

deh161

Table 1 Crystal data and structure refinement for deh161.

Identification code	deh161
Empirical formula	C ₇₅ H ₅₆ F ₁₃ N ₉ P ₂ Ru
Formula weight	1493.29
Temperature/K	150.0
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	13.6103(4)
b/Å	22.5386(8)
c/Å	22.1790(7)
α/°	90
β/°	106.6150(10)
γ/°	90
Volume/Å ³	6519.5(4)
Z	4
ρ _{calc} /g/cm ³	1.521
μ/mm ⁻¹	0.381
F(000)	3040.0
Crystal size/mm ³	0.16 × 0.05 × 0.04
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.486 to 49.622
Index ranges	-16 ≤ h ≤ 16, -26 ≤ k ≤ 26, -26 ≤ l ≤ 26
Reflections collected	112284
Independent reflections	11163 [R _{int} = 0.1894, R _{sigma} = 0.0771]
Data/restraints/parameters	11163/0/1032
Goodness-of-fit on F ²	1.032
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0752, wR ₂ = 0.1672
Final R indexes [all data]	R ₁ = 0.1226, wR ₂ = 0.1909
Largest diff. peak/hole / e Å ⁻³	4.00/-0.48

Table 2 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for deh161. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
C1	6957(4)	3457(3)	6396(3)	27.1(14)
C2	6995(5)	4074(3)	6480(3)	34.5(16)
C3	7749(6)	4406(3)	6355(4)	47(2)
C4	8489(6)	4136(4)	6112(4)	50(2)
C5	8460(5)	3532(3)	6034(4)	42.0(18)
C6	7717(5)	3182(3)	6190(3)	30.8(15)
C7	7761(5)	2537(3)	6181(3)	31.2(15)
C8	8522(6)	2224(3)	6002(4)	46.3(19)
C9	8613(7)	1627(4)	6064(5)	66(3)
C10	7991(8)	1323(4)	6354(6)	81(3)
C11	7230(7)	1614(4)	6529(5)	66(3)
C12	7047(6)	2217(3)	6397(3)	37.3(17)
C13	6216(5)	2545(3)	6511(3)	24.3(14)
C14	4646(5)	2639(3)	6769(3)	24.9(14)
C15	5044(6)	1681(3)	6594(4)	48(2)
C16	4164(6)	1684(3)	6737(4)	54(2)
C17	2991(5)	2431(3)	6997(3)	29.6(15)
C18	2950(5)	2374(3)	7608(3)	36.0(17)
C19	2090(5)	2557(3)	7766(4)	39.4(18)
C20	1252(5)	2785(3)	7319(4)	40.2(18)
C21	1301(5)	2821(3)	6701(4)	42.4(18)
C22	2160(5)	2639(3)	6539(4)	38.4(17)
C23	320(6)	3004(4)	7490(4)	63(3)
C24	3274(5)	3922(3)	7491(3)	27.1(14)
C25	3876(5)	3648(3)	8040(3)	30.1(15)
C26	3685(6)	3741(3)	8606(3)	35.4(16)
C27	2886(6)	4113(3)	8645(4)	42.3(19)
C28	2281(6)	4379(3)	8118(4)	40.1(18)
C29	2448(5)	4292(3)	7528(3)	34.6(16)
C30	1835(5)	4574(3)	6962(4)	38.2(17)
C31	1103(6)	5016(4)	6959(4)	50(2)
C32	605(6)	5307(4)	6425(5)	60(2)
C33	811(7)	5177(4)	5863(5)	61(2)
C34	1518(6)	4742(4)	5832(4)	50(2)
C35	2007(5)	4423(3)	6385(3)	33.5(16)
C36	2792(5)	3995(3)	6401(3)	27.9(15)
C37	3832(5)	3470(3)	5878(3)	28.7(14)
C38	2199(6)	3640(4)	5268(4)	48(2)

