

# deh148

**Table 1 Crystal data and structure refinement for deh148.**

Identification code	deh148
Empirical formula	$C_{70}H_{53}Cl_2F_{12}FeN_9P_2$
Formula weight	1436.90
Temperature/K	150.0
Crystal system	monoclinic
Space group	$P2_1/n$
$a/\text{\AA}$	13.8409(9)
$b/\text{\AA}$	22.4674(15)
$c/\text{\AA}$	21.2115(14)
$\alpha/^\circ$	90
$\beta/^\circ$	106.780(4)
$\gamma/^\circ$	90
Volume/ $\text{\AA}^3$	6315.3(7)
Z	4
$\rho_{\text{calc}}/\text{g cm}^{-3}$	1.511
$\mu/\text{mm}^{-1}$	0.462
F(000)	2936.0
Crystal size/ $\text{mm}^3$	$0.1 \times 0.08 \times 0.07$
Radiation	MoK $\alpha$ ( $\lambda = 0.71073$ )
$2\Theta$ range for data collection/ $^\circ$	4.402 to 55.11
Index ranges	$-18 \leq h \leq 17, -29 \leq k \leq 26, -27 \leq l \leq 27$
Reflections collected	132353
Independent reflections	14536 [ $R_{\text{int}} = 0.0986, R_{\text{sigma}} = 0.0661$ ]
Data/restraints/parameters	14536/0/868
Goodness-of-fit on $F^2$	1.019
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1 = 0.0560, wR_2 = 0.1043$
Final R indexes [all data]	$R_1 = 0.1077, wR_2 = 0.1215$
Largest diff. peak/hole / $e \text{\AA}^{-3}$	1.18/-0.99

**Table 2 Fractional Atomic Coordinates ( $\times 10^4$ ) and Equivalent Isotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for deh148.  $U_{\text{eq}}$  is defined as 1/3 of the trace of the orthogonalised  $U_{\text{IJ}}$  tensor.**

Atom	x	y	z	U(eq)
C1	6339(2)	7513.2(12)	1493.1(13)	19.4(6)
C2	7170(2)	7818.9(12)	1347.4(14)	22.2(6)
C3	7370(2)	8431.8(14)	1453.4(16)	32.2(7)
C4	8116(3)	8695.7(15)	1246.0(18)	40.3(9)
C5	8680(2)	8359.7(15)	926.2(17)	37.4(8)
C6	8548(2)	7759.6(15)	860.8(15)	31.5(7)
C7	7813(2)	7469.5(13)	1096.1(14)	23.0(6)
C8	7740(2)	6831.4(13)	1131.6(13)	21.2(6)
C9	6991(2)	6577.9(12)	1380.1(13)	18.4(6)
C10	6987(2)	5962.8(13)	1472.5(14)	23.8(6)
C11	7685(2)	5603.4(14)	1312.5(15)	29.8(7)
C12	8408(2)	5848.4(14)	1052.1(15)	30.6(7)
C13	8431(2)	6449.4(14)	966.9(15)	29.4(7)
C14	4838(2)	7490.3(12)	1804.2(13)	19.4(6)
C15	5193(2)	8413.4(13)	1460.3(15)	28.5(7)
C16	4318(2)	8446.3(13)	1604.6(16)	29.8(7)
C17	3159(2)	7760.8(12)	1947.0(14)	21.4(6)
C18	2321(2)	7629.1(13)	1430.5(15)	25.5(7)
C19	1428(2)	7486.3(14)	1558.2(16)	30.3(7)
C20	1355(2)	7482.6(14)	2197.0(16)	29.4(7)
C21	2193(2)	7643.7(14)	2703.1(15)	29.5(7)
C22	3098(2)	7783.3(13)	2583.5(15)	25.8(7)
C23	386(3)	7310(2)	2344(2)	53.6(11)
C24	3023(2)	6247.3(12)	1620.9(14)	21.0(6)
C25	2253(2)	5844.0(12)	1682.5(16)	25.1(7)
C26	1618(2)	5532.1(14)	1144.5(18)	32.9(8)
C27	932(2)	5126.6(15)	1245(2)	42.8(9)
C28	872(3)	5021.8(16)	1877(2)	48.3(10)
C29	1499(3)	5299.6(14)	2404(2)	39.9(9)
C30	2213(2)	5718.6(12)	2324.9(16)	27.3(7)
C31	2929(2)	6004.4(12)	2875.1(15)	24.6(7)
C32	3681(2)	6369.3(12)	2755.0(14)	20.9(6)
C33	4348(2)	6671.3(13)	3279.5(14)	24.7(6)
C34	4318(3)	6585.2(14)	3915.1(15)	32.1(7)
C35	3616(3)	6196.5(15)	4041.2(17)	38.8(8)
C36	2928(3)	5922.1(14)	3535.2(17)	34.8(8)
C37	4020(2)	6659.7(12)	986.7(13)	19.0(6)
C38	2370(2)	6512.5(14)	404.5(15)	29.7(7)

