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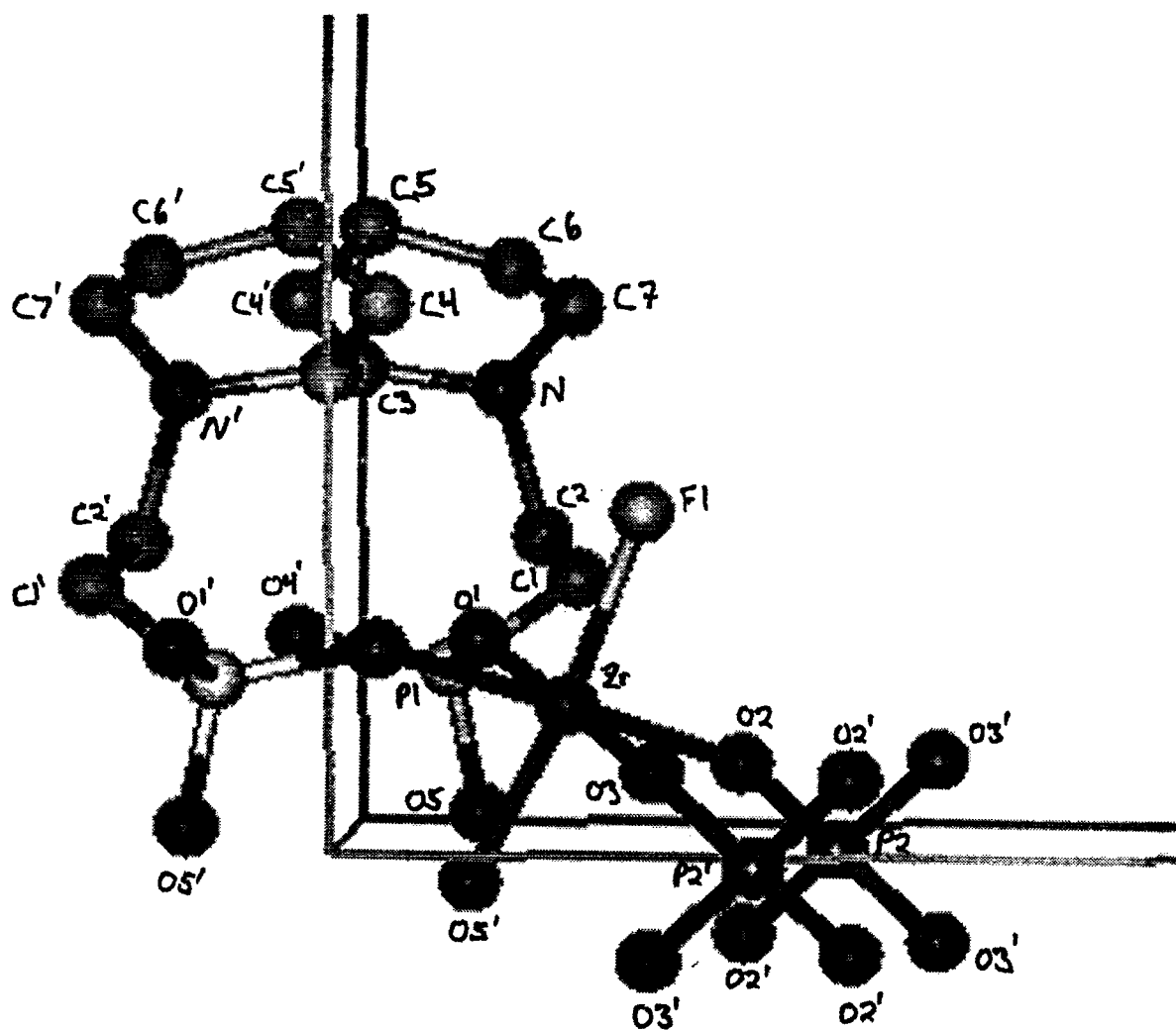
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Supplementary Materials for: Crystal Structure of a Porous Zirconium Phosphate/Phosphonate Compound and Photocatalytic Hydrogen Production From Related Materials.

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Selected bond lengths and angles for $Zr_2(PO_4)PVX_3$.