C39	2658(6)	3313(4)	4931(3)	46(2)
C40	4364(5)	2845(3)	5097(3)	31.6(15)
C41	5221(6)	3083(3)	4985(3)	39.7(17)
C42	5885(6)	2730(3)	4774(3)	39.6(17)
C43	5692(6)	2131(3)	4673(4)	44.7(19)
C44	4825(7)	1899(3)	4786(4)	52(2)
C45	4165(6)	2254(3)	4998(4)	48(2)
C46	6424(7)	1736(4)	4459(5)	67(3)
C47	4464(5)	4907(3)	6342(3)	30.4(15)
C48	4377(5)	4777(3)	5708(3)	36.1(17)
C49	3856(6)	5153(3)	5248(4)	45.1(19)
C50	3403(6)	5665(3)	5391(4)	47(2)
C51	3507(6)	5802(3)	6007(4)	42.5(19)
C52	4047(5)	5432(3)	6506(3)	32.7(16)
C53	4137(5)	5553(3)	7156(3)	36.2(17)
C54	3625(6)	6012(3)	7363(4)	45.9(19)
C55	3677(6)	6078(3)	7985(4)	49(2)
C56	4220(6)	5674(3)	8425(4)	45.3(19)
C57	4760(5)	5217(3)	8253(3)	34.2(16)
C58	4749(5)	5160(3)	7614(3)	30.5(15)
C59	5192(5)	4658(3)	7394(3)	25.6(14)
C60	5832(5)	3671(3)	7625(3)	23.2(14)
C61	6587(5)	4357(3)	8373(3)	38.5(17)
C62	7052(5)	3849(3)	8543(4)	41.4(18)
C63	6956(5)	2820(3)	8104(3)	28.9(15)
C64	6350(5)	2351(3)	8143(3)	34.0(16)
C65	6739(6)	1783(3)	8173(4)	42.8(18)
C66	7738(7)	1685(3)	8188(4)	48(2)
C67	8342(6)	2166(4)	8162(5)	60(2)
C68	7968(5)	2739(4)	8122(4)	46(2)
C69	8162(8)	1054(4)	8225(6)	86(3)
C70	3462(8)	5199(5)	10098(5)	71(3)
C71	4234(9)	5617(5)	10180(4)	76(3)
C72	3961(10)	6190(5)	9963(5)	76(3)
C73	2967(10)	6319(5)	9682(5)	82(3)
C74	2226(10)	5891(5)	9662(6)	92(4)
C75	2440(9)	5328(5)	9840(5)	81(3)
P2A	9493(4)	4928.8(18)	8590(4)	57.6(17)
F7A	9201(11)	4383(6)	8118(8)	104(4)
F8A	8440(20)	5256(13)	8240(9)	95(7)
F9A	10080(20)	5274(8)	8166(11)	127(11)
F10A	10543(7)	4617(4)	8931(7)	97(4)

F11A	8964(7)	4596(4)	9042(5)	67(3)
F12A	9765(8)	5466(3)	9082(5)	79(3)
P2B	9195(5)	4894(3)	8116(6)	58(2)
F7B	9153(16)	5408(8)	7621(11)	112(7)
F8B	8062(12)	4726(10)	7771(8)	107(7)
F9B	9631(13)	4475(8)	7715(11)	106(7)
F10B	9241(18)	4412(9)	8634(12)	104(7)
F11B	8800(30)	5325(17)	8546(16)	101(12)
F12B	10315(19)	5114(16)	8481(17)	125(14)
F13	3719(6)	4640(3)	10309(3)	109(2)
N1	6157(4)	3130(2)	6527(2)	24.7(12)
N2	5358(4)	2272(2)	6624(2)	26.6(12)
N3	3916(4)	2263(2)	6849(3)	31.9(13)
N4	3463(4)	3795(2)	6914(2)	24.9(12)
N5	2927(4)	3753(2)	5844(2)	29.9(13)
N6	3657(4)	3213(3)	5304(2)	32.5(13)
N7	5007(4)	4507(2)	6805(2)	25.3(12)
N8	5826(4)	4251(2)	7814(2)	24.7(12)
N9	6592(4)	3425(2)	8089(2)	28.0(12)
Ru1	4863.5(4)	3485.7(2)	6744.8(2)	21.74(15)
P1A	9362(9)	3064(6)	4453(7)	39(2)
F1A	10099(15)	2756(8)	5050(8)	76(5)
F2A	10350(17)	3312(11)	4224(9)	64(7)
F3A	9640(20)	2529(12)	3964(15)	83(7)
F4A	8633(19)	3392(8)	3875(9)	53(4)
F5A	8440(12)	2838(13)	4662(9)	115(8)
F6A	9400(20)	3613(8)	4871(11)	112(9)
P1B	9700(20)	2938(11)	4491(10)	65(5)
F2B	10700(30)	2650(9)	4920(11)	110(13)
F1B	9060(40)	2453(17)	4751(13)	156(17)
F3B	9740(20)	3430(20)	5031(15)	134(15)
F4B	9360(30)	2480(9)	4034(15)	103(13)
F6B	8660(20)	3210(20)	4050(20)	144(17)
F5B	10290(20)	3420(12)	4259(12)	72(9)

