5(11)	16.3(10)	-1.1(8)	-6.0(8)	0.8(9)
C64	25.6(10)	34.8(12)	22.3(11)	1.7(9)	0.9(8)	-0.6(9)
C65	37.1(12)	29.5(13)	30.9(12)	7.8(10)	2.0(10)	-6.5(10)
C66	34.4(12)	23.0(11)	31.1(12)	4.1(9)	-5.5(10)	1.8(9)
C67	24.0(10)	29.1(12)	26.2(11)	3.8(9)	-0.9(8)	3.6(9)
C68	26.0(10)	25.2(11)	21.5(10)	3.5(9)	-1.0(8)	-0.6(9)
C61	58.3(19)	28.4(15)	32.5(15)	-7.0(12)	-20.3(13)	11.9(14)
O1S	41.2(10)	40.9(11)	36.1(9)	-10.2(8)	-6.5(8)	15.8(8)
C1S	32.8(13)	42.9(16)	63.4(19)	-5.1(14)	-1.8(12)	-0.6(12)

Table 7.4 Bond Lengths for **7** [R/(S)-$NH_3CHMePh$] [B{Tar$(NHPh)_2$}$_2$].

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C1	1.228(3)	C31	C32	1.387(3)
O2	C2	1.408(2)	C31	C36	1.393(3)
O2	B1	1.475(3)	C32	C33	1.394(4)
O3	C3	1.399(2)	C33	C34	1.374(5)
O3	B1	1.478(3)	C34	C35	1.379(5)
O4	C4	1.232(3)	C35	C36	1.382(4)
O11	C11	1.230(2)	C41	C42	1.379(3)
O12	C12	1.401(2)	C41	C46	1.391(3)
O12	B1	1.465(3)	C42	C43	1.389(4)
O13	C13	1.399(2)	C43	C44	1.373(4)
O13	B1	1.470(3)	C44	C45	1.372(4)
O14	C14	1.234(3)	C45	C46	1.384(4)
N1	C1	1.346(3)	C51	C52	1.389(3)
N1	C21	1.412(3)	C51	C56	1.389(3)
N4	C4	1.344(3)	C52	C53	1.394(3)
N4	C31	1.411(3)	C53	C54	1.381(4)
N11	C11	1.346(3)	C54	C55	1.383(4)
N11	C41	1.418(3)	C55	C56	1.392(3)
N14	C14	1.344(3)	N62	C62	1.496(3)
N14	C51	1.419(3)	N62	C0AA	1.52(3)
C1	C2	1.527(3)	C62	C63	1.510(3)
C2	C3	1.555(3)	C62	C61	1.524(4)
C3	C4	1.524(3)	C63	C64	1.385(3)
C11	C12	1.531(3)	C63	C68	1.393(3)
C12	C13	1.567(3)	C63	C0AA	1.61(3)
C13	C14	1.531(3)	C64	C65	1.389(4)
C21	C22	1.392(3)	C65	C66	1.376(4)
C21	C26	1.391(3)	C66	C67	1.385(3)
C22	C23	1.388(3)	C67	C68	1.385(3)
C23	C24	1.378(4)	C61A	C0AA	1.57(4)
C24	C25	1.385(4)	O1S	C1S	1.408(4)
C25	C26	1.384(4)			

Table 7.5 Bond Angles for **7** [R/(S)-$NH_3CHMePh$] [B{Tar$(NHPh)_2$}$_2$].

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	O2	B1	110.77(16)	C31	C32	C33	119.1(3)

C3	O3	B1	109.91(15)	C34	C33	C32	121.1(3)
C12	O12	B1	111.04(15)	C33	C34	C35	119.6(2)
C13	O13	B1	109.31(15)	C34	C35	C36	120.3(3)
C1	N1	C21	129.2(2)	C35	C36	C31	120.2(3)
C4	N4	C31	128.8(2)	C42	C41	N11	124.1(2)
C11	N11	C41	128.36(18)	C42	C41	C46	119.6(2)
C14	N14	C51	127.64(18)	C46	C41	N11	116.2(2)
O1	C1	N1	124.8(2)	C41	C42	C43	119.3(2)
O1	C1	C2	122.0(2)	C44	C43	C42	121.2(3)
N1	C1	C2	113.16(18)	C45	C44	C43	119.4(3)
O2	C2	C1	111.34(16)	C44	C45	C46	120.4(3)
O2	C2	C3	105.16(16)	C45	C46	C41	120.1(2)
C1	C2	C3	110.75(17)	C52	C51	N14	117.60(19)
O3	C3	C2	105.34(16)	C52	C51	C56	120.2(2)
O3	C3	C4	112.48(17)	C56	C51	N14	122.16(18)
C4	C3	C2	111.90(16)	C51	C52	C53	119.5(2)
O4	C4	N4	125.4(2)	C54	C53	C52	120.8(2)
O4	C4	C3	120.95(18)	C53	C54	C55	119.1(2)
N4	C4	C3	113.67(18)	C54	C55	C56	121.2(2)
O11	C11	N11	124.06(18)	C51	C56	C55	119.2(2)
O11	C11	C12	121.61(18)	O2	B1	O3	104.62(17)
N11	C11	C12	114.31(17)	O12	B1	O2	112.78(17)
O12	C12	C11	109.81(15)	O12	B1	O3	112.73(17)
O12	C12	C13	105.04(15)	O12	B1	O13	104.53(17)
C11	C12	C13	113.08(16)	O13	B1	O2	110.80(17)
O13	C13	C12	104.74(15)	O13	B1	O3	111.57(16)
O13	C13	C14	112.70(16)	N62	C62	C63	112.07(19)
C14	C13	C12	109.95(16)	N62	C62	C61	109.8(3)
O14	C14	N14	124.44(19)	C63	C62	C61	111.1(2)
O14	C14	C13	120.84(18)	C64	C63	C62	117.9(2)
N14	C14	C13	114.73(18)	C64	C63	C68	119.0(2)
C22	C21	N1	124.0(2)	C64	C63	C0AA	132.5(12)
C26	C21	N1	116.2(2)	C68	C63	C62	123.0(2)
C26	C21	C22	119.7(2)	C68	C63	C0AA	106.2(12)
C23	C22	C21	119.2(2)	C63	C64	C65	120.7(2)
C24	C23	C22	121.3(2)	C66	C65	C64	119.9(2)
C23	C24	C25	119.3(3)	C65	C66	C67	120.1(2)
C26	C25	C24	120.3(3)	C68	C67	C66	120.0(2)
C25	C26	C21	120.2(2)	C67	C68	C63	120.3(2)
C32	C31	N4	123.5(2)	N62	C0AA	C63	105.6(19)
C32	C31	C36	119.7(2)	N62	C0AA	C61A	105(2)
C36	C31	N4	116.7(2)	C61A	C0AA	C63	108(2)

Table 7.6 Hydrogen Bonds for **7** [R/(S)-$NH_3CHMePh$] [B{$Tar(NHPh)_2$}$_2$].

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
O1S	H1S	O14	0.84	1.85	2.681(2)	168.3
N62	H62A	O1	0.92(3)	1.96(3)	2.821(3)	154(2)
N62	H62B	O13[1]	0.84(3)	2.26(3)	2.887(2)	131(3)
N62	H62C	O11	0.94(4)	1.82(4)	2.742(2)	168(3)
N14	H14	O13	0.88(3)	2.13(3)	2.636(2)	116(2)
N1	H1	O4	0.87(3)	1.99(3)	2.832(3)	161(3)
N4	H4	O3	0.89(3)	2.12(3)	2.620(2)	115(2)
N11	H11	O1S	0.87(3)	1.96(3)	2.823(3)	170(3)

[1]1+X,+Y,+Z

Table 7.7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **7** [R/(S)-$NH_3CHMePh$] [B{$Tar(NHPh)_2$}$_2$].

