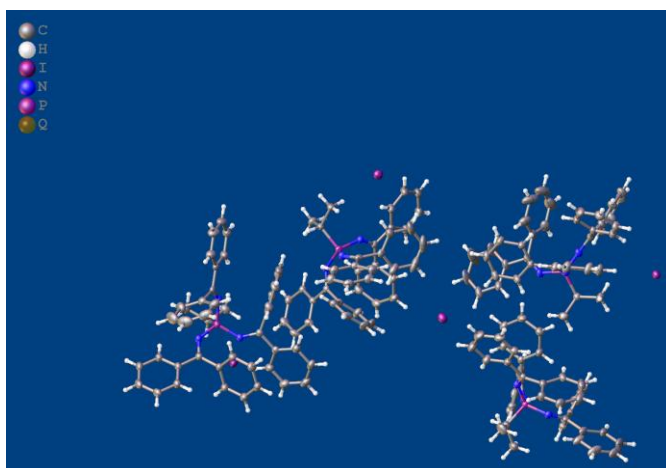


$R_1=3.54\%$

Crystal Data and Experimental



Experimental. A suitable crystal $0.19 \times 0.08 \times 0.07 \text{ mm}^3$ was selected and mounted on a suitable support on a Rigaku, XtaLAB Synergy, Dualflex, HyPix diffractometer diffractometer. The crystal was kept at a steady $T = 150.0(2) \text{ K}$ during data collection. The structure was solved with the help of ShelXT [1] structure solution program using the Intrinsic Phasing solution method and refined with ShelXL [1] refinement package using Least Squares minimisation.

Crystal Data. $\text{C}_{42}\text{H}_{37}\text{IN}_3\text{P}$, $M_r = 741.63$, triclinic, $P \bar{1}$ (No. 2), $a = 10.24441(6) \text{ \AA}$, $b = 24.65474(8) \text{ \AA}$, $c = 28.73312(8) \text{ \AA}$, $\alpha = 89.3291(2)^\circ$, $\beta = 85.1102(4)^\circ$, $\gamma = 87.9980(4)^\circ$, $V = 7226.11(5) \text{ \AA}^3$, $T = 150.0(2) \text{ K}$, $Z = 8$, $Z' = 4$, $\mu(\text{CuK}\alpha) = 7.628$, 185899 reflections measured, 30327 unique ($R_{\text{int}} = 0.0621$) which were used in all calculations. The final wR_2 was 0.0950 (all data) and R_1 was 0.0354 ($I > 2\sigma(I)$).

Compound	MP20_47
Formula	$\text{C}_{42}\text{H}_{37}\text{IN}_3\text{P}$
$D_{\text{calc.}} / \text{g cm}^{-3}$	1.363
μ / mm^{-1}	7.628
Formula Weight	741.63
Colour	Yellow
Shape	Parallelepiped
Size/ mm^3	$0.17 \times 0.12 \times 0.09$
T / K	150.0(2)
Crystal System	triclinic
Space Group	$P \bar{1}$
$a / \text{\AA}$	10.24441(6)
$b / \text{\AA}$	24.65474(8)
$c / \text{\AA}$	28.73312(8)
$\alpha / ^\circ$	89.3291(2)
$\beta / ^\circ$	85.1102(4)
$\gamma / ^\circ$	87.9980(4)
$V / \text{\AA}^3$	7226.11(5)
Z	8
Z'	4
Wavelength/ \AA	1.54184
Radiation type	$\text{CuK}\alpha$
$\Theta_{\text{min}} / ^\circ$	3.0
$2\Theta_{\text{max}} / ^\circ$	156.0
Measured Refl.	185899
Independent Refl.	30327
Reflections with $I > 2\sigma(I)$	29002
R_{int}	0.0621
Parameters	1701
Restraints	0
Largest Peak	2.057
Deepest Hole	-1.806
GooF	1.026
wR_2 (all data)	0.0950
wR_2	0.0941
R_1 (all data)	0.0366
R_1	0.0354

Structure Quality Indicators

Reflections:	d min (Cu) 0.79	I/ σ 33.8	Rint 6.21%	complete 99% (IUCr) 100%
Refinement:	Shift 0.005	Max Peak 1.1	Min Peak -1.8	Goof 1.026

Table 1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **MP20_47**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} .