C39	2830(2)	6775.2(14)	7.5(15)	31.9(7)
C40	4537(2)	7176.5(13)	95.0(13)	21.3(6)
C41	5279(2)	6870.4(13)	-85.0(14)	25.5(7)
C42	5939(2)	7185.8(13)	-345.3(14)	26.9(7)
C43	5865(2)	7798.9(13)	-426.0(14)	26.5(7)
C44	5099(2)	8093.2(14)	-245.9(15)	30.5(7)
C45	4434(2)	7785.8(13)	11.1(14)	27.4(7)
C46	6600(3)	8138.3(15)	-688.4(17)	36.5(8)
C47	5318(2)	5543.3(12)	2536.5(14)	19.5(6)
C48	4884(2)	5063.1(12)	2809.2(15)	21.8(6)
C49	4980(2)	5017.5(13)	3489.4(16)	29.5(7)
C50	4447(3)	4589.9(14)	3712.1(18)	37.9(8)
C51	3821(3)	4197.3(15)	3269(2)	44.0(9)
C52	3705(3)	4239.8(14)	2608.1(19)	37.5(8)
C53	4221(2)	4679.2(12)	2359.0(16)	26.5(7)
C54	4075(2)	4764.1(12)	1662.1(15)	24.2(7)
C55	4513(2)	5268.8(12)	1457.7(14)	21.7(6)
C56	4424(2)	5351.4(13)	788.5(15)	26.0(7)
C57	3875(2)	4960.0(14)	323.8(16)	32.7(8)
C58	3399(2)	4476.7(14)	522.1(18)	36.9(8)
C59	3502(2)	4378.0(14)	1171.3(18)	33.9(8)
C60	5999.9(19)	6526.8(12)	2691.7(13)	17.6(6)
C61	6747(2)	5871.8(14)	3516.0(15)	29.3(7)
C62	7239(2)	6386.7(14)	3647.9(15)	30.7(7)
C63	7161(2)	7378.4(12)	3134.8(13)	22.0(6)
C64	8166(2)	7442.9(14)	3159.1(15)	28.8(7)
C65	8584(2)	8002.0(14)	3209.2(16)	32.3(7)
C66	8023(2)	8505.5(14)	3230.2(16)	32.1(7)
C67	7014(2)	8435.2(13)	3198.0(15)	29.0(7)
C68	6579(2)	7873.1(13)	3157.7(14)	24.4(6)
C69	8518(3)	9112.0(15)	3300(2)	53.1(11)
Fe1	5037.4(3)	6666.6(2)	1828.9(2)	15.22(9)
N1	6240.4(16)	6932.5(10)	1520.9(11)	17.0(5)
N2	5527.6(17)	7825.3(10)	1599.6(11)	20.4(5)
N3	4105.3(18)	7887.7(10)	1817.2(12)	22.0(5)
N4	3756.0(16)	6458.8(10)	2112.3(11)	18.2(5)
N5	3108.7(16)	6430.4(10)	1002.3(11)	21.0(5)
N6	3839.0(17)	6863.8(11)	363.7(11)	22.1(5)
N7	5085.6(17)	5680.0(9)	1907.9(11)	19.0(5)
N8	5985.0(17)	5957.9(10)	2930.4(11)	20.1(5)
N9	6778.7(17)	6784.8(10)	3144.0(11)	21.6(5)
C70	10680(3)	4646.9(19)	6585.0(19)	55.2(11)

C11	10546.4(8)	4009.9(4)	7032.7(5)	55.5(3)
C12	11582.9(12)	5137.0(5)	7055.3(6)	84.9(4)
F1	8487(2)	4624.1(10)	5468.4(11)	70.3(7)
F2	7008.0(18)	5083.8(13)	5008.7(13)	78.2(8)
F3	9288.0(17)	5508.0(10)	5563.7(12)	62.9(6)
F4	8005(2)	5380.4(10)	6002.8(10)	67.6(7)
F5	7816.1(19)	5965.7(10)	5119.3(12)	65.6(7)
F6	8292.0(19)	5204.7(12)	4575.7(10)	69.7(7)
P1	8146.5(8)	5291.6(4)	5286.3(5)	43.1(2)
F7	3517.7(16)	8050.4(11)	4349.6(12)	64.8(7)
F8	4932.9(19)	7969.9(9)	4034.0(11)	60.8(7)
F9	3864.6(15)	8737.0(9)	3671.4(9)	45.5(5)
F10	5379.3(14)	8896.4(9)	4402.8(10)	50.7(6)
F11	3975.8(17)	8976.5(10)	4714.1(10)	57.3(6)
F12	5030.9(14)	8201.9(9)	5084.1(9)	39.8(5)
P2	4448.8(6)	8469.6(4)	4373.6(4)	28.79(19)