Atom	*x*	*y*	*z*	U(eq)
H2	-932	3827	8313	23
H3	1985	4207	7342	24
H12	2552	1192	6610	20
H13	-1169	576	7205	22
H22	6785	4895	9136	30
H23	9195	6031	9533	36
H24	7931	7453	9400	53
H25	4215	7752	8854	59
H26	1771	6629	8455	41
H32	-5448	5845	7278	42
H33	-8703	6612	6789	54
H34	-10149	6279	5803	53
H35	-8284	5195	5280	52
H36	-5050	4418	5755	39
H42	6891	-482	8101	44
H43	9399	-1677	8309	74
H44	9349	-2831	7642	82
H45	6846	-2786	6745	60
H46	4360	-1594	6520	46
H52	-7466	2814	6286	28
H53	-9840	3316	5432	33

H54	-8677	3051	4461	37
H55	-5153	2263	4344	36
H56	-2747	1753	5189	29
H62	4932	1726	9336	28
H64	5604	461	9833	33
H65	7652	-842	10019	39
H66	11086	-1157	9519	36
H67	12459	-179	8822	32
H68	10449	1131	8644	29
H61A	9562	2557	9362	62
H61B	8188	2324	9949	62
H61C	7075	3034	9480	62
H61D	5295	2880	9560	34
H61E	6177	2115	10011	34
H61F	3979	1960	9504	34
H1S	601	-120	5918	60
H1SA	2299	-440	5043	70
H1SB	4747	-524	5480	70
H1SC	3368	383	5412	70
H0AA	8946	2287	9185	35
H62A	5180(50)	2560(19)	8492(11)	23(6)
H62B	7410(60)	2140(20)	8368(14)	38(8)
H62C	5200(60)	1610(20)	8315(14)	43(8)
H14	-3740(50)	2186(19)	6703(13)	29(7)
H1	1060(50)	5190(20)	8312(13)	32(7)
H4	-2690(50)	4050(20)	6634(14)	37(8)
H11	3350(60)	-210(20)	6719(15)	46(9)

Compound 8 [S-NH_3CHEtPh][B{Tar$(NHPh)_2\}_2$] MeOH

Table 8.1 Crystal data & structure refinement for **8** [S-NH_3CHEtPh][B{Tar$(NHPh)_2\}_2$] MeOH

Identification code	lawr437CuLT
Empirical formula	$C_{41}H_{42}BN_5O_8$
Formula weight	743.60
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	C2
a/Å	28.6200(11)
b/Å	5.25819(14)
c/Å	28.6090(9)
α/°	90
β/°	113.834(4)
γ/°	90
Volume/Å^3	3938.2(3)
Z	4
ρ_{calc}g/cm^3	1.254
μ/mm^{-1}	0.716
F(000)	1568.0
Crystal size/mm^3	0.15 × 0.05 × 0.03
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.69 to 134.892
Index ranges	$-34 \le h \le 32$, $-6 \le k \le 6$, $-22 \le l \le 34$
Reflections collected	10916
Independent reflections	7008 [R_{int} = 0.0238, R_{sigma} = 0.0371]
Data/restraints/parameters	7008/2/564
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R_1 = 0.0364, wR_2 = 0.0950
Final R indexes [all data]	R_1 = 0.0396, wR_2 = 0.0972
Largest diff. peak/hole / e Å^{-3}	0.22/-0.16
Flack parameter	0.19(15)

Table 8.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **8** [S-NH_3CHEtPh][B{Tar$(NHPh)_2$}$_2$] MeOH.
U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
B1	1817.4(10)	2484(5)	2633.3(10)	25.4(5)
C1	515.5(9)	3644(5)	1848.2(9)	28.2(5)
N1	65.6(8)	2495(5)	1764.1(8)	34.2(5)
O1	598.7(7)	5031(4)	1545.8(7)	33.1(4)
C2	928.3(9)	3035(5)	2373.0(9)	27.9(5)
O2	1386.0(6)	4246(3)	2438.2(6)	27.6(4)
C3	1057.6(9)	137(5)	2446.3(9)	28.7(5)
O3	1590.2(7)	-7(3)	2652.1(7)	33.8(4)
C4	826.9(9)	-1049(5)	2786.8(9)	28.8(5)
N4	1162.1(8)	-2324(4)	3189.6(8)	30.3(4)
O4	368.6(7)	-820(4)	2677.6(7)	36.6(4)
C11	2883.5(9)	4326(5)	2387.4(9)	28.1(5)
O11	2641.3(7)	5902(4)	2064.3(7)	36.4(4)
C12	2617.8(9)	2328(5)	2577.6(8)	27.3(5)
O12	2089.5(6)	2395(4)	2292.9(6)	28.3(4)
C13	2693.3(10)	2915(5)	3142.9(9)	33.0(5)
O13	2205.3(7)	3208(3)	3131.0(6)	31.2(4)
C14	3001.4(11)	813(7)	3494.6(9)	41.0(7)
N14	2755.6(9)	-371(5)	3746.6(8)	35.4(5)
C21	-390.7(10)	2505(6)	1315.9(10)	33.0(5)
C22	-487.1(12)	4282(7)	931.9(11)	45.6(7)
C23	-947.4(12)	4188(7)	501.9(12)	50.7(8)
C24	-1307.6(11)	2345(7)	453.3(11)	44.5(7)
C25	-1209.1(12)	630(7)	841.0(14)	55.4(9)
C26	-755.7(12)	703(7)	1273.4(13)	52.1(8)
C31	1054.6(10)	-3699(5)	3559.4(9)	33.1(6)
C32	683.7(13)	-2898(7)	3722.9(12)	48.1(7)
C33	610.2(15)	-4264(8)	4104.1(13)	61.2(10)
C34	901.6(14)	-6386(7)	4322.0(11)	54.9(9)
C35	1267.3(13)	-7150(7)	4157.5(11)	50.6(8)
C36	1347.0(12)	-5833(6)	3775.5(10)	40.6(6)
C51	2907.6(11)	-2387(6)	4102.8(9)	38.7(6)
C52	2560.2(13)	-3228(6)	4291.9(10)	42.0(7)
C53	2676.5(14)	-5267(6)	4629.9(10)	48.2(8)
C54	3142.7(15)	-6447(6)	4781.8(11)	55.7(9)
C55	3492.2(14)	-5614(7)	4600.6(11)	55.0(9)
C56	3382.6(13)	-3560(7)	4257.5(11)	49.0(8)
N11	3387(9)	4150(40)	2557(8)	34(4)
O14	3436.1(9)	431(7)	3525.9(10)	53.1(7)
C42	3547(3)	8070(20)	2121(5)	45(3)
C41	3715(4)	6210(20)	2497(5)	43(3)
C46	4222(4)	6170(20)	2846(4)	83(4)

C45	4561(3)	8000(20)	2820(3)	75(4)
C44	4393(3)	9870(18)	2444(4)	58(3)
C43	3886(4)	9900(20)	2094(4)	62(3)
N11A	3401(9)	4380(40)	2674(9)	39(4)
O14A	3318(9)	-850(50)	3443(10)	46(6)
C41A	3770(3)	5910(20)	2638(4)	38(3)
C46A	4242(4)	5939(18)	3052(3)	62(3)
C45A	4615(3)	7659(18)	3062(3)	64(3)
C44A	4516(3)	9348(17)	2660(3)	53(3)
C43A	4044(4)	9317(19)	2246(3)	51(2)
C42A	3671(3)	7600(20)	2236(4)	43(2)
N2	1641.1(9)	7370(4)	1745.9(8)	28.4(4)
C61	706.6(14)	10372(10)	502.4(13)	67.8(12)
C62	1001.6(10)	9932(6)	1070.1(10)	36.5(6)
C63	1419.4(10)	7930(5)	1182.3(9)	29.2(5)
C64	1843.0(10)	8666(5)	1019.5(8)	27.8(5)
C65	2137.8(10)	10837(5)	1217.8(9)	31.1(5)
C66	2538.7(11)	11448(5)	1087.3(10)	34.4(6)
C67	2650.2(11)	9896(6)	750.6(10)	37.0(6)
C68	2355.1(11)	7770(6)	545.6(10)	39.2(6)
C69	1955.2(10)	7148(5)	682.5(9)	33.3(5)