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U_{eq}
I4	-158.1(2)	11494.1(2)	4491.2(2)	30.27(4)
I2	9343.1(2)	6342.3(2)	508.8(2)	34.35(4)
I3	3848.6(2)	5196.4(2)	3537.0(2)	39.10(5)
I1	4509.7(2)	272.5(2)	1454.5(2)	44.60(5)
P14	2147.7(5)	9210.2(2)	3701.2(2)	22.26(10)
P12	7604.2(5)	4148.0(2)	1259.4(2)	19.68(9)
P13	-2473.8(5)	6410.2(2)	4993.7(2)	23.14(10)
P11	3999.3(5)	1370.3(2)	-76.9(2)	24.22(10)
N12	8365.2(17)	4473.0(7)	1636.7(6)	23.5(3)
N33	-1951.9(18)	6681.9(8)	4491.4(7)	28.2(4)
N23	-1328.7(18)	6078.7(8)	5249.4(7)	25.8(4)
N24	3395.7(18)	9517.5(7)	3877.5(7)	27.4(4)
N22	6382.5(17)	4486.8(7)	1047.5(7)	24.9(4)
N32	7195.5(17)	3529.0(7)	1416.5(6)	23.1(3)
N11	4894.2(18)	1785.3(8)	-405.2(7)	27.4(4)
N21	2976.9(19)	1038.4(8)	-363.7(7)	28.7(4)
N31	3274.2(19)	1620.1(8)	404.8(7)	26.9(4)
N14	1230.7(18)	9590.1(7)	3388.3(6)	25.9(4)
N13	-3387.3(17)	6823.1(7)	5335.6(7)	25.1(4)
N34	2605.6(19)	8607.5(8)	3488.0(7)	29.1(4)
C2K	7401(2)	2437.4(9)	1679.3(7)	24.3(4)
C33	-2277(2)	7114.6(9)	4269.9(8)	25.5(4)
C22	5762(2)	4939.0(8)	1151.2(8)	24.5(4)
C42	8816(2)	4057.6(8)	773.9(7)	22.1(4)
C6H	8201(2)	3565.4(9)	2401.8(8)	26.8(4)
C1G	9400(2)	4920.9(8)	2219.3(7)	23.7(4)
C1E	2482(2)	2119.6(9)	1075.2(7)	24.7(4)
C32	6152(2)	3320.4(8)	1609.5(7)	21.2(4)
C1U	3393(2)	10429.0(9)	3506.1(8)	25.8(4)
C1N	-2284(2)	6792.4(9)	6057.7(7)	24.0(4)
C31	3261(2)	2076.5(9)	618.2(7)	23.5(4)
C6E	2145(2)	2625.4(10)	1271.6(8)	30.4(5)
C1T	129(2)	10152.4(9)	2872.4(8)	24.5(4)
C1A	5911(2)	2355.0(9)	-990.4(8)	27.6(4)
C12	8516(2)	4502.4(8)	2074.4(7)	21.5(4)
C3K	7434(2)	1882.0(9)	1751.5(8)	31.3(5)
C13	-3356(2)	6963.9(8)	5763.2(8)	23.7(4)
C1R	-3112(2)	7570.0(9)	4485.7(8)	27.2(4)
C1D	816(2)	1374.0(9)	-30.5(8)	26.3(4)
C1K	6201(2)	2732.5(8)	1721.2(7)	22.6(4)
C23	-69(2)	6048.9(9)	5203.0(7)	24.5(4)
C24	3876(2)	9991.6(9)	3819.4(8)	25.9(4)
C1L	4895(2)	3629.5(8)	1731.3(8)	24.6(4)
C1H	7925(2)	4123.6(9)	2436.2(7)	23.7(4)
C2P	1620(2)	6195.4(10)	4537.1(8)	28.6(4)
C6S	1972(2)	9422.7(9)	2174.0(8)	29.4(5)
C1I	6088(2)	5304.4(9)	1528.5(8)	27.1(4)
C1Q	-1828(2)	7157.2(10)	3765.2(8)	28.4(4)
C4J	2376(2)	5335.8(10)	434.8(9)	33.3(5)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{eq}
C14	918(2)	9655.2(8)	2968.1(7)	23.5(4)
C5J	3157(3)	4881.1(11)	303.7(9)	36.1(5)
C3D	-760(2)	1486.6(10)	633.4(9)	33.8(5)
C1S	1275(2)	9258.8(9)	2588.3(7)	24.5(4)
C6L	4101(2)	3808.6(9)	1388.3(9)	29.9(5)
C1C	1140(2)	611.6(9)	-629.3(8)	27.4(4)
C1F	4022(2)	2550.7(9)	432.9(7)	24.7(4)
C6U	2768(2)	10891.4(10)	3699.5(8)	30.3(5)
C44	1102(2)	9070.0(9)	4219.9(8)	25.9(4)
C1V	5026(2)	10110.1(9)	4077.1(9)	29.1(4)
C21	1716(2)	1015.8(9)	-335.1(8)	27.1(4)
C11	4808(2)	2020.9(8)	-804.4(7)	24.7(4)
C2N	-2347(2)	6292.4(9)	6289.5(8)	28.5(4)
C34	3655(2)	8437.4(9)	3250.6(8)	28.6(4)
C2J	3847(2)	5555.4(9)	1007.5(9)	31.0(5)
C6D	737(2)	1929.8(10)	-113.7(9)	32.5(5)
C6R	-2650(3)	7887.9(10)	4826.9(9)	33.0(5)
C52	9912(2)	3655.2(10)	898.4(9)	31.9(5)
C1O	589(2)	5633.3(9)	5487.9(8)	24.7(4)
C6T	-102(2)	10542.1(10)	3219.3(9)	33.6(5)
C3P	2332(2)	6540.4(11)	4235.0(8)	34.7(5)
C6P	630(2)	6971.7(10)	4951.3(8)	30.9(5)
C2E	2089(2)	1647.9(10)	1314.9(8)	31.7(5)
C5H	7660(2)	3214.7(10)	2740.5(9)	32.2(5)
C2U	3648(3)	10393.6(10)	3023.6(9)	34.5(5)
C1P	746(2)	6412.2(9)	4891.5(8)	24.9(4)
C6Q	-1941(2)	7646.4(10)	3522.3(9)	33.3(5)
C4C	97(3)	-139.7(10)	-1199.4(8)	34.5(5)
C2T	-420(2)	10237.3(10)	2447.7(8)	31.1(5)
C1J	4631(2)	5093.7(9)	884.8(8)	25.5(4)
C2G	9832(2)	4926.3(9)	2666.1(8)	28.6(4)
C5C	-730(3)	220.6(11)	-943.9(9)	34.9(5)
C2D	47(2)	1151.3(10)	341.7(8)	30.6(5)
C4D	-839(2)	2039.9(11)	551.0(9)	34.2(5)
C1M	-4449(2)	7313.1(9)	5975.4(9)	30.7(5)
C2O	-137(2)	5210.9(10)	5695.9(9)	31.3(5)
C2H	7101(2)	4322.4(10)	2813.7(8)	29.4(4)
C3G	10800(3)	5275.3(11)	2772.4(9)	36.2(5)
C4T	-1378(3)	11092.3(12)	2722.4(10)	43.3(6)
C6K	5054(2)	2458.4(10)	1846.6(9)	30.7(5)
C5U	2391(3)	11315.3(10)	3411.5(9)	35.8(5)
C4O	1745(3)	4887.7(10)	6078.6(8)	34.4(5)
C6G	9932(3)	5289.6(9)	1882.8(8)	32.7(5)
C5T	-840(3)	11012.5(11)	3142.8(10)	41.2(6)
C43	-3577(2)	5898.1(10)	4847.5(9)	32.7(5)
C6C	-221(2)	600.3(10)	-661.2(8)	31.7(5)
C5O	2472(2)	5301.4(10)	5871.7(8)	32.5(5)
C62	9373(2)	4600.7(9)	611.9(8)	31.1(5)
C3J	2727(2)	5672.2(10)	781.4(9)	34.5(5)
C5D	-93(3)	2261.8(10)	173.5(10)	35.8(5)
C6X	2646(3)	7540.1(10)	3158.9(9)	35.0(5)
C2S	943(2)	8716.9(9)	2648.5(8)	30.7(5)
C2C	1965(2)	243.6(10)	-889.5(9)	31.9(5)
C4P	2219(3)	7096.1(11)	4298.2(9)	36.1(5)
C2F	5306(2)	2595.1(9)	547.3(9)	30.0(5)
C5S	2340(3)	9046.7(11)	1829.7(9)	36.6(5)
C6N	-1210(2)	7117.1(10)	6093.7(9)	32.6(5)
C2A	7034(3)	2378.9(10)	-746.8(9)	34.3(5)
C3S	1305(3)	8344.7(10)	2300.2(9)	36.2(5)
C4K	6281(3)	1610.1(10)	1861.4(9)	35.9(5)
C6O	1906(2)	5670.7(9)	5574.5(8)	28.7(4)
C3H	6545(2)	3965.3(11)	3145.3(8)	34.8(5)
C6J	4282(2)	4763.4(10)	527.0(9)	32.2(5)
C5L	2949(2)	4106.5(11)	1514.8(12)	41.6(6)
C1W	4805(2)	8777.7(10)	3115.7(10)	33.7(5)

Atom	x	y	z	U_{eq}
C3T	-1169(3)	10704.9(12)	2377.2(9)	40.9(6)
C4I	5169(2)	868.4(9)	113.5(9)	29.4(5)
C4R	-4721(3)	8380.8(11)	4914.9(11)	45.8(7)
C4H	6835(3)	3415.2(11)	3112.1(9)	35.1(5)
C6A	5878(3)	2638.0(11)	-1413.7(10)	38.2(5)
C2V	5713(2)	10585.0(10)	3983.7(10)	35.3(5)
C1X	3734(3)	7862.6(10)	3097.6(10)	35.9(5)
C4U	2669(3)	11282.2(11)	2933.6(10)	39.1(6)
C3C	1446(3)	-128.1(10)	-1173.0(9)	35.2(5)
C1B	3673(2)	1974.1(10)	-1092.8(8)	31.4(5)
C5E	1413(2)	2661.5(12)	1699.4(9)	38.4(6)
C5Q	-1567(3)	7669.7(12)	3044.2(10)	41.5(6)
C3N	-1327(3)	6114.0(11)	6545.6(9)	37.2(5)
C2I	5554(3)	5232.7(12)	1984.1(9)	45.7(7)
C5F	4241(3)	3349.6(10)	-49.2(10)	40.9(6)
C5P	1380(3)	7314.1(10)	4657.8(9)	36.5(5)
C2Q	-1323(3)	6696.7(11)	3525.4(9)	39.3(6)
C3U	3290(3)	10823.1(12)	2737.6(9)	41.5(6)
C3O	444(3)	4838.7(10)	5986.6(9)	36.2(5)
C2L	4523(3)	3734.3(13)	2198.5(10)	42.9(6)
C4S	2004(3)	8508.6(11)	1889.5(9)	37.6(5)
C3V	6828(3)	10677.6(11)	4210.1(11)	40.1(6)
C6F	3480(3)	2932.1(10)	135.8(9)	33.7(5)
C4V	7270(3)	10302.6(11)	4524.2(11)	41.5(6)
C4F	5525(3)	3389.7(10)	57.1(10)	39.6(6)
C3E	1368(3)	1685.5(12)	1744.8(9)	40.5(6)
C54	-48(3)	8728.0(12)	4106.2(10)	40.6(6)
C2R	-4377(3)	7666.4(11)	4348.2(10)	37.3(5)
C64	625(3)	9598.3(11)	4459.9(9)	38.0(6)
C5R	-3452(3)	8294.9(10)	5035.1(10)	42.8(6)
C4G	11330(3)	5625.1(11)	2435.7(10)	41.5(6)
C5I	6095(3)	1124.5(10)	430.9(10)	36.8(5)
C4E	1024(3)	2192.5(13)	1935.8(9)	42.5(6)
C3F	6056(3)	3016.2(10)	357.8(10)	37.0(5)
C4N	-249(3)	6428.6(13)	6576.6(10)	42.8(6)
C5G	10882(3)	5639.1(11)	1993.9(10)	41.8(6)
C6V	5479(3)	9735.4(11)	4398.1(10)	41.7(6)
C5K	5096(3)	1898.6(10)	1913.8(10)	37.3(6)
C3A	8092(3)	2674.1(11)	-921.0(10)	41.4(6)
C2B	2793(3)	2415.2(13)	-1115.4(10)	42.3(6)
C4Q	-1086(3)	7212.7(14)	2812.3(10)	47.2(7)
C3R	-5182(3)	8066.7(11)	4568.3(12)	45.1(6)
C5N	-193(3)	6927.3(13)	6352.9(10)	43.5(6)
C6I	5921(3)	593.9(11)	-305.5(11)	41.5(6)
C4L	2601(3)	4223.4(13)	1975.9(14)	53.3(8)
C63	-4268(3)	5662.7(12)	5296.7(11)	45.4(6)
C2M	-5573(3)	7402.0(12)	5743.0(10)	43.1(6)
C6I	6914(3)	5727.9(11)	1417.9(11)	42.0(6)
C6W	5716(3)	8875.8(12)	3431.4(13)	46.9(7)
C4A	8042(3)	2953.2(11)	-1339.8(11)	45.3(7)
C6M	-4368(3)	7552.3(11)	6408.1(11)	43.7(6)
C5A	6947(3)	2935.9(12)	-1583.8(11)	48.7(7)
C5V	6600(3)	9829.1(12)	4619.4(11)	48.0(7)
C5X	2746(3)	6993.0(11)	3045.8(11)	45.6(6)
C6B	3501(3)	1502.5(13)	-1336.0(10)	44.7(6)
C53	-4558(3)	6114.2(14)	4512.8(12)	52.1(8)
C3L	3383(3)	4040.7(16)	2319.9(13)	59.2(9)
C2W	4946(3)	8998.8(14)	2665.9(12)	53.3(8)
C3M	-6600(3)	7728.8(14)	5939.6(13)	59.3(10)
C5M	-5393(4)	7882.3(12)	6599.5(14)	59.4(9)
C3Q	-961(3)	6723.7(13)	3051.1(10)	48.8(7)
C3B	1714(3)	2384.7(18)	-1370.2(12)	59.3(9)
C4I	6724(4)	5986.5(17)	2222.9(15)	71.9(13)
C3I	5878(4)	5576.8(17)	2330.2(11)	65.6(11)
C4B	1522(4)	1922(2)	-1602.3(13)	68.9(11)

