

# deh241

**Table 1 Crystal data and structure refinement for deh241.**

Identification code	deh241
Empirical formula	$C_{78}H_{60}F_{12}N_3P_5Ru$
Formula weight	1523.21
Temperature/K	150.0
Crystal system	triclinic
Space group	P-1
a/Å	13.8277(6)
b/Å	14.1535(7)
c/Å	21.4310(10)
$\alpha/^\circ$	71.268(2)
$\beta/^\circ$	78.496(2)
$\gamma/^\circ$	76.944(2)
Volume/Å <sup>3</sup>	3832.6(3)
Z	2
$\rho_{\text{calc}}/\text{cm}^3$	1.320
$\mu/\text{mm}^{-1}$	0.381
F(000)	1552.0
Crystal size/mm <sup>3</sup>	0.37 × 0.21 × 0.17
Radiation	MoK $\alpha$ ( $\lambda = 0.71073$ )
2 $\Theta$ range for data collection/ $^\circ$	4.62 to 55.264
Index ranges	$-18 \leq h \leq 18, -18 \leq k \leq 18, -27 \leq l \leq 27$
Reflections collected	105451
Independent reflections	17778 [ $R_{\text{int}} = 0.0759, R_{\text{sigma}} = 0.0552$ ]
Data/restraints/parameters	17778/27/900
Goodness-of-fit on $F^2$	1.044
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1 = 0.0770, wR_2 = 0.2125$
Final R indexes [all data]	$R_1 = 0.1056, wR_2 = 0.2327$
Largest diff. peak/hole / e Å <sup>-3</sup>	3.84/-1.65

**Table 2 Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for deh241.  $U_{\text{eq}}$  is defined as 1/3 of the trace of the orthogonalised  $U_{\text{IJ}}$  tensor.**

Atom	x	y	z	U(eq)
C1	3181(4)	7303(4)	6157(2)	31.9(11)
C2	2971(4)	8086(4)	5566(2)	35.7(12)
C3	3666(6)	8159(6)	4983(3)	51.6(16)
C4	3489(7)	8956(7)	4423(3)	72(2)
C5	2618(7)	9687(6)	4440(3)	67(2)
C6	1936(6)	9620(5)	4998(3)	49.7(16)
C7	2101(5)	8816(4)	5580(3)	35.8(12)
C8	1428(4)	8700(4)	6192(3)	31.5(11)
C9	1676(4)	7864(4)	6749(2)	25.0(10)
C10	1005(4)	7720(4)	7344(2)	25.1(10)
C11	142(4)	8414(4)	7399(3)	31.0(11)
C12	-94(4)	9277(4)	6866(3)	35.0(12)
C13	536(4)	9393(4)	6276(3)	36.6(12)
C14	-1031(5)	10050(5)	6947(4)	48.4(16)
C15	515(3)	5738(4)	7983(2)	24.3(9)
C16	389(4)	4858(4)	8505(2)	28.4(10)
C17	-179(4)	4197(4)	8466(3)	35.7(12)
C18	-615(4)	4378(5)	7908(3)	43.5(14)
C19	-506(4)	5245(5)	7388(3)	42.9(14)
C20	49(4)	5928(4)	7419(3)	34.8(12)
C21	752(4)	6954(4)	8756(2)	24.8(10)
C22	1286(4)	7415(4)	9029(3)	30.4(11)
C23	863(5)	7752(4)	9577(3)	37.4(12)
C24	-109(5)	7619(4)	9864(3)	38.4(13)
C25	-647(5)	7182(5)	9598(3)	42.4(14)
C26	-210(4)	6844(4)	9036(3)	31.3(11)
C27	4811(4)	4950(4)	6895(2)	29.0(10)
C28	5810(4)	4617(4)	6627(3)	33.3(11)
C29	6053(5)	3757(5)	6392(3)	46.1(15)
C30	7006(5)	3435(6)	6139(4)	59.8(19)
C31	7759(5)	3997(6)	6097(4)	61(2)
C32	7544(5)	4823(6)	6325(3)	50.1(16)
C33	6565(4)	5154(4)	6601(3)	35.6(12)
C34	6280(4)	6004(4)	6874(2)	30.2(11)
C35	5266(4)	6245(4)	7147(2)	24.9(9)
C36	5000(4)	7025(4)	7454(2)	25.2(10)
C37	5709(4)	7530(4)	7496(3)	30.2(11)
C38	6715(4)	7309(4)	7226(3)	33.9(12)