Table 8.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **8**
[S-NH_3CHEtPh][B{Tar$(NHPh)_2$}$_2$] MeOH.
Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
B1	33.2(13)	20.1(12)	27.1(12)	-1.2(11)	16.5(11)	-6.0(11)
C1	30.6(12)	24.0(11)	34.1(12)	-2.8(10)	17.4(10)	-4.8(9)
N1	33.6(11)	37.7(12)	32.4(11)	4.2(10)	14.4(9)	-9.4(10)
O1	34.2(9)	32.3(9)	33.8(8)	2.9(7)	14.9(7)	-6.1(7)
C2	31.9(12)	25.6(12)	31.3(11)	-3.2(10)	18.1(10)	-9.5(10)
O2	28.3(8)	24.1(8)	32.7(8)	-1.2(7)	14.6(7)	-8.8(7)
C3	34.3(12)	24.8(11)	32.4(12)	-2.0(10)	19.1(10)	-8.3(10)
O3	34.0(9)	22.3(8)	52.1(11)	0.1(8)	24.7(8)	-5.2(7)
C4	34.9(13)	25.1(11)	30.5(11)	-3.3(10)	17.4(10)	-11.7(10)
N4	33.8(11)	29.6(11)	30.8(10)	-2.5(9)	16.3(9)	-7.8(9)
O4	32.4(9)	40.5(10)	39.7(9)	5.1(9)	17.3(7)	-10.4(8)
C11	29.6(12)	26.8(12)	32.0(11)	-5.5(10)	16.7(10)	-5.6(10)
O11	35.2(9)	34.9(10)	39.4(9)	6.8(8)	15.4(8)	-7.3(8)
C12	27.9(11)	27.6(11)	25.3(11)	-2.9(9)	9.3(9)	-7.1(10)
O12	25.9(8)	37.4(9)	22.2(7)	-5.4(7)	10.4(6)	-11.2(7)
C13	34.5(12)	37.0(14)	25.4(11)	-5.4(10)	9.9(10)	-9.5(11)
O13	37.3(9)	33.4(9)	22.9(7)	-3.3(7)	12.1(7)	-1.0(7)
C14	36.4(14)	58.6(18)	24.4(11)	-4.0(12)	8.4(10)	2.5(14)

N14	38.1(12)	41.7(13)	20.9(9)	-2.0(9)	6.4(9)	2.9(10)
C21	30.6(12)	35.7(13)	35.4(12)	-4.9(11)	16.2(10)	-5.0(11)
C22	41.9(15)	48.6(17)	42.1(15)	6.0(14)	12.6(12)	-14.4(14)
C23	45.1(16)	59(2)	40.6(15)	9.7(15)	10.0(13)	-5.9(15)
C24	31.8(13)	55.2(18)	41.2(14)	-8.3(14)	9.3(11)	-1.3(13)
C25	37.8(15)	52.3(19)	65(2)	3.4(17)	8.9(14)	-16.7(15)
C26	39.2(15)	47.6(18)	60.1(18)	15.0(16)	10.5(14)	-11.8(14)
C31	42.6(14)	30.2(13)	26.2(11)	-1.8(10)	13.6(11)	-12.3(11)
C32	59.4(19)	51.2(18)	43.4(15)	6.7(14)	30.7(14)	-2.2(15)
C33	76(2)	73(3)	50.1(17)	12.7(19)	41.1(18)	-4(2)
C34	68(2)	63(2)	32.5(13)	10.1(14)	19.3(14)	-18.0(18)
C35	60.7(19)	46.6(17)	33.2(13)	11.0(13)	7.3(14)	-7.0(15)
C36	45.4(15)	40.3(15)	32.4(12)	1.0(12)	11.9(11)	-6.5(13)
C51	49.2(15)	36.0(14)	20.1(10)	-5.4(11)	2.6(11)	2.9(13)
C52	57.4(18)	38.8(15)	24.3(11)	-3.2(11)	10.6(12)	0.8(13)
C53	67(2)	39.6(16)	27.7(12)	-3.2(12)	8.8(13)	-2.5(15)
C54	79(2)	36.7(15)	32.2(13)	-5.7(12)	2.6(15)	3.0(16)
C55	59.7(19)	48.8(18)	34.4(14)	-6.4(14)	-3.8(14)	9.0(16)
C56	49.5(17)	50.6(18)	32.4(13)	-5.1(13)	1.5(12)	6.6(14)
N11	32(4)	23(3)	51(10)	-10(5)	21(6)	-12(3)
O14	35.4(12)	81(2)	40.4(12)	10.0(14)	12.2(10)	9.3(14)
C42	42(5)	46(6)	55(5)	0(4)	30(4)	-14(5)
C41	27(4)	36(5)	69(8)	4(5)	24(4)	-6(4)
C46	32(5)	75(7)	131(11)	39(7)	21(6)	-4(4)
C45	27(4)	69(8)	117(10)	16(8)	19(5)	-15(5)
C44	46(6)	38(5)	114(10)	-12(6)	55(7)	-16(4)
C43	64(7)	47(6)	85(7)	12(5)	42(6)	-15(5)
N11A	25(4)	48(7)	44(8)	-11(5)	13(5)	-3(4)
C41A	32(5)	25(4)	60(6)	-6(4)	23(4)	-4(3)
C46A	28(4)	30(3)	112(8)	14(5)	12(4)	-7(3)
C45A	34(4)	41(4)	105(8)	4(6)	17(5)	-4(3)
C44A	39(5)	31(5)	95(8)	-1(6)	35(5)	-13(4)
C43A	53(7)	41(5)	74(6)	1(4)	42(5)	-13(5)
C42A	37(4)	40(5)	59(7)	2(5)	26(4)	-7(5)
N2	35.4(11)	24.7(10)	27.5(10)	2.7(9)	15.1(9)	-1.1(10)
C61	48.4(18)	109(3)	43.2(16)	26(2)	15.4(14)	24(2)
C62	35.6(13)	40.5(14)	34.7(13)	7.6(11)	15.6(11)	0.5(12)
C63	34.8(12)	26.9(12)	24.6(10)	-1.0(9)	10.7(9)	-5.1(10)
C64	35.5(12)	26.9(12)	19.4(9)	1.0(9)	9.3(9)	-1.5(10)
C65	43.2(14)	27.6(12)	25.3(10)	-1.1(10)	16.9(10)	-4.0(11)
C66	42.4(14)	32.2(13)	31.8(12)	0.8(10)	18.2(11)	-7.9(11)
C67	43.3(14)	43.2(15)	31.8(12)	5.3(11)	22.7(11)	-0.9(12)
C68	51.3(16)	41.4(15)	30.1(12)	-3.0(11)	21.9(12)	2.3(13)
C69	41.6(14)	31.7(13)	25.9(11)	-3.5(10)	12.9(10)	-4.9(11)

Table 8.4 Bond Lengths for **8** [S-NH_3CHEtPh][B{Tar$(NHPh)_2\}_2$] MeOH.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
B1	O2	1.462(3)	C32	C33	1.391(4)
B1	O3	1.473(3)	C33	C34	1.382(6)
B1	O12	1.473(3)	C34	C35	1.370(6)
B1	O13	1.458(3)	C35	C36	1.388(4)
C1	N1	1.353(3)	C51	C52	1.383(5)
C1	O1	1.226(3)	C51	C56	1.392(4)
C1	C2	1.523(3)	C52	C53	1.391(4)
N1	C21	1.413(3)	C53	C54	1.373(5)
C2	O2	1.399(3)	C54	C55	1.371(6)
C2	C3	1.562(3)	C55	C56	1.407(5)
C3	O3	1.397(3)	N11	C41	1.49(2)
C3	C4	1.514(3)	C42	C41	1.3900
C4	N4	1.343(3)	C42	C43	1.3900
C4	O4	1.225(3)	C41	C46	1.3900
N4	C31	1.414(3)	C46	C45	1.3900
C11	O11	1.226(3)	C45	C44	1.3900
C11	C12	1.521(3)	C44	C43	1.3900
C11	N11	1.32(2)	N11A	C41A	1.36(3)
C11	N11A	1.37(2)	C41A	C46A	1.3900
C12	O12	1.399(3)	C41A	C42A	1.3900
C12	C13	1.573(3)	C46A	C45A	1.3900
C13	O13	1.392(3)	C45A	C44A	1.3900
C13	C14	1.515(4)	C44A	C43A	1.3900
C14	N14	1.346(4)	C43A	C42A	1.3900
C14	O14	1.227(4)	N2	C63	1.504(3)
C14	O14A	1.31(2)	C61	C62	1.515(4)
N14	C51	1.411(4)	C62	C63	1.527(4)
C21	C22	1.382(4)	C63	C64	1.514(4)
C21	C26	1.379(4)	C64	C65	1.396(3)
C22	C23	1.393(4)	C64	C69	1.385(4)
C23	C24	1.381(5)	C65	C66	1.380(4)
C24	C25	1.367(5)	C66	C67	1.394(4)
C25	C26	1.385(5)	C67	C68	1.381(4)
C31	C32	1.387(4)	C68	C69	1.390(4)
C31	C36	1.387(4)			

