

deh265

Table 1 Crystal data and structure refinement for deh265.

Identification code	deh265
Empirical formula	$C_{114}H_{94}B_2FeN_3P_3$
Formula weight	1676.30
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/c$
$a/\text{\AA}$	15.2667(14)
$b/\text{\AA}$	15.9297(14)
$c/\text{\AA}$	40.090(4)
$\alpha/^\circ$	90
$\beta/^\circ$	99.585(3)
$\gamma/^\circ$	90
Volume/ \AA^3	9613.5(15)
Z	4
$\rho_{\text{calc}}/\text{g cm}^{-3}$	1.158
μ/mm^{-1}	0.256
F(000)	3520.0
Crystal size/ mm^3	$0.3 \times 0.28 \times 0.08$
Radiation	MoK α ($\lambda = 0.71073$)
2Θ range for data collection/ $^\circ$	4.85 to 47.036
Index ranges	$-17 \leq h \leq 17, -17 \leq k \leq 17, -44 \leq l \leq 44$
Reflections collected	168875
Independent reflections	14172 [$R_{\text{int}} = 0.0920, R_{\text{sigma}} = 0.0419$]
Data/restraints/parameters	14172/0/1111
Goodness-of-fit on F^2	1.162
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.1071, wR_2 = 0.2394$
Final R indexes [all data]	$R_1 = 0.1228, wR_2 = 0.2484$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	0.83/-0.80

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for deh265. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
B1	1719(6)	2279(6)	2259(2)	32(2)
C91	2714(5)	2329(5)	2499.6(19)	37.0(19)
C92	3414(5)	1788(5)	2478.6(19)	36.3(19)
C93	4225(6)	1827(5)	2693.9(19)	41(2)
C94	4351(6)	2439(6)	2949(2)	43(2)
C95	3674(6)	2969(5)	2980(2)	42(2)
C96	2882(5)	2898(5)	2762.7(17)	33.9(18)
C97	1444(5)	3124(5)	2022.8(17)	27.5(16)
C98	1689(5)	3935(5)	2128.0(19)	34.9(18)
C99	1453(6)	4639(5)	1935(2)	45(2)
C100	929(6)	4558(5)	1611.8(19)	42(2)
C101	677(5)	3759(5)	1507.2(19)	36.3(19)
C102	925(5)	3063(5)	1705.3(17)	33.6(18)
C103	1012(5)	2173(5)	2530.4(16)	26.9(16)
C104	291(5)	2693(5)	2539.8(18)	35.1(18)
C105	-257(6)	2609(6)	2780(2)	46(2)
C106	-102(6)	1987(6)	3025(2)	48(2)
C107	598(5)	1452(5)	3016.3(19)	39(2)
C108	1139(6)	1553(5)	2779.3(19)	38.5(19)
C109	1651(5)	1465(4)	2007.1(17)	31.3(18)
C110	1008(5)	824(5)	1985.1(19)	37.4(19)
C111	962(7)	175(6)	1761(2)	51(2)
C112	1565(7)	98(6)	1549(2)	53(3)
C113	2200(7)	690(6)	1553(2)	56(3)
C114	2257(6)	1380(5)	1783(2)	41(2)
B2	8580(6)	7462(5)	5237(2)	28.3(19)
C67	8490(5)	7449(5)	4822.3(17)	28.6(17)
C68	8474(5)	8181(5)	4620.2(19)	35.0(18)
C69	8382(6)	8146(6)	4271.6(19)	42(2)
C70	8288(5)	7403(6)	4103.5(19)	42(2)
C71	8267(5)	6660(6)	4296.2(19)	41(2)
C72	8350(5)	6721(5)	4643.7(19)	36.8(19)
C73	9182(5)	6676(4)	5406.7(18)	27.6(16)
C74	9829(5)	6261(5)	5256.3(18)	33.6(18)
C75	10361(5)	5618(5)	5410(2)	37.1(19)
C76	10269(5)	5352(5)	5731(2)	41(2)
C77	9641(5)	5757(5)	5892.3(19)	34.9(18)
C78	9123(6)	6394(5)	5732.4(18)	36.1(19)

