

Table 3S. Bond lengths [Å] and angles [°] for 2:5.

P(1)-F(10)	1.564(4)
P(1)-F(12)	1.569(4)
P(1)-F(8)	1.574(4)
P(1)-F(7')	1.583(8)
P(1)-F(9)	1.582(4)
P(1)-F(11)	1.587(4)
P(1)-F(7)	1.656(9)
P(2)-F(2)	1.487(8)
P(2)-F(3'')	1.524(10)
P(2)-F(4)	1.559(5)
P(2)-F(6)	1.568(5)
P(2)-F(3)	1.590(11)
P(2)-F(1)	1.601(6)
P(2)-F(5)	1.621(5)
P(2)-F(2')	1.752(13)
P(2)-F(3')	1.844(13)
O(1)-C(27)	1.381(5)
O(1)-C(1)	1.423(5)
O(2)-C(3)	1.421(6)
O(2)-C(2)	1.433(6)
O(3)-C(4)	1.428(6)
O(3)-C(5)	1.428(5)
O(4)-C(7)	1.415(5)
O(4)-C(6)	1.428(5)
O(5)-C(9)	1.394(5)
O(5)-C(8)	1.438(5)
O(6)-C(11)	1.370(5)
O(6)-C(15)	1.436(5)
O(7)-C(16)	1.421(5)
O(7)-C(17)	1.431(5)
O(8)-C(18)	1.421(6)
O(8)-C(19)	1.436(6)
O(9)-C(21)	1.424(6)
O(9)-C(20)	1.441(5)
O(10)-C(23)	1.382(5)
O(10)-C(22)	1.424(6)
O(11)-C(55)	1.213(8)
O(12)-C(52)	1.217(14)
N(1)-C(36)	1.460(5)
N(1)-C(35)	1.516(5)
N(2)-C(43)	1.504(5)
N(2)-C(44)	1.503(5)
C(1)-C(2)	1.503(6)
C(3)-C(4)	1.491(7)
C(5)-C(6)	1.492(7)
C(7)-C(8)	1.506(6)
C(9)-C(10)	1.387(6)
C(9)-C(14)	1.393(6)
C(10)-C(11)	1.395(6)
C(11)-C(12)	1.389(6)
C(12)-C(13)	1.397(6)
C(13)-C(14)	1.376(6)
C(15)-C(16)	1.496(6)
C(17)-C(18)	1.493(7)
C(19)-C(20)	1.496(7)
C(21)-C(22)	1.509(7)

C(23)-C(24)	1.385(7)
C(23)-C(28)	1.384(6)
C(24)-C(25)	1.382(7)
C(25)-C(26)	1.395(7)
C(26)-C(27)	1.376(6)
C(27)-C(28)	1.395(6)
C(29)-C(30)	1.366(9)
C(29)-C(34)	1.372(6)
C(30)-C(31)	1.342(12)
C(31)-C(32)	1.394(12)
C(32)-C(33)	1.400(10)
C(33)-C(34)	1.375(6)
C(34)-C(35)	1.501(6)
C(36)-C(37)	1.516(5)
C(37)-C(42)	1.388(6)
C(37)-C(38)	1.389(5)
C(38)-C(39)	1.391(5)
C(39)-C(40)	1.389(6)
C(39)-C(43)	1.511(5)
C(40)-C(41)	1.381(6)
C(41)-C(42)	1.391(6)
C(44)-C(45)	1.509(6)
C(45)-C(50)	1.384(7)
C(45)-C(46)	1.387(6)
C(46)-C(47)	1.387(7)
C(47)-C(48)	1.376(8)
C(48)-C(49)	1.378(7)
C(49)-C(50)	1.389(7)
C(52)-C(51')	1.26(2)
C(52)-C(53')	1.44(2)
C(52)-C(53)	1.60(2)
C(52)-C(51)	1.76(2)
C(54)-C(55)	1.485(11)
C(55)-C(56)	1.470(9)

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F(10)-P(1)-F(12)	90.4(2)
F(10)-P(1)-F(8)	92.9(3)
F(12)-P(1)-F(8)	91.6(2)
F(10)-P(1)-F(7')	96.7(4)
F(12)-P(1)-F(7')	165.7(4)
F(8)-P(1)-F(7')	100.4(4)
F(10)-P(1)-F(9)	87.9(3)
F(12)-P(1)-F(9)	87.9(3)
F(8)-P(1)-F(9)	179.0(3)
F(7')-P(1)-F(9)	80.0(4)
F(10)-P(1)-F(11)	178.8(2)
F(12)-P(1)-F(11)	89.4(2)
F(8)-P(1)-F(11)	88.3(2)
F(7')-P(1)-F(11)	83.2(4)
F(9)-P(1)-F(11)	90.9(2)
F(10)-P(1)-F(7)	82.5(4)
F(12)-P(1)-F(7)	167.3(4)
F(8)-P(1)-F(7)	78.4(4)
F(9)-P(1)-F(7)	102.3(4)
F(11)-P(1)-F(7)	98.0(4)
F(2)-P(2)-F(3'')	89.5(5)
F(2)-P(2)-F(4)	103.5(4)
F(3'')-P(2)-F(4)	92.4(5)
F(2)-P(2)-F(6)	94.6(4)