Table 8.5 Bond Angles for **8** [S-NH_3CHEtPh][B{Tar$(NHPh)_2\}_2$] MeOH.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O2	B1	O3	105.09(19)	C21	C26	C25	120.1(3)
O2	B1	O12	110.99(19)	C32	C31	N4	121.6(3)
O12	B1	O3	110.8(2)	C32	C31	C36	120.1(3)
O13	B1	O2	113.6(2)	C36	C31	N4	118.2(3)

O13	B1	O3	111.7(2)	C31	C32	C33	119.1(3)
O13	B1	O12	104.87(19)	C34	C33	C32	121.1(4)
N1	C1	C2	112.6(2)	C35	C34	C33	119.2(3)
O1	C1	N1	125.6(2)	C34	C35	C36	121.0(3)
O1	C1	C2	121.8(2)	C31	C36	C35	119.5(3)
C1	N1	C21	128.6(2)	C52	C51	N14	117.5(3)
C1	C2	C3	112.6(2)	C52	C51	C56	119.9(3)
O2	C2	C1	110.32(19)	C56	C51	N14	122.6(3)
O2	C2	C3	105.5(2)	C51	C52	C53	120.7(3)
C2	O2	B1	111.29(18)	C54	C53	C52	119.8(4)
O3	C3	C2	105.57(19)	C55	C54	C53	120.0(3)
O3	C3	C4	113.1(2)	C54	C55	C56	121.2(3)
C4	C3	C2	110.3(2)	C51	C56	C55	118.4(4)
C3	O3	B1	111.05(19)	C11	N11	C41	123.5(16)
N4	C4	C3	114.3(2)	C41	C42	C43	120.0
O4	C4	C3	119.7(2)	C42	C41	N11	124.4(11)
O4	C4	N4	126.0(2)	C42	C41	C46	120.0
C4	N4	C31	126.9(2)	C46	C41	N11	115.6(11)
O11	C11	C12	121.6(2)	C45	C46	C41	120.0
O11	C11	N11	121.5(9)	C44	C45	C46	120.0
O11	C11	N11A	125.4(11)	C45	C44	C43	120.0
N11	C11	C12	116.6(9)	C44	C43	C42	120.0
N11A	C11	C12	112.1(11)	C41A	N11A	C11	131(2)
C11	C12	C13	110.6(2)	N11A	C41A	C46A	117.3(12)
O12	C12	C11	110.7(2)	N11A	C41A	C42A	122.3(12)
O12	C12	C13	105.12(19)	C46A	C41A	C42A	120.0
C12	O12	B1	110.59(17)	C45A	C46A	C41A	120.0
O13	C13	C12	106.08(19)	C46A	C45A	C44A	120.0
O13	C13	C14	114.0(2)	C43A	C44A	C45A	120.0
C14	C13	C12	110.0(2)	C42A	C43A	C44A	120.0
C13	O13	B1	110.82(18)	C43A	C42A	C41A	120.0
N14	C14	C13	113.8(2)	C61	C62	C63	112.4(3)
O14	C14	C13	118.0(3)	N2	C63	C62	108.4(2)
O14	C14	N14	128.2(3)	N2	C63	C64	109.7(2)
O14A	C14	C13	131.0(12)	C64	C63	C62	114.6(2)
O14A	C14	N14	106.6(12)	C65	C64	C63	120.8(2)
C14	N14	C51	131.2(3)	C69	C64	C63	120.4(2)
C22	C21	N1	122.6(2)	C69	C64	C65	118.8(2)
C26	C21	N1	117.8(3)	C66	C65	C64	120.8(2)
C26	C21	C22	119.6(3)	C65	C66	C67	119.9(3)
C21	C22	C23	119.4(3)	C68	C67	C66	119.7(2)
C24	C23	C22	121.0(3)	C67	C68	C69	120.2(2)
C25	C24	C23	118.7(3)	C64	C69	C68	120.6(2)
C24	C25	C26	121.2(3)				

Table 8.6 Hydrogen Bonds for **8** [S-NH_3CHEtPh][B{Tar$(NHPh)_2$}$_2$] MeOH.

D	**H**	**A**	**d(D-H)/Å**	**d(H-A)/Å**	**d(D-A)/Å**	**D-H-A/°**
N2	H2A	O3[1]	0.91(4)	2.36(3)	2.992(3)	127(2)
N4	H4	O3	0.85(3)	2.14(3)	2.622(3)	115(3)
N14	H14	O13	0.88(3)	2.14(3)	2.623(3)	114(3)
N2	H2B	O11	0.90(4)	1.89(3)	2.741(3)	157(3)
N2	H2B	O12	0.90(4)	2.44(3)	3.052(3)	125(3)
N2	H2C	O1	0.91(4)	2.26(3)	3.060(3)	146(3)
N2	H2C	O2	0.91(4)	2.14(3)	2.885(3)	139(3)
N1	H1	O4	0.84(4)	2.16(4)	2.964(3)	159(3)

[1]+X,1+Y,+Z

Table 8.7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **8** [S-NH_3CHEtPh][B{Tar(NHPh)$_2$}$_2$] MeOH.

Atom	*x*	*y*	*z*	U(eq)
H2	816	3627	2643	33
H3	916	-725	2106	34
H12	2754	600	2557	33
H13	2883	4555	3253	40
H22	-242	5557	961	55
H23	-1014	5411	238	61
H24	-1618	2269	156	53
H25	-1456	-634	813	67
H26	-696	-489	1541	62
H32	483	-1436	3577	58
H33	356	-3730	4216	73
H34	849	-7304	4583	66
H35	1469	-8604	4307	61
H36	1600	-6390	3663	49
H52	2239	-2405	4190	50
H53	2434	-5842	4755	58
H54	3223	-7841	5012	67
H55	3814	-6439	4709	66
H56	3627	-2987	4134	59
H11	3535	2749	2715	41
H42	3201	8096	1882	54
H46	4337	4899	3103	100
H45	4907	7981	3059	89
H44	4624	11121	2426	70
H43	3771	11178	1837	74
H11A	3513	3253	2922	47
H46A	4310	4784	3327	74
H45A	4938	7680	3345	76
H44A	4771	10524	2667	63
H43A	3976	10472	1971	61
H42A	3349	7576	1953	52
H61A	449	11694	449	102
H61B	538	8790	340	102
H61C	942	10917	351	102
H62A	762	9380	1221	44
H62B	1159	11554	1235	44
H63	1257	6337	997	35
H65	2061	11906	1445	37
H66	2738	12923	1227	41
H67	2928	10300	663	44
H68	2426	6730	310	47
H69	1757	5669	544	40
H2A	1728(11)	8860(70)	1921(11)	29(7)

H4	1455(12)	-2480(70)	3179(11)	34(8)
H14	2444(13)	170(70)	3675(12)	36(8)
H2B	1932(13)	6450(70)	1838(12)	35(8)
H2C	1411(12)	6480(60)	1825(12)	34(8)
H1	69(12)	1590(70)	2008(13)	40(9)

Compound 9 [S-$NH_3CH(CH_2OH)Ph$][$B\{Tar(NHPh)_2\}_2$] MeOH

Table 9.1 Crystal data & structure refinement for **9** [S-$NH_3CH(CH_2OH)Ph$][$B\{Tar(NHPh)_2\}_2$]