C39	6969(4)	6554(4)	6919(3)	35.1(12)
C40	7481(5)	7883(5)	7279(3)	46.8(15)
C41	3276(4)	8606(4)	7285(3)	31.1(11)
C42	2385(4)	9181(4)	7492(3)	35.2(12)
C43	2023(5)	10123(4)	7085(4)	46.9(15)
C44	2547(6)	10502(5)	6462(4)	57.4(19)
C45	3436(6)	9944(5)	6255(3)	52.8(17)
C46	3797(5)	9007(4)	6662(3)	37.5(12)
C47	3782(4)	7519(4)	8576(2)	25.9(10)
C48	3756(4)	6728(4)	9158(3)	31.2(11)
C49	3781(4)	6861(5)	9764(3)	39.7(13)
C50	3872(5)	7797(5)	9794(3)	48.0(16)
C51	3946(5)	8582(5)	9213(4)	51.8(17)
C52	3889(5)	8462(4)	8611(3)	39.9(13)
C53	2235(4)	5105(4)	6764(2)	27.1(10)
C54	1793(4)	4435(4)	6583(3)	32.8(11)
C55	1441(5)	4740(5)	5959(3)	42.7(14)
C56	944(6)	4112(5)	5819(3)	53.2(18)
C57	776(6)	3205(5)	6278(4)	54.4(18)
C58	1112(5)	2887(5)	6888(3)	44.9(15)
C59	1648(4)	3503(4)	7044(3)	31.7(11)
C60	2035(4)	3246(4)	7670(2)	27.1(10)
C61	2478(3)	3954(3)	7797(2)	23.0(9)
C62	2847(3)	3718(4)	8404(2)	23.6(9)
C63	2780(4)	2789(4)	8873(3)	29.4(10)
C64	2338(4)	2071(4)	8758(3)	31.8(11)
C65	1969(4)	2315(4)	8162(3)	32.8(11)
C66	2297(5)	1047(4)	9270(3)	44.7(14)
C67	4792(3)	4083(4)	8439(2)	24.6(9)
C68	5493(4)	4596(4)	8519(2)	29.6(10)
C69	6511(4)	4205(4)	8437(3)	36.4(12)
C70	6838(4)	3298(5)	8285(3)	43.6(14)
C71	6160(4)	2777(5)	8211(3)	45.5(15)
C72	5137(4)	3164(4)	8289(3)	35.3(12)
C73	3147(4)	4446(4)	9418(2)	24.2(9)
C74	2236(4)	4924(4)	9670(2)	29.8(10)
C75	1970(4)	4775(4)	10349(3)	37.3(12)
C76	2606(5)	4140(5)	10782(3)	39.4(13)
C77	3513(5)	3651(5)	10541(3)	46.1(15)
C78	3789(4)	3801(5)	9868(3)	38.5(13)
N1	2588(3)	7188(3)	6730.8(19)	24.4(8)
N2	4531(3)	5708(3)	7138.9(19)	23.6(8)

N3	2544(3)	4916(3)	7340.9(19)	21.4(8)
P1	1337.0(9)	6570.4(9)	8005.3(6)	20.6(2)
P2	3685.9(9)	7313.3(9)	7795.9(6)	22.5(3)
P3	3462.6(9)	4648.6(9)	8516.2(6)	21.0(2)
Ru1	3011.7(3)	6062.3(3)	7639.8(2)	19.77(12)
F1	-922(4)	8020(4)	5884(2)	78.5(14)
F2	-1122(3)	7886(3)	4903(2)	61.7(11)
F3	-728(4)	6486(4)	5747(3)	81.3(15)
F4	403(3)	6910(4)	4858(2)	81.1(16)
F5	624(3)	7069(3)	5819.1(18)	50.1(9)
F6	198(3)	8484(3)	5003(2)	73.0(13)
P4	-251.1(11)	7480.8(12)	5361.7(7)	35.3(3)
P5A	5304(3)	8770(3)	2652.1(19)	42.5(10)
F7A	5267(8)	8486(9)	3422(4)	74.1(15)
F8A	5735(8)	7628(7)	2724(6)	74.1(15)
F9A	6350(7)	9006(9)	2543(6)	74.1(15)
F10A	5299(8)	9007(9)	1892(4)	74.1(15)
F11A	4685(8)	9824(7)	2576(6)	74.1(15)
F12A	4186(7)	8597(9)	2753(6)	74.1(15)
P5B	672(3)	-788(2)	11184.9(17)	52.0(8)
F7B	1202(7)	-1396(6)	11845(4)	84.0(12)
F8B	556(7)	-1766(6)	11149(4)	84.0(12)
F9B	1682(7)	-1145(6)	10804(4)	84.0(12)
F10B	308(7)	-219(6)	10551(4)	84.0(12)
F11B	-265(7)	-367(6)	11590(4)	84.0(12)
F12B	908(7)	214(6)	11242(4)	84.0(12)