Table 3 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for deh161. 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}
C1	21 (3)	33 (4)	26 (3)	0 (3)	6 (3)	0 (3)
C2	34 (4)	33 (4)	41 (4)	-7 (3)	17 (3)	-3 (3)
C3	53 (5)	30 (4)	63 (5)	-9 (4)	28 (4)	-6 (4)
C4	44 (5)	44 (5)	67 (6)	-1 (4)	25 (4)	-9 (4)
C5	32 (4)	48 (5)	52 (5)	1 (4)	22 (3)	-1 (4)
C6	25 (3)	37 (4)	30 (4)	0 (3)	7 (3)	2 (3)
C7	26 (3)	35 (4)	35 (4)	-1 (3)	12 (3)	5 (3)
C8	44 (5)	41 (5)	60 (5)	-2 (4)	26 (4)	3 (4)
C9	61 (6)	49 (6)	106 (8)	4 (5)	52 (6)	23 (4)
C10	89 (7)	33 (5)	145 (10)	5 (6)	72 (8)	25 (5)
C11	73 (6)	34 (5)	108 (8)	8 (5)	56 (6)	13 (4)
C12	42 (4)	28 (4)	45 (4)	6 (3)	19 (4)	8 (3)
C13	28 (3)	23 (3)	23 (3)	1 (3)	9 (3)	7 (3)
C14	33 (4)	23 (3)	21 (3)	-2 (3)	10 (3)	1 (3)
C15	42 (5)	22 (4)	86 (6)	-5 (4)	29 (4)	-1 (3)
C16	53 (5)	17 (4)	99 (7)	-5 (4)	31 (5)	-3 (3)
C17	26 (4)	22 (3)	42 (4)	2 (3)	13 (3)	-10 (3)
C18	30 (4)	25 (4)	49 (5)	-1 (3)	5 (3)	-7 (3)
C19	37 (4)	37 (4)	47 (5)	-3 (3)	16 (4)	-14 (3)
C20	31 (4)	43 (4)	52 (5)	-8 (4)	20 (4)	-11 (3)
C21	27 (4)	42 (4)	56 (5)	-2 (4)	8 (4)	-8 (3)
C22	35 (4)	35 (4)	47 (5)	0 (3)	13 (4)	-9 (3)
C23	44 (5)	80 (7)	71 (6)	-2 (5)	27 (5)	-1 (5)
C24	26 (3)	24 (3)	32 (4)	-5 (3)	9 (3)	-7 (3)
C25	30 (4)	23 (3)	40 (4)	-5 (3)	14 (3)	-5 (3)
C26	47 (4)	32 (4)	27 (4)	-5 (3)	10 (3)	-10 (3)
C27	55 (5)	35 (4)	46 (5)	-10 (4)	30 (4)	-6 (4)
C28	42 (4)	38 (4)	48 (5)	-8 (4)	24 (4)	-2 (3)
C29	35 (4)	23 (3)	50 (4)	-7 (3)	19 (3)	-7 (3)
C30	28 (4)	32 (4)	57 (5)	-1 (4)	17 (4)	3 (3)
C31	48 (5)	46 (5)	64 (6)	-5 (4)	26 (4)	12 (4)
C32	47 (5)	48 (5)	84 (7)	2 (5)	16 (5)	21 (4)
C33	54 (5)	50 (5)	69 (6)	10 (5)	3 (5)	18 (4)
C34	36 (4)	59 (5)	55 (5)	10 (4)	13 (4)	17 (4)
C35	24 (3)	35 (4)	44 (4)	2 (3)	13 (3)	3 (3)
C36	19 (3)	26 (3)	39 (4)	-1 (3)	8 (3)	0 (3)
C37	31 (3)	26 (3)	30 (4)	3 (3)	10 (3)	2 (3)
C38	33 (4)	61 (5)	41 (4)	0 (4)	-6 (4)	8 (4)
C39	42 (4)	66 (6)	26 (4)	-9 (4)	2 (3)	9 (4)