Identification code	lawr434CuLT
Empirical formula	$C_{41}H_{43.95}BN_5O_{10}$
Formula weight	777.57
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	5.51895(7)
b/Å	15.5145(2)
c/Å	22.2271(3)
α/°	90
β/°	94.4499(12)
γ/°	90
Volume/Å^3	1897.44(4)
Z	2
ρ_{calc}g/cm^3	1.361
μ/mm^{-1}	0.808
F(000)	820.0
Crystal size/mm^3	0.1 × 0.07 × 0.05
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.98 to 134.994
Index ranges	$-3 \le h \le 6$, $-18 \le k \le 18$, $-25 \le l \le 26$
Reflections collected	10612
Independent reflections	6701 [R_{int} = 0.0292, R_{sigma} = 0.0444]
Data/restraints/parameters	6701/1/518
Goodness-of-fit on F^2	1.042
Final R indexes [I>=2σ (I)]	R_1 = 0.0414, wR_2 = 0.1029
Final R indexes [all data]	R_1 = 0.0434, wR_2 = 0.1045
Largest diff. peak/hole / e Å^{-3}	0.34/-0.24
Flack parameter	0.08(15)

Table 9.2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **9** [S-$NH_3CH(CH_2OH)Ph$][B{$Tar(NHPh)_2$}$_2$].
U_{eq} is defined as 1/3 of of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
B1	4492(6)	6141(2)	2507.2(15)	24.3(7)
C1	2124(6)	7848(2)	1568.9(14)	26.7(6)
N1	2417(5)	8702.8(19)	1523.7(13)	30.3(6)
O1	303(4)	7440.2(16)	1384.8(11)	33.3(5)
C2	4332(5)	7403(2)	1897.2(14)	24.9(6)
O2	4059(4)	6499.1(15)	1892.5(9)	26.9(5)
C3	4586(5)	7658(2)	2578.7(14)	24.7(6)
O3	5195(4)	6892.3(14)	2887.8(9)	25.0(4)
C4	6470(6)	8364(2)	2700.2(14)	25.9(6)
N4	8003(5)	8213.5(18)	3184.0(12)	27.4(5)
O4	6475(5)	9009.5(16)	2375.5(11)	37.0(6)
C11	1655(5)	4166(2)	2586.6(14)	23.1(6)
N11	1089(5)	3472.5(17)	2912.6(12)	27.1(5)
O11	1134(4)	4241.8(15)	2043.8(10)	28.3(5)
C12	3005(5)	4880.0(18)	2953.3(14)	21.8(6)
O12	2359(4)	5686.3(13)	2702.7(9)	22.8(4)
C13	5835(5)	4828(2)	2931.6(14)	24.1(6)
O13	6412(4)	5483.3(14)	2533.2(10)	24.9(4)
C14	7058(5)	4954(2)	3571.9(15)	26.7(6)
N14	8576(5)	5629.3(17)	3630.9(12)	25.2(5)
O14	6631(4)	4459.9(17)	3979.9(12)	37.9(6)
C21	806(6)	9331(2)	1261.3(14)	29.1(7)
C22	-1412(6)	9129(2)	943.1(14)	29.8(7)
C23	-2798(6)	9790(3)	677.0(17)	36.3(8)
C24	-2031(7)	10634(3)	713.7(19)	43.6(9)
C25	164(8)	10827(3)	1039(2)	45.2(9)
C26	1575(7)	10178(2)	1310.2(17)	37.0(8)
C31	9890(6)	8745(2)	3442.0(16)	30.5(7)
C32	10901(8)	9415(3)	3134.3(18)	45.9(10)
C33	12843(9)	9872(3)	3426(2)	58.7(13)
C34	13727(8)	9676(3)	4000(2)	54.7(12)
C35	12702(8)	9017(3)	4302(2)	51.1(11)
C36	10784(7)	8553(2)	4028.2(18)	39.2(8)
C41	-368(6)	2758(2)	2727.5(16)	31.4(7)
C42	-1677(7)	2687(2)	2174.0(17)	39.1(8)
C43	-3153(10)	1975(3)	2049.8(19)	54.9(12)
C44	-3310(12)	1327(3)	2467(2)	69.8(17)
C45	-1941(11)	1384(3)	3010(2)	63.3(14)
C46	-487(9)	2090(3)	3144(2)	51.6(11)
C51	9952(6)	5909(2)	4162.3(15)	25.8(6)
C52	12072(6)	6379(2)	4092.1(16)	29.5(7)
C53	13439(6)	6680(2)	4597.5(17)	35.2(8)

C54	12725(7)	6528(2)	5173.4(17)	37.5(8)
C55	10642(7)	6059(3)	5236.1(16)	37.0(8)
C56	9231(6)	5744(2)	4735.1(15)	31.4(7)
C1S	1919(8)	3452(3)	4598(2)	51.1(10)
O1S	3238(5)	3235(2)	4099.0(13)	46.5(7)
N2	-908(5)	5654.1(19)	1484.7(11)	27.3(6)
C62	-1389(6)	5394(2)	840.0(14)	28.9(7)
C63	-2623(5)	4529(2)	771.4(14)	26.1(6)
C64	-4631(6)	4308(2)	1081.3(14)	29.6(7)
C65	-5848(6)	3536(2)	959.0(16)	35.2(8)
C66	-5082(7)	2980(2)	526.8(18)	39.1(8)
C67	-3073(7)	3186(3)	222.3(16)	38.6(8)
C68	-1840(6)	3956(2)	345.6(15)	32.7(7)
O5	-5334(5)	6177(2)	663.6(13)	47.2(7)
C61	-2876(8)	6111(3)	500.6(17)	41.8(9)

Table 9.3 Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for **9** [S-$NH_3CH(CH_2OH)Ph$][B{$Tar(NHPh)_2$}$_2$]. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
B1	20.4(15)	30.3(18)	21.5(15)	-0.4(13)	-2.4(12)	-5.6(13)
C1	22.8(14)	35.1(17)	21.9(14)	1.7(12)	-0.5(11)	-5.3(13)
N1	25.0(12)	34.4(15)	30.2(13)	6.6(11)	-6.0(10)	-7.3(11)
O1	26.9(11)	35.0(13)	36.6(12)	3.5(10)	-7.4(10)	-6.8(9)
C2	21.2(14)	29.4(16)	23.7(15)	3.5(12)	-0.8(11)	-7.6(12)
O2	27.3(10)	29.7(11)	22.6(10)	-0.4(9)	-3.8(8)	-5.7(9)
C3	22.2(14)	28.9(16)	22.6(14)	1.5(12)	0.3(11)	-6.7(12)
O3	26.6(10)	26.6(11)	21.0(10)	2.2(8)	-3.1(8)	-7.1(9)
C4	28.0(15)	26.1(15)	23.6(14)	0.0(12)	1.6(12)	-6.5(12)
N4	27.7(12)	27.4(13)	26.3(13)	-0.7(11)	-1.9(10)	-6.0(11)
O4	40.8(13)	33.1(13)	35.6(13)	7.2(10)	-6.8(10)	-14.6(10)
C11	17.8(12)	24.4(15)	26.7(15)	-0.1(12)	-1.3(11)	-0.4(11)
N11	29.9(13)	24.7(13)	25.3(13)	1.6(10)	-7.0(10)	-3.7(10)
O11	30.6(11)	28.8(11)	24.7(11)	-0.4(9)	-2.4(8)	-6.4(9)
C12	16.2(13)	22.4(14)	26.5(15)	0.7(12)	-1.2(11)	-0.3(11)
O12	18.2(9)	21.9(10)	27.7(10)	2.1(8)	-2.6(8)	-2.5(8)
C13	17.0(13)	27.4(15)	27.4(16)	-1.3(12)	-1.2(11)	-0.9(11)
O13	17.5(9)	31.8(11)	25.2(10)	-0.4(9)	0.5(8)	-4.4(8)
C14	19.4(14)	30.5(16)	29.4(16)	1.8(13)	-3.1(12)	0.8(12)
N14	22.2(12)	28.3(13)	24.6(12)	0.4(10)	-2.2(10)	-1.5(10)
O14	33.0(12)	40.8(14)	37.6(13)	11.4(11)	-12.0(10)	-11.2(11)
C21	27.4(15)	38.0(18)	21.5(14)	6.0(13)	-0.4(12)	-1.8(13)
C22	24.8(14)	38.9(18)	25.1(15)	2.9(13)	-0.8(12)	-3.3(13)
C23	27.5(17)	47(2)	32.9(18)	2.3(15)	-4.4(14)	0.6(15)