**Table 3 Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for deh241. 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	43 (3)	27 (3)	25 (2)	-9 (2)	-6 (2)	-4 (2)
C2	44 (3)	43 (3)	19 (2)	-4 (2)	-6 (2)	-11 (2)
C3	62 (4)	62 (4)	24 (3)	-7 (3)	0 (3)	-12 (3)
C4	83 (6)	89 (6)	23 (3)	2 (3)	4 (3)	-9 (5)
C5	92 (6)	65 (5)	31 (3)	10 (3)	-17 (4)	-19 (4)
C6	65 (4)	45 (4)	30 (3)	3 (3)	-14 (3)	-7 (3)
C7	50 (3)	31 (3)	25 (2)	0 (2)	-11 (2)	-11 (2)
C8	44 (3)	24 (2)	26 (2)	-2 (2)	-16 (2)	-4 (2)
C9	28 (2)	21 (2)	25 (2)	-4.1 (18)	-8.3 (19)	-1.5 (18)
C10	30 (2)	21 (2)	24 (2)	-3.6 (18)	-9.8 (19)	-2.5 (18)
C11	34 (3)	28 (3)	30 (3)	-7 (2)	-10 (2)	0 (2)
C12	37 (3)	24 (3)	44 (3)	-7 (2)	-15 (2)	0 (2)
C13	42 (3)	27 (3)	38 (3)	0 (2)	-20 (2)	-2 (2)
C14	41 (3)	30 (3)	65 (4)	-6 (3)	-21 (3)	11 (2)
C15	20 (2)	28 (2)	25 (2)	-9.7 (19)	-4.2 (18)	-1.6 (18)
C16	28 (2)	29 (3)	27 (2)	-10 (2)	-2 (2)	-2 (2)
C17	35 (3)	28 (3)	44 (3)	-16 (2)	9 (2)	-9 (2)
C18	32 (3)	47 (3)	63 (4)	-29 (3)	-1 (3)	-15 (3)
C19	39 (3)	53 (4)	46 (3)	-20 (3)	-19 (3)	-7 (3)
C20	39 (3)	35 (3)	33 (3)	-12 (2)	-15 (2)	-2 (2)
C21	28 (2)	23 (2)	22 (2)	-5.6 (18)	-5.5 (19)	-0.2 (18)
C22	29 (3)	32 (3)	33 (3)	-14 (2)	-6 (2)	-1 (2)
C23	47 (3)	38 (3)	34 (3)	-20 (2)	-13 (2)	1 (2)
C24	47 (3)	35 (3)	29 (3)	-14 (2)	-1 (2)	3 (2)
C25	36 (3)	50 (4)	42 (3)	-26 (3)	7 (3)	-3 (3)
C26	30 (3)	34 (3)	31 (3)	-15 (2)	-1 (2)	-3 (2)
C27	30 (3)	29 (3)	30 (3)	-13 (2)	-3 (2)	-4 (2)
C28	31 (3)	36 (3)	34 (3)	-19 (2)	1 (2)	-1 (2)
C29	39 (3)	50 (4)	59 (4)	-36 (3)	5 (3)	-6 (3)
C30	48 (4)	66 (5)	76 (5)	-50 (4)	11 (4)	-6 (3)
C31	36 (3)	81 (5)	74 (5)	-49 (4)	11 (3)	-1 (3)
C32	36 (3)	68 (4)	57 (4)	-39 (4)	8 (3)	-11 (3)
C33	30 (3)	45 (3)	33 (3)	-17 (2)	-1 (2)	-3 (2)
C34	30 (3)	34 (3)	26 (2)	-9 (2)	-2 (2)	-6 (2)
C35	28 (2)	22 (2)	24 (2)	-5.9 (18)	-3.9 (19)	-2.6 (18)
C36	29 (2)	24 (2)	22 (2)	-7.4 (18)	-4.3 (19)	-3.0 (19)
C37	32 (3)	29 (3)	29 (3)	-9 (2)	-2 (2)	-7 (2)
C38	30 (3)	39 (3)	33 (3)	-9 (2)	2 (2)	-14 (2)
C39	28 (3)	45 (3)	32 (3)	-13 (2)	3 (2)	-10 (2)