C79	9077(5)	8311(4)	5413.7(18)	30.8(17)
C80	9730(5)	8746(5)	5280(2)	38.8(19)
C81	10172(6)	9454(5)	5431(2)	47(2)
C82	9977(6)	9732(5)	5730(2)	44(2)
C83	9357(6)	9322(5)	5880(2)	48(2)
C84	8927(6)	8624(5)	5723.4(19)	39(2)
C85	7566(5)	7381(5)	5314.0(16)	29.3(17)
C86	7027(5)	8060(6)	5361(2)	43(2)
C87	6137(6)	7978(7)	5399(3)	60(3)
C88	5741(7)	7198(9)	5385(3)	71(3)
C89	6284(7)	6501(7)	5341(2)	56(3)
C90	7152(6)	6593(5)	5302.9(19)	39(2)
C1	1106(4)	6862(4)	3767.8(17)	22.2(15)
C2	437(5)	6868(5)	3974.3(19)	32.0(17)
C3	560(5)	7330(5)	4262.6(18)	32.1(18)
C4	1317(5)	7838(5)	4339.1(18)	34.2(18)
C5	1960(5)	7817(4)	4116.5(16)	25.4(16)
C6	2701(5)	8334(4)	4184.7(16)	22.6(15)
C7	2841(5)	8830(4)	4469.7(16)	28.4(17)
C8	2222(6)	8860(5)	4692(2)	41(2)
C9	1475(6)	8368(5)	4622.5(18)	37.4(19)
C10	2349(8)	9458(7)	4989(2)	67(3)
C11	4547(5)	8470(5)	4138.3(18)	31.9(17)
C12	4936(6)	9257(5)	4184(2)	46(2)
C13	5751(7)	9366(6)	4387(2)	59(3)
C14	6192(6)	8688(6)	4554(2)	53(2)
C15	5825(5)	7902(5)	4511.2(19)	41(2)
C16	5024(5)	7796(5)	4305.5(18)	34.5(18)
C17	3296(5)	9325(4)	3673.6(17)	24.4(16)
C18	3792(5)	9513(5)	3423.1(19)	33.7(18)
C19	3683(6)	10277(5)	3264(2)	44(2)
C20	3107(6)	10866(5)	3347(2)	42(2)
C21	2594(6)	10686(5)	3586(2)	40(2)
C22	2673(5)	9938(5)	3752.0(19)	33.9(18)
C23	1617(5)	6419(4)	2981.1(17)	25.3(16)
C24	1127(5)	5802(5)	2785.2(19)	33.3(18)
C25	1168(5)	4989(5)	2887.4(17)	29.1(17)
C26	1722(5)	4796(4)	3196.3(17)	25.8(16)
C27	2214(4)	5450(4)	3381.8(15)	17.5(14)
C28	2777(5)	5246(4)	3688.5(15)	19.9(15)
C29	2830(5)	4413(4)	3789.0(16)	22.9(16)
C30	2399(5)	3777(4)	3618.8(18)	29.0(17)

C31	1821(5)	3958(4)	3326.5(18)	30.3(17)
C32	2533(6)	2874(4)	3733(2)	40(2)
C33	4469(5)	5652(4)	4044.1(18)	28.5(17)
C34	4944(5)	5649(5)	4371.8(18)	38(2)
C35	5794(7)	5297(6)	4437(3)	59(3)
C36	6165(6)	4946(6)	4179(3)	59(3)
C37	5673(6)	4955(6)	3849(2)	56(3)
C38	4861(5)	5295(5)	3786.6(19)	37(2)
C39	2931(5)	6109(4)	4330.4(16)	24.8(16)
C40	3292(5)	6639(4)	4597.8(17)	27.8(16)
C41	2952(6)	6638(5)	4894.6(18)	36.0(19)
C42	2247(5)	6137(5)	4935.6(18)	36.4(19)
C43	1870(5)	5614(4)	4676.6(18)	29.7(17)
C44	2205(5)	5602(4)	4375.7(18)	31.1(17)
C45	1573(5)	8514(4)	3268.7(17)	25.0(16)
C46	1146(5)	9123(4)	3040.5(17)	28.0(16)
C47	1462(5)	9283(5)	2749.4(19)	31.6(18)
C48	2170(5)	8789(5)	2675.9(19)	33.5(18)
C49	2583(5)	8209(4)	2918.5(17)	26.3(16)
C50	3292(5)	7712(5)	2841.3(18)	32.2(17)
C51	3530(5)	7744(5)	2522.7(18)	35.4(18)
C52	3094(5)	8307(5)	2278.6(18)	32.9(18)
C53	2469(5)	8840(5)	2357.1(18)	32.6(18)
C54	3347(6)	8309(5)	1927.0(18)	40(2)
C55	4954(5)	7627(4)	3297.7(18)	29.5(17)
C56	5496(5)	7467(5)	3605.3(17)	30.0(17)
C57	6299(5)	7799(6)	3688(2)	42(2)
C58	6638(6)	8336(6)	3473(2)	46(2)
C59	6132(6)	8503(5)	3167(2)	46(2)
C60	5284(5)	8170(5)	3075(2)	37.6(19)
C61	4203(5)	6161(4)	2988.6(17)	27.7(16)
C62	3579(5)	5694(5)	2786(2)	37.1(19)
C63	3806(6)	4992(5)	2623(2)	41(2)
C64	4685(6)	4730(5)	2669(2)	44(2)
C65	5324(6)	5205(5)	2873(2)	41(2)
C66	5082(5)	5909(5)	3035.8(18)	32.8(18)
Fe1	2871.1(6)	7195.1(6)	3558.2(2)	19.1(2)
N1	1851(4)	7298(3)	3835.8(13)	21.1(12)
N2	2155(4)	6274(3)	3271.0(13)	20.4(12)
N3	2275(4)	8079(3)	3218.8(13)	20.4(12)
P1	3460.5(13)	8304.5(10)	3879.9(4)	22.4(4)
P2	3346.1(12)	6117.3(10)	3926.8(4)	20.9(4)