Atom	x	y	z	U_{eq}
C4M	-6494(4)	7966.6(13)	6367.6(14)	64.0(11)
C5W	6758(3)	9210.6(17)	3291(2)	74.9(13)
C5B	2409(4)	1478.1(19)	-1592.2(13)	69.8(11)
C5I	7235(4)	6067.1(14)	1768.7(16)	63.9(10)
C2X	4913(3)	7642.9(15)	2900(2)	83.9(16)
C3W	5971(4)	9335.9(18)	2539.5(19)	80.0(14)
C4W	6866(4)	9435.3(17)	2849(2)	87.4(17)
C4X	3933(4)	6771.8(14)	2870.7(19)	78.5(14)
C3X	5006(4)	7095.4(19)	2788(3)	123(3)

Table 2. Anisotropic Displacement Parameters ($\times 10^4$) **MP20_47**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2} \times U_{11} + \dots + 2hka^* \times b^* \times U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
I4	33.61(8)	26.75(7)	31.01(7)	-1.46(5)	-4.37(5)	-4.73(5)
I2	32.02(8)	28.95(8)	41.60(8)	1.71(6)	-3.14(6)	5.27(6)
I3	44.21(9)	30.86(8)	43.31(9)	-0.12(6)	-8.98(7)	-3.96(6)
I1	55.29(11)	36.30(9)	39.86(9)	-8.08(7)	14.15(7)	-10.16(7)
P14	24.0(2)	16.6(2)	26.3(2)	-2.24(19)	-3.85(19)	1.17(18)
P12	19.2(2)	17.0(2)	22.7(2)	1.31(18)	-1.97(17)	1.69(17)
P13	21.9(2)	23.5(2)	23.9(2)	-1.58(19)	-2.26(18)	3.12(19)
P11	26.4(2)	20.9(2)	25.4(2)	-2.32(19)	-1.15(19)	-2.49(19)
N12	25.0(8)	22.7(8)	22.6(8)	-0.8(7)	-2.3(6)	1.5(7)
N33	25.9(9)	31.6(10)	26.7(9)	0.2(7)	-1.9(7)	4.6(7)
N23	24.7(9)	24.9(9)	27.1(9)	-0.2(7)	-0.6(7)	4.2(7)
N24	26.2(9)	20.7(9)	35.6(10)	-3.2(7)	-5.0(7)	0.7(7)
N22	21.9(8)	20.7(8)	32.3(9)	1.1(7)	-4.7(7)	2.5(6)
N32	22.6(8)	19.6(8)	26.8(9)	1.9(7)	-2.2(7)	1.7(6)
N11	29.1(9)	24.5(9)	28.4(9)	-0.6(7)	-1.0(7)	-1.0(7)
N21	28.5(9)	27.8(9)	29.9(9)	-5.2(7)	-1.9(7)	-2.6(7)
N31	29.8(9)	24.7(9)	26.5(9)	-1.4(7)	-2.3(7)	-4.0(7)
N14	29.3(9)	23.1(9)	25.5(9)	-0.6(7)	-3.5(7)	1.1(7)
N13	21.4(8)	24.5(9)	28.8(9)	0.2(7)	-0.8(7)	3.9(7)
N34	30.0(9)	20.3(9)	37.0(10)	-5.7(8)	-3.6(8)	2.4(7)
C2K	26.1(10)	22.2(10)	24.4(10)	0.5(8)	-2.0(8)	0.6(8)
C33	22.9(10)	26.7(10)	27.5(10)	-1.6(8)	-4.6(8)	-2.3(8)
C22	23.4(10)	20.3(10)	28.9(10)	6.5(8)	1.6(8)	0.7(7)
C42	22.9(9)	21.2(10)	22.2(9)	-0.1(7)	-2.3(7)	-0.2(7)
C6H	32.7(11)	24.0(10)	24.2(10)	1.4(8)	-6.4(8)	3.6(8)
C1G	25.3(10)	19.2(9)	26.4(10)	-2.6(8)	-2.6(8)	3.6(8)
C1E	20.9(9)	29.5(11)	24.5(10)	-0.7(8)	-6.2(8)	0.6(8)
C32	22.2(9)	21.5(10)	20.2(9)	0.4(7)	-4.3(7)	-0.5(7)
C1U	26.8(10)	21.6(10)	29.6(11)	-2.4(8)	-4.3(8)	-2.5(8)
C1N	28.3(10)	20.5(10)	22.7(9)	-3.6(8)	0.4(8)	-0.2(8)
C31	22.6(9)	23.2(10)	25.3(10)	0.3(8)	-5.9(8)	1.1(8)
C6E	26.6(10)	33.5(12)	30.9(11)	-2.9(9)	-3.2(9)	3.5(9)
C1T	23.2(9)	23.5(10)	26.6(10)	1.9(8)	-0.6(8)	0.1(8)
C1A	33.0(11)	20.4(10)	28.3(11)	-2.8(8)	3.6(8)	1.6(8)
C12	22.5(9)	18.8(9)	22.6(9)	-0.1(7)	-0.4(7)	5.5(7)
C3K	37.2(12)	23.6(11)	32.8(11)	1.2(9)	-3.4(9)	5.1(9)
C13	24.9(10)	16.6(9)	28.6(10)	2.4(8)	3.4(8)	-1.2(7)
C1R	32.1(11)	21.1(10)	28.0(10)	-0.6(8)	-0.9(8)	-1.5(8)
C1D	25.6(10)	25.9(11)	27.8(10)	-2.7(8)	-3.3(8)	-1.5(8)
C1K	23.8(10)	21.1(10)	23.3(9)	2.6(8)	-4.4(7)	-1.9(8)
C23	26.0(10)	22.0(10)	25.1(10)	-4.8(8)	-1.9(8)	4.8(8)
C24	26.2(10)	20.3(10)	30.8(11)	-4.2(8)	-0.3(8)	0.4(8)
C1L	21.6(9)	19.4(9)	32.4(11)	-0.4(8)	-0.5(8)	-0.3(7)
C1H	25.0(10)	24.1(10)	22.4(9)	1.8(8)	-3.8(8)	0.4(8)
C2P	28.0(10)	28.5(11)	29.0(11)	-2.4(9)	-3.4(8)	4.4(8)
C6S	30.9(11)	24.0(10)	32.0(11)	1.7(9)	2.7(9)	1.7(8)
C1I	29.9(11)	21.6(10)	28.8(11)	0.6(8)	-1.6(8)	10.5(8)
C1Q	25.2(10)	32.0(12)	28.1(11)	0.8(9)	-3.3(8)	-0.6(8)
C4J	24.7(10)	36.1(12)	38.8(12)	11.1(10)	-4.0(9)	4.7(9)
C14	24.5(10)	20.2(10)	25.7(10)	2.4(8)	-1.0(8)	-4.6(8)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C5J	35.1(12)	38.0(13)	35.4(12)	3.3(10)	-7.7(10)	4.8(10)
C3D	35.9(12)	36.0(13)	29.0(11)	-1.9(10)	2.0(9)	-3.2(10)
C1S	26.6(10)	22.4(10)	24.5(10)	-0.6(8)	-3.2(8)	1.0(8)
C6L	23.0(10)	25.6(11)	41.3(13)	3.5(9)	-4.2(9)	-1.7(8)
C1C	30.3(11)	25.1(10)	27.4(10)	-1.6(8)	-4.2(8)	-3.1(8)
C1F	29.5(10)	21.5(10)	23.0(9)	-4.4(8)	-2.1(8)	-0.1(8)
C6U	34.0(11)	28.5(11)	28.1(11)	-3.2(9)	-2.9(9)	3.7(9)
C44	28.0(10)	24.9(10)	25.2(10)	1.5(8)	-5.2(8)	0.7(8)
C1V	29.2(11)	22.2(10)	36.6(12)	-2.3(9)	-5.6(9)	-1.6(8)
C21	29.5(11)	24.8(10)	27.0(10)	-0.9(8)	-1.7(8)	-2.7(8)
C11	30.1(10)	19.2(9)	23.8(10)	-4.9(8)	1.1(8)	4.7(8)
C2N	30.8(11)	25.3(11)	29.7(11)	2.9(9)	-2.9(9)	-3.0(8)
C34	29.4(11)	23.1(10)	34.0(11)	-4.4(9)	-9.1(9)	7.0(8)
C2J	30.6(11)	24.0(11)	37.8(12)	3.4(9)	-2.9(9)	6.2(9)
C6D	34.8(12)	27.9(11)	34.1(12)	3.6(9)	1.3(9)	-1.8(9)
C6R	42.7(13)	24.9(11)	32.4(12)	1.5(9)	-6.2(10)	-6.5(9)
C52	26.0(10)	34.2(12)	34.0(12)	1.6(9)	2.2(9)	7.8(9)
C1O	27.2(10)	20.7(10)	25.7(10)	-3.3(8)	-1.1(8)	4.8(8)
C6T	34.5(12)	35.3(13)	31.2(11)	-5.0(10)	-7.8(9)	8.5(10)
C3P	31.7(12)	44.4(14)	27.0(11)	-1.5(10)	2.9(9)	2.2(10)
C6P	32.1(11)	26.7(11)	32.7(11)	-2.1(9)	1.5(9)	4.1(9)
C2E	32.3(11)	33.7(12)	29.8(11)	2.7(9)	-4.8(9)	-5.2(9)
C5H	41.1(13)	24.2(11)	32.8(11)	5.8(9)	-11.3(10)	-3.0(9)
C2U	43.3(13)	27.3(11)	31.7(12)	-5.5(9)	5.4(10)	-2.9(10)
C1P	22.2(9)	25.1(10)	27.5(10)	-0.5(8)	-3.4(8)	3.2(8)
C6Q	31.7(11)	33.4(12)	34.9(12)	3.3(10)	-3.9(9)	-2.3(9)
C4C	47.4(14)	33.2(12)	24.3(10)	-2.2(9)	-8.0(10)	-11.2(10)
C2T	38.2(12)	29.8(11)	24.4(10)	0.4(9)	-1.2(9)	6.8(9)
C1J	22.4(10)	23.2(10)	30.0(10)	7.3(8)	-0.6(8)	2.5(8)
C2G	32.1(11)	27.1(11)	26.7(10)	-1.7(8)	-3.4(8)	1.5(9)
C5C	35.7(12)	38.3(13)	32.4(12)	-0.5(10)	-10.2(10)	-8.3(10)
C2D	35.3(12)	25.5(11)	30.5(11)	-0.1(9)	0.6(9)	-2.4(9)
C4D	32.4(12)	35.7(13)	34.3(12)	-7.2(10)	-2.4(9)	5.1(9)
C1M	34.9(12)	18.1(10)	36.3(12)	4.0(9)	10.9(9)	5.8(8)
C2O	29.2(11)	27.7(11)	36.3(12)	2.1(9)	-1.2(9)	2.6(9)
C2H	32.1(11)	29.2(11)	26.5(10)	-3.0(9)	0.7(9)	0.1(9)
C3G	37.9(13)	35.8(13)	36.2(12)	-8.2(10)	-9.2(10)	-3.0(10)
C4T	51.7(16)	41.3(15)	35.0(13)	-0.1(11)	-3.3(11)	24.3(12)
C6K	24.0(10)	29.5(11)	39.6(12)	8.1(9)	-7.9(9)	-3.9(8)
C5U	41.1(13)	26.3(11)	39.3(13)	-1.3(10)	-3.1(10)	7.1(10)