C40	42(3)	58(4)	51(4)	-24(3)	4(3)	-27(3)
C41	37(3)	22(2)	36(3)	-9(2)	-14(2)	-1(2)
C42	37(3)	26(3)	47(3)	-12(2)	-11(2)	-5(2)
C43	47(3)	23(3)	69(4)	-12(3)	-17(3)	2(2)
C44	69(5)	24(3)	67(5)	7(3)	-26(4)	2(3)
C45	68(5)	38(3)	44(4)	7(3)	-10(3)	-16(3)
C46	44(3)	28(3)	37(3)	-4(2)	-8(2)	-6(2)
C47	24(2)	26(2)	30(2)	-13(2)	-3.9(19)	-0.2(18)
C48	31(3)	37(3)	31(3)	-12(2)	-10(2)	-6(2)
C49	36(3)	55(4)	31(3)	-12(3)	-11(2)	-9(3)
C50	43(3)	66(4)	48(4)	-36(3)	-18(3)	6(3)
C51	55(4)	45(4)	74(5)	-43(4)	-28(3)	10(3)
C52	46(3)	30(3)	50(3)	-18(3)	-14(3)	-1(2)
C53	32(3)	26(2)	26(2)	-10.7(19)	-9(2)	0(2)
C54	38(3)	32(3)	35(3)	-19(2)	-14(2)	4(2)
C55	58(4)	36(3)	38(3)	-16(2)	-24(3)	6(3)
C56	75(5)	45(4)	54(4)	-25(3)	-38(4)	2(3)
C57	69(5)	46(4)	65(4)	-30(3)	-32(4)	-3(3)
C58	53(4)	36(3)	61(4)	-29(3)	-23(3)	-2(3)
C59	32(3)	29(3)	40(3)	-20(2)	-10(2)	3(2)
C60	27(2)	27(2)	30(2)	-16(2)	-4(2)	1.6(19)
C61	21(2)	21(2)	27(2)	-9.4(18)	-3.8(18)	0.1(17)
C62	21(2)	22(2)	25(2)	-6.4(18)	-4.9(18)	0.6(18)
C63	31(3)	23(2)	32(3)	-3(2)	-9(2)	-2(2)
C64	32(3)	21(2)	39(3)	-8(2)	-3(2)	-2(2)
C65	30(3)	25(2)	46(3)	-16(2)	-6(2)	1(2)
C66	60(4)	18(3)	51(4)	-3(2)	-9(3)	-7(2)
C67	21(2)	24(2)	27(2)	-4.9(19)	-8.0(18)	1.3(18)
C68	29(3)	28(3)	29(2)	-6(2)	-6(2)	-2(2)
C69	28(3)	41(3)	37(3)	-4(2)	-10(2)	-6(2)
C70	27(3)	45(3)	53(4)	-14(3)	-4(3)	4(2)
C71	32(3)	41(3)	62(4)	-23(3)	-6(3)	7(2)
C72	31(3)	34(3)	46(3)	-20(2)	-9(2)	0(2)
C73	27(2)	24(2)	21(2)	-5.0(18)	-6.3(18)	-4.5(19)
C74	35(3)	27(2)	27(2)	-7(2)	-6(2)	-5(2)
C75	43(3)	37(3)	32(3)	-13(2)	4(2)	-10(2)
C76	56(4)	47(3)	20(2)	-7(2)	-2(2)	-25(3)
C77	44(3)	61(4)	25(3)	5(3)	-14(2)	-10(3)
C78	32(3)	47(3)	32(3)	-5(2)	-10(2)	-1(2)
N1	27(2)	24(2)	20.6(19)	-6.3(16)	-3.4(16)	-2.4(16)
N2	25(2)	22.2(19)	22.1(19)	-6.6(15)	-1.8(16)	-2.9(16)
N3	22.2(19)	20.3(19)	22.0(18)	-8.5(15)	-6.7(15)	2.4(15)

P1	22.1(6)	19.7(6)	19.0(5)	-5.1(4)	-4.7(4)	-0.9(4)
P2	25.9(6)	18.3(6)	23.6(6)	-7.1(5)	-4.5(5)	-2.4(5)
P3	21.4(6)	19.9(6)	21.3(6)	-5.7(4)	-5.8(4)	-0.7(4)
Ru1	22.13(19)	18.44(19)	18.44(18)	-5.92(13)	-4.32(13)	-0.75(13)
F1	93(3)	91(3)	49(2)	-39(2)	-7(2)	17(3)
F2	50(2)	77(3)	66(3)	-33(2)	-32(2)	12(2)
F3	74(3)	59(3)	107(4)	-2(3)	-20(3)	-27(2)
F4	60(3)	132(4)	62(3)	-68(3)	-26(2)	34(3)
F5	71(2)	40.2(19)	45(2)	-9.8(16)	-33.4(18)	-2.9(17)
F6	67(3)	62(3)	73(3)	23(2)	-32(2)	-20(2)
P4	38.6(8)	41.1(8)	27.8(7)	-13.3(6)	-9.3(6)	-1.0(6)
P5A	52(2)	40(2)	45(2)	-24.1(17)	1.0(17)	-16.7(17)
F7A	62(3)	78(3)	74(3)	-21(2)	-4(2)	-1(2)
F8A	62(3)	78(3)	74(3)	-21(2)	-4(2)	-1(2)
F9A	62(3)	78(3)	74(3)	-21(2)	-4(2)	-1(2)
F10A	62(3)	78(3)	74(3)	-21(2)	-4(2)	-1(2)
F11A	62(3)	78(3)	74(3)	-21(2)	-4(2)	-1(2)
F12A	62(3)	78(3)	74(3)	-21(2)	-4(2)	-1(2)
P5B	56.5(19)	49.4(17)	56.1(18)	-20.9(14)	-5.6(14)	-14.8(14)
F7B	110(3)	58(2)	76(2)	-24.6(17)	-19(2)	14.5(18)
F8B	110(3)	58(2)	76(2)	-24.6(17)	-19(2)	14.5(18)
F9B	110(3)	58(2)	76(2)	-24.6(17)	-19(2)	14.5(18)
F10B	110(3)	58(2)	76(2)	-24.6(17)	-19(2)	14.5(18)
F11B	110(3)	58(2)	76(2)	-24.6(17)	-19(2)	14.5(18)
F12B	110(3)	58(2)	76(2)	-24.6(17)	-19(2)	14.5(18)