C40	35(4)	37(4)	21(3)	-6(3)	5(3)	-2(3)
C41	49(5)	32(4)	37(4)	-6(3)	10(4)	-7(3)
C42	46(4)	34(4)	45(4)	-8(3)	23(4)	-6(3)
C43	49(5)	46(5)	41(5)	-8(4)	16(4)	3(4)
C44	69(6)	30(4)	59(5)	-13(4)	22(5)	-4(4)
C45	48(5)	41(5)	55(5)	-11(4)	16(4)	-11(4)
C46	74(6)	54(5)	78(7)	-21(5)	33(5)	6(5)
C47	32(4)	20(3)	41(4)	5(3)	14(3)	-2(3)
C48	47(4)	25(4)	41(4)	4(3)	19(3)	5(3)
C49	58(5)	38(4)	43(5)	7(4)	20(4)	3(4)
C50	58(5)	37(4)	48(5)	14(4)	20(4)	5(4)
C51	55(5)	24(4)	55(5)	13(3)	24(4)	8(3)
C52	38(4)	22(3)	40(4)	4(3)	15(3)	1(3)
C53	35(4)	24(4)	51(5)	-2(3)	15(3)	-4(3)
C54	60(5)	23(4)	54(5)	-1(4)	16(4)	7(4)
C55	60(5)	30(4)	58(5)	-11(4)	20(4)	15(4)
C56	56(5)	45(5)	41(4)	-17(4)	23(4)	-4(4)
C57	40(4)	27(4)	35(4)	-4(3)	11(3)	-4(3)
C58	31(4)	20(3)	42(4)	-10(3)	13(3)	-4(3)
C59	24(3)	18(3)	36(4)	-4(3)	9(3)	-7(3)
C60	24(3)	24(3)	25(3)	-1(3)	13(3)	0(3)
C61	35(4)	33(4)	42(4)	-11(3)	2(3)	-3(3)
C62	31(4)	43(5)	41(4)	-7(4)	-5(3)	2(3)
C63	28(4)	30(4)	27(4)	6(3)	6(3)	6(3)
C64	30(4)	34(4)	36(4)	9(3)	6(3)	4(3)
C65	45(5)	35(4)	47(5)	11(3)	9(4)	0(3)
C66	58(5)	33(4)	54(5)	14(4)	15(4)	12(4)
C67	37(5)	49(5)	99(7)	13(5)	29(5)	14(4)
C68	31(4)	45(5)	67(6)	13(4)	20(4)	7(3)
C69	87(8)	47(6)	122(10)	21(6)	27(7)	30(5)
C70	78(7)	63(6)	60(6)	4(5)	2(5)	3(6)
C71	78(7)	91(8)	53(6)	-1(6)	11(5)	-3(6)
C72	111(9)	68(7)	53(6)	-6(5)	30(6)	5(6)
C73	90(8)	75(8)	82(8)	5(6)	27(7)	21(7)
C74	84(8)	66(7)	127(11)	-10(7)	29(8)	15(7)
C75	78(8)	89(9)	70(7)	-13(6)	9(6)	-6(6)
P2A	54(3)	30(2)	100(5)	7(2)	39(3)	6.7(19)
F7A	138(12)	59(8)	124(12)	-20(8)	54(11)	20(7)
F8A	101(14)	101(14)	87(13)	36(12)	32(10)	59(11)
F9A	200(20)	61(7)	190(20)	21(11)	170(20)	10(10)
F10A	54(6)	53(6)	183(12)	10(7)	29(7)	9(5)
F11A	63(6)	58(6)	79(7)	14(5)	16(5)	-26(5)

F12A	86(7)	35(5)	126(9)	2(5)	47(7)	-13(5)
P2B	41(4)	53(5)	80(7)	-12(4)	17(4)	-3(3)
F7B	116(15)	88(13)	150(18)	45(13)	69(14)	2(11)
F8B	78(12)	156(18)	86(12)	19(12)	20(9)	-47(12)
F9B	84(12)	85(12)	167(19)	-57(12)	62(13)	-12(9)
F10B	129(18)	61(13)	93(16)	6(12)	-13(15)	-5(11)
F11B	120(30)	62(13)	150(30)	30(20)	90(30)	30(19)
F12B	62(13)	170(40)	160(30)	-60(20)	46(16)	-58(18)
F13	132(6)	83(5)	100(5)	17(4)	14(4)	3(4)
N1	26(3)	25(3)	21(3)	0(2)	4(2)	2(2)
N2	30(3)	19(3)	31(3)	-3(2)	10(2)	2(2)
N3	28(3)	21(3)	48(4)	-3(3)	12(3)	-6(2)
N4	26(3)	21(3)	26(3)	-1(2)	4(2)	-5(2)
N5	22(3)	37(3)	28(3)	3(2)	2(2)	6(2)
N6	32(3)	40(3)	22(3)	-4(2)	2(2)	5(3)
N7	32(3)	19(3)	28(3)	3(2)	14(2)	-1(2)
N8	22(3)	25(3)	25(3)	-6(2)	4(2)	1(2)
N9	23(3)	30(3)	29(3)	-1(2)	5(2)	1(2)
Ru1	22.4(3)	18.2(2)	24.8(3)	-0.1(2)	7.00(19)	0.8(2)
P1A	37(6)	39(4)	41(3)	-8(2)	9(4)	-7(3)
F1A	74(11)	88(11)	57(8)	13(7)	3(7)	-2(8)
F2A	51(10)	110(16)	40(9)	-15(9)	28(8)	1(9)
F3A	95(10)	91(14)	64(10)	-2(8)	21(8)	-36(8)
F4A	50(8)	50(7)	56(7)	-5(5)	10(5)	12(6)
F5A	59(9)	180(20)	115(11)	39(12)	36(8)	-47(10)
F6A	230(30)	52(9)	61(10)	-7(7)	53(13)	19(11)
P1B	81(12)	71(10)	48(6)	-15(7)	28(9)	-43(8)
F2B	160(30)	51(10)	65(12)	30(9)	-53(15)	-43(13)
F1B	220(40)	190(30)	111(18)	-44(17)	120(20)	-130(30)
F3B	91(15)	250(40)	86(18)	-120(20)	69(14)	-100(20)
F4B	190(30)	17(8)	59(15)	-14(8)	-37(17)	11(12)
F6B	29(13)	170(30)	230(40)	-80(30)	20(20)	-11(18)
F5B	48(13)	49(9)	85(17)	41(10)	-33(10)	-23(8)

