

## Supplementary materials

# New Data on the Reactions of Zirconium and Hafnium Tetrachlorides with Aliphatic Acids

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**Table S1.** Bond lengths [Å] for complex IV.

Complex IV	Bond Lengths [Å]
Hf(1)-O(6)	2.039(6)
Hf(1)-O(3)	2.096(7)
Hf(1)-O(1)	2.189(6)
Hf(1)-O(7)	2.191(6)
Hf(1)-O(10)	2.205(7)
Hf(1)-O(35)	2.207(6)
Hf(1)-O(14)	2.270(6)
Hf(1)-O(13)	2.276(7)
Hf(1)-C(9)	2.654(10)
Hf(1)-Hf(5)	3.4646(5)
Hf(1)-Hf(2)	3.4713(5)
Hf(1)-Hf(6)	3.4971(5)
Hf(2)-O(6)	2.030(6)
Hf(2)-O(2)	2.055(7)
Hf(2)-O(34)	2.166(7)
Hf(2)-O(18)	2.180(6)
Hf(2)-O(38)	2.217(6)
Hf(2)-O(24)	2.224(6)
Hf(2)-O(4)	2.253(6)
Hf(2)-O(1)	2.372(6)
Hf(2)-Hf(4)	3.4549(5)
Hf(2)-Hf(5)	3.5166(5)
Hf(2)-Hf(3)	3.5584(5)
Hf(2)-H(2)	2.35(10)
Hf(3)-O(8)	2.058(6)
Hf(3)-O(2)	2.078(6)
Hf(3)-O(29)	2.115(6)
Hf(3)-O(36)	2.151(6)
Hf(3)-O(25)	2.201(6)
Hf(3)-O(4)	2.253(7)
Hf(3)-O(12)	2.283(6)
Hf(3)-O(5)	2.375(6)
Hf(3)-Hf(6)	3.4762(5)
Hf(3)-Hf(4)	3.4768(5)
Hf(3)-Hf(5)	3.5390(6)

Hf(3)-H(2)	2.30(10)
Hf(4)-O(2)	2.024(6)
Hf(4)-O(3)	2.087(6)
Hf(4)-O(26)	2.185(7)
Hf(4)-O(1)	2.195(7)
Hf(4)-O(5)	2.198(6)
Hf(4)-O(17)	2.205(6)
Hf(4)-O(16)	2.239(6)
Hf(4)-O(15)	2.312(6)
Hf(4)-C(13)	2.672(9)
Hf(5)-O(8)	2.035(7)
Hf(5)-O(6)	2.049(6)
Hf(5)-O(23)	2.171(6)
Hf(5)-O(11)	2.171(7)
Hf(5)-O(21)	2.178(6)
Hf(5)-O(9)	2.194(7)
Hf(5)-O(7)	2.350(6)
Hf(5)-O(4)	2.390(7)
Hf(5)-Hf(6)	3.4611(5)
Hf(6)-O(8)	2.032(6)
Hf(6)-O(3)	2.100(6)
Hf(6)-O(22)	2.201(7)
Hf(6)-O(5)	2.201(7)
Hf(6)-O(7)	2.223(6)
Hf(6)-O(37)	2.227(7)
Hf(6)-O(19)	2.251(6)
Hf(6)-O(20)	2.261(6)
Hf(6)-C(21)	2.608(10)
O(2)-H(2)	0.95(2)
O(4)-H(4)	0.85(2)
O(5)-H(5)	0.85(2)
O(7)-H(7)	0.893(17)
C(1)-O(10)	1.257(11)
C(1)-O(9)	1.262(11)
C(1)-C(2)	1.515(14)
C(2)-C(4)	1.50(2)
C(2)-C(3)	1.475(16)
C(2)-H(2A)	1.0000
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-O(12)	1.250(12)
C(5)-O(11)	1.277(12)
C(5)-C(6)	1.529(13)
C(6)-C(7)	1.496(15)
C(6)-C(8)	1.515(15)
C(6)-H(6A)	1.0000
C(7)-H(7A)	0.9800