**Table 4 Bond Lengths for deh241.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.420(7)	C48	C49	1.379(7)
C1	N1	1.319(6)	C49	C50	1.382(9)
C2	C3	1.406(8)	C50	C51	1.381(10)
C2	C7	1.400(8)	C51	C52	1.373(9)
C3	C4	1.377(10)	C53	C54	1.420(7)
C4	C5	1.401(12)	C53	N3	1.315(6)
C5	C6	1.358(10)	C54	C55	1.415(7)
C6	C7	1.410(8)	C54	C59	1.400(8)
C7	C8	1.435(8)	C55	C56	1.372(9)
C8	C9	1.419(7)	C56	C57	1.380(10)
C8	C13	1.411(8)	C57	C58	1.378(9)
C9	C10	1.406(7)	C58	C59	1.413(8)
C9	N1	1.402(6)	C59	C60	1.451(7)
C10	C11	1.375(7)	C60	C61	1.404(7)
C10	P1	1.819(5)	C60	C65	1.408(7)
C11	C12	1.406(7)	C61	C62	1.405(6)
C12	C13	1.369(8)	C61	N3	1.408(6)
C12	C14	1.515(8)	C62	C63	1.384(7)
C15	C16	1.400(7)	C62	P3	1.820(5)
C15	C20	1.403(7)	C63	C64	1.404(7)
C15	P1	1.829(5)	C64	C65	1.380(8)
C16	C17	1.381(7)	C64	C66	1.516(7)
C17	C18	1.371(9)	C67	C68	1.400(7)
C18	C19	1.382(9)	C67	C72	1.397(7)
C19	C20	1.389(8)	C67	P3	1.829(5)
C21	C22	1.396(7)	C68	C69	1.390(7)
C21	C26	1.368(7)	C69	C70	1.380(8)
C21	P1	1.838(5)	C70	C71	1.376(9)
C22	C23	1.381(7)	C71	C72	1.394(8)
C23	C24	1.389(9)	C73	C74	1.384(7)
C24	C25	1.366(9)	C73	C78	1.400(7)
C25	C26	1.412(7)	C73	P3	1.836(5)
C27	C28	1.422(7)	C74	C75	1.386(7)
C27	N2	1.291(6)	C75	C76	1.369(8)
C28	C29	1.411(8)	C76	C77	1.377(9)
C28	C33	1.407(8)	C77	C78	1.377(8)
C29	C30	1.357(9)	N1	Ru1	2.172(4)
C30	C31	1.420(10)	N2	Ru1	2.188(4)
C31	C32	1.359(9)	N3	Ru1	2.183(4)
C32	C33	1.405(8)	P1	Ru1	2.3193(12)
C33	C34	1.447(8)	P2	Ru1	2.3166(12)



C34	C35	1.417(7)	P3	Ru1	2.3258(12)
C34	C39	1.395(8)	F1	P4	1.585(4)
C35	C36	1.405(6)	F2	P4	1.595(4)
C35	N2	1.406(6)	F3	P4	1.598(5)
C36	C37	1.369(7)	F4	P4	1.573(4)
C36	P2	1.825(5)	F5	P4	1.598(4)
C37	C38	1.402(7)	F6	P4	1.581(4)
C38	C39	1.374(8)	P5A	F7A	1.562(9)
C38	C40	1.513(8)	P5A	F8A	1.560(9)
C41	C42	1.392(8)	P5A	F9A	1.515(9)
C41	C46	1.392(8)	P5A	F10A	1.556(9)
C41	P2	1.833(5)	P5A	F11A	1.518(9)
C42	C43	1.385(8)	P5A	F12A	1.580(9)
C43	C44	1.387(10)	P5B	F7B	1.621(9)
C44	C45	1.378(10)	P5B	F8B	1.456(9)
C45	C46	1.379(8)	P5B	F9B	1.538(10)
C47	C48	1.383(7)	P5B	F10B	1.462(9)
C47	C52	1.402(7)	P5B	F11B	1.524(9)
C47	P2	1.821(5)	P5B	F12B	1.572(10)