Table 4 Bond Lengths for deh161.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.401(9)	C47	N7	1.406(8)
C1	C6	1.390(9)	C48	C49	1.360(10)
C1	N1	1.413(8)	C49	C50	1.385(11)
C2	C3	1.361(10)	C50	C51	1.369(10)
C3	C4	1.409(10)	C51	C52	1.412(9)
C4	C5	1.371(11)	C52	C53	1.438(10)
C5	C6	1.401(9)	C53	C54	1.397(10)
C6	C7	1.456(9)	C53	C58	1.424(10)
C7	C8	1.401(9)	C54	C55	1.368(11)
C7	C12	1.401(9)	C55	C56	1.383(11)
C8	C9	1.355(11)	C56	C57	1.379(10)
C9	C10	1.384(13)	C57	C58	1.419(9)
C10	C11	1.372(11)	C58	C59	1.430(9)
C11	C12	1.398(10)	C59	N7	1.303(8)
C12	C13	1.433(9)	C59	N8	1.412(8)
C13	N1	1.322(8)	C60	N8	1.374(8)
C13	N2	1.405(8)	C60	N9	1.351(8)
C14	N2	1.381(8)	C60	Ru1	2.063(6)
C14	N3	1.356(8)	C61	C62	1.310(10)
C14	Ru1	1.934(6)	C61	N8	1.390(8)
C15	C16	1.324(11)	C62	N9	1.401(9)
C15	N2	1.394(8)	C63	C64	1.359(9)
C16	N3	1.388(9)	C63	C68	1.378(9)
C17	C18	1.380(10)	C63	N9	1.447(8)
C17	C22	1.369(10)	C64	C65	1.380(10)
C17	N3	1.439(8)	C65	C66	1.368(11)
C18	C19	1.377(10)	C66	C67	1.373(11)
C19	C20	1.379(10)	C66	C69	1.528(11)
C20	C21	1.394(10)	C67	C68	1.381(11)
C20	C23	1.508(10)	C70	C71	1.384(14)
C21	C22	1.380(10)	C70	C75	1.376(14)
C24	C25	1.401(9)	C70	F13	1.355(11)
C24	C29	1.421(9)	C71	C72	1.390(14)
C24	N4	1.404(8)	C72	C73	1.350(14)
C25	C26	1.369(9)	C73	C74	1.387(15)
C26	C27	1.396(10)	C74	C75	1.335(15)
C27	C28	1.360(10)	P2A	F7A	1.590(14)
C28	C29	1.405(10)	P2A	F8A	1.60(2)
C29	C30	1.443(10)	P2A	F9A	1.602(16)
C30	C31	1.407(10)	P2A	F10A	1.578(11)
C30	C35	1.407(10)	P2A	F11A	1.580(10)

C31	C32	1.353(12)	P2A	F12A	1.601(11)
C32	C33	1.385(12)	P2B	F7B	1.59(2)
C33	C34	1.388(11)	P2B	F8B	1.560(17)
C34	C35	1.415(10)	P2B	F9B	1.529(19)
C35	C36	1.432(9)	P2B	F10B	1.57(2)
C36	N4	1.318(8)	P2B	F11B	1.56(4)
C36	N5	1.409(8)	P2B	F12B	1.59(2)
C37	N5	1.368(8)	N1	Ru1	2.112(5)
C37	N6	1.356(8)	N4	Ru1	2.161(5)
C37	Ru1	2.031(6)	N7	Ru1	2.311(5)
C38	C39	1.325(11)	P1A	F1A	1.58(2)
C38	N5	1.399(9)	P1A	F2A	1.66(2)
C39	N6	1.393(9)	P1A	F3A	1.74(3)
C40	C41	1.370(10)	P1A	F4A	1.56(2)
C40	C45	1.365(10)	P1A	F5A	1.544(18)
C40	N6	1.441(8)	P1A	F6A	1.54(2)
C41	C42	1.382(10)	P1B	F2B	1.55(3)
C42	C43	1.381(10)	P1B	F1B	1.60(3)
C43	C44	1.378(11)	P1B	F3B	1.62(3)
C43	C46	1.508(11)	P1B	F4B	1.43(3)
C44	C45	1.382(11)	P1B	F6B	1.60(3)
C47	C48	1.407(9)	P1B	F5B	1.52(3)
C47	C52	1.405(9)			