**Table 3 Anisotropic Displacement Parameters ( $\text{\AA}^2 \times 10^3$ ) for deh148. 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	19.3(14)	22.6(15)	15.1(14)	0.3(11)	3.2(11)	-3.0(12)
C2	22.3(15)	23.1(15)	19.5(15)	0.6(12)	3.2(12)	-6.0(12)
C3	34.4(18)	28.0(17)	35.9(18)	-4.5(14)	12.9(15)	-9.9(14)
C4	41(2)	31.6(19)	48(2)	-2.6(16)	13.6(17)	-19.6(16)
C5	32.2(18)	42(2)	40(2)	4.6(16)	14.4(16)	-14.7(16)
C6	24.8(16)	40.8(19)	29.7(18)	5.8(15)	9.0(14)	-4.3(14)
C7	17.0(14)	31.3(16)	19.7(15)	1.8(12)	3.6(12)	-5.1(12)
C8	15.5(14)	29.0(16)	17.8(14)	2.7(12)	2.8(11)	-0.2(12)
C9	15.6(13)	22.6(15)	15.4(13)	0.2(11)	1.9(11)	0.8(11)
C10	21.4(15)	25.5(16)	24.9(16)	4.1(13)	7.1(13)	1.6(12)
C11	29.2(17)	27.7(17)	33.2(18)	4.5(14)	10.2(14)	5.2(14)
C12	25.5(16)	35.5(18)	34.1(18)	1.6(14)	13.7(14)	9.1(14)
C13	23.1(16)	39.1(18)	28.6(17)	1.8(14)	11.6(13)	-2.9(14)
C14	17.6(14)	23.3(15)	15.8(14)	0.1(11)	2.5(11)	-1.7(11)
C15	34.9(18)	16.5(15)	35.1(18)	1.7(13)	11.7(14)	-1.0(13)
C16	36.9(18)	14.2(15)	39.7(19)	1.9(13)	13.1(15)	4.0(13)
C17	20.2(15)	16.9(14)	28.3(16)	0.4(12)	8.8(13)	5.6(11)
C18	25.5(16)	29.2(16)	22.2(16)	-1.3(13)	7.4(13)	7.6(13)
C19	22.7(16)	34.6(18)	30.2(18)	-4.1(14)	2.4(13)	3.6(14)
C20	22.0(16)	32.4(17)	33.6(18)	4.4(14)	7.5(14)	4.9(13)
C21	31.8(18)	33.2(17)	25.6(17)	1.6(14)	11.4(14)	6.9(14)
C22	25.1(16)	23.6(16)	26.7(16)	-3.4(13)	4.4(13)	4.3(13)
C23	34(2)	79(3)	50(2)	11(2)	16.3(18)	-7(2)
C24	16.1(14)	18.6(14)	30.3(16)	-0.6(12)	9.8(12)	1.8(11)
C25	17.7(15)	18.1(15)	42.2(19)	-3.2(13)	12.8(14)	1.2(12)
C26	20.5(16)	28.4(17)	49(2)	-7.3(15)	9.1(15)	-2.5(13)
C27	25.1(18)	28.8(18)	72(3)	-11.2(18)	9.3(18)	-6.8(14)
C28	28.7(19)	33(2)	87(3)	2(2)	23(2)	-9.5(16)
C29	33.6(19)	28.8(18)	65(3)	3.3(17)	27.3(19)	-1.8(15)
C30	23.9(16)	15.2(14)	49(2)	3.0(13)	20.6(15)	4.1(12)
C31	25.3(16)	18.7(15)	35.7(18)	4.8(13)	17.9(14)	6.1(12)
C32	23.2(15)	15.6(14)	28.5(16)	3.5(12)	14.8(13)	7.3(12)
C33	28.0(16)	22.9(15)	26.6(16)	1.7(13)	13.1(13)	4.4(13)
C34	42.0(19)	31.7(18)	25.8(17)	0.6(14)	14.7(15)	9.2(15)
C35	57(2)	37.3(19)	31.4(19)	7.7(16)	28.5(18)	9.8(17)
C36	41(2)	28.9(17)	45(2)	6.8(16)	30.3(17)	5.7(15)
C37	18.3(14)	16.3(13)	22.4(15)	-1.6(12)	5.7(11)	1.3(11)
C38	16.1(15)	40.5(19)	27.2(17)	-4.9(14)	-2.2(13)	0.6(13)
C39	24.7(16)	42(2)	21.9(16)	-1.1(14)	-4.3(13)	3.1(14)