**Table 5 Bond Angles for deh241.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	C1	C2	124.3(5)	C65	C64	C66	121.5(5)
C3	C2	C1	119.9(6)	C64	C65	C60	122.3(5)
C7	C2	C1	119.5(5)	C68	C67	P3	119.1(4)
C7	C2	C3	120.5(5)	C72	C67	C68	118.6(4)
C4	C3	C2	119.7(7)	C72	C67	P3	122.2(4)
C3	C4	C5	119.7(7)	C69	C68	C67	120.4(5)
C6	C5	C4	121.2(6)	C70	C69	C68	120.1(5)
C5	C6	C7	120.4(7)	C71	C70	C69	120.4(5)
C2	C7	C6	118.6(5)	C70	C71	C72	120.0(6)
C2	C7	C8	117.6(5)	C71	C72	C67	120.5(5)
C6	C7	C8	123.8(6)	C74	C73	C78	118.2(5)
C9	C8	C7	118.9(5)	C74	C73	P3	119.5(4)
C13	C8	C7	123.2(5)	C78	C73	P3	122.3(4)
C13	C8	C9	117.9(5)	C73	C74	C75	120.9(5)
C10	C9	C8	119.4(4)	C76	C75	C74	120.2(5)
N1	C9	C8	121.9(4)	C75	C76	C77	119.8(5)
N1	C9	C10	118.7(4)	C76	C77	C78	120.5(5)
C9	C10	P1	116.1(4)	C77	C78	C73	120.4(5)
C11	C10	C9	120.3(4)	C1	N1	C9	117.5(4)
C11	C10	P1	123.5(4)	C1	N1	Ru1	122.6(3)
C10	C11	C12	121.2(5)	C9	N1	Ru1	119.8(3)
C11	C12	C14	120.2(5)	C27	N2	C35	117.9(4)
C13	C12	C11	118.4(5)	C27	N2	Ru1	122.4(3)
C13	C12	C14	121.4(5)	C35	N2	Ru1	119.3(3)
C12	C13	C8	122.6(5)	C53	N3	C61	117.1(4)
C16	C15	C20	118.1(5)	C53	N3	Ru1	122.8(3)
C16	C15	P1	121.1(4)	C61	N3	Ru1	119.9(3)
C20	C15	P1	120.7(4)	C10	P1	C15	103.6(2)
C17	C16	C15	120.9(5)	C10	P1	C21	102.1(2)
C18	C17	C16	120.6(5)	C10	P1	Ru1	101.81(16)
C17	C18	C19	119.6(5)	C15	P1	C21	102.0(2)
C18	C19	C20	120.8(5)	C15	P1	Ru1	113.87(15)
C19	C20	C15	120.0(5)	C21	P1	Ru1	130.10(16)
C22	C21	P1	119.2(4)	C36	P2	C41	103.3(2)
C26	C21	C22	119.0(5)	C36	P2	Ru1	102.17(16)
C26	C21	P1	121.7(4)	C41	P2	Ru1	115.61(17)
C23	C22	C21	121.2(5)	C47	P2	C36	102.1(2)
C22	C23	C24	119.2(5)	C47	P2	C41	102.0(2)
C25	C24	C23	120.4(5)	C47	P2	Ru1	128.32(17)
C24	C25	C26	120.0(5)	C62	P3	C67	103.8(2)
C21	C26	C25	120.2(5)	C62	P3	C73	100.9(2)

