

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
=====	=====	=====	=====	=====	=====
W	P	2.495(2)	C1	C2	1.48(1)
W	C13	2.005(9)	C1	C3	1.48(1)
W	C14	2.058(9)	C1	C4	1.49(1)
W	C15	2.054(9)	C2	C5	1.50(1)
W	C16	2.040(9)	C2	C6	1.51(1)
W	C17	2.022(9)	C3	C4	1.51(1)
P	C1	1.807(8)	C5	C6	1.53(1)
P	C2	1.820(8)	C7	C8	1.35(1)
P	C7	1.833(8)	C7	C12	1.41(1)
O1	C13	1.12(1)	C8	C9	1.41(1)
O2	C14	1.12(1)	C9	C10	1.30(2)
O3	C15	1.12(1)	C10	C11	1.38(2)
O4	C16	1.13(1)	C11	C12	1.37(1)
O5	C17	1.15(1)			

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
=====	=====	=====	=====	=====	=====	=====	=====
P	W	C13	178.8 (3)	P	C1	C2	66.4 (5)
P	W	C14	91.1 (2)	P	C1	C3	138.6 (6)
P	W	C15	89.0 (2)	P	C1	C4	137.8 (6)
P	W	C16	91.2 (2)	C2	C1	C3	133.9 (7)
P	W	C17	91.7 (3)	C2	C1	C4	133.9 (7)
C13	W	C14	89.5 (4)	C3	C1	C4	61.2 (7)
C13	W	C15	89.9 (3)	P	C2	C1	65.5 (4)
C13	W	C16	88.3 (4)	P	C2	C5	140.4 (7)
C13	W	C17	89.4 (4)	P	C2	C6	135.9 (7)
C14	W	C15	90.9 (3)	C1	C2	C5	136.0 (8)
C14	W	C16	177.3 (3)	C1	C2	C6	132.6 (8)
C14	W	C17	88.0 (3)	C5	C2	C6	61.4 (6)
C15	W	C16	90.5 (3)	C1	C3	C4	59.8 (6)
C15	W	C17	178.7 (4)	C1	C4	C3	59.0 (6)
C16	W	C17	90.5 (4)	C2	C5	C6	59.6 (6)
W	P	C1	126.0 (3)	C2	C6	C5	59.0 (6)
W	P	C2	125.3 (3)	P	C7	C8	120.8 (6)
W	P	C7	122.3 (3)	P	C7	C12	120.6 (7)
C1	P	C2	48.1 (4)	C8	C7	C12	118.6 (8)
C1	P	C7	106.4 (4)	C7	C8	C9	119.7 (8)
C2	P	C7	106.4 (4)	C8	C9	C10	122.1 (1)

Bond Angles (cont.)

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
=====	=====	=====	=====	=====	=====	=====	=====
C9	C10	C11	120.1(1)	W	C14	O2	177.6(7)
C10	C11	C12	120.3(9)	W	C15	O3	176.8(8)
C7	C12	C11	119.6(9)	W	C16	O4	178.6(7)
W	C13	O1	178.6(9)	W	C17	O5	177.7(8)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B (A2)
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W	0.35997(5)	0.59207(2)	0.10668(2)	1.910(5)
P	0.4408(3)	0.4532(1)	0.1720(1)	2.03(3)
O1	0.254(2)	0.7666(6)	0.0262(6)	7.6(2)
O2	0.774(1)	0.6720(5)	0.1571(5)	4.9(2)
O3	0.162(1)	0.6579(5)	0.2658(4)	4.7(2)
O4	-0.052(1)	0.5203(6)	0.0454(4)	5.0(2)
O5	0.570(1)	0.5357(6)	-0.0533(3)	5.0(2)
C1	0.651(1)	0.4325(5)	0.2353(4)	2.5(1)
C2	0.461(1)	0.4363(5)	0.2784(4)	2.7(2)
C3	0.824(2)	0.3743(7)	0.2382(7)	4.4(2)
C4	0.852(1)	0.4696(7)	0.2496(5)	3.6(2)
C5	0.365(2)	0.3867(6)	0.3439(5)	3.7(2)