C40	22.4(15)	27.3(16)	12.4(14)	2.1(12)	2.0(11)	-0.1(12)
C41	30.5(17)	23.1(15)	21.7(15)	2.0(12)	5.4(13)	2.8(13)
C42	25.9(16)	29.7(17)	25.5(16)	0.0(13)	8.4(13)	2.5(13)
C43	31.0(17)	28.1(17)	17.6(15)	5.6(13)	2.8(13)	-1.5(13)
C44	39.3(19)	22.6(16)	25.8(17)	5.0(13)	3.4(14)	3.7(14)
C45	28.2(17)	29.1(17)	23.9(16)	1.3(13)	5.8(13)	9.1(13)
C46	43(2)	33.7(18)	34.1(19)	4.7(15)	12.2(16)	-6.2(15)
C47	17.9(14)	15.8(13)	25.6(16)	1.1(12)	7.5(12)	5.2(11)
C48	22.0(15)	13.4(13)	33.0(17)	5.5(12)	12.7(13)	5.7(11)
C49	34.3(18)	21.3(16)	35.7(19)	8.8(13)	14.5(15)	9.7(13)
C50	49(2)	28.7(18)	44(2)	15.2(16)	26.7(18)	9.5(16)
C51	48(2)	26.3(18)	69(3)	13.9(18)	34(2)	-1.3(16)
C52	35.3(19)	19.7(16)	64(3)	2.8(16)	24.2(18)	-2.5(14)
C53	22.4(15)	14.3(14)	46(2)	1.0(13)	15.0(14)	3.1(12)
C54	15.9(14)	16.5(14)	41.3(19)	-2.9(13)	9.7(13)	3.1(11)
C55	15.6(14)	18.0(14)	30.7(17)	-2.2(12)	5.4(12)	4.5(11)
C56	24.8(16)	23.1(15)	29.8(17)	-4.2(13)	7.4(13)	1.0(12)
C57	32.0(18)	34.1(18)	30.2(18)	-10.0(14)	5.8(15)	4.2(15)
C58	31.8(19)	27.6(18)	45(2)	-15.3(16)	1.3(16)	-2.7(14)
C59	23.2(16)	20.2(16)	57(2)	-8.7(15)	9.1(16)	-4.7(13)
C60	16.1(13)	18.1(14)	19.6(14)	0.8(11)	6.8(11)	0.6(11)
C61	28.7(17)	29.9(17)	24.3(16)	9.5(13)	-0.3(13)	2.5(14)
C62	27.8(17)	33.6(18)	23.4(17)	6.9(14)	-4.1(13)	0.4(14)
C63	24.4(15)	22.0(15)	16.5(14)	-2.9(12)	1.0(12)	-4.7(12)
C64	24.6(16)	25.7(16)	34.3(18)	-3.4(14)	5.9(14)	0.0(13)
C65	22.5(16)	34.4(18)	40.4(19)	-3.3(15)	9.6(15)	-5.1(14)
C66	30.5(17)	27.0(17)	34.6(18)	-4.2(14)	2.6(14)	-8.6(14)
C67	29.0(17)	24.3(16)	31.9(17)	-6.1(13)	6.0(14)	0.7(13)
C68	20.5(15)	30.3(16)	20.8(15)	-2.6(13)	3.2(12)	-1.4(13)
C69	42(2)	30(2)	84(3)	-10(2)	12(2)	-12.7(17)
Fe1	14.20(19)	14.45(19)	16.82(19)	0.76(16)	4.17(15)	-0.52(16)
N1	14.7(11)	19.2(12)	15.4(12)	-0.1(9)	1.8(9)	-1.6(9)
N2	24.1(13)	15.7(12)	22.6(13)	0.1(10)	8.9(10)	-2.2(10)
N3	23.2(13)	16.1(12)	27.9(13)	-0.4(10)	9.4(11)	1.5(10)
N4	18.5(12)	14.4(11)	23.1(13)	0.9(9)	8.1(10)	1.1(9)
N5	15.2(12)	23.8(12)	22.4(13)	-2.3(10)	2.8(10)	-0.1(10)
N6	18.8(12)	27.7(13)	17.1(12)	0.3(10)	0.9(10)	2.4(10)
N7	17.4(12)	15.6(11)	24.4(13)	-1.9(10)	6.9(10)	0.3(9)
N8	18.8(12)	20.3(12)	19.6(12)	3.6(10)	3.1(10)	-0.5(10)
N9	20.8(12)	20.8(13)	20.0(12)	1.2(10)	0.6(10)	-2.7(10)
C70	47(2)	70(3)	43(2)	5(2)	3.8(19)	-5(2)
Cl1	63.9(7)	42.4(5)	62.9(7)	-0.3(5)	22.5(5)	-0.4(5)