N2	C27	C28	125.0(5)	C62	P3	Ru1	101.78(15)
C29	C28	C27	121.0(5)	C67	P3	C73	101.8(2)
C33	C28	C27	119.2(5)	C67	P3	Ru1	114.83(16)
C33	C28	C29	119.8(5)	C73	P3	Ru1	130.09(16)
C30	C29	C28	121.2(6)	N1	Ru1	N2	90.51(15)
C29	C30	C31	118.7(6)	N1	Ru1	N3	89.53(14)
C32	C31	C30	121.1(6)	N1	Ru1	P1	80.78(11)
C31	C32	C33	120.8(6)	N1	Ru1	P2	85.60(11)
C28	C33	C34	117.3(5)	N1	Ru1	P3	169.81(11)
C32	C33	C28	118.4(5)	N2	Ru1	P1	171.04(11)
C32	C33	C34	124.3(5)	N2	Ru1	P2	81.81(11)
C35	C34	C33	118.4(5)	N2	Ru1	P3	86.43(11)
C39	C34	C33	122.8(5)	N3	Ru1	N2	90.26(14)
C39	C34	C35	118.7(5)	N3	Ru1	P1	87.59(10)
C36	C35	C34	118.5(5)	N3	Ru1	P2	170.65(11)
C36	C35	N2	119.3(4)	N3	Ru1	P3	80.77(10)
N2	C35	C34	122.2(4)	P1	Ru1	P3	101.80(4)
C35	C36	P2	117.1(4)	P2	Ru1	P1	99.48(4)
C37	C36	C35	120.6(5)	P2	Ru1	P3	103.54(4)
C37	C36	P2	122.3(4)	F1	P4	F2	89.9(2)
C36	C37	C38	121.9(5)	F1	P4	F3	89.1(3)
C37	C38	C40	120.6(5)	F1	P4	F5	90.4(2)
C39	C38	C37	117.3(5)	F2	P4	F3	90.0(3)
C39	C38	C40	122.0(5)	F2	P4	F5	179.7(2)
C38	C39	C34	123.0(5)	F4	P4	F1	178.0(3)
C42	C41	P2	120.1(4)	F4	P4	F2	90.4(2)
C46	C41	C42	118.4(5)	F4	P4	F3	88.9(3)
C46	C41	P2	121.4(4)	F4	P4	F5	89.3(2)
C43	C42	C41	120.7(6)	F4	P4	F6	93.4(3)
C42	C43	C44	120.0(6)	F5	P4	F3	89.9(2)
C45	C44	C43	119.8(6)	F6	P4	F1	88.6(3)
C44	C45	C46	120.1(6)	F6	P4	F2	90.2(2)
C45	C46	C41	121.0(6)	F6	P4	F3	177.7(3)
C48	C47	C52	118.0(5)	F6	P4	F5	89.9(2)
C48	C47	P2	119.8(4)	F7A	P5A	F12A	89.8(6)
C52	C47	P2	122.2(4)	F8A	P5A	F7A	86.3(6)
C49	C48	C47	121.8(5)	F8A	P5A	F12A	92.5(6)
C48	C49	C50	119.7(6)	F9A	P5A	F7A	91.0(6)
C51	C50	C49	119.1(5)	F9A	P5A	F8A	91.0(7)
C52	C51	C50	121.4(6)	F9A	P5A	F10A	91.9(6)
C51	C52	C47	120.0(6)	F9A	P5A	F11A	100.4(7)
N3	C53	C54	124.9(5)	F9A	P5A	F12A	176.4(7)

C55	C54	C53	120.0(5)	F10A P5A	F7A	176.6(7)
C59	C54	C53	119.4(5)	F10A P5A	F8A	91.9(6)
C59	C54	C55	120.5(5)	F10A P5A	F12A	87.4(6)
C56	C55	C54	118.9(6)	F11A P5A	F7A	95.7(6)
C55	C56	C57	120.9(6)	F11A P5A	F8A	168.4(7)
C58	C57	C56	121.6(6)	F11A P5A	F10A	85.5(6)
C57	C58	C59	119.1(6)	F11A P5A	F12A	76.1(6)
C54	C59	C58	119.1(5)	F8B P5B	F7B	87.5(5)
C54	C59	C60	117.0(5)	F8B P5B	F9B	77.1(5)
C58	C59	C60	123.8(5)	F8B P5B	F10B	94.5(5)
C61	C60	C59	119.2(5)	F8B P5B	F11B	108.6(6)
C61	C60	C65	118.5(5)	F8B P5B	F12B	174.1(6)
C65	C60	C59	122.3(5)	F9B P5B	F7B	84.9(5)
C60	C61	C62	119.6(4)	F9B P5B	F12B	98.6(5)
C60	C61	N3	122.2(4)	F10B P5B	F7B	173.4(6)
C62	C61	N3	118.1(4)	F10B P5B	F9B	89.4(5)
C61	C62	P3	117.1(3)	F10B P5B	F11B	93.2(5)
C63	C62	C61	120.2(4)	F10B P5B	F12B	89.4(5)
C63	C62	P3	122.6(4)	F11B P5B	F7B	92.1(5)
C62	C63	C64	121.1(5)	F11B P5B	F9B	173.5(6)
C63	C64	C66	120.3(5)	F11B P5B	F12B	75.5(5)
C65	C64	C63	118.2(5)	F12B P5B	F7B	88.1(5)

**Table 6 Hydrogen Atom Coordinates ( $\text{\AA}\times 10^4$ ) and  
Isotropic Displacement Parameters ( $\text{\AA}^2\times 10^3$ ) for deh241.**