P3	3880.6(12)	7126.8(11)	3198.8(4)	20.9(4)
----	------------	------------	-----------	---------

Table 3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for deh265. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B1	45 (5)	34 (5)	18 (4)	-2 (4)	6 (4)	9 (4)
C91	48 (5)	36 (5)	29 (4)	4 (4)	14 (4)	7 (4)
C92	45 (5)	39 (5)	26 (4)	1 (3)	8 (4)	0 (4)
C93	44 (5)	46 (5)	33 (4)	7 (4)	6 (4)	1 (4)
C94	46 (5)	53 (5)	31 (4)	13 (4)	6 (4)	-11 (4)
C95	64 (6)	27 (4)	29 (4)	5 (3)	-4 (4)	-6 (4)
C96	50 (5)	34 (4)	17 (4)	2 (3)	2 (3)	1 (4)
C97	28 (4)	34 (4)	22 (4)	-2 (3)	11 (3)	-3 (3)
C98	47 (5)	32 (4)	24 (4)	7 (3)	2 (3)	-1 (4)
C99	45 (5)	31 (5)	57 (6)	-9 (4)	6 (4)	-5 (4)
C100	67 (6)	33 (5)	27 (4)	6 (3)	9 (4)	5 (4)
C101	45 (5)	41 (5)	23 (4)	-1 (3)	6 (3)	-1 (4)
C102	50 (5)	28 (4)	22 (4)	-2 (3)	3 (3)	4 (4)
C103	30 (4)	35 (4)	15 (3)	-2 (3)	2 (3)	-3 (3)
C104	43 (5)	35 (4)	28 (4)	10 (3)	6 (4)	6 (4)
C105	57 (6)	46 (5)	37 (5)	0 (4)	11 (4)	10 (4)
C106	51 (6)	66 (6)	30 (4)	6 (4)	13 (4)	1 (5)
C107	43 (5)	46 (5)	29 (4)	10 (4)	7 (4)	-3 (4)
C108	46 (5)	35 (4)	33 (4)	0 (4)	5 (4)	9 (4)
C109	53 (5)	24 (4)	16 (4)	4 (3)	4 (3)	12 (4)
C110	27 (4)	49 (5)	33 (4)	0 (4)	-2 (3)	1 (4)
C111	59 (6)	40 (5)	47 (5)	-7 (4)	-17 (5)	-6 (4)
C112	83 (7)	31 (5)	38 (5)	-8 (4)	-8 (5)	19 (5)
C113	88 (8)	49 (6)	26 (5)	-10 (4)	-5 (5)	18 (6)
C114	48 (5)	36 (5)	41 (5)	-3 (4)	11 (4)	3 (4)
B2	33 (5)	32 (5)	20 (4)	1 (4)	8 (4)	0 (4)
C67	34 (4)	29 (4)	24 (4)	1 (3)	9 (3)	-1 (3)
C68	43 (5)	31 (4)	33 (4)	0 (3)	11 (4)	6 (4)
C69	48 (5)	51 (5)	29 (4)	17 (4)	6 (4)	13 (4)
C70	35 (5)	69 (6)	21 (4)	1 (4)	-1 (3)	9 (4)
C71	44 (5)	50 (5)	28 (4)	-13 (4)	7 (4)	9 (4)
C72	41 (5)	38 (5)	31 (4)	3 (4)	4 (4)	-1 (4)
C73	32 (4)	20 (4)	31 (4)	-3 (3)	5 (3)	-3 (3)
C74	50 (5)	27 (4)	25 (4)	7 (3)	9 (4)	-3 (4)
C75	32 (4)	41 (5)	39 (5)	1 (4)	9 (4)	1 (4)
C76	35 (5)	34 (4)	52 (5)	11 (4)	5 (4)	5 (4)
C77	45 (5)	34 (4)	25 (4)	11 (3)	5 (4)	-3 (4)
C78	49 (5)	34 (4)	26 (4)	2 (3)	6 (4)	1 (4)
C79	42 (5)	23 (4)	28 (4)	-1 (3)	7 (3)	1 (3)