Cl2	138.8(12)	41.8(6)	59.5(7)	7.4(5)	5.5(8)	-20.5(7)
F1	107(2)	36.8(13)	53.2(15)	4.5(11)	0.9(14)	-8.9(13)
F2	52.5(15)	107(2)	70.1(17)	-17.8(16)	8.7(13)	-27.3(15)
F3	52.4(14)	52.0(14)	72.3(16)	9.6(12)	-1.1(12)	-7.9(11)
F4	115(2)	54.4(14)	36.7(12)	0.8(11)	26.6(13)	-31.3(14)
F5	74.3(17)	57.3(15)	62.1(15)	26.7(12)	14.8(13)	15.4(13)
F6	73.9(17)	101(2)	34.0(13)	15.2(13)	15.8(12)	23.6(15)
P1	51.8(6)	43.6(6)	28.8(5)	10.6(4)	3.6(4)	-8.4(5)
F7	38.1(12)	71.5(16)	71.8(16)	20.1(13)	-5.1(11)	-22.2(11)
F8	95.0(18)	44.3(13)	50.2(14)	4.0(10)	32.2(13)	30.7(12)
F9	56.4(13)	39.7(11)	28.7(11)	0.9(9)	-6.4(9)	3.3(10)
F10	33.9(11)	56.5(13)	55.2(14)	18.6(11)	2.7(10)	-8.6(10)
F11	69.1(15)	62.9(15)	44.4(13)	0.9(11)	23.5(11)	29.2(12)
F12	30.0(10)	56.7(13)	30.3(10)	11.8(9)	4.8(8)	5.0(9)
P2	25.8(4)	33.1(5)	25.4(4)	-1.1(3)	4.1(3)	1.3(3)

**Table 4 Bond Lengths for deh148.**

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.447(4)	C40	C45	1.383(4)
C1	N1	1.315(3)	C40	N6	1.439(4)
C1	N2	1.397(3)	C41	C42	1.390(4)
C2	C3	1.410(4)	C42	C43	1.388(4)
C2	C7	1.402(4)	C43	C44	1.393(4)
C3	C4	1.369(4)	C43	C46	1.501(4)
C4	C5	1.394(5)	C44	C45	1.382(4)
C5	C6	1.362(5)	C47	C48	1.435(4)
C6	C7	1.414(4)	C47	N7	1.314(3)
C7	C8	1.441(4)	C47	N8	1.404(4)
C8	C9	1.412(4)	C48	C49	1.414(4)
C8	C13	1.402(4)	C48	C53	1.411(4)
C9	C10	1.396(4)	C49	C50	1.375(4)
C9	N1	1.408(3)	C50	C51	1.393(5)
C10	C11	1.375(4)	C51	C52	1.368(5)
C11	C12	1.389(4)	C52	C53	1.407(4)
C12	C13	1.364(4)	C53	C54	1.446(4)
C14	Fe1	1.870(3)	C54	C55	1.412(4)
C14	N2	1.380(3)	C54	C59	1.410(4)
C14	N3	1.357(3)	C55	C56	1.401(4)
C15	C16	1.334(4)	C55	N7	1.399(4)
C15	N2	1.403(4)	C56	C57	1.375(4)
C16	N3	1.394(4)	C57	C58	1.396(5)
C17	C18	1.379(4)	C58	C59	1.361(5)
C17	C22	1.378(4)	C60	Fe1	1.953(3)
C17	N3	1.442(3)	C60	N8	1.377(3)
C18	C19	1.378(4)	C60	N9	1.350(3)
C19	C20	1.388(4)	C61	C62	1.331(4)
C20	C21	1.382(4)	C61	N8	1.391(4)
C20	C23	1.512(4)	C62	N9	1.398(4)
C21	C22	1.384(4)	C63	C64	1.385(4)
C24	C25	1.433(4)	C63	C68	1.382(4)
C24	N4	1.316(4)	C63	N9	1.437(3)
C24	N5	1.413(4)	C64	C65	1.374(4)
C25	C26	1.410(4)	C65	C66	1.381(4)
C25	C30	1.408(4)	C66	C67	1.388(4)
C26	C27	1.375(4)	C66	C69	1.513(4)
C27	C28	1.388(5)	C67	C68	1.391(4)
C28	C29	1.354(5)	Fe1	N1	2.046(2)
C29	C30	1.410(4)	Fe1	N4	2.083(2)
C30	C31	1.445(4)	Fe1	N7	2.222(2)