F(3''')-P(2)-F(6)	175.4(6)
F(4)-P(2)-F(6)	88.8(3)
F(2)-P(2)-F(3)	101.5(5)
F(3''')-P(2)-F(3)	25.5(5)
F(4)-P(2)-F(3)	110.9(5)
F(6)-P(2)-F(3)	150.5(5)
F(2)-P(2)-F(1)	80.3(4)
F(3''')-P(2)-F(1)	93.4(6)
F(4)-P(2)-F(1)	173.1(4)
F(6)-P(2)-F(1)	85.2(3)
F(3)-P(2)-F(1)	73.5(5)
F(2)-P(2)-F(5)	168.9(4)
F(3''')-P(2)-F(5)	91.9(5)
F(4)-P(2)-F(5)	87.4(3)
F(6)-P(2)-F(5)	83.7(3)
F(3)-P(2)-F(5)	75.8(5)
F(1)-P(2)-F(5)	88.7(4)
F(4)-P(2)-F(2')	78.5(5)
F(6)-P(2)-F(2')	81.3(5)
F(1)-P(2)-F(2')	103.7(5)
F(5)-P(2)-F(2')	159.6(5)
F(4)-P(2)-F(3')	72.6(4)
F(6)-P(2)-F(3')	149.2(5)
F(1)-P(2)-F(3')	114.2(5)
F(5)-P(2)-F(3')	118.7(5)
F(2')-P(2)-F(3')	71.2(6)
C(27)-O(1)-C(1)	118.3(3)
C(3)-O(2)-C(2)	114.6(4)
C(4)-O(3)-C(5)	111.6(3)
C(7)-O(4)-C(6)	112.9(3)
C(9)-O(5)-C(8)	116.9(3)
C(11)-O(6)-C(15)	118.4(3)
C(16)-O(7)-C(17)	113.3(3)
C(18)-O(8)-C(19)	112.3(3)
C(21)-O(9)-C(20)	112.0(4)
C(23)-O(10)-C(22)	117.6(3)
C(36)-N(1)-C(35)	115.3(4)
C(43)-N(2)-C(44)	111.6(3)
O(1)-C(1)-C(2)	106.4(4)
O(2)-C(2)-C(1)	108.6(3)
O(2)-C(3)-C(4)	110.3(4)
O(3)-C(4)-C(3)	110.8(4)
O(3)-C(5)-C(6)	110.1(4)
O(4)-C(6)-C(5)	108.0(4)
O(4)-C(7)-C(8)	107.4(4)
O(5)-C(8)-C(7)	107.7(3)
C(10)-C(9)-O(5)	122.8(4)
C(10)-C(9)-C(14)	121.3(4)
O(5)-C(9)-C(14)	115.9(4)
C(9)-C(10)-C(11)	118.6(4)
O(6)-C(11)-C(12)	125.2(4)
O(6)-C(11)-C(10)	113.5(4)
C(12)-C(11)-C(10)	121.4(4)
C(11)-C(12)-C(13)	118.3(4)
C(14)-C(13)-C(12)	121.5(4)
C(13)-C(14)-C(9)	118.9(4)
O(6)-C(15)-C(16)	106.0(3)
O(7)-C(16)-C(15)	109.5(3)
O(7)-C(17)-C(18)	108.5(4)
O(8)-C(18)-C(17)	108.6(4)

O(8)-C(19)-C(20)	108.4(4)
O(9)-C(20)-C(19)	108.7(4)
O(9)-C(21)-C(22)	108.7(4)
O(10)-C(22)-C(21)	108.4(4)
O(10)-C(23)-C(24)	115.6(4)
O(10)-C(23)-C(28)	123.4(4)
C(24)-C(23)-C(28)	121.0(4)
C(23)-C(24)-C(25)	118.8(4)
C(24)-C(25)-C(26)	121.6(5)
C(27)-C(26)-C(25)	118.3(5)
C(26)-C(27)-O(1)	124.8(4)
C(26)-C(27)-C(28)	121.3(4)
O(1)-C(27)-C(28)	113.9(4)
C(23)-C(28)-C(27)	118.9(4)
C(30)-C(29)-C(34)	120.4(6)
C(31)-C(30)-C(29)	121.4(7)
C(30)-C(31)-C(32)	119.4(6)
C(33)-C(32)-C(31)	119.9(6)
C(34)-C(33)-C(32)	118.9(6)
C(29)-C(34)-C(33)	120.0(5)
C(29)-C(34)-C(35)	120.6(5)
C(33)-C(34)-C(35)	119.5(5)
C(34)-C(35)-N(1)	112.8(4)
N(1)-C(36)-C(37)	114.2(4)
C(42)-C(37)-C(38)	118.9(4)
C(42)-C(37)-C(36)	123.4(4)
C(38)-C(37)-C(36)	117.7(4)
C(37)-C(38)-C(39)	121.4(4)
C(40)-C(39)-C(38)	119.0(4)
C(40)-C(39)-C(43)	122.7(4)
C(38)-C(39)-C(43)	118.0(4)
C(41)-C(40)-C(39)	119.9(4)
C(40)-C(41)-C(42)	120.7(4)
C(37)-C(42)-C(41)	120.0(4)
N(2)-C(43)-C(39)	112.8(3)
N(2)-C(44)-C(45)	112.0(3)
C(50)-C(45)-C(46)	118.6(4)
C(50)-C(45)-C(44)	120.5(4)
C(46)-C(45)-C(44)	120.9(4)
C(45)-C(46)-C(47)	121.0(5)
C(48)-C(47)-C(46)	119.6(5)
C(47)-C(48)-C(49)	120.4(5)
C(50)-C(49)-C(48)	119.8(5)
C(49)-C(50)-C(45)	120.7(4)
O(12)-C(52)-C(51')	116(2)
O(12)-C(52)-C(53')	109(2)
C(51')-C(52)-C(53')	131(2)
O(12)-C(52)-C(53)	128.6(13)
O(12)-C(52)-C(51)	128.7(12)
C(53)-C(52)-C(51)	99.9(12)
O(11)-C(55)-C(56)	121.1(7)
O(11)-C(55)-C(54)	121.5(7)
C(56)-C(55)-C(54)	117.3(7)