C80	48(5)	36(5)	34(4)	-7(4)	12(4)	-8(4)
C81	59(6)	43(5)	40(5)	-4(4)	11(4)	-27(4)
C82	52(6)	37(5)	45(5)	-11(4)	11(4)	-6(4)
C83	64(6)	45(5)	36(5)	-16(4)	15(4)	-7(5)
C84	53(5)	39(5)	28(4)	-3(4)	18(4)	-9(4)
C85	42(5)	30(4)	16(3)	1(3)	4(3)	0(3)
C86	36(5)	44(5)	45(5)	2(4)	-4(4)	4(4)
C87	46(6)	65(7)	68(7)	14(5)	3(5)	15(5)
C88	42(6)	116(10)	55(6)	15(7)	10(5)	-15(7)
C89	62(7)	65(7)	39(5)	11(5)	5(5)	-17(5)
C90	47(5)	38(5)	28(4)	8(3)	-1(4)	-7(4)
C1	24(4)	21(3)	23(4)	2(3)	7(3)	-1(3)
C2	30(4)	29(4)	36(4)	8(3)	1(3)	4(3)
C3	38(5)	34(4)	25(4)	5(3)	10(3)	3(4)
C4	48(5)	33(4)	23(4)	1(3)	11(3)	5(4)
C5	32(4)	25(4)	19(3)	0(3)	5(3)	2(3)
C6	36(4)	12(3)	20(3)	-2(3)	5(3)	4(3)
C7	41(5)	27(4)	18(4)	-1(3)	6(3)	-3(3)
C8	53(6)	40(5)	32(4)	-14(4)	13(4)	-1(4)
C9	49(5)	42(5)	26(4)	-3(4)	21(4)	0(4)
C10	101(9)	65(7)	43(5)	-27(5)	38(6)	-26(6)
C11	42(5)	26(4)	26(4)	0(3)	3(3)	-6(3)
C12	50(6)	37(5)	45(5)	-3(4)	-11(4)	3(4)
C13	65(7)	44(6)	61(6)	1(5)	-8(5)	-20(5)
C14	41(5)	68(7)	45(5)	6(5)	-9(4)	-19(5)
C15	41(5)	48(5)	32(4)	10(4)	-1(4)	-1(4)
C16	41(5)	36(4)	27(4)	2(3)	7(3)	-1(4)
C17	37(4)	14(3)	21(4)	-1(3)	2(3)	2(3)
C18	38(5)	24(4)	43(5)	4(3)	18(4)	3(3)
C19	57(6)	23(4)	51(5)	14(4)	6(4)	-1(4)
C20	58(6)	25(4)	42(5)	3(4)	6(4)	-6(4)
C21	46(5)	21(4)	52(5)	-2(4)	9(4)	16(4)
C22	35(5)	40(5)	28(4)	-5(3)	8(3)	-15(4)
C23	29(4)	24(4)	22(4)	2(3)	1(3)	4(3)
C24	44(5)	28(4)	26(4)	1(3)	2(3)	4(4)
C25	31(4)	32(4)	24(4)	-11(3)	3(3)	-5(3)
C26	30(4)	24(4)	25(4)	-3(3)	10(3)	1(3)
C27	20(4)	17(3)	18(3)	-1(3)	10(3)	-2(3)
C28	38(4)	16(3)	8(3)	-1(3)	10(3)	-1(3)
C29	42(4)	18(4)	11(3)	3(3)	11(3)	17(3)
C30	42(5)	22(4)	27(4)	5(3)	16(3)	10(3)
C31	44(5)	18(4)	32(4)	-5(3)	17(4)	5(3)

C32	68(6)	16(4)	39(5)	-4(3)	15(4)	0(4)
C33	41(5)	17(4)	27(4)	6(3)	7(3)	-2(3)
C34	50(5)	38(4)	22(4)	-1(3)	-9(4)	11(4)
C35	57(6)	60(6)	54(6)	-4(5)	-6(5)	20(5)
C36	44(6)	66(7)	67(7)	15(5)	6(5)	23(5)
C37	52(6)	77(7)	47(6)	17(5)	29(5)	23(5)
C38	35(5)	57(5)	23(4)	13(4)	13(3)	12(4)
C39	33(4)	26(4)	15(3)	4(3)	5(3)	5(3)
C40	31(4)	29(4)	24(4)	1(3)	5(3)	-4(3)
C41	54(5)	33(4)	22(4)	-4(3)	8(4)	-8(4)
C42	53(5)	43(5)	18(4)	-2(3)	18(4)	1(4)
C43	39(5)	26(4)	29(4)	-2(3)	20(3)	-2(3)
C44	49(5)	19(4)	27(4)	-1(3)	9(3)	-11(3)
C45	28(4)	25(4)	25(4)	3(3)	11(3)	1(3)
C46	31(4)	26(4)	28(4)	4(3)	9(3)	8(3)
C47	31(4)	30(4)	35(4)	17(3)	7(3)	10(3)
C48	36(5)	30(4)	33(4)	6(3)	1(3)	4(4)
C49	34(4)	23(4)	22(4)	2(3)	5(3)	5(3)
C50	38(4)	30(4)	28(4)	8(3)	3(3)	2(4)
C51	46(5)	32(4)	29(4)	3(3)	8(4)	-2(4)
C52	45(5)	31(4)	23(4)	4(3)	7(3)	1(4)
C53	36(4)	34(4)	28(4)	9(3)	5(3)	-6(4)
C54	57(5)	41(5)	23(4)	9(3)	10(4)	9(4)
C55	35(4)	28(4)	27(4)	0(3)	11(3)	-1(3)
C56	32(4)	38(4)	21(4)	-2(3)	8(3)	3(3)
C57	37(5)	57(5)	31(4)	1(4)	0(4)	-4(4)
C58	53(6)	47(5)	37(5)	1(4)	9(4)	-2(4)
C59	42(5)	43(5)	56(6)	10(4)	13(4)	-11(4)
C60	35(5)	40(5)	37(4)	11(4)	4(4)	-3(4)
C61	38(5)	25(4)	22(4)	3(3)	9(3)	0(3)
C62	31(4)	33(4)	50(5)	-13(4)	13(4)	-7(4)
C63	44(5)	33(5)	44(5)	-12(4)	3(4)	-3(4)
C64	52(6)	28(4)	55(5)	-10(4)	19(4)	-3(4)
C65	38(5)	34(5)	55(5)	2(4)	18(4)	8(4)
C66	43(5)	28(4)	26(4)	-3(3)	0(3)	5(4)
Fe1	27.3(5)	14.8(5)	15.7(5)	0.9(4)	5.1(4)	-0.3(4)
N1	30(3)	17(3)	17(3)	5(2)	4(2)	3(3)
N2	25(3)	19(3)	19(3)	-4(2)	7(2)	-1(2)
N3	22(3)	22(3)	17(3)	-1(2)	4(2)	0(2)
P1	34.8(11)	15.2(9)	17.8(9)	0.3(7)	6.4(8)	0.1(8)
P2	32.2(10)	15.4(9)	16.0(9)	0.1(7)	6.2(7)	-0.2(8)
P3	25.7(10)	19.9(9)	17.3(8)	1.7(7)	4.1(7)	0.1(8)