C31	C32	1.405(4)	C70	Cl1	1.756(4)
C31	C36	1.413(4)	C70	Cl2	1.747(4)
C32	C33	1.399(4)	F1	P1	1.586(2)
C32	N4	1.411(3)	F2	P1	1.585(2)
C33	C34	1.375(4)	F3	P1	1.594(2)
C34	C35	1.389(5)	F4	P1	1.600(2)
C35	C36	1.359(5)	F5	P1	1.592(2)
C37	Fe1	1.929(3)	F6	P1	1.589(2)
C37	N5	1.372(3)	F7	P2	1.585(2)
C37	N6	1.352(3)	F8	P2	1.583(2)
C38	C39	1.332(4)	F9	P2	1.593(2)
C38	N5	1.393(4)	F10	P2	1.593(2)
C39	N6	1.397(4)	F11	P2	1.587(2)
C40	C41	1.378(4)	F12	P2	1.6066(19)

**Table 5 Bond Angles for deh148.**

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	C1	C2	125.4(3)	N7	C55	C56	118.1(3)
N1	C1	N2	113.1(2)	C57	C56	C55	120.7(3)
N2	C1	C2	121.5(2)	C56	C57	C58	119.5(3)
C3	C2	C1	124.1(3)	C59	C58	C57	120.7(3)
C7	C2	C1	116.5(2)	C58	C59	C54	121.2(3)
C7	C2	C3	119.4(3)	N8	C60	Fe1	114.53(19)
C4	C3	C2	120.2(3)	N9	C60	Fe1	141.8(2)
C3	C4	C5	120.1(3)	N9	C60	N8	103.4(2)
C6	C5	C4	120.5(3)	C62	C61	N8	106.1(3)
C5	C6	C7	120.6(3)	C61	C62	N9	107.6(3)
C2	C7	C6	118.4(3)	C64	C63	N9	117.8(3)
C2	C7	C8	118.4(2)	C68	C63	C64	120.3(3)
C6	C7	C8	123.0(3)	C68	C63	N9	121.7(3)
C9	C8	C7	119.4(2)	C65	C64	C63	119.6(3)
C13	C8	C7	122.2(3)	C64	C65	C66	121.5(3)
C13	C8	C9	118.3(3)	C65	C66	C67	118.3(3)
C10	C9	C8	119.0(3)	C65	C66	C69	119.8(3)
C10	C9	N1	119.8(2)	C67	C66	C69	121.9(3)
N1	C9	C8	121.2(2)	C66	C67	C68	121.2(3)
C11	C10	C9	121.0(3)	C63	C68	C67	119.1(3)
C10	C11	C12	120.3(3)	C14	Fe1	C37	85.39(11)
C13	C12	C11	119.5(3)	C14	Fe1	C60	103.93(11)
C12	C13	C8	122.0(3)	C14	Fe1	N1	80.16(10)
N2	C14	Fe1	116.01(19)	C14	Fe1	N4	95.67(10)
N3	C14	Fe1	139.1(2)	C14	Fe1	N7	172.02(10)
N3	C14	N2	103.7(2)	C37	Fe1	C60	169.86(11)
C16	C15	N2	105.7(3)	C37	Fe1	N1	98.65(10)
C15	C16	N3	108.4(3)	C37	Fe1	N4	79.09(10)
C18	C17	N3	119.5(3)	C37	Fe1	N7	93.43(10)
C22	C17	C18	120.7(3)	C60	Fe1	N1	87.04(10)
C22	C17	N3	119.7(3)	C60	Fe1	N4	95.78(10)
C19	C18	C17	119.4(3)	C60	Fe1	N7	76.79(10)
C18	C19	C20	121.0(3)	N1	Fe1	N4	175.45(9)
C19	C20	C23	121.4(3)	N1	Fe1	N7	107.82(9)
C21	C20	C19	118.4(3)	N4	Fe1	N7	76.36(8)
C21	C20	C23	120.2(3)	C1	N1	C9	117.4(2)
C20	C21	C22	121.2(3)	C1	N1	Fe1	114.13(18)
C17	C22	C21	119.1(3)	C9	N1	Fe1	128.37(17)
N4	C24	C25	125.4(3)	C1	N2	C15	132.1(2)
N4	C24	N5	112.2(2)	C14	N2	C1	116.0(2)
N5	C24	C25	122.2(3)	C14	N2	C15	111.3(2)