C4O	44.1(13)	30.7(12)	27.8(11)	-0.7(9)	-4.9(10)	13.5(10)
C6G	45.8(13)	23.7(11)	28.4(11)	-0.1(9)	-2.1(10)	-3.3(9)
C5T	46.1(14)	38.7(14)	37.9(13)	-11.8(11)	-5.1(11)	17.7(11)
C43	33.5(12)	30.8(12)	34.5(12)	-6.4(9)	-4.9(9)	-1.9(9)
C6C	32.7(12)	31.4(12)	31.5(11)	-3.9(9)	-4.6(9)	-0.9(9)
C5O	31.5(11)	35.9(12)	30.4(11)	-3.9(9)	-6.7(9)	8.8(9)
C62	35.5(12)	27.0(11)	30.1(11)	2.0(9)	3.0(9)	-7.6(9)
C3J	31.2(11)	28.0(12)	43.1(13)	7.1(10)	-2.5(10)	11.4(9)
C5D	38.5(13)	25.4(11)	42.9(13)	0.6(10)	-2.8(10)	4.3(9)
C6X	47.2(14)	25.8(11)	31.8(12)	-3.8(9)	-4.1(10)	2.3(10)
C2S	41.4(12)	25.4(11)	26.7(11)	1.3(9)	-8.2(9)	-7.4(9)
C2C	33.7(12)	29.3(11)	32.9(11)	-5.1(9)	-2.2(9)	-2.2(9)
C4P	36.3(12)	38.3(13)	33.3(12)	6.2(10)	-0.2(10)	-7.5(10)
C2F	32.2(11)	24.2(11)	34.3(11)	-3.5(9)	-4.9(9)	-3.2(9)
C5S	37.3(13)	39.0(13)	31.8(12)	-3.4(10)	2.7(10)	7.0(10)
C6N	35.8(12)	30.0(12)	32.2(11)	-1.6(9)	-1.1(9)	-8.5(9)
C2A	41.1(13)	30.7(12)	31.0(11)	-2.2(9)	0.2(10)	-5.7(10)
C3S	51.1(15)	24.1(11)	35.7(12)	-3.4(9)	-16.0(11)	-3.8(10)
C4K	45.3(14)	20.7(11)	43.1(13)	7.2(10)	-11.8(11)	-3.5(9)
C6O	27.9(11)	28.2(11)	29.5(11)	-2.6(9)	-1.8(8)	4.4(8)
C3H	34.5(12)	44.0(14)	25.5(11)	0.0(10)	1.8(9)	-5.3(10)
C6J	32.1(11)	29.3(11)	34.6(12)	3.3(9)	-3.4(9)	7.7(9)
C5L	21.1(11)	31.6(13)	71.5(19)	8.7(12)	-3.0(11)	3.4(9)
C1W	25.9(11)	25.7(11)	48.9(14)	-8.8(10)	-3.0(10)	9.0(9)
C3T	50.2(15)	44.1(15)	27.3(11)	2.3(10)	-5.4(10)	18.8(12)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C4I	30.8(11)	21.7(10)	36.0(12)	1.7(9)	-4.7(9)	-2.8(8)
C4R	62.4(18)	23.7(12)	47.1(15)	0.8(11)	14.8(13)	8.9(11)
C4H	40.5(13)	37.7(13)	28.1(11)	8.3(10)	-5.9(9)	-10.8(10)
C6A	39.0(13)	35.1(13)	39.4(13)	7.7(11)	1.1(10)	3.0(10)
C2V	31.8(12)	26.5(11)	48.6(14)	2.4(10)	-8.5(10)	-2.9(9)
C1X	35.5(12)	26.2(12)	46.8(14)	-12.0(10)	-11.8(10)	8.8(9)
C4U	47.3(14)	31.8(13)	38.7(13)	10.3(10)	-7.1(11)	-3.1(11)
C3C	45.7(14)	30.6(12)	29.5(11)	-6.6(9)	-1.3(10)	-4.4(10)
C1B	31.2(11)	37.8(13)	24.8(10)	2.4(9)	-1.0(9)	-1.5(9)
C5E	32.8(12)	46.1(15)	35.3(13)	-7.9(11)	-1.1(10)	11.1(10)
C5Q	39.8(13)	46.5(15)	38.1(14)	14.2(12)	-2.7(11)	-6.4(11)
C3N	41.4(13)	38.9(13)	31.6(12)	7.5(10)	-7.9(10)	1.7(10)
C2I	60.0(17)	42.1(15)	31.1(13)	4.5(11)	10.1(12)	17.6(13)
C5F	59.7(17)	23.9(12)	39.1(13)	4.6(10)	-4.7(12)	-1.3(11)
C5P	40.4(13)	28.0(12)	40.7(13)	1.4(10)	-1.2(10)	-3.1(10)
C2Q	45.2(14)	38.6(14)	32.6(12)	0.8(10)	2.8(10)	5.2(11)
C3U	55.1(16)	40.9(14)	27.7(12)	2.5(10)	3.0(11)	-9.0(12)
C3O	41.1(13)	27.6(12)	38.5(13)	5.0(10)	1.4(10)	3.7(10)
C2L	34.1(13)	58.7(17)	34.7(13)	-7.5(12)	2.5(10)	6.9(12)
C4S	46.1(14)	32.5(12)	34.7(12)	-10.8(10)	-8.5(10)	7.8(10)
C3V	30.3(12)	32.7(13)	59.2(17)	-1.8(12)	-10.8(11)	-8.2(10)
C6F	39.4(13)	25.4(11)	37.0(12)	3.0(9)	-8.5(10)	-0.2(9)
C4V	33.8(13)	40.6(14)	52.3(16)	-7.1(12)	-15.2(11)	-1.8(10)
C4F	51.0(15)	22.8(11)	42.9(14)	-5.0(10)	11.6(11)	-9.2(10)
C3E	38.2(13)	50.1(16)	32.6(12)	7.2(11)	0.5(10)	-4.6(11)
C54	36.3(13)	50.3(16)	36.0(13)	2.0(11)	-3.1(10)	-15.0(11)
C2R	33.2(12)	32.1(12)	46.9(14)	-8.5(11)	-6.2(10)	3.5(10)
C64	49.0(15)	32.8(13)	29.9(12)	-1.3(10)	5.5(10)	9.7(11)
C5R	68.9(19)	23.8(12)	35.4(13)	-3.2(10)	0.5(12)	-6.3(11)
C4G	43.6(14)	32.6(13)	48.8(15)	-12.5(11)	-1.5(11)	-10.7(11)
C51	37.2(13)	31.5(12)	43.3(14)	4.2(10)	-12.7(10)	-2.0(10)
C4E	33.1(12)	63.9(18)	29.2(12)	-0.4(12)	2.9(10)	5.0(12)
C3F	33.3(12)	27.4(12)	50.0(15)	-9.4(10)	2.3(10)	-7.2(9)
C4N	37.2(13)	56.1(17)	36.9(13)	2.5(12)	-14.2(11)	-2.3(12)
C5G	56.4(16)	28.8(12)	40.0(14)	-3.3(10)	3.1(12)	-14.5(11)
C6V	46.8(15)	32.5(13)	49.0(15)	5.4(11)	-19.2(12)	-10.9(11)
C5K	34.2(12)	30.1(12)	49.4(15)	12.3(11)	-10.6(11)	-11.7(10)
C3A	41.9(14)	36.8(14)	45.6(15)	-3.6(11)	-0.4(11)	-10.7(11)
C2B	36.1(13)	52.8(16)	36.8(13)	5.7(12)	-0.9(10)	8.4(11)
C4Q	47.7(15)	64.3(19)	28.1(12)	5.5(12)	5.8(11)	-5.0(13)
C3R	36.3(13)	36.1(14)	61.0(18)	-2.1(13)	2.1(12)	9.7(11)
C5N	36.7(13)	52.3(16)	43.4(14)	-2.9(12)	-9.0(11)	-14.3(12)
C61	39.8(14)	32.0(13)	52.0(16)	-10.3(11)	-2.0(11)	7.0(10)
C4L	28.5(13)	42.6(16)	85(2)	-7.2(15)	12.2(14)	10.7(11)
C63	45.8(15)	43.2(15)	47.9(16)	-4.6(12)	-0.4(12)	-17.2(12)
C2M	38.6(13)	46.5(15)	40.4(14)	15.6(12)	8.8(11)	17.9(11)
C6I	43.2(14)	33.1(13)	49.3(15)	-6.2(11)	0.3(12)	-4.9(11)
C6W	30.3(13)	43.7(15)	67.7(19)	-14.6(14)	-10.2(12)	6.5(11)
C4A	45.0(15)	30.2(13)	57.8(17)	5.7(12)	13.2(13)	-5.9(11)
C6M	44.0(14)	28.4(12)	55.7(17)	-13.1(11)	14.8(12)	-2.8(11)
C5A	52.8(17)	37.6(14)	52.8(17)	18.3(13)	8.7(13)	0.9(12)
C5V	52.5(16)	40.9(15)	54.8(17)	6.2(13)	-27.8(14)	-6.3(12)
C5X	65.3(18)	26.2(12)	46.7(15)	-7.3(11)	-12.3(13)	-1.2(12)
C6B	55.4(17)	46.9(16)	33.6(13)	-2.8(11)	-10.5(12)	-8.3(13)
C53	51.3(17)	51.8(17)	58.1(18)	-2.7(14)	-28.5(14)	-13.1(13)
C3L	43.9(16)	73(2)	56.8(19)	-20.4(17)	16.1(14)	10.8(15)
C2W	39.7(15)	58.2(19)	58.1(18)	9.2(15)	10.2(13)	16.7(13)
C3M	48.6(17)	56.2(19)	66(2)	27.8(16)	18.0(15)	30.4(15)
C5M	64(2)	33.2(15)	75(2)	-20.6(15)	29.0(18)	0.8(14)
C3Q	57.3(17)	51.0(17)	35.4(14)	-3.0(12)	8.3(12)	6.7(14)
C3B	38.1(15)	89(3)	50.3(18)	19.7(18)	-7.3(13)	7.6(16)
C4I	82(3)	64(2)	72(2)	-44(2)	-32(2)	38(2)
C3I	91(3)	70(2)	32.4(14)	-12.5(15)	-4.5(15)	48(2)
C4B	50.4(19)	106(3)	54(2)	23(2)	-25.6(16)	-16(2)
C4M	67(2)	32.7(15)	83(3)	6.3(15)	36.7(19)	22.1(14)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C5W	30.0(15)	65(2)	131(4)	-32(3)	-12.3(19)	0.2(15)
C5B	86(3)	85(3)	44.0(18)	-0.8(17)	-24.2(18)	-33(2)
C5I	62(2)	42.8(17)	89(3)	-35.0(18)	-14.1(18)	2.8(15)
C2X	36.7(16)	44.7(19)	170(5)	-52(2)	-10(2)	12.0(14)
C3W	47(2)	73(3)	112(4)	33(2)	31(2)	15.9(18)
C4W	43(2)	54(2)	157(5)	8(3)	32(3)	-2.5(16)
C4X	70(2)	32.0(16)	136(4)	-42(2)	-31(2)	17.6(16)
C3X	49(2)	63(3)	258(8)	-93(4)	-12(3)	19.9(19)