Table 4 Bond Lengths for deh265.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
B1	C91	1.662(12)	C12	C13	1.380(12)
B1	C97	1.657(11)	C13	C14	1.384(13)
B1	C103	1.665(11)	C14	C15	1.371(12)
B1	C109	1.634(11)	C15	C16	1.367(11)
C91	C92	1.385(11)	C17	C18	1.388(10)
C91	C96	1.383(11)	C17	C22	1.434(10)
C92	C93	1.388(11)	C17	P1	1.822(7)
C93	C94	1.403(12)	C18	C19	1.371(10)
C94	C95	1.356(12)	C19	C20	1.364(12)
C95	C96	1.372(11)	C20	C21	1.367(12)
C97	C98	1.391(10)	C21	C22	1.360(11)
C97	C102	1.386(10)	C23	C24	1.395(10)
C98	C99	1.378(11)	C23	N2	1.327(8)
C99	C100	1.409(12)	C24	C25	1.356(10)
C100	C101	1.376(11)	C25	C26	1.413(10)
C101	C102	1.380(11)	C26	C27	1.420(9)
C103	C104	1.384(10)	C26	C31	1.433(10)
C103	C108	1.393(10)	C27	C28	1.416(9)
C104	C105	1.382(11)	C27	N2	1.383(8)
C105	C106	1.387(12)	C28	C29	1.386(9)
C106	C107	1.371(12)	C28	P2	1.821(6)
C107	C108	1.368(11)	C29	C30	1.331(10)
C109	C110	1.409(11)	C30	C31	1.375(10)
C109	C114	1.399(11)	C30	C32	1.514(10)
C110	C111	1.365(12)	C33	C34	1.391(10)
C111	C112	1.355(14)	C33	C38	1.397(10)
C112	C113	1.351(14)	C33	P2	1.855(8)
C113	C114	1.428(12)	C34	C35	1.397(12)
B2	C67	1.646(10)	C35	C36	1.378(13)
B2	C73	1.632(11)	C36	C37	1.409(13)
B2	C79	1.652(11)	C37	C38	1.338(11)
B2	C85	1.633(11)	C39	C40	1.403(10)
C67	C68	1.417(10)	C39	C44	1.408(10)
C67	C72	1.361(11)	C39	P2	1.833(7)
C68	C69	1.382(11)	C40	C41	1.375(10)
C69	C70	1.358(12)	C41	C42	1.371(11)
C70	C71	1.417(12)	C42	C43	1.380(10)
C71	C72	1.381(11)	C43	C44	1.386(10)
C73	C74	1.406(10)	C45	C46	1.416(10)
C73	C78	1.398(10)	C45	N3	1.319(9)
C74	C75	1.387(11)	C46	C47	1.359(10)

C75	C76	1.383(11)	C47	C48	1.408(10)
C76	C77	1.400(11)	C48	C49	1.412(10)
C77	C78	1.377(11)	C48	C53	1.429(10)
C79	C80	1.390(11)	C49	C50	1.415(10)
C79	C84	1.391(10)	C49	N3	1.379(8)
C80	C81	1.399(11)	C50	C51	1.386(10)
C81	C82	1.355(12)	C50	P3	1.818(7)
C82	C83	1.369(12)	C51	C52	1.410(10)
C83	C84	1.387(11)	C52	C53	1.352(11)
C85	C86	1.391(11)	C52	C54	1.523(10)
C85	C90	1.403(11)	C55	C56	1.390(10)
C86	C87	1.398(13)	C55	C60	1.397(10)
C87	C88	1.379(15)	C55	P3	1.805(7)
C88	C89	1.414(15)	C56	C57	1.324(11)
C89	C90	1.366(13)	C57	C58	1.377(12)
C1	C2	1.418(10)	C58	C59	1.364(12)
C1	N1	1.322(9)	C59	C60	1.389(11)
C2	C3	1.357(10)	C61	C62	1.365(10)
C3	C4	1.403(11)	C61	C66	1.384(11)
C4	C5	1.433(10)	C61	P3	1.860(7)
C4	C9	1.403(11)	C62	C63	1.368(11)
C5	C6	1.389(10)	C63	C64	1.388(12)
C5	N1	1.384(9)	C64	C65	1.389(12)
C6	C7	1.377(9)	C65	C66	1.379(11)
C6	P1	1.820(7)	Fe1	N1	2.066(5)
C7	C8	1.404(11)	Fe1	N2	2.063(5)
C8	C9	1.374(11)	Fe1	N3	2.061(5)
C8	C10	1.510(11)	Fe1	P1	2.283(2)
C11	C12	1.386(11)	Fe1	P2	2.3024(19)
C11	C16	1.404(11)	Fe1	P3	2.2809(19)
C11	P1	1.823(8)			

