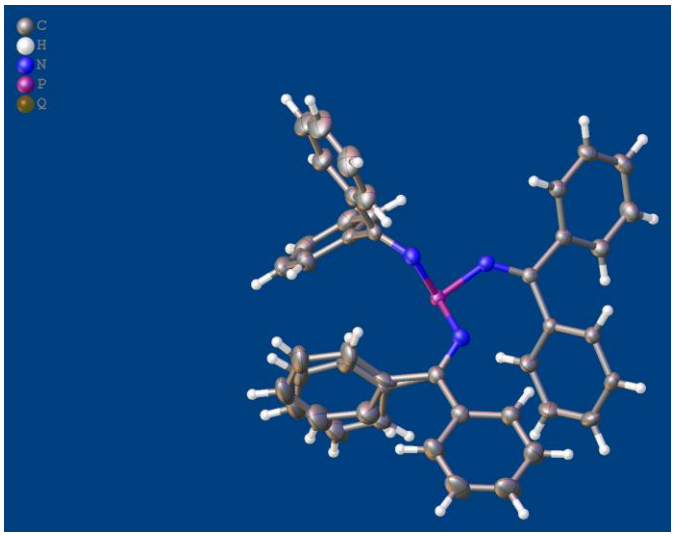
MP20_16

R_1=3.68%

Crystal Data and Experimental



Experimental. A suitable crystal 0.18×0.12×0.11 mm^3 was selected and mounted on a suitable support on a Rigaku, XtaLAB Synergy, Dualflex, HyPix diffractometer diffractometer. The crystal was kept at a steady T = 150.0(1) K during data collection. The structure was solved with the help of ShelXT [1] structure solution program using the Intrinsic Phasing solution method. The model was refined with version of the program olex2.refine using Levenberg-Marquardt minimisation [2].

Crystal Data. $C_{39}H_{30}N_3P$, M_r = 571.63, monoclinic, $P2_1/c$ (No. 14), a = 15.6467(1), b = 13.6318(1), c = 15.1950(1) Å, β = 104.357(1)°, V = 3139.76(4) Å^3, T = 150.0(1) K, Z = 4, Z' = 1, μ(CuK$_\alpha$) = 1.010, 39465 reflections measured, 6618 unique (R_{int} = 0.0345) which were used in all calculations. The final wR_2 was 0.0943 (all data) and R_1 was 0.0349 (I > 2σ(I)).

Compound	**MP20_16**
Formula	$C_{39}H_{30}N_3P$
$D_{calc.}$/ g cm^{-3}	1.209
μ/mm^{-1}	1.010
Formula Weight	571.63
Colour	Red
Shape	Block
Size/mm^3	0.18×0.12×0.11
T/K	150.0(1)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	15.6467(1)
b/Å	13.6318(1)
c/Å	15.1950(1)
α/°	90
β/°	104.357(1)
γ/°	90
V/Å^3	3139.76(4)
Z	4
Z'	1
Wavelength/Å	1.54184
Radiation type	CuK$_\alpha$
Θ$_{min}$/°	2.9
2Θ$_{max}$/°	155.0
Measured Refl.	39465
Independent Refl.	6618
Reflections with I > 2σ(I)	6378
R_{int}	0.0345
Parameters	443
Restraints	0
Largest Peak	0.201
Deepest Hole	-0.416
GooF	1.0448
wR_2 (all data)	0.0966
wR_2	0.0939
R_1 (all data)	0.0377
R_1	0.0368

Structure Quality Indicators

Reflections:	d min (Cu) 0.79	I/σ 44.9	Rint 3.45%	complete 99% (IUCr) 100%
Refinement:	Shift -0.002	Max Peak 0.3	Min Peak -0.3	GooF 1.061

Table 1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **MP20_16**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij}.