C26	C25	C24	123.2(3)	C14	N3	C16	110.9(2)
C30	C25	C24	116.9(3)	C14	N3	C17	126.8(2)
C30	C25	C26	119.6(3)	C16	N3	C17	121.9(2)
C27	C26	C25	120.1(3)	C24	N4	C32	117.3(2)
C26	C27	C28	119.9(3)	C24	N4	Fe1	112.24(18)
C29	C28	C27	121.1(3)	C32	N4	Fe1	128.10(18)
C28	C29	C30	120.9(4)	C37	N5	C24	117.1(2)
C25	C30	C29	118.3(3)	C37	N5	C38	111.5(2)
C25	C30	C31	118.9(3)	C38	N5	C24	130.4(2)
C29	C30	C31	122.8(3)	C37	N6	C39	110.8(2)
C32	C31	C30	118.9(3)	C37	N6	C40	126.6(2)
C32	C31	C36	117.9(3)	C39	N6	C40	122.4(2)
C36	C31	C30	123.1(3)	C47	N7	C55	117.6(2)
C31	C32	N4	121.6(3)	C47	N7	Fe1	107.62(17)
C33	C32	C31	119.5(3)	C55	N7	Fe1	127.48(18)
C33	C32	N4	118.9(2)	C60	N8	C47	118.3(2)
C34	C33	C32	120.8(3)	C60	N8	C61	111.7(2)
C33	C34	C35	119.9(3)	C61	N8	C47	129.6(2)
C36	C35	C34	120.2(3)	C60	N9	C62	111.3(2)
C35	C36	C31	121.5(3)	C60	N9	C63	127.6(2)
N5	C37	Fe1	114.28(19)	C62	N9	C63	121.0(2)
N6	C37	Fe1	141.4(2)	Cl2	C70	Cl1	112.0(2)
N6	C37	N5	103.8(2)	F1	P1	F3	90.30(14)
C39	C38	N5	105.9(3)	F1	P1	F4	89.76(13)
C38	C39	N6	107.9(3)	F1	P1	F5	178.78(15)
C41	C40	C45	121.1(3)	F1	P1	F6	90.26(14)
C41	C40	N6	120.3(3)	F2	P1	F1	90.33(15)
C45	C40	N6	118.6(3)	F2	P1	F3	179.37(16)
C40	C41	C42	118.9(3)	F2	P1	F4	90.48(14)
C43	C42	C41	121.4(3)	F2	P1	F5	90.38(15)
C42	C43	C44	118.2(3)	F2	P1	F6	89.77(14)
C42	C43	C46	121.1(3)	F3	P1	F4	89.51(14)
C44	C43	C46	120.8(3)	F5	P1	F3	88.99(13)
C45	C44	C43	121.1(3)	F5	P1	F4	89.24(14)
C44	C45	C40	119.3(3)	F6	P1	F3	90.24(14)
N7	C47	C48	125.2(3)	F6	P1	F4	179.74(17)
N7	C47	N8	112.0(2)	F6	P1	F5	90.73(14)
N8	C47	C48	122.6(3)	F7	P2	F9	90.32(12)
C49	C48	C47	122.6(3)	F7	P2	F10	179.32(15)
C53	C48	C47	116.9(3)	F7	P2	F11	90.15(14)
C53	C48	C49	119.8(3)	F7	P2	F12	89.46(11)
C50	C49	C48	120.0(3)	F8	P2	F7	90.63(14)

C49	C50	C51	120.1(3)	F8	P2	F9	90.53(12)
C52	C51	C50	120.9(3)	F8	P2	F10	90.05(13)
C51	C52	C53	120.8(3)	F8	P2	F11	179.22(15)
C48	C53	C54	118.9(3)	F8	P2	F12	89.87(11)
C52	C53	C48	118.4(3)	F9	P2	F12	179.54(13)
C52	C53	C54	122.7(3)	F10	P2	F9	89.76(11)
C55	C54	C53	118.3(3)	F10	P2	F12	90.46(11)
C59	C54	C53	123.8(3)	F11	P2	F9	89.44(11)
C59	C54	C55	117.9(3)	F11	P2	F10	89.17(13)
C56	C55	C54	119.8(3)	F11	P2	F12	90.16(11)
N7	C55	C54	122.0(3)				