Table 5 Bond Angles for deh265.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C91	B1	C103	104.7(6)	N2	C23	C24	124.5(7)
C97	B1	C91	114.4(7)	C25	C24	C23	120.6(7)
C97	B1	C103	109.0(6)	C24	C25	C26	117.6(7)
C109	B1	C91	110.7(6)	C25	C26	C27	119.1(6)
C109	B1	C97	108.0(6)	C25	C26	C31	122.3(7)
C109	B1	C103	110.0(7)	C27	C26	C31	118.6(6)
C92	C91	B1	125.1(7)	C28	C27	C26	118.6(6)
C96	C91	B1	120.7(7)	N2	C27	C26	121.9(6)
C96	C91	C92	114.0(8)	N2	C27	C28	119.6(6)
C91	C92	C93	123.5(8)	C27	C28	P2	116.6(5)
C92	C93	C94	118.9(8)	C29	C28	C27	118.0(6)
C95	C94	C93	119.0(8)	C29	C28	P2	125.3(5)
C94	C95	C96	119.7(8)	C30	C29	C28	125.4(6)
C95	C96	C91	124.8(8)	C29	C30	C31	118.0(6)
C98	C97	B1	123.5(6)	C29	C30	C32	122.5(7)
C102	C97	B1	121.2(7)	C31	C30	C32	119.5(7)
C102	C97	C98	115.3(7)	C30	C31	C26	121.3(7)
C99	C98	C97	123.6(7)	C34	C33	C38	118.4(7)
C98	C99	C100	119.8(8)	C34	C33	P2	123.8(6)
C101	C100	C99	116.9(7)	C38	C33	P2	117.8(6)
C100	C101	C102	122.1(7)	C33	C34	C35	120.0(8)
C101	C102	C97	122.2(7)	C36	C35	C34	120.5(9)
C104	C103	B1	124.2(6)	C35	C36	C37	118.6(9)
C104	C103	C108	114.9(7)	C38	C37	C36	120.8(8)
C108	C103	B1	120.9(7)	C37	C38	C33	121.7(8)
C105	C104	C103	122.5(7)	C40	C39	C44	117.6(6)
C104	C105	C106	120.7(8)	C40	C39	P2	121.4(5)
C107	C106	C105	117.9(8)	C44	C39	P2	120.9(5)
C108	C107	C106	120.4(8)	C41	C40	C39	120.3(7)
C107	C108	C103	123.6(8)	C42	C41	C40	121.4(7)
C110	C109	B1	125.8(7)	C41	C42	C43	119.9(7)
C114	C109	B1	119.5(7)	C42	C43	C44	119.7(7)
C114	C109	C110	114.7(7)	C43	C44	C39	121.1(7)
C111	C110	C109	123.3(8)	N3	C45	C46	124.1(6)
C112	C111	C110	121.0(9)	C47	C46	C45	119.5(7)
C113	C112	C111	119.3(8)	C46	C47	C48	118.0(7)
C112	C113	C114	120.8(9)	C47	C48	C49	119.5(7)
C109	C114	C113	120.8(9)	C47	C48	C53	121.8(7)
C67	B2	C79	113.4(6)	C49	C48	C53	118.7(7)
C73	B2	C67	110.9(6)	C48	C49	C50	119.0(6)
C73	B2	C79	105.3(6)	N3	C49	C48	121.4(6)