Atom	*x*	*y*	*z*	U_{eq}
P1	2310.0(2)	6400.5(2)	3459.3(2)	23.77(9)
N1	3325.6(6)	6817.5(7)	3340.8(6)	28.01(19)
N2	1714.3(5)	6868.4(6)	2462.6(6)	23.54(17)
N3	2438.3(6)	5179.5(7)	3201.7(6)	27.91(19)
C1A	3304.9(7)	8113.9(8)	4471.7(7)	28.5(2)
C2A	3636.9(9)	7987.6(10)	5405.7(8)	39.4(3)
C3A	3262.5(10)	8481.5(10)	6013.9(9)	44.1(3)
C4A	2583.3(9)	9136.1(9)	5706.4(9)	40.9(3)
C5A	2260.4(8)	9282.9(9)	4784.1(9)	40.1(3)
C6A	2610.5(8)	8760.5(9)	4166.0(8)	34.0(2)
C1	3693.2(7)	7551.8(8)	3815.1(7)	27.7(2)
C1B	4562.9(7)	7894.3(9)	3694.0(7)	33.8(2)
C2B	5056.2(8)	7301.1(12)	3258.0(9)	44.9(3)
C3B	5832.7(9)	7655.3(15)	3085.5(11)	60.9(4)
C4B	6113.4(10)	8597.1(15)	3336.6(12)	64.0(5)
C5B	5639.6(10)	9180.2(14)	3782.1(11)	58.1(4)
C6B	4866.4(8)	8832.0(11)	3966.0(9)	43.5(3)
C1C	577.3(6)	7175.7(7)	1130.3(6)	22.88(19)
C2C	1068.9(7)	7841.4(7)	758.5(7)	25.9(2)
C3C	647.9(8)	8471.2(8)	69.1(7)	31.2(2)
C4C	-265.0(8)	8451.6(9)	-245.1(8)	35.4(3)
C5C	-756.9(8)	7789.7(9)	115.5(8)	36.3(3)
C6C	-338.7(7)	7145.8(8)	795.9(7)	29.3(2)
C2	1024.4(6)	6533.9(7)	1905.0(6)	21.57(19)
C1D	586.5(6)	5569.9(7)	1973.3(6)	22.58(19)
C2D	405.7(7)	4918.0(8)	1246.9(7)	26.1(2)
C3D	-30.2(7)	4041.2(8)	1303.9(8)	32.4(2)
C4D	-298.4(8)	3819.3(9)	2082.8(9)	37.8(3)
C5D	-125.0(9)	4464.1(10)	2804.9(8)	40.7(3)
C6D	320.3(8)	5335.9(9)	2754.3(7)	33.1(2)
C1E	2636.8(7)	3493.9(8)	3637.2(7)	29.2(2)
C2E	2062.8(8)	3179.2(8)	2834.2(8)	33.4(2)
C3E	1942.5(10)	2186.4(10)	2644.4(9)	45.0(3)
C4E	2395.0(12)	1499.7(10)	3252.0(10)	52.5(4)
C5E	2967.6(12)	1799.8(10)	4044.0(10)	56.0(4)
C6E	3091.2(10)	2792.4(10)	4243.3(9)	44.1(3)
C1F	2982(5)	4846(7)	4879(5)	24.9(13)
C2F	2375(3)	4700(4)	5380(4)	37.5(9)
C3F	2584(4)	4985(3)	6281(3)	57.1(9)
C4F	3404(5)	5387(4)	6657(3)	66.1(13)
C5F	3990(4)	5546(4)	6144(4)	64.6(14)
C6F	3767(3)	5297(4)	5218(3)	45.9(10)
C3	2710.5(7)	4562.6(8)	3845.3(7)	26.9(2)
C1G	3155(7)	4856(8)	4746(7)	34.7(16)
C2G	2737(3)	4764(5)	5468(4)	52.0(12)
C3G	3118(5)	5067(4)	6352(3)	66.9(13)
C4G	3973(5)	5426(4)	6564(4)	65.4(14)
C5G	4421(3)	5492(3)	5896(3)	60.2(10)
C6G	4030(3)	5214(4)	5004(3)	44.6(9)