<u>Bond</u>	<u>Bond Distance</u>
Zr_O1	2.085(13)
Zr_O4	2.030(12)
Zr_O5	2.044(13)
Zr_O2	2.095(13)
Zr_O3	1.992(14)
Zr_F1	2.029(14)
P1_O1	1.538(15)
P1_O2	1.574(15)
P1_O3	1.517(16)
P1_C1	1.795(16)
O1_O4	2.898(17)
O1_O2	2.599(15)
O1_O2	2.887(16)
O1_O3	2.547(17)
O1_O3	2.796(17)
O1_C1	2.689(18)
O1_F1	2.908(18)
O4_O4	2.530(19)
O4_O4	3.47(5)
O4_O5	2.561(15)
O4_O5	2.610(15)
O4_O3	2.927(17)
O4_F1	2.938(17)
O4_P2	1.555(12)
O5_O4	2.908(16)
O5_O5	2.52(4)
O5_O2	2.978(16)
O5_O3	2.915(17)
O5_F1	2.904(18)
O5_P2	1.588(13)
C7_C6	1.416(18)
O2_O3	2.487(18)
O2_O3	2.737(28)
O2_C1	2.826(17)
O2_F1	2.907(18)
O3_O3	3.42(6)
O3_O3	2.96(5)
O3_C1	2.578(19)
F1_F2	3.462(20)
N1_O2	3.586(30)
N1_C1	2.349(19)
N1_C2	1.550(9)
N1_C3	1.424(15)
N1_C4	2.405(15)
N1_C5	2.882(13)
N1_C6	2.373(15)
N1_C7	1.346(15)

C1_C2	1.509(18)
C4_C3	1.363(15)
C4_C5	1.357(15)
C4_F2	2.763(26)
C5_C5	1.547(13)
C5_C6	1.429(16)
C6_C7	1.416(18)
C2_O(W2)	2.863(34)
O(W1)_F1	2.658(20)
O(W1)_N1	2.704(20)
O(W1)_C6	2.634(32)
O(W1)_C7	2.864(34)
O(W1)_O(W2)	2.383(34)
O(W1)_F2	2.816(29)
O(W2)_O1	3.58(4)
O(W2)_O4	3.20(5)
O(W2)_F1	3.29(5)
O(W2)_F1	2.362(34)
O(W2)_C2	2.863(34)
O(W2)_N1	3.143(25)
O(W2)_O(W1)	2.383(34)
O(W2)_F2	3.26(6)
F2_C4	2.763(26)
F2_O(W1)	2.816(29)
F2_O(W2)	3.26(6)

Bond Angle

O1_Zr_O4	89.5(7)
O1_Zr_O5	178.9(9)
O1_Zr_O2	87.3(7)
O1_Zr_O3	86.6(7)
O1_Zr_F1	90.0(8)
O4_Zr_O5	91.1(7)
O4_Zr_O2	176.1(9)
O4_Zr_O3	93.4(8)
O4_Zr_F1	92.7(8)
O5_Zr_O2	92.0(7)
O5_Zr_O3	92.5(8)
O5_Zr_F1	91.0(8)
O2_Zr_O3	84.0(9)
O2_Zr_F1	89.6(8)
O3_Zr_F1	172.9(10)
O1_P1_O2	113.2(13)
O1_P1_O3	113.0(13)
O1_P1_C1	107.3(12)
O2_P1_O3	107.1(12)
O2_P1_C1	113.9(11)

O3_P1_C1	101.9(13)
Zr_O1_P1	148.2(15)
Zr_O4_P2	158.7(11)
Zr_O5_P2	155.0(16)
Zr_O2_P1	150.6(16)
Zr_O3_P1	162.1(16)
P1_C1_C2	118.6(16)
O4_P2_O4	108.9(15)
O4_P2_O5	109.1(6)
O4_P2_O5	112.3(10)
O4_P2_O5	112.3(10)
O4_P2_O5	109.1(6)
O5_P2_O5	105.2(22)
C1_C2_N1	100.3(13)
C2_N1_C3	113.1(13)
C2_N1_C7	122.4(15)
C3_N1_C7	113.8(10)
N1_C3_C4	119.3(11)
C3_C4_C5	126.6(11)
C4_C5_C5	128.8(14)
C4_C5_C6	109.8(9)
C5_C5_C6	121.0(14)
C5_C6_C7	118.3(15)
N1_C7_C6	118.5(14)