C24	38.2(19)	44(2)	48(2)	7.2(17)	-4.0(16)	6.6(16)
C25	43(2)	36(2)	55(2)	8.8(17)	-6.9(17)	-3.7(16)
C26	33.8(18)	37.2(18)	38.6(19)	5.3(15)	-6.8(15)	-5.7(14)
C31	25.8(15)	31.1(16)	34.4(17)	-12.4(13)	1.4(13)	-2.2(13)
C32	45(2)	54(2)	38.3(19)	-9.4(18)	4.6(16)	-26.3(19)
C33	51(3)	62(3)	64(3)	-19(2)	12(2)	-33(2)
C34	36(2)	62(3)	65(3)	-30(2)	-6.6(19)	-11.0(19)
C35	47(2)	49(2)	53(2)	-21(2)	-20.7(19)	0.9(19)
C36	38.4(19)	34.7(19)	42(2)	-8.0(15)	-10.1(16)	2.1(15)
C41	34.1(17)	27.6(16)	31.5(17)	-0.2(13)	-2.6(14)	-6.2(13)
C42	48(2)	35.3(19)	32.2(18)	3.0(15)	-6.0(16)	-15.3(16)
C43	77(3)	50(2)	33.5(19)	2.0(18)	-19.4(19)	-29(2)
C44	107(4)	54(3)	44(2)	7(2)	-14(3)	-51(3)
C45	92(4)	47(2)	47(2)	14(2)	-15(2)	-34(3)
C46	67(3)	43(2)	41(2)	7.1(18)	-16.4(19)	-20(2)
C51	23.7(14)	25.0(15)	27.5(15)	-2.3(12)	-5.7(12)	3.4(12)
C52	25.0(14)	29.0(16)	34.2(17)	-4.4(13)	0.5(12)	-3.5(12)
C53	27.4(16)	32.4(17)	44(2)	-8.5(15)	-5.5(14)	0.0(13)
C54	38.9(18)	34.2(18)	36.7(18)	-8.9(15)	-15.1(15)	7.4(15)
C55	41.1(19)	42.9(19)	25.9(16)	-2.7(15)	-4.0(14)	4.7(16)
C56	26.8(15)	36.5(17)	30.3(16)	1.4(14)	-1.2(13)	0.4(13)
C1S	42(2)	50(2)	59(3)	5(2)	-7.4(18)	0.0(18)
O1S	47.3(15)	49.4(16)	41.1(14)	8.6(12)	-7.4(12)	-14.4(13)
N2	25.3(12)	34.0(14)	21.9(12)	0.5(11)	-2.2(10)	-10.5(11)
C62	26.6(15)	39.1(18)	20.2(14)	-0.2(13)	-2.5(12)	-6.2(13)
C63	22.5(14)	33.1(17)	21.3(14)	0.6(12)	-7.3(11)	1.0(12)
C64	29.1(15)	34.1(17)	24.7(15)	-3.1(13)	-3.1(12)	-2.5(13)
C65	31.6(17)	39.7(19)	33.2(17)	0.4(14)	-4.1(14)	-8.2(14)
C66	45(2)	32.7(18)	37.6(19)	-2.8(15)	-12.8(15)	-7.3(15)
C67	47(2)	37.2(19)	30.7(17)	-8.1(15)	-4.8(15)	7.9(16)
C68	30.9(16)	40.9(19)	25.6(15)	-2.1(14)	-2.8(12)	4.1(14)
O5	46.7(15)	56.6(18)	36.1(14)	-9.7(13)	-10.9(11)	15.1(13)
C61	53(2)	36.7(19)	32.4(18)	2.3(15)	-15.7(16)	-4.1(17)

Table 9.4 Bond Lengths for **9** [S-$NH_3CH(CH_2OH)Ph$][$B\{Tar(NHPh)_2\}_2$]

Atom	Atom	Length/Å	Atom	Atom	Length/Å
B1	O2	1.477(4)	C25	C26	1.383(6)
B1	O3	1.474(4)	C31	C32	1.385(6)
B1	O12	1.467(4)	C31	C36	1.389(5)
B1	O13	1.469(4)	C32	C33	1.401(6)
C1	N1	1.341(5)	C33	C34	1.364(8)
C1	O1	1.230(4)	C34	C35	1.369(8)
C1	C2	1.535(4)	C35	C36	1.382(5)
N1	C21	1.414(4)	C41	C42	1.382(5)

C2	O2	1.410(4)	C41	C46	1.394(5)
C2	C3	1.561(4)	C42	C43	1.387(5)
C3	O3	1.399(4)	C43	C44	1.376(6)
C3	C4	1.521(4)	C44	C45	1.375(7)
C4	N4	1.336(4)	C45	C46	1.377(6)
C4	O4	1.234(4)	C51	C52	1.397(5)
N4	C31	1.414(4)	C51	C56	1.387(5)
C11	N11	1.347(4)	C52	C53	1.385(5)
C11	O11	1.224(4)	C53	C54	1.388(6)
C11	C12	1.534(4)	C54	C55	1.377(6)
N11	C41	1.412(4)	C55	C56	1.397(5)
C12	O12	1.404(4)	C1S	O1S	1.414(6)
C12	C13	1.569(4)	N2	C62	1.493(4)
C13	O13	1.401(4)	C62	C63	1.508(5)
C13	C14	1.540(4)	C62	C61	1.543(5)
C14	N14	1.341(4)	C63	C64	1.392(5)
C14	O14	1.224(4)	C63	C68	1.391(5)
N14	C51	1.422(4)	C64	C65	1.389(5)
C21	C22	1.401(5)	C65	C66	1.381(6)
C21	C26	1.383(5)	C66	C67	1.380(6)
C22	C23	1.385(5)	C67	C68	1.392(5)
C23	C24	1.377(6)	O5	C61	1.435(5)
C24	C25	1.395(6)			

Table 9.5 Bond Angles for **9** [S-$NH_3CH(CH_2OH)Ph$][B{Tar$(NHPh)_2$}$_2$]

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
O3	B1	O2	104.5(3)	C23	C22	C21	118.8(3)
O12	B1	O2	112.3(2)	C24	C23	C22	121.5(3)
O12	B1	O3	113.0(3)	C23	C24	C25	119.0(4)
O12	B1	O13	104.3(3)	C26	C25	C24	120.4(4)
O13	B1	O2	111.2(3)	C21	C26	C25	120.0(3)
O13	B1	O3	111.7(2)	C32	C31	N4	123.3(3)
N1	C1	C2	112.6(3)	C32	C31	C36	119.8(3)
O1	C1	N1	125.7(3)	C36	C31	N4	116.9(3)
O1	C1	C2	121.7(3)	C31	C32	C33	118.3(4)
C1	N1	C21	129.5(3)	C34	C33	C32	121.7(5)
C1	C2	C3	110.8(3)	C33	C34	C35	119.6(4)
O2	C2	C1	111.3(2)	C34	C35	C36	120.3(4)
O2	C2	C3	105.1(2)	C35	C36	C31	120.3(4)
C2	O2	B1	111.0(2)	C42	C41	N11	124.6(3)
O3	C3	C2	105.2(2)	C42	C41	C46	119.0(3)
O3	C3	C4	112.9(2)	C46	C41	N11	116.4(3)
C4	C3	C2	111.3(2)	C41	C42	C43	119.9(4)
C3	O3	B1	110.3(2)	C44	C43	C42	120.9(4)
N4	C4	C3	113.5(3)	C45	C44	C43	119.1(4)
O4	C4	C3	120.9(3)	C44	C45	C46	120.8(4)