Table 2. Anisotropic Displacement Parameters ($\times 10^4$) **MP20_16**. The anisotropic displacement factor exponent takes the form: form: $-2\pi^2[h^2a^{*2} \times U_{11} + ... + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	26.80(14)	24.49(14)	19.97(13)	-0.75(9)	5.71(10)	-2.87(9)
N1	26.9(4)	33.9(5)	22.5(4)	1.1(3)	4.8(3)	-2.0(3)
N2	25.9(4)	22.3(4)	23.2(4)	-1.3(3)	7.6(3)	-1.2(3)
N3	31.3(4)	27.0(4)	24.7(4)	1.2(3)	5.5(3)	1.8(3)
C1A	30.1(5)	27.8(5)	27.1(5)	-0.6(4)	6.0(4)	-9.5(4)
C2A	47.3(7)	40.4(6)	28.1(6)	1.8(5)	5.2(5)	-0.9(5)
C3A	58.8(8)	47.3(7)	28.4(6)	-2.9(5)	14.6(5)	-14.1(6)
C4A	44.4(7)	38.9(6)	46.5(7)	-12.6(5)	24.7(6)	-19.3(5)
C5A	34.0(6)	35.7(6)	52.0(7)	-7.6(5)	13.4(5)	-6.9(5)
C6A	32.3(5)	34.7(6)	33.6(6)	-0.9(5)	5.7(4)	-5.4(4)
C1	25.8(5)	33.1(5)	21.9(5)	4.7(4)	1.5(4)	-2.2(4)
C1B	25.8(5)	46.5(6)	26.6(5)	4.0(5)	1.9(4)	-5.1(4)
C2B	29.9(6)	61.1(8)	43.5(7)	-4.8(6)	8.7(5)	-4.2(6)
C3B	33.0(7)	96.7(13)	56.0(9)	-10.3(9)	16.5(6)	-6.5(7)
C4B	34.0(7)	99.8(14)	59.8(9)	-3.1(9)	14.5(7)	-25.2(8)
C5B	40.6(7)	71.3(10)	62.2(9)	-2.7(8)	12.4(7)	-25.8(7)
C6B	33.6(6)	52.2(7)	43.5(7)	-1.2(6)	7.3(5)	-13.6(5)
C1C	27.7(5)	22.6(4)	19.6(4)	-2.1(3)	8.3(4)	1.4(4)
C2C	28.7(5)	26.4(5)	24.2(5)	-0.5(4)	9.7(4)	0.6(4)
C3C	39.8(6)	31.5(5)	24.8(5)	4.2(4)	13.1(4)	0.5(4)
C4C	40.7(6)	39.9(6)	25.0(5)	8.6(4)	6.8(4)	7.7(5)
C5C	29.1(5)	45.2(7)	32.7(6)	5.7(5)	4.0(4)	4.1(5)
C6C	28.1(5)	32.3(5)	28.5(5)	2.6(4)	8.8(4)	-0.1(4)
C2	24.5(4)	21.6(4)	20.6(4)	-1.8(3)	9.4(4)	0.4(3)
C1D	23.3(4)	23.6(5)	20.6(4)	1.2(4)	5.2(3)	-1.2(4)
C2D	28.8(5)	27.5(5)	21.4(5)	-0.5(4)	5.4(4)	-2.6(4)
C3D	35.1(6)	26.3(5)	31.6(5)	-2.5(4)	0.3(4)	-5.6(4)
C4D	37.5(6)	31.4(6)	40.9(6)	8.8(5)	2.8(5)	-12.7(5)
C5D	46.6(7)	47.0(7)	31.1(6)	8.5(5)	14.8(5)	-14.6(5)
C6D	41.3(6)	37.1(6)	23.4(5)	-2.4(4)	12.6(4)	-9.3(5)
C1E	31.5(5)	28.8(5)	27.7(5)	3.0(4)	8.0(4)	3.4(4)
C2E	37.6(6)	29.4(5)	31.6(5)	1.1(4)	5.5(4)	1.9(4)
C3E	60.6(8)	34.2(6)	38.0(6)	-5.7(5)	8.2(6)	-2.2(6)
C4E	87.2(11)	27.0(6)	45.8(7)	-1.6(5)	21.1(7)	6.0(6)
C5E	87.1(11)	34.3(7)	43.3(7)	9.2(6)	10.1(7)	19.7(7)
C6E	58.2(8)	36.1(6)	33.0(6)	4.1(5)	1.6(5)	10.5(6)
C1F	43(3)	23.6(14)	8(2)	2.2(14)	6(2)	-5.1(18)
C2F	54(2)	34.7(15)	25.0(15)	1.7(11)	12.9(19)	-5.2(19)
C3F	93(3)	49.7(19)	30.6(16)	1.7(12)	18(2)	0(2)
C4F	114(5)	46(2)	26(2)	0.6(15)	-5(3)	-9(3)
C5F	77(3)	59(2)	40(3)	2(2)	-20(3)	-18(2)
C6F	42(2)	52(2)	36(2)	6.4(17)	-5.0(16)	-8.7(19)
C3	25.0(5)	29.9(5)	25.3(5)	1.8(4)	5.2(4)	-0.1(4)
C1G	56(4)	31.4(16)	22(3)	9.2(16)	20.7(18)	4(2)
C2G	63(3)	55(2)	40(3)	-2.1(15)	17(3)	-11(3)
C3G	105(4)	68(3)	30(2)	-6.1(18)	21(3)	-10(3)
C4G	106(4)	50(2)	28(2)	-4.4(18)	-7(3)	-1(2)
C5G	65(2)	58(2)	42(2)	-1.7(16)	-16.2(18)	-2(2)
C6G	36(2)	59(2)	32(2)	1.1(16)	-5.9(13)	-0.9(17)