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B (A2)
C6	0.396(2)	0.4835(6)	0.3518(5)	4.2(2)
C7	0.370(1)	0.3500(5)	0.1290(5)	2.8(1)
C8	0.298(1)	0.3451(5)	0.0548(5)	3.3(2)
C9	0.243(2)	0.2650(8)	0.0233(7)	6.0(2)
C10	0.259(2)	0.1948(7)	0.0643(8)	5.6(3)
C11	0.331(2)	0.1976(6)	0.1408(7)	5.1(3)
C12	0.389(2)	0.2736(6)	0.1733(6)	4.1(2)
C13	0.290(1)	0.7040(5)	0.0559(5)	3.3(2)
C14	0.628(1)	0.6427(5)	0.1408(5)	2.7(1)
C15	0.231(1)	0.6322(5)	0.2105(5)	2.8(1)
C16	0.095(1)	0.5454(6)	0.0682(5)	2.9(2)
C17	0.491(1)	0.5548(6)	0.0045(5)	3.0(2)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$$(4/3) * [a2*B(1,1) + b2*B(2,2) + c2*B(3,3) + ab(\cos \gamma)*B(1,2) + ac(\cos \beta)*B(1,3) + bc(\cos \alpha)*B(2,3)]$$

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
W	0.0235(1)	0.0250(1)	0.0241(1)	0.0037(1)	-0.0021(1)	0.0034(1)
P	0.0275(8)	0.0238(7)	0.0258(7)	-0.0009(8)	-0.0016(8)	0.0025(7)
O1	0.104(7)	0.066(4)	0.121(6)	0.024(5)	-0.036(5)	0.050(4)
O2	0.037(3)	0.065(4)	0.084(5)	-0.001(4)	-0.018(4)	-0.022(4)
O3	0.060(5)	0.063(4)	0.054(3)	0.005(4)	0.016(4)	-0.020(3)
O4	0.028(3)	0.106(6)	0.055(4)	-0.002(5)	-0.003(3)	-0.018(4)
O5	0.059(4)	0.104(6)	0.027(3)	0.003(5)	0.010(3)	-0.017(3)
C1	0.030(4)	0.037(3)	0.026(3)	-0.003(4)	-0.001(3)	0.010(3)
C2	0.039(5)	0.032(3)	0.031(3)	0.005(4)	0.003(4)	0.009(3)
C3	0.045(6)	0.049(5)	0.072(6)	0.005(5)	-0.012(5)	0.020(4)
C4	0.033(4)	0.062(5)	0.040(4)	-0.009(5)	-0.006(4)	0.016(4)
C5	0.051(5)	0.051(4)	0.039(4)	-0.005(5)	0.017(4)	0.015(3)

Table of General Anisotropic Displacement Parameter Expressions - U's (Cont.)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C6	0.079(7)	0.041(4)	0.038(4)	-0.007(6)	0.020(5)	0.002(4)
C7	0.040(4)	0.027(3)	0.041(4)	-0.002(4)	0.002(4)	0.003(3)
C8	0.036(4)	0.034(4)	0.054(4)	-0.002(4)	-0.014(4)	-0.017(3)
C9	0.062(6)	0.070(6)	0.096(6)	0.008(6)	-0.040(5)	-0.051(4)
C10	0.067(7)	0.042(5)	0.105(8)	-0.025(5)	-0.007(7)	-0.025(5)
C11	0.098(9)	0.032(4)	0.065(6)	-0.020(6)	0.014(7)	0.004(4)
C12	0.058(6)	0.033(4)	0.066(5)	-0.005(5)	0.009(6)	0.008(4)
C13	0.039(4)	0.035(4)	0.051(4)	0.011(4)	-0.008(4)	0.014(3)
C14	0.035(4)	0.029(3)	0.038(3)	0.004(4)	-0.010(4)	-0.010(3)
C15	0.034(4)	0.032(3)	0.042(4)	0.003(4)	-0.001(4)	-0.006(3)
C16	0.037(4)	0.045(4)	0.030(3)	0.006(4)	-0.005(3)	-0.004(3)
C17	0.034(4)	0.044(4)	0.036(3)	-0.003(4)	0.001(4)	0.001(4)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi i \{h^2a^2U(1,1) + k^2b^2U(2,2) + l^2c^2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)\}]$ where a,b, and c are reciprocal lattice constants.