Table 5 Bond Angles for deh161.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	C1	N1	119.4(5)	C66	C67	C68	121.8(7)
C6	C1	C2	118.9(6)	C63	C68	C67	118.2(7)
C6	C1	N1	121.7(6)	C75	C70	C71	123.4(10)
C3	C2	C1	121.3(6)	F13	C70	C71	118.5(10)
C2	C3	C4	120.3(7)	F13	C70	C75	118.1(10)
C5	C4	C3	118.6(7)	C70	C71	C72	118.0(11)
C4	C5	C6	121.6(7)	C73	C72	C71	119.5(11)
C1	C6	C5	119.2(6)	C72	C73	C74	119.2(11)
C1	C6	C7	119.2(6)	C75	C74	C73	123.8(12)
C5	C6	C7	121.6(6)	C74	C75	C70	115.6(11)
C8	C7	C6	122.9(6)	F7A	P2A	F8A	91.0(12)
C8	C7	C12	118.6(6)	F7A	P2A	F9A	93.6(11)
C12	C7	C6	118.4(6)	F7A	P2A	F12A	177.8(8)
C9	C8	C7	121.8(7)	F8A	P2A	F9A	91.2(14)
C8	C9	C10	119.2(8)	F8A	P2A	F12A	89.0(10)
C11	C10	C9	120.4(8)	F10A	P2A	F7A	89.6(7)
C10	C11	C12	120.7(8)	F10A	P2A	F8A	178.9(13)
C7	C12	C13	117.0(6)	F10A	P2A	F9A	87.7(9)
C11	C12	C7	118.2(7)	F10A	P2A	F11A	89.9(7)
C11	C12	C13	124.7(7)	F10A	P2A	F12A	90.5(7)
N1	C13	C12	125.3(6)	F11A	P2A	F7A	88.7(7)
N1	C13	N2	111.8(5)	F11A	P2A	F8A	91.1(11)
N2	C13	C12	122.9(6)	F11A	P2A	F9A	176.7(12)
N2	C14	Ru1	117.5(4)	F11A	P2A	F12A	89.2(6)
N3	C14	N2	104.2(5)	F12A	P2A	F9A	88.6(9)
N3	C14	Ru1	138.1(5)	F7B	P2B	F12B	88.0(16)
C16	C15	N2	105.7(6)	F8B	P2B	F7B	90.2(11)
C15	C16	N3	109.2(6)	F8B	P2B	F10B	91.0(11)
C18	C17	N3	118.9(6)	F8B	P2B	F11B	89.1(15)
C22	C17	C18	120.3(6)	F8B	P2B	F12B	175.5(17)
C22	C17	N3	120.8(6)	F9B	P2B	F7B	89.6(12)
C19	C18	C17	119.9(7)	F9B	P2B	F8B	93.4(12)
C18	C19	C20	121.1(7)	F9B	P2B	F10B	93.3(14)
C19	C20	C21	117.9(7)	F9B	P2B	F11B	177.4(17)
C19	C20	C23	121.5(7)	F9B	P2B	F12B	90.8(14)
C21	C20	C23	120.6(7)	F10B	P2B	F7B	176.8(15)
C22	C21	C20	121.3(7)	F10B	P2B	F12B	90.6(17)
C17	C22	C21	119.4(7)	F11B	P2B	F7B	90.9(15)
C25	C24	C29	118.8(6)	F11B	P2B	F10B	86.1(18)
C25	C24	N4	119.2(6)	F11B	P2B	F12B	86.8(19)
N4	C24	C29	121.8(6)	C1	N1	Ru1	126.3(4)