O4	C4	N4	125.6(3)	C45	C46	C41	120.2(4)
C4	N4	C31	128.6(3)	C52	C51	N14	117.7(3)
N11	C11	C12	114.5(3)	C56	C51	N14	122.2(3)
O11	C11	N11	124.1(3)	C56	C51	C52	120.1(3)
O11	C11	C12	121.4(3)	C53	C52	C51	119.6(3)
C11	N11	C41	128.4(3)	C52	C53	C54	121.0(3)
C11	C12	C13	112.9(2)	C55	C54	C53	118.8(3)
O12	C12	C11	109.6(2)	C54	C55	C56	121.5(3)
O12	C12	C13	104.9(2)	C51	C56	C55	119.0(3)
C12	O12	B1	111.2(2)	N2	C62	C63	112.5(3)
O13	C13	C12	104.9(2)	N2	C62	C61	108.8(3)
O13	C13	C14	112.8(2)	C63	C62	C61	111.9(3)
C14	C13	C12	109.3(2)	C64	C63	C62	122.7(3)
C13	O13	B1	109.3(2)	C68	C63	C62	118.4(3)
N14	C14	C13	114.5(3)	C68	C63	C64	118.7(3)
O14	C14	C13	120.6(3)	C65	C64	C63	120.4(3)
O14	C14	N14	124.8(3)	C66	C65	C64	120.3(3)
C14	N14	C51	127.5(3)	C67	C66	C65	119.9(3)
C22	C21	N1	123.5(3)	C66	C67	C68	120.0(3)
C26	C21	N1	116.3(3)	C63	C68	C67	120.6(3)
C26	C21	C22	120.2(3)	O5	C61	C62	113.9(3)

Table 9.6 Hydrogen Bonds for **9** [S-$NH_3CH(CH_2OH)Ph$][B{$Tar(NHPh)_2$}$_2$]

D	H	A	d(D-H)/Å	d(H-A)/Å	d(D-A)/Å	D-H-A/°
N4	H4	O3	0.88	2.15	2.623(3)	113.1
N11	H11	O1S	0.88	1.96	2.830(4)	169.9
N14	H14	O12[1]	0.88	2.52	3.048(3)	119.6
N14	H14	O13	0.88	2.17	2.642(3)	112.8
O1S	H1S	O14	0.84	1.88	2.695(4)	164.8
N2	H2A	O13[2]	0.91	2.13	2.868(3)	137.5
N2	H2B	O1	0.91	2.00	2.863(4)	158.9
N2	H2C	O11	0.91	1.84	2.720(4)	161.0
O5	H5	O2[2]	0.84	1.99	2.822(4)	168.9

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

Table 9.7 Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for **9** [S-$NH_3CH(CH_2OH)Ph$][B{$Tar(NHPh)_2$}$_2$]

Atom	*x*	*y*	*z*	U(eq)
H1	3819	8903	1681	36
H2	5842	7565	1703	30
H3	2979	7866	2699	30
H4	7814	7717	3366	33
H11	1707	3464	3290	33
H12	2574	4857	3382	26
H13	6299	4255	2769	29
H14	8738	5934	3303	30
H22	-1956	8549	911	36
H23	-4312	9659	464	44
H24	-2985	11079	520	52
H25	695	11409	1074	54
H26	3071	10313	1530	44
H32	10293	9561	2736	55
H33	13562	10329	3219	70
H34	15046	9994	4189	66
H35	13312	8879	4702	61
H36	10073	8100	4242	47
H42	-1567	3125	1879	47
H43	-4069	1934	1671	66
H44	-4350	847	2382	84
H45	-1998	930	3295	76
H46	437	2123	3522	62
H52	12573	6491	3700	35
H53	14887	6995	4549	42
H54	13657	6744	5518	45
H55	10154	5947	5629	44

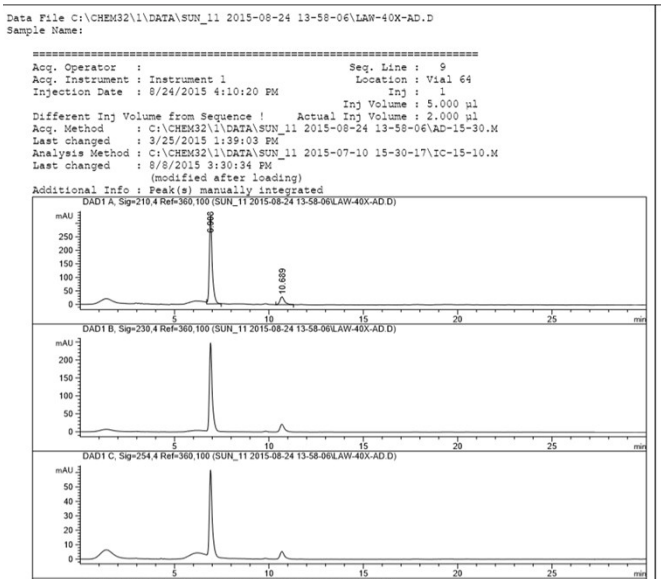
H56	7797	5422	4786	38
H1SA	2869	3295	4973	77
H1SB	373	3138	4571	77
H1SC	1599	4074	4596	77
H1S	4470	3553	4096	70
H2A	-2338	5686	1661	41
H2B	-166	6178	1504	41
H2C	74	5257	1681	41
H62	212	5351	660	35
H64	-5173	4687	1378	36
H65	-7213	3390	1174	42
H66	-5936	2458	439	47
H67	-2530	2801	-71	46
H68	-451	4092	137	39
H5	-5333	6309	1030	71
H61A	-2050	6670	582	50
H61B	-2898	5999	62	50

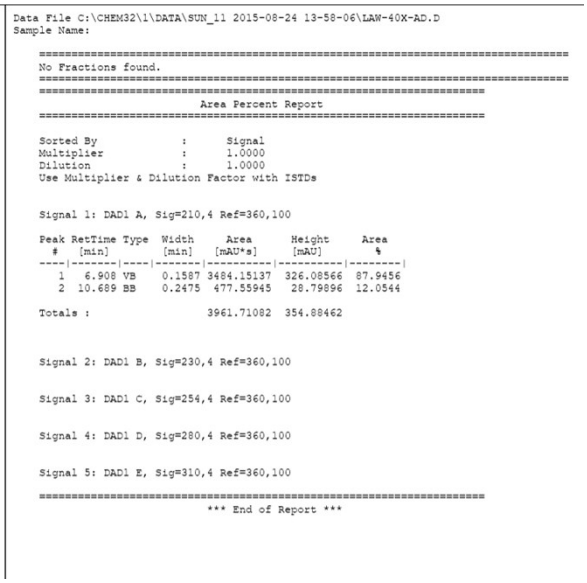
S3. Chiral HPLC Data

Compound 7 (a-methylbenzylamine) gem 64 76%ee (87.9R:12.1S)

Peaks eluted at 6.9 and 10.7 min were for R- and S-$PhCONH_2CHMePh$ obtained from derivatizing the amine by reaction with PhCOCl.

The column is CHIRALPAK® AD-H eluted with 85: 15 hexane: i-propanol with flow rate 1mL min^{-1}.





Compound 8 (a-ethylbenzylamine) lawr 437 91% ee (95.7S: 4.3R)

The chiral HPLC traces at 8.4 and 8.9 min are due to R- and S-PhCONH2CHEtPh respectively.