Table 3. Bond Lengths in Å for **MP20_16**.

Atom	Atom	Length/Å
P1	N2	1.6937(9)
P1	N3	1.7329(9)
P1	N1	1.7387(9)
N1	C1	1.2831(14)
N2	C2	1.2798(13)
N3	C3	1.2799(14)
C1A	C6A	1.3867(17)
C1A	C2A	1.3957(16)

Atom	Atom	Length/Å
C1A	C1	1.5009(15)
C2A	C3A	1.3851(19)
C3A	C4A	1.378(2)
C4A	C5A	1.3814(19)
C5A	C6A	1.3943(17)
C1	C1B	1.4926(15)
C1B	C6B	1.3902(19)
C1B	C2B	1.3936(19)

Atom	Atom	Length/Å
C2B	C3B	1.3915(19)
C3B	C4B	1.380(3)
C4B	C5B	1.374(3)
C5B	C6B	1.3910(18)
C1C	C2C	1.3964(14)
C1C	C6C	1.3974(15)
C1C	C2	1.4940(13)
C2C	C3C	1.3878(15)
C3C	C4C	1.3895(17)
C4C	C5C	1.3841(17)
C5C	C6C	1.3900(16)
C2	C1D	1.4974(13)
C1D	C6D	1.3889(14)
C1D	C2D	1.3904(14)
C2D	C3D	1.3893(15)
C3D	C4D	1.3837(17)
C4D	C5D	1.3794(18)
C5D	C6D	1.3893(16)
C1E	C2E	1.3914(16)
C1E	C6E	1.3941(16)
C1E	C3	1.4892(15)
C2E	C3E	1.3867(17)
C3E	C4E	1.380(2)
C4E	C5E	1.372(2)
C5E	C6E	1.390(2)
C1F	C6F	1.357(10)
C1F	C2F	1.370(7)
C1F	C3	1.570(8)
C2F	C3F	1.382(7)
C3F	C4F	1.381(7)
C4F	C5F	1.361(9)
C5F	C6F	1.405(7)
C3	C1G	1.430(11)
C1G	C6G	1.413(11)
C1G	C2G	1.416(7)
C2G	C3G	1.390(8)
C3G	C4G	1.385(10)
C4G	C5G	1.371(8)
C5G	C6G	1.394(6)

Table 4. Bond Angles in ° for **MP20_16**.