C73	B2	C85	110.3(6)	N3	C49	C50	119.4(6)
C85	B2	C67	105.5(6)	C49	C50	P3	114.2(5)
C85	B2	C79	111.5(6)	C51	C50	C49	120.6(7)
C68	C67	B2	123.9(6)	C51	C50	P3	125.0(6)
C72	C67	B2	121.4(6)	C50	C51	C52	119.8(7)
C72	C67	C68	114.4(6)	C51	C52	C54	118.7(7)
C69	C68	C67	122.3(7)	C53	C52	C51	120.5(7)
C70	C69	C68	121.4(8)	C53	C52	C54	120.8(7)
C69	C70	C71	117.9(7)	C52	C53	C48	121.0(7)
C72	C71	C70	119.0(8)	C56	C55	C60	117.1(7)
C67	C72	C71	124.8(8)	C56	C55	P3	119.9(5)
C74	C73	B2	124.7(6)	C60	C55	P3	123.0(6)
C78	C73	B2	121.1(6)	C57	C56	C55	122.6(7)
C78	C73	C74	114.1(7)	C56	C57	C58	121.3(8)
C75	C74	C73	123.9(7)	C59	C58	C57	118.0(8)
C76	C75	C74	119.8(7)	C58	C59	C60	121.8(8)
C75	C76	C77	118.1(7)	C59	C60	C55	119.1(7)
C78	C77	C76	120.6(7)	C62	C61	C66	119.3(7)
C77	C78	C73	123.4(7)	C62	C61	P3	120.7(6)
C80	C79	B2	123.4(6)	C66	C61	P3	120.1(6)
C80	C79	C84	113.6(7)	C61	C62	C63	121.5(8)
C84	C79	B2	122.9(7)	C62	C63	C64	119.9(8)
C79	C80	C81	124.1(7)	C63	C64	C65	119.0(7)
C82	C81	C80	118.9(8)	C66	C65	C64	120.3(8)
C81	C82	C83	120.2(8)	C65	C66	C61	120.1(7)
C82	C83	C84	119.5(8)	N1	Fe1	P1	84.02(16)
C83	C84	C79	123.7(8)	N1	Fe1	P2	84.18(15)
C86	C85	B2	124.4(7)	N1	Fe1	P3	173.38(16)
C86	C85	C90	115.2(7)	N2	Fe1	N1	88.9(2)
C90	C85	B2	120.1(7)	N2	Fe1	P1	171.38(16)
C85	C86	C87	123.3(9)	N2	Fe1	P2	84.75(16)
C88	C87	C86	120.6(10)	N2	Fe1	P3	87.96(15)
C87	C88	C89	116.7(9)	N3	Fe1	N1	90.7(2)
C90	C89	C88	122.0(9)	N3	Fe1	N2	89.0(2)
C89	C90	C85	122.2(9)	N3	Fe1	P1	86.18(16)
N1	C1	C2	123.7(6)	N3	Fe1	P2	171.99(16)
C3	C2	C1	119.4(7)	N3	Fe1	P3	83.46(16)
C2	C3	C4	119.4(7)	P1	Fe1	P2	99.34(7)
C3	C4	C5	118.4(7)	P3	Fe1	P1	98.60(7)
C3	C4	C9	123.2(7)	P3	Fe1	P2	101.31(7)
C9	C4	C5	118.4(7)	C1	N1	C5	117.7(6)
C6	C5	C4	118.9(6)	C1	N1	Fe1	123.1(4)

N1	C5	C4	121.2(6)	C5	N1	Fe1	119.1(4)
N1	C5	C6	119.9(6)	C23	N2	C27	116.3(6)
C5	C6	P1	116.2(5)	C23	N2	Fe1	123.9(5)
C7	C6	C5	120.8(6)	C27	N2	Fe1	119.7(4)
C7	C6	P1	123.0(6)	C45	N3	C49	117.2(6)
C6	C7	C8	121.2(7)	C45	N3	Fe1	122.6(4)
C7	C8	C10	120.7(8)	C49	N3	Fe1	120.1(4)
C9	C8	C7	118.4(7)	C6	P1	C11	103.7(3)
C9	C8	C10	120.8(8)	C6	P1	C17	103.1(3)
C8	C9	C4	122.2(7)	C6	P1	Fe1	99.4(2)
C12	C11	C16	116.9(7)	C11	P1	Fe1	132.0(3)
C12	C11	P1	122.3(6)	C17	P1	C11	99.9(3)
C16	C11	P1	120.7(6)	C17	P1	Fe1	115.0(2)
C13	C12	C11	121.0(8)	C28	P2	C33	99.7(3)
C12	C13	C14	120.4(9)	C28	P2	C39	104.6(3)
C15	C14	C13	119.7(8)	C28	P2	Fe1	99.2(2)
C16	C15	C14	119.6(8)	C33	P2	Fe1	129.8(2)
C15	C16	C11	122.3(8)	C39	P2	C33	102.4(3)
C18	C17	C22	118.3(6)	C39	P2	Fe1	117.0(2)
C18	C17	P1	118.0(5)	C50	P3	C61	101.6(3)
C22	C17	P1	123.7(5)	C50	P3	Fe1	100.1(3)
C19	C18	C17	119.3(7)	C55	P3	C50	105.0(3)
C20	C19	C18	121.9(8)	C55	P3	C61	99.6(3)
C19	C20	C21	119.7(7)	C55	P3	Fe1	121.6(2)
C22	C21	C20	120.8(7)	C61	P3	Fe1	125.7(2)
C21	C22	C17	119.8(7)				

**Table 6 Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and
Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for deh265.**

Atom	x	y	z	U(eq)
H92	3334.36	1368.97	2307.64	44
H93	4687.5	1444.26	2668.99	49
H94	4902.7	2481.6	3097.74	52
H95	3748.49	3387.64	3150.87	50
H96	2415.52	3267.27	2795.52	41
H98	2038.94	4007.15	2345.35	42
H99	1642.32	5178.7	2018.49	54
H100	758.6	5033.31	1472.93	51
H101	319.17	3683.52	1291.56	44
H102	734.62	2523.84	1621.29	40
H104	168.13	3124.74	2375.11	42
H105	-744.85	2980.39	2776.59	56
H106	-468.7	1933.38	3192.79	58
H107	708.26	1009.05	3176.21	47
H108	1626.86	1180.9	2784.67	46
H110	585.51	844.62	2134.02	45
H111	501.04	-228.12	1752.06	62
H112	1540.51	-368.33	1400.29	63
H113	2614.04	645.87	1401.68	67
H114	2712.27	1787.35	1783.87	49
H68	8528.29	8713.59	4728.12	42
H69	8384.85	8653.37	4147.01	51
H70	8238.79	7382.16	3864.29	51
H71	8196.77	6128.1	4188.08	49
H72	8304.88	6218.47	4767.15	44
H74	9907.59	6431.61	5036.1	40
H75	10787.48	5359.99	5295.97	45
H76	10621.37	4906.58	5839	49
H77	9571.2	5591.63	6114.02	42
H78	8704.49	6655.47	5849.59	43
H80	9884.46	8549.55	5074.17	47
H81	10602.43	9734.93	5325.89	56
H82	10271.18	10212.17	5835.1	53
H83	9222.71	9513.8	6090.19	57
H84	8506.59	8343.43	5833.72	47
H86	7275.99	8607.29	5367.61	52
H87	5802.36	8463.21	5433.5	72
H88	5133.06	7131.51	5405.45	85
H89	6037.78	5952.91	5336.87	67