**Table 6 Hydrogen Atom Coordinates ( $\text{\AA}\times 10^4$ ) and  
Isotropic Displacement Parameters ( $\text{\AA}^2\times 10^3$ ) for deh148.**

Atom	x	y	z	U(eq)
H3	6985.45	8662.5	1669.44	39
H4	8250.29	9108.54	1320.17	48
H5	9159.39	8550.72	752.51	45
H6	8952.46	7533.91	655.21	38
H10	6494.5	5789.87	1648.75	29
H11	7672.62	5185.84	1380.28	36
H12	8882.94	5599.36	934.21	37
H13	8930	6614.14	790.73	35
H15	5521.04	8723.59	1297.14	34
H16	3909.65	8791.66	1568.48	36
H18	2358.79	7636.65	990.43	31
H19	852.39	7388.93	1203.25	36
H21	2147.63	7658.73	3141.12	35
H22	3669.39	7893.22	2935.43	31
H23A	-130.29	7612.22	2165.06	80
H23B	507.09	7281.41	2821.67	80
H23C	154.81	6923.98	2140.94	80
H26	1663.05	5602.07	712.27	39
H27	501.3	4918.53	881.44	51
H28	381.81	4750.67	1940.95	58
H29	1457.36	5210.85	2833.39	48
H33	4827.56	6938.91	3195.32	30
H34	4776.16	6791.37	4267.66	39
H35	3615.85	6122.17	4482.11	47
H36	2435.67	5669.3	3627.71	42
H38	1678.42	6403.46	300.98	36
H39	2526.44	6883.26	-438.87	38
H41	5338.04	6450.81	-32.18	31
H42	6451.41	6977.25	-470.53	32
H44	5032.46	8512.32	-300.57	37
H45	3911.33	7991.18	128.83	33
H46A	7161.32	7877.37	-700.38	55
H46B	6858.62	8479.64	-401.74	55
H46C	6258.55	8279.61	-1134.29	55
H49	5412.13	5282.1	3792.41	35
H50	4505.6	4562.17	4168.55	45
H51	3470.85	3895.99	3428.39	53
H52	3271.22	3969.63	2313.65	45
H56	4746.71	5681.26	654.52	31

H57	3819.52	5017.88	-128.95	39
H58	2999.62	4213.77	200.43	44
H59	3180.84	4042.82	1296.22	41
H61	6887.69	5517.21	3770.08	35
H62	7801.22	6469.08	4017.63	37
H64	8564.74	7102.46	3141.29	35
H65	9276.08	8042.92	3229.77	39
H67	6612.68	8777.22	3203.7	35
H68	5890.91	7829.89	3145.95	29
H69A	9199.39	9086.02	3606.79	80
H69B	8117.32	9395.86	3470.26	80
H69C	8559.56	9246.87	2869.48	80
H70A	10877.91	4525.13	6191.19	66
H70B	10021.88	4854.01	6432.77	66

## deh148

**Table 1 Crystal data and structure refinement for deh148.**

Identification code	deh148
Empirical formula	C <sub>70</sub> H <sub>53</sub> Cl <sub>2</sub> F <sub>12</sub> FeN <sub>9</sub> P <sub>2</sub>
Formula weight	1436.90
Temperature/K	150.0
Crystal system	monoclinic
Space group	P2 <sub>1</sub> /n
a/Å	13.8409(9)
b/Å	22.4674(15)
c/Å	21.2115(14)
α/°	90
β/°	106.780(4)
γ/°	90
Volume/Å <sup>3</sup>	6315.3(7)
Z	4
ρ <sub>calc</sub> /cm <sup>3</sup>	1.511
μ/mm <sup>-1</sup>	0.462
F(000)	2936.0
Crystal size/mm <sup>3</sup>	0.1 × 0.08 × 0.07
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	4.402 to 55.11
Index ranges	-18 ≤ h ≤ 17, -29 ≤ k ≤ 26, -27 ≤ l ≤ 27
Reflections collected	132353

Independent reflections	14536 [ $R_{\text{int}} = 0.0986$ , $R_{\text{sigma}} = 0.0661$ ]
Data/restraints/parameters	14536/0/868
Goodness-of-fit on $F^2$	1.019
Final R indexes [ $I \geq 2\sigma(I)$ ]	$R_1 = 0.0560$ , $wR_2 = 0.1043$
Final R indexes [all data]	$R_1 = 0.1077$ , $wR_2 = 0.1215$
Largest diff. peak/hole / e $\text{\AA}^{-3}$	1.18/-0.99