Atom	x	y	z	U(eq)
H1	3787.75	6831.15	6138.18	38
H3	4254.17	7660.41	4975.39	62
H4	3954.44	9011.21	4027.61	86
H5	2503.1	10240.24	4054.24	80
H6	1345.73	10117.03	4995.81	60
H11	-303.12	8308.81	7804.96	37
H13	367.38	9961.25	5909.49	44
H14A	-1555.09	9706.54	7255.41	73
H14B	-1264.18	10392.68	6513.8	73
H14C	-879.07	10549.9	7123.94	73
H16	697.69	4714.13	8891.36	34
H17	-267.84	3610.86	8829.79	43
H18	-989.13	3911.03	7880.04	52
H19	-814.57	5374.47	7003.13	51
H20	113.59	6524.31	7059.88	42
H22	1953.43	7497.42	8835.21	37
H23	1231.46	8071.35	9754.89	45
H24	-401.04	7834.47	10246.79	46
H25	-1315.62	7103.65	9791.99	51
H26	-585.97	6540.37	8851.64	38
H27	4311.48	4587.32	6893.42	35
H29	5539.78	3397.37	6410.84	55
H30	7166.82	2845.11	5992.15	72
H31	8424.35	3791.95	5907.12	73
H32	8062.6	5181.94	6297.45	60
H37	5514.16	8044.45	7714.83	36
H39	7646.05	6399.91	6728.43	42
H40A	7184.24	8600.85	7205.23	70
H40B	8065.99	7812.7	6943.18	70
H40C	7687.84	7606.31	7723.39	70
H42	2022.67	8923.72	7917.83	42
H43	1415.3	10510.65	7231.76	56
H44	2294.17	11143.42	6178.94	69
H45	3800.67	10206.43	5831.17	63
H46	4411.84	8629.93	6515.26	45
H48	3719.93	6075.7	9139.13	37
H49	3736.53	6311.37	10158.33	48
H50	3882.69	7899.84	10209.28	58
H51	4037.7	9218	9229.73	62

H52	3922.18	9016.8	8219.14	48
H53	2314.6	5737.5	6443.74	33
H55	1547.34	5367.74	5643.51	51
H56	711.56	4305.18	5399.43	64
H57	420.49	2789.09	6171.16	65
H58	984.79	2262.86	7200.51	54
H63	3036.82	2635.25	9280.6	35
H65	1658.97	1838.45	8082.27	39
H66A	2980.83	681.64	9327.92	67
H66B	1941.52	654.13	9118.8	67
H66C	1943.95	1143.88	9695.52	67
H68	5271.02	5215.85	8629.6	36
H69	6983.28	4562.06	8485.26	44
H70	7534.31	3031.4	8231.81	52
H71	6389.73	2153.11	8106.32	55
H72	4671.94	2800.78	8238.96	42
H74	1786.77	5360.16	9373.77	36
H75	1345.37	5113.74	10514.14	45
H76	2422.14	4037.78	11247.3	47
H77	3950.88	3207.18	10842.61	55
H78	4419.22	3464.47	9706.94	46

**Table 7 Atomic Occupancy for deh241.**

<b>Atom</b>	<b><i>Occupancy</i></b>	<b>Atom</b>	<b><i>Occupancy</i></b>	<b>Atom</b>	<b><i>Occupancy</i></b>
P5A	0.417(4)	F7A	0.417(4)	F8A	0.417(4)
F9A	0.417(4)	F10A	0.417(4)	F11A	0.417(4)
F12A	0.417(4)	P5B	0.583(4)	F7B	0.583(4)
F8B	0.583(4)	F9B	0.583(4)	F10B	0.583(4)
F11B	0.583(4)	F12B	0.583(4)		

**Table 8 Solvent masks information for deh241.**

Number	X	Y	Z	Volume	Electron count Content
1	0.500	0.000	0.000	229.5	58.5 ?
2	0.500	-0.228	0.500	291.7	65.6 ?

# deh241

**Table 1 Crystal data and structure refinement for deh241.**

Identification code	deh241
Empirical formula	C <sub>78</sub> H <sub>60</sub> F <sub>12</sub> N <sub>3</sub> P <sub>5</sub> Ru
Formula weight	1523.21
Temperature/K	150.0
Crystal system	triclinic
Space group	P-1
a/Å	13.8277(6)
b/Å	14.1535(7)
c/Å	21.4310(10)
$\alpha$ /°	71.268(2)
$\beta$ /°	78.496(2)
$\gamma$ /°	76.944(2)
Volume/Å <sup>3</sup>	3832.6(3)
Z	2
$\rho_{\text{calc}}$ /cm <sup>3</sup>	1.320
$\mu$ /mm <sup>-1</sup>	0.381
F(000)	1552.0
Crystal size/mm <sup>3</sup>	0.37 × 0.21 × 0.17
Radiation	MoK $\alpha$ ( $\lambda$ = 0.71073)
2 $\Theta$ range for data collection/°	4.62 to 55.264
Index ranges	-18 ≤ h ≤ 18, -18 ≤ k ≤ 18, -27 ≤ l ≤ 27
Reflections collected	105451
Independent reflections	17778 [R <sub>int</sub> = 0.0759, R <sub>sigma</sub> = 0.0552]
Data/restraints/parameters	17778/27/900
Goodness-of-fit on F <sup>2</sup>	1.044
Final R indexes [I ≥ 2 $\sigma$ (I)]	R <sub>1</sub> = 0.0770, wR <sub>2</sub> = 0.2125
Final R indexes [all data]	R <sub>1</sub> = 0.1056, wR <sub>2</sub> = 0.2327
Largest diff. peak/hole / e Å <sup>-3</sup>	3.84/-1.65