C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-O(14)	1.270(12)
C(9)-O(13)	1.273(12)
C(9)-C(10)	1.512(16)
C(10)-C(11)	1.444(18)
C(10)-C(12)	1.506(16)
C(10)-H(10A)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-O(15)	1.279(11)
C(13)-O(16)	1.285(11)
C(13)-C(14)	1.509(13)
C(14)-C(15)	1.526(14)
C(14)-C(16)	1.547(14)
C(14)-H(14A)	1.0000
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-O(18)	1.262(11)
C(17)-O(17)	1.268(11)
C(17)-C(18)	1.509(12)
C(18)-C(19)	1.531(15)
C(18)-C(20)	1.538(15)
C(18)-H(18A)	1.0000
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-O(20)	1.274(12)
C(21)-O(19)	1.273(12)
C(21)-C(22)	1.512(13)
C(22)-C(24)	1.519(15)
C(22)-C(23)	1.528(14)
C(22)-H(22A)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800

C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-O(21)	1.254(11)
C(25)-O(22)	1.268(12)
C(25)-C(26)	1.538(13)
C(26)-C(27)	1.535(16)
C(26)-C(28)	1.543(16)
C(26)-H(26A)	1.0000
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-O(23)	1.267(10)
C(29)-O(24)	1.278(11)
C(29)-C(30)	1.502(13)
C(30)-C(31)	1.519(15)
C(30)-C(32)	1.531(14)
C(30)-H(30A)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-O(25)	1.260(11)
C(33)-O(26)	1.270(11)
C(33)-C(34)	1.524(14)
C(34)-C(36)	1.516(15)
C(34)-C(35)	1.533(14)
C(34)-H(34A)	1.0000
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
C(37)-O(27)	1.210(12)
C(37)-O(28)	1.333(11)
C(37)-C(38)	1.517(14)
O(28)-H(28)	0.8400
C(38)-C(39)	1.528(16)
C(38)-C(40)	1.543(16)
C(38)-H(38A)	1.0000
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(40)-H(40A)	0.9800
C(40)-H(40B)	0.9800
C(40)-H(40C)	0.9800

C(41)-O(42)	1.244(12)
C(41)-O(29)	1.254(11)
C(41)-C(43)	1.524(13)
C(43)-C(45)	1.538(14)
C(43)-C(44)	1.566(15)
C(43)-H(43A)	1.0000
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-O(30)	1.195(14)
C(46)-O(31)	1.332(14)
C(46)-C(47)	1.504(16)
C(47)-C(48)	1.507(19)
C(47)-C(49)	1.52(2)
C(47)-H(47A)	1.0000
O(31)-H(31)	0.8400
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(50)-O(32)	1.221(13)
C(50)-O(33)	1.312(13)
C(50)-C(51)	1.520(15)
O(32)-H(32)	0.8400
O(33)-H(33)	0.8400
C(51)-C(53)	1.46(2)
C(51)-C(52)	1.496(18)
C(51)-H(51A)	1.0000
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-O(35)	1.246(11)
C(54)-O(34)	1.270(12)
C(54)-C(55)	1.509(14)
C(55)-C(57)	1.539(16)
C(55)-C(56)	1.543(15)
C(55)-H(55A)	1.0000
C(56)-H(56A)	0.9800
C(56)-H(56B)	0.9800
C(56)-H(56C)	0.9800
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800
C(57)-H(57C)	0.9800

C(58)-O(37)	1.249(11)
C(58)-O(36)	1.258(11)
C(58)-C(59)	1.542(13)
C(59)-C(60)	1.513(15)
C(59)-C(61)	1.515(15)
C(59)-H(59A)	1.0000
O(38)-H(38C)	0.959(10)
O(38)-H(38D)	0.958(10)
C(60)-H(60A)	0.9800
C(60)-H(60B)	0.9800
C(60)-H(60C)	0.9800
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800