Table 3. Bond Lengths in Å for **MP20_47**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
P14	N14	1.6222(19)	C31	C1F	1.495(3)
P14	N24	1.6286(19)	C6E	C5E	1.386(3)
P14	N34	1.6514(19)	C1T	C6T	1.393(3)
P14	C44	1.797(2)	C1T	C2T	1.397(3)
P12	N12	1.6230(19)	C1T	C14	1.481(3)
P12	N22	1.6371(18)	C1A	C6A	1.397(3)
P12	N32	1.6445(18)	C1A	C2A	1.401(4)
P12	C42	1.797(2)	C1A	C11	1.481(3)
P13	N23	1.6277(19)	C12	C1H	1.493(3)
P13	N13	1.6362(19)	C3K	C4K	1.389(4)
P13	N33	1.640(2)	C13	C1M	1.482(3)
P13	C43	1.801(2)	C1R	C6R	1.387(3)
P11	N31	1.631(2)	C1R	C2R	1.399(3)
P11	N21	1.634(2)	C1D	C6D	1.389(3)
P11	N11	1.6347(19)	C1D	C2D	1.392(3)
P11	C41	1.805(2)	C1D	C2I	1.490(3)
N12	C12	1.283(3)	C1K	C6K	1.395(3)
N33	C33	1.284(3)	C23	C1O	1.483(3)
N23	C23	1.286(3)	C23	C1P	1.485(3)
N24	C24	1.287(3)	C24	C1V	1.484(3)
N22	C22	1.289(3)	C1L	C2L	1.389(3)
N32	C32	1.283(3)	C1L	C6L	1.389(3)
N11	C11	1.288(3)	C1H	C2H	1.399(3)
N21	C21	1.290(3)	C2P	C3P	1.388(3)
N31	C31	1.287(3)	C2P	C1P	1.396(3)
N14	C14	1.282(3)	C6S	C5S	1.383(3)
N13	C13	1.284(3)	C6S	C1S	1.398(3)
N34	C34	1.283(3)	C1I	C6I	1.384(4)
C2K	C3K	1.382(3)	C1I	C2I	1.387(3)
C2K	C1K	1.403(3)	C1Q	C6Q	1.393(3)
C33	C1Q	1.487(3)	C1Q	C2Q	1.396(4)
C33	C1R	1.495(3)	C4J	C3J	1.382(4)
C22	C1J	1.479(3)	C4J	C5J	1.391(4)
C22	C1I	1.484(3)	C14	C1S	1.487(3)
C42	C62	1.526(3)	C5J	C6J	1.387(3)
C42	C52	1.535(3)	C3D	C4D	1.383(4)
C6H	C5H	1.387(3)	C3D	C2D	1.385(3)
C6H	C1H	1.398(3)	C1S	C2S	1.396(3)
C1G	C2G	1.393(3)	C6L	C5L	1.392(3)
C1G	C6G	1.408(3)	C1C	C2C	1.397(3)
C1G	C12	1.482(3)	C1C	C6C	1.407(3)
C1E	C6E	1.395(3)	C1C	C2I	1.484(3)
C1E	C2E	1.399(3)	C1F	C2F	1.391(3)
C1E	C31	1.480(3)	C1F	C6F	1.395(3)
C32	C1K	1.481(3)	C6U	C5U	1.390(3)
C32	C1L	1.491(3)	C44	C64	1.526(3)
C1U	C6U	1.386(3)	C44	C54	1.532(3)
C1U	C2U	1.392(3)	C1V	C6V	1.394(4)
C1U	C24	1.495(3)	C1V	C2V	1.398(3)
C1N	C6N	1.394(3)	C11	C1B	1.493(3)
C1N	C2N	1.395(3)	C2N	C3N	1.384(3)
C1N	C13	1.489(3)	C34	C1X	1.486(3)