Atom	Atom	Atom	Angle/°
N2	P1	N3	103.22(4)
N2	P1	N1	95.67(4)
N3	P1	N1	97.51(4)
C1	N1	P1	119.40(8)
C2	N2	P1	130.14(7)
C3	N3	P1	119.58(8)
C6A	C1A	C2A	118.83(11)
C6A	C1A	C1	120.97(10)
C2A	C1A	C1	120.20(10)
C3A	C2A	C1A	120.40(12)
C4A	C3A	C2A	120.45(12)
C3A	C4A	C5A	119.68(12)
C4A	C5A	C6A	120.23(12)
C1A	C6A	C5A	120.33(11)
N1	C1	C1B	118.05(10)
N1	C1	C1A	124.94(9)
C1B	C1	C1A	117.00(9)
C6B	C1B	C2B	119.09(11)
C6B	C1B	C1	120.38(11)
C2B	C1B	C1	120.42(11)
C3B	C2B	C1B	120.03(14)
C4B	C3B	C2B	120.25(15)
C5B	C4B	C3B	120.06(14)
C4B	C5B	C6B	120.25(15)
C1B	C6B	C5B	120.27(14)
C2C	C1C	C6C	119.34(9)
C2C	C1C	C2	120.14(9)
C6C	C1C	C2	120.47(9)
C3C	C2C	C1C	120.10(10)
C2C	C3C	C4C	120.17(10)
C5C	C4C	C3C	120.11(10)
C4C	C5C	C6C	120.04(11)
C5C	C6C	C1C	120.22(10)
N2	C2	C1C	117.80(9)
N2	C2	C1D	126.31(9)
C1C	C2	C1D	115.83(8)
C6D	C1D	C2D	119.10(9)
C6D	C1D	C2	120.01(9)
C2D	C1D	C2	120.83(9)
C3D	C2D	C1D	120.45(10)
C4D	C3D	C2D	119.94(10)
C5D	C4D	C3D	119.97(10)
C4D	C5D	C6D	120.23(11)
C1D	C6D	C5D	120.30(10)
C2E	C1E	C6E	118.71(11)
C2E	C1E	C3	119.14(10)
C6E	C1E	C3	122.06(10)
C3E	C2E	C1E	120.53(11)
C4E	C3E	C2E	120.14(13)
C5E	C4E	C3E	119.96(13)
C4E	C5E	C6E	120.44(13)
C5E	C6E	C1E	120.22(12)
C6F	C1F	C2F	122.8(6)
C6F	C1F	C3	119.1(5)
C2F	C1F	C3	117.9(6)
C1F	C2F	C3F	118.9(5)
C4F	C3F	C2F	119.3(4)
C5F	C4F	C3F	121.0(4)
C4F	C5F	C6F	120.0(4)
C1F	C6F	C5F	117.8(5)
N3	C3	C1G	122.6(4)
N3	C3	C1E	119.14(10)
C1G	C3	C1E	118.1(4)
N3	C3	C1F	124.0(4)
C1E	C3	C1F	116.1(3)
C6G	C1G	C2G	114.6(8)
C6G	C1G	C3	124.8(6)
C2G	C1G	C3	120.5(8)
C3G	C2G	C1G	123.5(7)
C4G	C3G	C2G	119.2(5)
C5G	C4G	C3G	119.5(4)
C4G	C5G	C6G	121.3(5)
C5G	C6G	C1G	121.7(6)

Table 5. Torsion Angles in ° for **MP20_16**.