The column is CHIRALPAK® IC eluted with 4: 1 hexane:i-propanol with flow rate 1mL min^{-1}.

```
Data File C:\CHEM32\1\DATA\QDY 2018-04-30 14-03-48\LAWR437B-IC-20.D
Sample Name:

    ==================================================================
    Acq. Operator   :                          Seq. Line :   4
    Acq. Instrument : Instrument 1              Location : Vial 8
    Injection Date  : 4/30/2018 2:59:18 PM          Inj :   1
                                               Inj Volume : 5.000 µl
    Different Inj Volume from Sequence !     Actual Inj Volume : 3.000 µl
    Acq. Method     : C:\CHEM32\1\DATA\QDY 2018-04-30 14-03-48\IC-20-20.M
    Last changed    : 4/30/2018 2:16:16 PM
                      (modified after loading)
    Analysis Method : C:\CHEM32\1\METHODS\IC-10-10.M
    Last changed    : 4/27/2018 8:32:05 PM
                      (modified after loading)
    Additional Info : Peak(s) manually integrated
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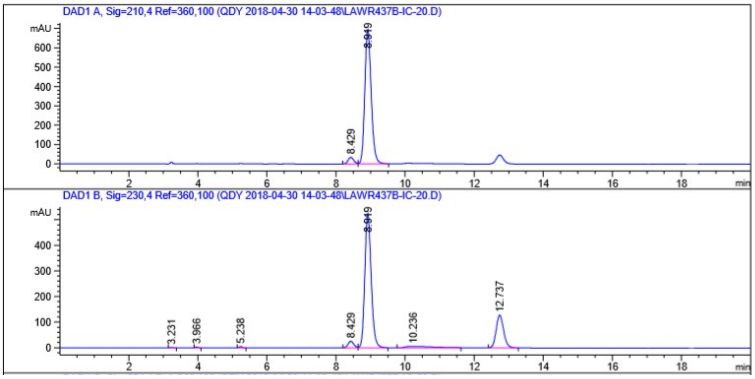


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    ==================================================================
                            Area Percent Report
    ==================================================================

    Sorted By             :      Signal
    Multiplier            :      1.0000
    Dilution              :      1.0000
    Use Multiplier & Dilution Factor with ISTDs


    Signal 1: DAD1 A, Sig=210,4 Ref=360,100

    Peak RetTime Type  Width     Area      Height     Area
      #   [min]        [min]   [mAU*s]     [mAU]       %
    ----|-------|----|-------|----------|----------|--------|
       1   8.429 BV    0.1799  399.33630   34.27179   4.2828
       2   8.919 VB    0.1979 8924.82813  694.84668  95.7172

    Totals :                   9324.16443  729.11847
```

Compound 9 (S-phenylglycinol) lawr 434 95% ee (97.5S: 2.5R)

from isolated solid (single step)

The peaks at 8.7 and 11.6 mins are R- & S- [$PhCONH_2CH(CH_2OCOPh)Ph$] respectively.

These are from double derivatization of phenylglycinol with PhCOCl the column was CHIRALPAK® IC eluted with 4:1 hexane: i-propanol with flow rate 1mL min^{-1}.

Data File C:\CHEM32\1\DATA\QDY 2016-08-31 22-18-20\LAWR434B.D
Sample Name:

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==================================================================
Acq. Operator   :                          Seq. Line :   3
Acq. Instrument : Instrument 1              Location : Vial 22
Injection Date  : 8/31/2016 10:53:27 PM          Inj :   1
                                          Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\QDY 2016-08-31 22-18-20\IC-20-20.M
Last changed    : 8/31/2016 11:10:11 PM
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\OD-2.5-30.M
Last changed    : 8/31/2016 11:47:11 PM
                  (modified after loading)
Additional Info : Peak(s) manually integrated
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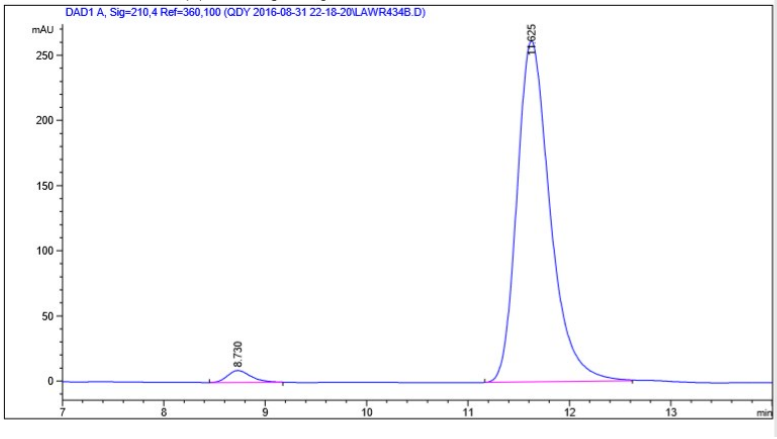


```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=210,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.730 BB    0.2480  150.17807    9.21985   2.4686
   2  11.625 BB    0.3447 5933.34375  261.51462  97.5314

Totals :                  6083.52182  270.73447
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Supplementary Figures:

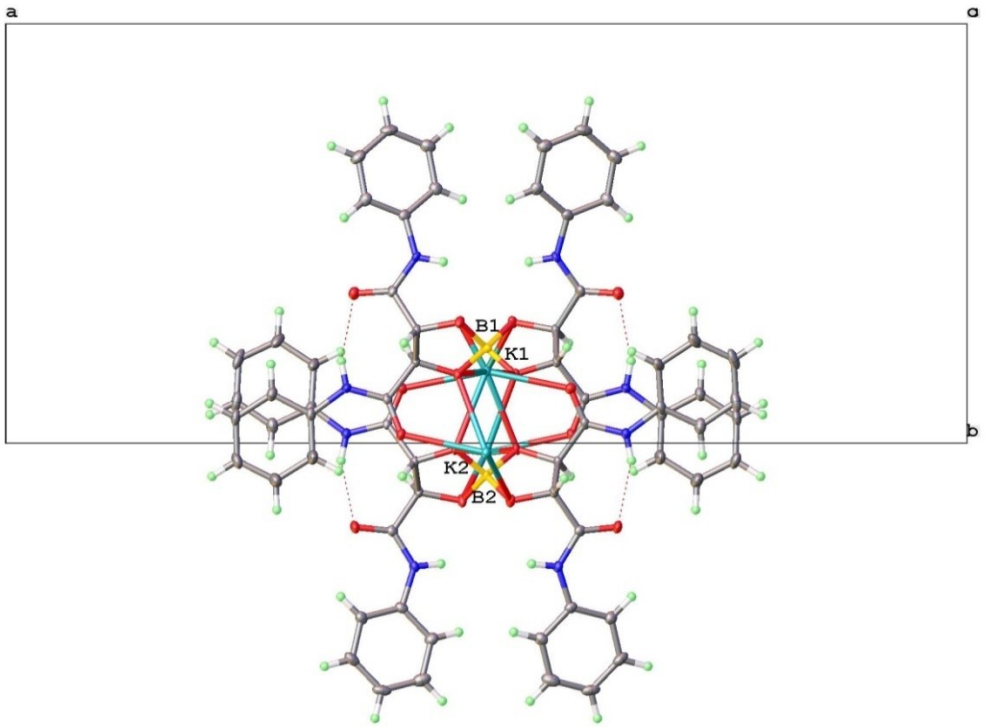

Figure S1. Molecular ion stack of K[B{L-Tar(NHPh)$_2$}$_2$] **2** viewed along [001].

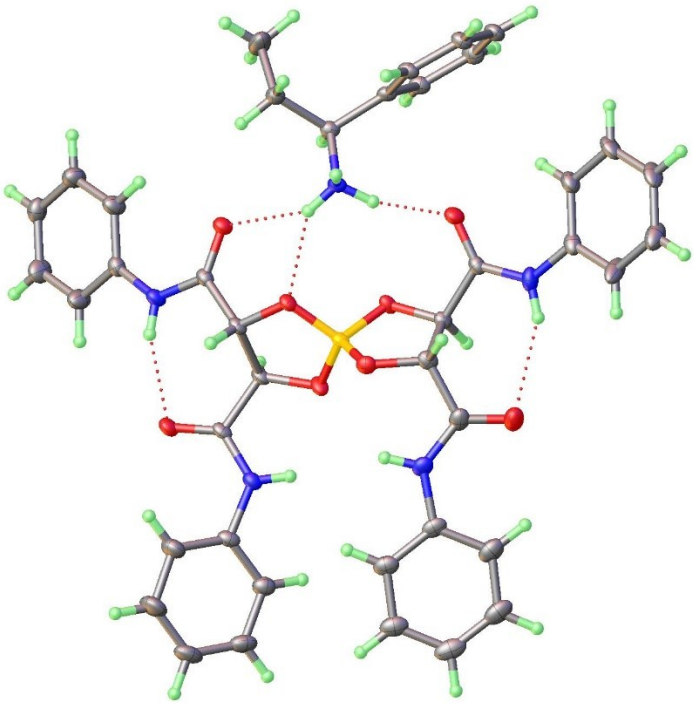

Figure S2. Ion pair in **8** [S-NH$_3$CHEtPh][B{L-Tar(NHPh)$_2$}$_2$].MeOH.