Atom	Atom	Length/Å
C34	C1W	1.492(3)
C2J	C3J	1.387(3)
C2J	C1J	1.401(3)
C6D	C5D	1.386(4)
C6R	C5R	1.383(4)
C1O	C6O	1.399(3)
C1O	C2O	1.400(3)
C6T	C5T	1.388(4)
C3P	C4P	1.384(4)
C6P	C5P	1.390(3)
C6P	C1P	1.392(3)
C2E	C3E	1.387(4)
C5H	C4H	1.388(4)
C2U	C3U	1.391(4)
C6Q	C5Q	1.395(4)
C4C	C5C	1.380(4)
C4C	C3C	1.391(4)
C2T	C3T	1.385(3)
C1J	C6J	1.397(4)
C2G	C3G	1.391(3)
C5C	C6C	1.390(3)
C4D	C5D	1.390(4)
C1M	C2M	1.389(4)
C1M	C6M	1.392(4)
C2O	C3O	1.386(3)
C2H	C3H	1.390(3)
C3G	C4G	1.378(4)
C4T	C5T	1.379(4)
C4T	C3T	1.383(4)
C6K	C5K	1.391(3)
C5U	C4U	1.381(4)
C4O	C5O	1.382(4)
C4O	C3O	1.391(4)
C6G	C5G	1.382(4)
C43	C53	1.527(4)
C43	C63	1.536(4)
C5O	C6O	1.387(3)
C6X	C5X	1.390(4)
C6X	C1X	1.390(4)
C2S	C3S	1.384(4)
C2C	C3C	1.383(3)
C4P	C5P	1.387(4)
C2F	C3F	1.391(3)
C5S	C4S	1.387(4)
C6N	C5N	1.397(4)
C2A	C3A	1.381(4)
C3S	C4S	1.391(4)
C4K	C5K	1.384(4)
C3H	C4H	1.381(4)
C5L	C4L	1.374(5)
C1W	C6W	1.384(4)

Atom	Atom	Length/Å
C1W	C2W	1.395(4)
C4I	C6I	1.525(4)
C4I	C5I	1.527(3)
C4R	C5R	1.382(5)
C4R	C3R	1.393(5)
C6A	C5A	1.391(4)
C2V	C3V	1.389(4)
C1X	C2X	1.386(4)
C4U	C3U	1.381(4)
C1B	C6B	1.388(4)
C1B	C2B	1.393(4)
C5E	C4E	1.387(4)
C5Q	C4Q	1.371(5)
C3N	C4N	1.381(4)
C2I	C3I	1.384(5)
C5F	C4F	1.383(4)
C5F	C6F	1.387(4)
C2Q	C3Q	1.383(4)
C2L	C3L	1.390(4)
C3V	C4V	1.377(4)
C4V	C5V	1.388(4)
C4F	C3F	1.385(4)
C3E	C4E	1.393(4)
C2R	C3R	1.387(4)
C4G	C5G	1.386(4)
C4N	C5N	1.381(4)
C6V	C5V	1.387(4)
C3A	C4A	1.383(4)
C2B	C3B	1.381(4)
C4Q	C3Q	1.388(4)
C4L	C3L	1.386(5)
C2M	C3M	1.388(4)
C6I	C5I	1.385(4)
C6W	C5W	1.402(5)
C4A	C5A	1.375(5)
C6M	C5M	1.385(4)
C5X	C4X	1.373(5)
C6B	C5B	1.394(5)
C2W	C3W	1.383(5)
C3M	C4M	1.382(6)
C5M	C4M	1.367(6)
C3B	C4B	1.357(6)
C4I	C3I	1.370(7)
C4I	C5I	1.379(7)
C4B	C5B	1.400(7)
C5W	C4W	1.376(8)
C2X	C3X	1.389(5)
C3W	C4W	1.362(8)
C4X	C3X	1.384(7)

Table 4. Bond Angles in ° for **MP20_47**.

Atom	Atom	Atom	Angle/°
N14	P14	N24	113.91(10)
N14	P14	N34	116.50(10)
N24	P14	N34	110.71(10)
N14	P14	C44	103.86(10)
N24	P14	C44	105.73(10)
N34	P14	C44	104.84(10)
N12	P12	N22	115.17(9)
N12	P12	N32	115.21(9)

Atom	Atom	Atom	Angle/°
N22	P12	N32	111.41(9)
N12	P12	C42	103.64(10)
N22	P12	C42	105.23(10)
N32	P12	C42	104.73(9)
N23	P13	N13	114.41(10)
N23	P13	N33	113.40(10)
N13	P13	N33	113.93(10)
N23	P13	C43	104.68(11)

Atom	Atom	Atom	Angle/°
N13	P13	C43	104.14(11)
N33	P13	C43	104.83(11)
N31	P11	N21	111.09(10)
N31	P11	N11	116.41(10)
N21	P11	N11	113.50(10)
N31	P11	C41	104.69(11)
N21	P11	C41	105.91(11)
N11	P11	C41	103.99(10)
C12	N12	P12	142.81(17)
C33	N33	P13	133.76(17)
C23	N23	P13	135.96(17)
C24	N24	P14	135.81(17)
C22	N22	P12	134.31(17)
C32	N32	P12	134.32(16)
C11	N11	P11	135.73(18)
C21	N21	P11	133.57(17)
C31	N31	P11	135.79(17)
C14	N14	P14	141.50(17)
C13	N13	P13	133.38(16)
C34	N34	P14	131.86(18)
C3K	C2K	C1K	120.2(2)
N33	C33	C1Q	118.0(2)
N33	C33	C1R	123.9(2)
C1Q	C33	C1R	118.12(19)
N22	C22	C1J	117.6(2)
N22	C22	C1I	124.18(19)
C1J	C22	C1I	118.20(19)
C62	C42	C52	110.99(18)
C62	C42	P12	110.82(15)
C52	C42	P12	110.91(15)
C5H	C6H	C1H	119.9(2)
C2G	C1G	C6G	118.5(2)
C2G	C1G	C12	122.04(19)
C6G	C1G	C12	119.1(2)
C6E	C1E	C2E	119.6(2)
C6E	C1E	C31	120.8(2)
C2E	C1E	C31	119.7(2)
N32	C32	C1K	117.75(18)
N32	C32	C1L	124.51(19)
C1K	C32	C1L	117.74(18)
C6U	C1U	C2U	119.7(2)
C6U	C1U	C24	119.6(2)
C2U	C1U	C24	120.5(2)
C6N	C1N	C2N	120.0(2)
C6N	C1N	C13	120.9(2)
C2N	C1N	C13	119.09(19)
N31	C31	C1E	117.48(19)
N31	C31	C1F	123.11(19)
C1E	C31	C1F	119.38(19)
C5E	C6E	C1E	120.3(2)
C6T	C1T	C2T	118.8(2)
C6T	C1T	C14	119.2(2)
C2T	C1T	C14	122.0(2)
C6A	C1A	C2A	118.6(2)
C6A	C1A	C11	121.5(2)
C2A	C1A	C11	119.8(2)
N12	C12	C1G	117.02(19)
N12	C12	C1H	124.16(19)
C1G	C12	C1H	118.71(18)
C2K	C3K	C4K	120.4(2)
N13	C13	C1M	118.2(2)
N13	C13	C1N	123.52(19)
C1M	C13	C1N	118.3(2)
C6R	C1R	C2R	120.1(2)
C6R	C1R	C33	120.4(2)