H90	7485.45	6106.69	5267.91	46
H1	1013.84	6525.33	3569.41	27
H2	-92.83	6552.35	3911.31	38
H3	136.48	7309.76	4411.44	39
H7	3366.75	9158.57	4516.84	34
H9	1051.63	8386.7	4771.1	45
H10A	2396.26	9138.35	5199.68	100
H10B	1838.5	9838.92	4969.38	100
H10C	2892.57	9784.79	4988.98	100
H12	4636.32	9729.56	4073.91	56
H13	6010.84	9908.7	4412.8	70
H14	6747.67	8767.54	4697.14	64
H15	6125.9	7433.63	4623.96	49
H16	4781.43	7246.84	4274.72	41
H18	4203.88	9116.84	3362.81	40
H19	4017.99	10399.29	3090.05	53
H20	3062.98	11398.12	3238.69	50
H21	2177.39	11089.03	3637.69	48
H22	2315.7	9821.79	3919.3	41
H23	1561.24	6981.05	2901.63	30
H24	762.19	5952.28	2578.26	40
H25	835.09	4565.35	2755.94	35
H29	3204.31	4284.02	3996.45	27
H31	1480.92	3517.74	3208.5	36
H32A	3034.11	2633.04	3642.13	61
H32B	1993.64	2551.32	3651.36	61
H32C	2657.66	2853.39	3981.17	61
H34	4691.51	5886.3	4551.37	46
H35	6117.98	5298.71	4660.66	71
H36	6741.67	4703.45	4222.43	71
H37	5920.54	4716.99	3667.94	68
H38	4542.07	5293.43	3561.87	45
H40	3773.48	6998.91	4573.86	33
H41	3210.71	6991.69	5075.04	43
H42	2018.75	6150.64	5141.93	44
H43	1383.55	5264.16	4704.46	36
H44	1939.41	5245.58	4197.15	37
H45	1340.05	8412.6	3470.39	30
H46	642.26	9417.82	3090.61	34
H47	1211.57	9715.62	2599.95	38
H51	3985.14	7387.6	2468.96	43
H53	2224.93	9254.1	2197.78	39

H54A	3967.36	8485.02	1942.51	60
H54B	2961.98	8700.84	1781.41	60
H54C	3273.63	7743.21	1830.6	60
H56	5283.4	7105.85	3762.42	36
H57	6646.93	7663.09	3900.4	51
H58	7208.35	8583.15	3535.68	55
H59	6364.27	8856.95	3011.81	56
H60	4934.95	8310.21	2863.37	45
H62	2973.55	5860.81	2756.53	44
H63	3362.23	4684.33	2478.67	49
H64	4846.47	4234.98	2561.9	53
H65	5931.21	5042.58	2901.45	49
H66	5519.87	6222.94	3180.33	39

Table 7 Solvent masks information for deh265.

Number	X	Y	Z	Volume	Electron count Content
1	-0.500	0.500	1.000	771.9	167.6 ?
2	-0.500	0.000	0.500	771.9	167.6 ?

deh265

Table 1 Crystal data and structure refinement for deh265.

Identification code	deh265
Empirical formula	C ₁₁₄ H ₉₄ B ₂ FeN ₃ P ₃
Formula weight	1676.30
Temperature/K	150.0
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	15.2667(14)
b/Å	15.9297(14)
c/Å	40.090(4)
α /°	90
β /°	99.585(3)
γ /°	90
Volume/Å ³	9613.5(15)
Z	4
ρ_{calc} /g/cm ³	1.158
μ /mm ⁻¹	0.256
F(000)	3520.0
Crystal size/mm ³	0.3 × 0.28 × 0.08
Radiation	MoK α (λ = 0.71073)
2 Θ range for data collection/°	4.85 to 47.036
Index ranges	-17 ≤ h ≤ 17, -17 ≤ k ≤ 17, -44 ≤ l ≤ 44
Reflections collected	168875
Independent reflections	14172 [R _{int} = 0.0920, R _{sigma} = 0.0419]
Data/restraints/parameters	14172/0/1111
Goodness-of-fit on F ²	1.162
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.1071, wR ₂ = 0.2394
Final R indexes [all data]	R ₁ = 0.1228, wR ₂ = 0.2484
Largest diff. peak/hole / e Å ⁻³	0.83/-0.80