C26	C25	C24	120.8(6)	C13	N1	C1	117.3(5)
C25	C26	C27	120.3(7)	C13	N1	Ru1	116.5(4)
C28	C27	C26	120.1(7)	C14	N2	C13	117.0(5)
C27	C28	C29	121.2(7)	C14	N2	C15	110.9(5)
C24	C29	C30	118.5(6)	C15	N2	C13	132.0(5)
C28	C29	C24	118.6(7)	C14	N3	C16	109.9(6)
C28	C29	C30	122.8(6)	C14	N3	C17	125.8(5)
C31	C30	C29	123.3(7)	C16	N3	C17	124.2(6)
C31	C30	C35	118.0(7)	C24	N4	Ru1	128.6(4)
C35	C30	C29	118.7(6)	C36	N4	C24	117.1(5)
C32	C31	C30	121.6(8)	C36	N4	Ru1	112.8(4)
C31	C32	C33	120.3(8)	C37	N5	C36	118.2(5)
C32	C33	C34	121.1(8)	C37	N5	C38	110.9(6)
C33	C34	C35	118.4(8)	C38	N5	C36	129.4(6)
C30	C35	C34	120.4(6)	C37	N6	C39	111.5(6)
C30	C35	C36	117.3(6)	C37	N6	C40	126.2(5)
C34	C35	C36	121.8(6)	C39	N6	C40	122.1(5)
N4	C36	C35	125.4(6)	C47	N7	Ru1	125.3(4)
N4	C36	N5	113.1(5)	C59	N7	C47	118.4(5)
N5	C36	C35	121.5(6)	C59	N7	Ru1	107.9(4)
N5	C37	Ru1	114.3(4)	C60	N8	C59	118.3(5)
N6	C37	N5	103.5(5)	C60	N8	C61	111.5(5)
N6	C37	Ru1	141.6(5)	C61	N8	C59	129.4(5)
C39	C38	N5	106.9(6)	C60	N9	C62	110.7(5)
C38	C39	N6	107.1(6)	C60	N9	C63	126.0(5)
C41	C40	N6	120.9(6)	C62	N9	C63	123.2(5)
C45	C40	C41	119.6(7)	C14	Ru1	C37	86.5(3)
C45	C40	N6	119.5(6)	C14	Ru1	C60	103.6(2)
C40	C41	C42	120.6(7)	C14	Ru1	N1	77.1(2)
C43	C42	C41	120.4(7)	C14	Ru1	N4	99.4(2)
C42	C43	C46	121.1(7)	C14	Ru1	N7	172.8(2)
C44	C43	C42	118.2(7)	C37	Ru1	C60	169.0(3)
C44	C43	C46	120.7(7)	C37	Ru1	N1	100.0(2)
C43	C44	C45	121.1(7)	C37	Ru1	N4	76.4(2)
C40	C45	C44	120.1(7)	C37	Ru1	N7	95.5(2)
C52	C47	C48	120.6(6)	C60	Ru1	N1	86.8(2)
C52	C47	N7	121.1(6)	C60	Ru1	N4	97.3(2)
N7	C47	C48	118.2(6)	C60	Ru1	N7	73.9(2)
C49	C48	C47	119.7(7)	N1	Ru1	N4	175.20(19)
C48	C49	C50	121.3(7)	N1	Ru1	N7	109.20(19)
C51	C50	C49	119.4(7)	N4	Ru1	N7	74.47(18)
C50	C51	C52	122.0(7)	F1A	P1A	F2A	91.6(11)

C47	C52	C51	117.0(6)	F1A	P1A	F3A	91.0(13)
C47	C52	C53	119.6(6)	F2A	P1A	F3A	72.5(13)
C51	C52	C53	123.3(6)	F4A	P1A	F1A	177.8(14)
C54	C53	C52	124.3(7)	F4A	P1A	F2A	88.3(14)
C54	C53	C58	118.1(7)	F4A	P1A	F3A	91.0(14)
C58	C53	C52	117.5(6)	F5A	P1A	F1A	88.8(11)
C55	C54	C53	121.7(7)	F5A	P1A	F2A	179.6(15)
C54	C55	C56	120.1(7)	F5A	P1A	F3A	107.7(16)
C57	C56	C55	121.1(7)	F5A	P1A	F4A	91.3(11)
C56	C57	C58	119.3(7)	F6A	P1A	F1A	86.8(12)
C53	C58	C59	117.7(6)	F6A	P1A	F2A	91.3(14)
C57	C58	C53	119.5(6)	F6A	P1A	F3A	163.6(15)
C57	C58	C59	121.9(6)	F6A	P1A	F4A	91.0(12)
N7	C59	C58	124.7(6)	F6A	P1A	F5A	88.5(16)
N7	C59	N8	113.4(5)	F2B	P1B	F1B	87.8(17)
N8	C59	C58	121.7(6)	F2B	P1B	F3B	89.9(17)
N8	C60	Ru1	115.0(4)	F2B	P1B	F6B	177(2)
N9	C60	N8	103.3(5)	F1B	P1B	F3B	95.9(16)
N9	C60	Ru1	141.3(5)	F4B	P1B	F2B	101(2)
C62	C61	N8	106.4(6)	F4B	P1B	F1B	70(2)
C61	C62	N9	108.1(6)	F4B	P1B	F3B	162(3)
C64	C63	C68	121.0(6)	F4B	P1B	F6B	77(2)
C64	C63	N9	121.6(6)	F4B	P1B	F5B	112(3)
C68	C63	N9	117.3(6)	F6B	P1B	F1B	90(2)
C63	C64	C65	119.6(7)	F6B	P1B	F3B	91(2)
C66	C65	C64	121.0(7)	F5B	P1B	F2B	93.3(15)
C65	C66	C67	118.3(7)	F5B	P1B	F1B	177(2)
C65	C66	C69	120.6(8)	F5B	P1B	F3B	81.8(16)
C67	C66	C69	121.1(8)	F5B	P1B	F6B	89.4(18)

**Table 6 Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and
Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for deh161.**