Atom	Atom	Atom	Angle/°
C2R	C1R	C33	119.5(2)
C6D	C1D	C2D	119.5(2)
C6D	C1D	C21	120.6(2)
C2D	C1D	C21	119.9(2)
C6K	C1K	C2K	118.9(2)
C6K	C1K	C32	120.72(19)
C2K	C1K	C32	120.27(18)
N23	C23	C1O	117.2(2)
N23	C23	C1P	123.71(19)
C1O	C23	C1P	119.09(18)
N24	C24	C1V	117.2(2)
N24	C24	C1U	125.6(2)
C1V	C24	C1U	117.11(19)
C2L	C1L	C6L	120.2(2)
C2L	C1L	C32	118.6(2)
C6L	C1L	C32	121.2(2)
C6H	C1H	C2H	119.4(2)
C6H	C1H	C12	120.06(19)
C2H	C1H	C12	120.55(19)
C3P	C2P	C1P	119.7(2)
C5S	C6S	C1S	119.9(2)
C6I	C1I	C2I	120.1(3)
C6I	C1I	C22	119.0(2)
C2I	C1I	C22	120.9(2)
C6Q	C1Q	C2Q	119.1(2)
C6Q	C1Q	C33	121.1(2)
C2Q	C1Q	C33	119.7(2)
C3J	C4J	C5J	120.3(2)
N14	C14	C1T	116.3(2)
N14	C14	C1S	123.77(19)
C1T	C14	C1S	119.87(19)
C6J	C5J	C4J	119.6(2)
C4D	C3D	C2D	120.6(2)
C2S	C1S	C6S	119.6(2)
C2S	C1S	C14	120.0(2)
C6S	C1S	C14	120.39(19)
C1L	C6L	C5L	119.6(2)
C2C	C1C	C6C	119.2(2)
C2C	C1C	C21	119.5(2)
C6C	C1C	C21	121.3(2)
C2F	C1F	C6F	120.2(2)
C2F	C1F	C31	118.76(19)
C6F	C1F	C31	121.0(2)
C1U	C6U	C5U	120.0(2)
C64	C44	C54	111.5(2)
C64	C44	P14	110.32(16)
C54	C44	P14	110.83(16)
C6V	C1V	C2V	119.1(2)
C6V	C1V	C24	120.3(2)
C2V	C1V	C24	120.5(2)
N21	C21	C1C	117.4(2)
N21	C21	C1D	123.9(2)
C1C	C21	C1D	118.61(19)
N11	C11	C1A	117.8(2)
N11	C11	C1B	124.2(2)
C1A	C11	C1B	118.00(19)
C3N	C2N	C1N	119.9(2)
N34	C34	C1X	118.0(2)
N34	C34	C1W	124.5(2)
C1X	C34	C1W	117.5(2)
C3J	C2J	C1J	119.9(2)
C5D	C6D	C1D	120.3(2)
C5R	C6R	C1R	119.7(3)
C6O	C1O	C2O	119.1(2)
C6O	C1O	C23	121.3(2)

Atom	Atom	Atom	Angle/°
C2O	C1O	C23	119.5(2)
C5T	C6T	C1T	120.8(2)
C4P	C3P	C2P	120.1(2)
C5P	C6P	C1P	120.1(2)
C3E	C2E	C1E	119.9(2)
C6H	C5H	C4H	120.3(2)
C3U	C2U	C1U	120.1(2)
C6P	C1P	C2P	119.8(2)
C6P	C1P	C23	119.8(2)
C2P	C1P	C23	120.3(2)
C1Q	C6Q	C5Q	120.0(2)
C5C	C4C	C3C	120.2(2)
C3T	C2T	C1T	119.9(2)
C6J	C1J	C2J	119.1(2)
C6J	C1J	C22	120.4(2)
C2J	C1J	C22	120.4(2)
C3G	C2G	C1G	120.7(2)
C4C	C5C	C6C	120.2(2)
C3D	C2D	C1D	119.8(2)
C3D	C4D	C5D	119.6(2)
C2M	C1M	C6M	119.3(2)
C2M	C1M	C13	119.9(2)
C6M	C1M	C13	120.7(2)
C3O	C2O	C1O	120.2(2)
C3H	C2H	C1H	120.0(2)
C4G	C3G	C2G	120.0(2)
C5T	C4T	C3T	119.8(2)
C5K	C6K	C1K	120.4(2)
C4U	C5U	C6U	120.1(2)
C5O	C4O	C3O	119.9(2)
C5G	C6G	C1G	120.3(2)
C4T	C5T	C6T	119.9(2)
C53	C43	C63	111.8(2)
C53	C43	P13	112.01(19)
C63	C43	P13	109.62(18)
C5C	C6C	C1C	119.9(2)
C4O	C5O	C6O	120.3(2)
C4J	C3J	C2J	120.4(2)
C6D	C5D	C4D	120.0(2)
C5X	C6X	C1X	120.6(3)
C3S	C2S	C1S	120.1(2)
C3C	C2C	C1C	120.2(2)
C3P	C4P	C5P	120.5(2)
C1F	C2F	C3F	119.7(2)
C6S	C5S	C4S	120.4(2)
C1N	C6N	C5N	119.0(2)
C3A	C2A	C1A	120.9(2)
C2S	C3S	C4S	120.2(2)
C5K	C4K	C3K	119.9(2)
C5O	C6O	C1O	120.3(2)
C4H	C3H	C2H	120.2(2)
C5J	C6J	C1J	120.7(2)
C4L	C5L	C6L	120.2(3)
C6W	C1W	C2W	120.4(3)
C6W	C1W	C34	120.7(3)
C2W	C1W	C34	118.9(3)
C4T	C3T	C2T	120.8(2)
C6I	C4I	C5I	111.5(2)
C6I	C4I	P11	110.56(18)
C5I	C4I	P11	110.55(16)
C5R	C4R	C3R	119.6(2)
C3H	C4H	C5H	120.1(2)
C5A	C6A	C1A	119.9(3)
C3V	C2V	C1V	119.9(2)
C2X	C1X	C6X	119.6(3)

Atom	Atom	Atom	Angle/°
C2X	C1X	C34	119.6(3)
C6X	C1X	C34	120.8(2)
C5U	C4U	C3U	120.4(2)
C2C	C3C	C4C	120.2(2)
C6B	C1B	C2B	120.6(3)
C6B	C1B	C11	120.8(2)
C2B	C1B	C11	118.6(2)
C6E	C5E	C4E	119.9(2)
C4Q	C5Q	C6Q	120.3(3)
C4N	C3N	C2N	120.6(2)
C3I	C2I	C1I	119.8(3)
C4F	C5F	C6F	120.7(2)
C4P	C5P	C6P	119.7(2)
C3Q	C2Q	C1Q	120.4(3)
C4U	C3U	C2U	119.8(2)
C2O	C3O	C4O	120.2(2)
C1L	C2L	C3L	119.7(3)
C5S	C4S	C3S	119.8(2)
C4V	C3V	C2V	120.4(2)
C5F	C6F	C1F	119.3(2)
C3V	C4V	C5V	120.2(2)
C5F	C4F	C3F	120.0(2)
C2E	C3E	C4E	120.1(3)
C3R	C2R	C1R	119.6(3)
C4R	C5R	C6R	120.8(3)
C3G	C4G	C5G	120.2(2)
C5E	C4E	C3E	120.2(2)
C4F	C3F	C2F	120.1(2)
C3N	C4N	C5N	119.7(2)
C6G	C5G	C4G	120.3(2)
C5V	C6V	C1V	120.6(2)
C4K	C5K	C6K	120.1(2)
C2A	C3A	C4A	119.8(3)
C3B	C2B	C1B	120.5(3)
C5Q	C4Q	C3Q	120.3(3)
C2R	C3R	C4R	120.2(3)
C4N	C5N	C6N	120.8(2)
C5L	C4L	C3L	120.5(2)
C3M	C2M	C1M	120.2(3)
C1I	C6I	C5I	119.4(3)
C1W	C6W	C5W	118.4(4)
C5A	C4A	C3A	120.2(3)
C5M	C6M	C1M	120.1(3)
C4A	C5A	C6A	120.6(3)
C6V	C5V	C4V	119.7(3)
C4X	C5X	C6X	119.4(3)
C1B	C6B	C5B	118.2(3)
C4L	C3L	C2L	119.8(3)
C3W	C2W	C1W	120.0(4)
C4M	C3M	C2M	119.5(3)
C4M	C5M	C6M	120.1(3)
C2Q	C3Q	C4Q	119.9(3)
C4B	C3B	C2B	119.5(3)
C3I	C4I	C5I	120.4(3)
C4I	C3I	C2I	120.0(3)
C3B	C4B	C5B	121.0(3)
C5M	C4M	C3M	120.8(3)
C4W	C5W	C6W	120.4(4)
C6B	C5B	C4B	120.2(4)
C4I	C5I	C6I	120.2(4)
C1X	C2X	C3X	119.3(4)
C4W	C3W	C2W	119.8(4)
C3W	C4W	C5W	120.9(4)
C5X	C4X	C3X	120.3(3)
C4X	C3X	C2X	120.5(4)