Atom	Atom	Atom	Atom	Angle/°
N2	P1	N1	C1	105.42(8)
N3	P1	N1	C1	-150.41(8)
N3	P1	N2	C2	46.40(10)
N1	P1	N2	C2	145.50(9)
N2	P1	N3	C3	-166.35(8)
N1	P1	N3	C3	95.99(9)
C6A	C1A	C2A	C3A	1.66(18)
C1	C1A	C2A	C3A	-177.96(11)
C1A	C2A	C3A	C4A	-2.87(19)
C2A	C3A	C4A	C5A	1.53(19)
C3A	C4A	C5A	C6A	0.97(18)
C2A	C1A	C6A	C5A	0.83(17)
C1	C1A	C6A	C5A	-179.55(10)
C4A	C5A	C6A	C1A	-2.16(17)
P1	N1	C1	C1B	-179.72(7)
P1	N1	C1	C1A	-1.27(14)
C6A	C1A	C1	N1	-74.16(14)
C2A	C1A	C1	N1	105.46(13)
C6A	C1A	C1	C1B	104.31(12)
C2A	C1A	C1	C1B	-76.07(13)
N1	C1	C1B	C6B	160.76(11)
C1A	C1	C1B	C6B	-17.82(15)
N1	C1	C1B	C2B	-15.38(16)
C1A	C1	C1B	C2B	166.04(11)
C6B	C1B	C2B	C3B	-1.2(2)
C1	C1B	C2B	C3B	175.03(12)
C1B	C2B	C3B	C4B	-0.6(2)
C2B	C3B	C4B	C5B	1.9(3)
C3B	C4B	C5B	C6B	-1.3(3)
C2B	C1B	C6B	C5B	1.7(2)
C1	C1B	C6B	C5B	-174.45(12)
C4B	C5B	C6B	C1B	-0.5(2)
C6C	C1C	C2C	C3C	0.54(15)
C2	C1C	C2C	C3C	-176.81(9)
C1C	C2C	C3C	C4C	0.91(16)
C2C	C3C	C4C	C5C	-1.33(18)
C3C	C4C	C5C	C6C	0.28(18)
C4C	C5C	C6C	C1C	1.19(18)
C2C	C1C	C6C	C5C	-1.59(16)
C2	C1C	C6C	C5C	175.75(10)
P1	N2	C2	C1C	172.63(7)
P1	N2	C2	C1D	-4.21(15)
C2C	C1C	C2	N2	30.87(13)
C6C	C1C	C2	N2	-146.45(10)
C2C	C1C	C2	C1D	-151.96(9)
C6C	C1C	C2	C1D	30.73(13)
N2	C2	C1D	C6D	55.27(14)
C1C	C2	C1D	C6D	-121.64(10)
N2	C2	C1D	C2D	-127.58(11)
C1C	C2	C1D	C2D	55.51(12)
C6D	C1D	C2D	C3D	-0.42(16)
C2	C1D	C2D	C3D	-177.60(9)
C1D	C2D	C3D	C4D	0.93(16)
C2D	C3D	C4D	C5D	-0.65(18)
C3D	C4D	C5D	C6D	-0.1(2)
C2D	C1D	C6D	C5D	-0.37(17)
C2	C1D	C6D	C5D	176.83(11)
C4D	C5D	C6D	C1D	0.6(2)
C6E	C1E	C2E	C3E	0.35(18)
C3	C1E	C2E	C3E	-176.40(12)
C1E	C2E	C3E	C4E	-0.2(2)
C2E	C3E	C4E	C5E	-0.2(2)