Atom	x	y	z	U(eq)
H2	6485.85	4263.65	6628.5	41
H3	7775.66	4820.92	6430.66	56
H4	8998.09	4367.04	6004.75	60
H5	8955.1	3345.95	5869.63	50
H8	8985.44	2435.99	5833.21	56
H9	9098.87	1419.62	5909	79
H10	8092.4	909.8	6433.98	98
H11	6823.37	1403.06	6740.67	79
H15	5389.26	1346.8	6491.64	58
H16	3765.41	1342.68	6759.52	65
H18	3513.8	2209.25	7920.24	43
H19	2074.07	2526.4	8190.26	47
H21	731.01	2974.69	6384.1	51
H22	2174	2657.27	6113.53	46
H23A	474.89	3026.45	7949.4	94
H23B	-251.06	2728.91	7325.05	94
H23C	131.91	3398.44	7308.66	94
H25	4422.89	3394.8	8018.86	36
H26	4098.36	3551.64	8973.54	42
H27	2763.66	4180.82	9040.14	51
H28	1736.42	4629.39	8150.41	48
H31	954.26	5111.85	7340.33	60
H32	112.82	5602.64	6436.25	72
H33	461.84	5387.39	5492.99	73
H34	1670.47	4662.17	5447.37	60
H38	1507.61	3772.74	5141.69	58
H39	2361.42	3173.92	4514.65	56
H41	5360.33	3494.92	5051.69	48
H42	6478.47	2899.44	4699.57	48
H44	4677.71	1488.64	4716.44	62
H45	3572.63	2086.22	5075.96	57
H46A	6735.86	1450.97	4792.37	100
H46B	6961.31	1979.38	4368.55	100
H46C	6048.88	1522.2	4078.35	100
H48	4682.21	4427.74	5601.97	43
H49	3800.18	5063.93	4821.39	54
H50	3024.96	5918.01	5064.18	56
H51	3207.38	6157.73	6102.86	51
H54	3231.41	6285.65	7065.31	55

H55	3339.2	6401.35	8115.15	58
H56	4222.24	5711.49	8851.59	54
H57	5134.25	4943.9	8559.5	41
H61	6739.34	4725.1	8588.27	46
H62	7604.4	3781.28	8910.1	50
H64	5662.58	2413.72	8149.6	41
H65	6305.88	1454.24	8182.76	51
H67	9036.15	2103.62	8170.77	72
H68	8396.97	3067.91	8108.27	56
H69A	8754.75	1047.6	8057.94	129
H69B	7630.04	787.61	7976.49	129
H69C	8372.52	922.54	8664.65	129
H71	4929.18	5515.97	10377.75	91
H72	4471.13	6488.13	10012.12	91
H73	2776.26	6698.55	9500.08	98
H74	1525.66	6004.37	9513.78	111
H75	1919.66	5035.88	9790.97	97

Table 7 Atomic Occupancy for deh161.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
P2A	0.612(9)	F7A	0.612(9)	F8A	0.612(9)
F9A	0.612(9)	F10A	0.612(9)	F11A	0.612(9)
F12A	0.612(9)	P2B	0.388(9)	F7B	0.388(9)
F8B	0.388(9)	F9B	0.388(9)	F10B	0.388(9)
F11B	0.388(9)	F12B	0.388(9)	P1A	0.55(3)
F1A	0.55(3)	F2A	0.55(3)	F3A	0.55(3)
F4A	0.55(3)	F5A	0.55(3)	F6A	0.55(3)
P1B	0.45(3)	F2B	0.45(3)	F1B	0.45(3)
F3B	0.45(3)	F4B	0.45(3)	F6B	0.45(3)
F5B	0.45(3)				

deh161

Table 1 Crystal data and structure refinement for deh161.

Identification code	deh161
Empirical formula	C ₇₅ H ₅₆ F ₁₃ N ₉ P ₂ Ru
Formula weight	1493.29
Temperature/K	150.0
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	13.6103(4)
b/Å	22.5386(8)
c/Å	22.1790(7)
α /°	90
β /°	106.6150(10)
γ /°	90
Volume/Å ³	6519.5(4)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.521
μ/mm^{-1}	0.381
F(000)	3040.0
Crystal size/mm ³	0.16 × 0.05 × 0.04
Radiation	MoK α (λ = 0.71073)
2 Θ range for data collection/°	4.486 to 49.622
Index ranges	-16 ≤ h ≤ 16, -26 ≤ k ≤ 26, -26 ≤ l ≤ 26
Reflections collected	112284
Independent reflections	11163 [R _{int} = 0.1894, R _{sigma} = 0.0771]
Data/restraints/parameters	11163/0/1032

Goodness-of-fit on F^2 1.032
Final R indexes [$I \geq 2\sigma(I)$] $R_1 = 0.0752$, $wR_2 = 0.1672$
Final R indexes [all data] $R_1 = 0.1226$, $wR_2 = 0.1909$
Largest diff. peak/hole / $e \text{ \AA}^{-3}$ 4.00/-0.48