Table 5. Hydrogen Fractional Atomic Coordinates ($\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for MP20_47.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H2K	8175.46	2615.95	1602.73	29
H42	8387.53	3905.63	515.04	27
H6H	8748.01	3429.34	2152.11	32
H6E	2413.05	2939.83	1114.9	36
H3K	8233.07	1689.06	1726.25	38
H2P	1724.22	5821.35	4503.47	34
H6S	2188.69	9783.95	2129.86	35
H4J	1614.65	5413.63	288.67	40
H5J	2926.3	4657.48	67.74	43
H3D	-1252.71	1338	887.2	41
H6L	4338.01	3729.93	1076.04	36
H6U	2602.11	10918.17	4021.81	36
H44	1618.92	8860.01	4435.1	31
H2N	-3071.81	6079.23	6271.9	34
H2J	4078.42	5783.33	1240.46	37
H6D	1243.09	2080	-363.47	39
H6R	-1803.93	7827.67	4915.35	40
H52A	10314.11	3785.99	1163.42	48
H52B	10558.69	3620.27	637.31	48
H52C	9549.73	3307.76	972.38	48
H6T	242.1	10486.4	3505.92	40
H3P	2885.83	6397.89	3989.98	42
H6P	50.51	7116.66	5187.89	37
H2E	2310.4	1309.4	1185.99	38
H5H	7849.42	2843.84	2718.58	39
H2U	4058.44	10082.41	2892.32	41
H6Q	-2265.98	7957.36	3678.55	40
H4C	-247.41	-391.14	-1389.94	41
H2T	-282.22	9980.26	2212.64	37
H2G	9468.86	4694.17	2895.63	34
H5C	-1631.22	209.38	-960.8	42
H2D	74.95	778.35	394.36	37
H4D	-1387.29	2262.29	746.82	41
H2O	-1011.15	5179.86	5639.07	38
H2H	6925.31	4693.71	2842.66	35
H3G	11089.38	5272.43	3070.56	43
H4T	-1879.69	11405.64	2671.12	52
H6K	4256.45	2651.15	1885.56	37
H5U	1950.75	11621.44	3540.68	43
H4O	2126.9	4642.22	6279.27	41
H6G	9642.71	5298	1584.55	39
H5T	-971.05	11273.56	3374.69	49
H43	-3052.09	5603.75	4689.8	39
H6C	-780.07	846.67	-493.32	38
H5O	3343.42	5332.27	5932.1	39
H62A	8665.65	4855.59	563.76	47
H62B	9911.79	4552.24	324.45	47
H62C	9890.1	4736.12	845.57	47
H3J	2207.54	5978.94	863.44	41
H5D	-151.59	2633.04	113.64	43
H6X	1842.84	7691.86	3276.66	42
H2S	477.11	8605.72	2923.01	37
H2C	2867.05	248.54	-872.13	38
H4P	2709.12	7325.22	4098.03	43
H2F	5661.41	2344.39	749.63	36
H5S	2815.75	9155.28	1556.4	44
H6N	-1172.31	7455.26	5947.22	39
H2A	7069.03	2193.6	-464.09	41
H3S	1079.56	7984	2340.95	43

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H4K	6306.44	1234.94	1899.77	43
H6O	2404.75	5944.37	5432.17	34
H3H	5974.96	4097.18	3390.48	42
H6J	4809.73	4461.45	437.57	39
H5L	2413.65	4226.77	1286.47	50
H3T	-1536.4	10758.99	2094.57	49
H4I	4683	590.38	294.79	35
H4R	-5263.1	8646.99	5064.56	55
H4H	6477.2	3178.67	3339.04	42
H6A	5141.79	2627.21	-1581.51	46
H2V	5422.81	10838.62	3770.05	42
H4U	2436.36	11570.83	2742.76	47
H3C	1999.36	-371.23	-1346.66	42
H5E	1182.32	2999.64	1827.56	46
H5Q	-1643.47	7996.53	2882.37	50
H3N	-1369.02	5779.49	6698.07	45
H2I	4980.34	4954.07	2056.73	55
H5F	3883.71	3605.35	-246.96	49
H5P	1320.17	7687.43	4702.42	44
H2Q	-1228.89	6369.64	3685.56	47
H3U	3467.57	10801.01	2415.45	50
H3O	-38.12	4555.48	6120.35	43
H2L	5034.07	3600.06	2429.14	52
H4S	2245.44	8258.2	1655.6	45
H3V	7278.98	10995.06	4149.17	48
H6F	2617.07	2906.56	62.69	40
H4V	8020.61	10366.91	4672.96	50
H4F	6031.6	3667.62	-73.25	47
H3E	1114.04	1371.84	1905.88	49
H54A	-583.43	8651.93	4388.37	61
H54B	283	8393.18	3966.76	61
H54C	-562.73	8924.38	3892.2	61
H2R	-4676.61	7463.38	4110.63	45
H64A	27.84	9790.27	4271.63	57
H64B	1361.59	9818.93	4498.75	57
H64C	187.25	9517.95	4760.21	57
H5R	-3133.54	8513.29	5258.71	51
H4G	11990.65	5852.71	2505.19	50
H51A	6695.72	850.73	534.83	55
H51B	5594.68	1282.19	696.3	55
H51C	6575.11	1401.41	260.98	55
H4E	532.38	2216.73	2222.69	51
H3F	6915.39	3046.71	433.09	44
H4N	435.07	6305.34	6747.24	51
H5G	11222.95	5884.53	1771.19	50
H6V	5025.17	9419.74	4464.48	50
H5K	4325.43	1718.02	1993.99	45
H3A	8834.94	2685.24	-757.13	50
H2B	2932.54	2732.52	-957.82	51
H4Q	-842.2	7230.41	2493.33	57
H3R	-6032.96	8125.47	4484.24	54
H5N	532.23	7139.28	6375.17	52
H61A	6431.27	856.82	-482.07	62
H61B	5312.82	441.38	-499.71	62
H61C	6492.24	310.79	-198.42	62
H4L	1835.94	4426.57	2057.71	64
H63A	-3623.43	5515.86	5491.62	68
H63B	-4830.65	5380.33	5218.47	68
H63C	-4780.2	5944.62	5460.98	68
H2M	-5636.84	7242.05	5454.74	52
H6I	7250.8	5784.28	1110.89	50
H6W	5637.44	8723.22	3729.62	56
H4A	8751.75	3153.25	-1456.86	54
H6M	-3625.59	7490.42	6568.67	52
H5A	6920.5	3125.05	-1864.93	58

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H5V	6902.12	9575.54	4830.84	58
H5X	2015.59	6778.49	3088.38	55
H6B	4098.7	1210.42	-1328.26	54
H53A	-5103.42	6396.8	4662.27	78
H53B	-5093.02	5824.79	4429.13	78
H53C	-4092.27	6256.8	4236.51	78
H3L	3145	4122.91	2631.39	71
H2W	4351.9	8919.53	2451.18	64
H3M	-7353.32	7787.52	5784.62	71
H5M	-5331.11	8046.71	6886.11	71
H3Q	-634.67	6414.54	2892.44	59
H3B	1124.85	2679.01	-1382.62	71
H4I	6955.52	6211.71	2457.68	86
H3I	5520.01	5529.93	2635.89	79
H4B	789.64	1899.51	-1770.63	83
H4M	-7180.74	8186.53	6499.29	77
H5W	7380.85	9281.37	3497.92	90
H5B	2269.36	1165.84	-1756.93	84
H5I	7797.68	6350.04	1697.72	77
H2X	5635.26	7859.79	2842.09	101
H3W	6048.09	9494.32	2243.5	96
H4W	7560.29	9658.16	2761.39	105
H4X	4015.65	6402.57	2807.4	94
H3X	5795.73	6945.24	2656.37	148

Citation

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