Atom	Atom	Atom	Atom	Angle/°
C3E	C4E	C5E	C6E	0.5(3)
C4E	C5E	C6E	C1E	-0.3(2)
C2E	C1E	C6E	C5E	-0.1(2)
C3	C1E	C6E	C5E	176.54(13)
C6F	C1F	C2F	C3F	-2.9(11)
C3	C1F	C2F	C3F	-177.1(5)
C1F	C2F	C3F	C4F	-1.5(8)
C2F	C3F	C4F	C5F	3.0(7)
C3F	C4F	C5F	C6F	-0.3(8)
C2F	C1F	C6F	C5F	5.6(11)
C3	C1F	C6F	C5F	179.7(5)
C4F	C5F	C6F	C1F	-3.9(9)
P1	N3	C3	C1G	-18.7(4)
P1	N3	C3	C1E	166.98(8)
P1	N3	C3	C1F	-2.7(3)
C2E	C1E	C3	N3	-18.21(16)
C6E	C1E	C3	N3	165.15(11)
C2E	C1E	C3	C1G	167.2(4)
C6E	C1E	C3	C1G	-9.4(4)
C2E	C1E	C3	C1F	152.3(3)
C6E	C1E	C3	C1F	-24.4(3)
C6F	C1F	C3	N3	-75.5(8)
C2F	C1F	C3	N3	98.9(7)
C6F	C1F	C3	C1E	114.5(6)
C2F	C1F	C3	C1E	-71.1(7)
N3	C3	C1G	C6G	-72.7(10)
C1E	C3	C1G	C6G	101.7(9)
N3	C3	C1G	C2G	109.9(8)
C1E	C3	C1G	C2G	-75.8(9)
C6G	C1G	C2G	C3G	4.7(12)
C3	C1G	C2G	C3G	-177.6(6)
C1G	C2G	C3G	C4G	-4.0(10)
C2G	C3G	C4G	C5G	1.2(8)
C3G	C4G	C5G	C6G	0.6(7)
C4G	C5G	C6G	C1G	0.2(9)
C2G	C1G	C6G	C5G	-2.7(11)
C3	C1G	C6G	C5G	179.7(6)

Table 6. Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($Å^2 \times 10^3$) for **MP20_16**.

Atom	*x*	*y*	*z*	U_{iso}
H2A	4112.38	7569.39	5621.07	47
H3A	3471.14	8370.3	6634.01	53
H4A	2343.37	9477.67	6117.79	49
H5A	1808.02	9731.65	4574.64	48
H6A	2377.09	8846.19	3545.61	41
H2B	4866.2	6668.04	3082.28	54
H3B	6163.8	7255.71	2799.92	73
H4B	6623.67	8837.46	3204.18	77
H5B	5836.7	9810.14	3961.23	70
H6B	4551.23	9227.99	4272.17	52
H2C	1679.29	7862.86	973.18	31
H3C	977.62	8907.4	-183.28	37
H4C	-545.98	8883.9	-698.4	43
H5C	-1367.66	7775.86	-97.53	44
H6C	-669.52	6693.58	1029.31	35
H2D	577.76	5069.77	719.38	31
H3D	-141.51	3603.95	819.04	39
H4D	-595.52	3235.7	2119.3	45
H5D	-306.76	4314.74	3327.52	49
H6D	440.6	5764.75	3245.66	40
H2E	1757.37	3638.31	2421.38	40

Atom	*x*	*y*	*z*	U_{iso}
H3E	1556.18	1982.86	2106.77	54
H4E	2311.83	834.19	3124.7	63
H5E	3274.93	1335.67	4449.96	67
H6E	3478.36	2989.35	4782.86	53
H2F	1832.18	4414.12	5118.01	45
H3F	2177.67	4906.99	6629.67	69
H4F	3557.04	5550.35	7270.27	79
H5F	4538.27	5820.14	6406.15	78
H6F	4145.54	5437.6	4849.13	55
H2G	2177	4486.44	5344.07	62
H3G	2802.96	5029.46	6795.19	80
H4G	4241.85	5619.99	7154.55	79
H5G	4996.78	5726.89	6040.97	72
H6G	4352.22	5265.94	4568.3	54

Table 7. Atomic Occupancies for all atoms that are not fully occupied in **MP20_16**.

Atom	Occupancy	Atom	Occupancy	Atom	Occupancy	Atom	Occupancy
C1F	0.5	H4F	0.5	C2G	0.5	C5G	0.5
C2F	0.5	C5F	0.5	H2G	0.5	H5G	0.5
H2F	0.5	H5F	0.5	C3G	0.5	C6G	0.5
C3F	0.5	C6F	0.5	H3G	0.5	H6G	0.5
H3F	0.5	H6F	0.5	C4G	0.5		
C4F	0.5	C1G	0.5	H4G	0.5		

Citations

[1] Sheldrick, G.M. (2015). Acta Cryst. A71, 3-8.

[2] Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H. (2009), J. Appl. Cryst. 42, 339-341.