**Table S2.** Bond angles [deg.] for complex **IV**.

<b>Complex IV</b>	<b>Bond Angles [deg.]</b>
O(6)-Hf(1)-O(3)	94.7(3)
O(6)-Hf(1)-O(1)	73.6(2)
O(3)-Hf(1)-O(1)	70.0(2)
O(6)-Hf(1)-O(7)	73.9(2)
O(3)-Hf(1)-O(7)	71.4(2)
O(1)-Hf(1)-O(7)	126.2(2)
O(6)-Hf(1)-O(10)	83.6(3)
O(3)-Hf(1)-O(10)	144.8(2)
O(1)-Hf(1)-O(10)	140.8(2)
O(7)-Hf(1)-O(10)	74.4(2)
O(6)-Hf(1)-O(35)	83.2(2)
O(3)-Hf(1)-O(35)	142.2(2)
O(1)-Hf(1)-O(35)	73.3(2)
O(7)-Hf(1)-O(35)	141.6(2)
O(10)-Hf(1)-O(35)	72.7(2)
O(6)-Hf(1)-O(14)	149.7(2)
O(3)-Hf(1)-O(14)	91.2(3)
O(1)-Hf(1)-O(14)	135.8(2)
O(7)-Hf(1)-O(14)	80.0(2)
O(10)-Hf(1)-O(14)	74.8(2)
O(35)-Hf(1)-O(14)	109.4(2)
O(6)-Hf(1)-O(13)	152.2(2)
O(3)-Hf(1)-O(13)	90.0(3)
O(1)-Hf(1)-O(13)	82.4(2)
O(7)-Hf(1)-O(13)	133.1(2)
O(10)-Hf(1)-O(13)	107.8(3)
O(35)-Hf(1)-O(13)	76.5(2)
O(14)-Hf(1)-O(13)	57.2(2)
O(6)-Hf(1)-C(9)	173.3(3)
O(3)-Hf(1)-C(9)	91.9(3)
O(1)-Hf(1)-C(9)	109.9(3)
O(7)-Hf(1)-C(9)	107.3(3)
O(10)-Hf(1)-C(9)	90.4(3)

O(35)-Hf(1)-C(9)	92.2(3)
O(14)-Hf(1)-C(9)	28.6(3)
O(13)-Hf(1)-C(9)	28.6(3)
O(6)-Hf(1)-Hf(5)	32.15(16)
O(3)-Hf(1)-Hf(5)	86.00(17)
O(1)-Hf(1)-Hf(5)	99.47(16)
O(7)-Hf(1)-Hf(5)	42.00(16)
O(10)-Hf(1)-Hf(5)	73.89(16)
O(35)-Hf(1)-Hf(5)	108.81(16)
O(14)-Hf(1)-Hf(5)	119.33(16)
O(13)-Hf(1)-Hf(5)	174.64(18)
C(9)-Hf(1)-Hf(5)	147.9(2)
O(6)-Hf(1)-Hf(2)	31.38(17)
O(3)-Hf(1)-Hf(2)	85.75(17)
O(1)-Hf(1)-Hf(2)	42.44(16)
O(7)-Hf(1)-Hf(2)	99.40(16)
O(10)-Hf(1)-Hf(2)	107.99(17)
O(35)-Hf(1)-Hf(2)	72.95(16)
O(14)-Hf(1)-Hf(2)	176.95(19)
O(13)-Hf(1)-Hf(2)	122.34(17)
C(9)-Hf(1)-Hf(2)	151.0(2)
Hf(5)-Hf(1)-Hf(2)	60.930(11)
O(6)-Hf(1)-Hf(6)	81.41(17)
O(3)-Hf(1)-Hf(6)	33.59(17)
O(1)-Hf(1)-Hf(6)	95.58(17)
O(7)-Hf(1)-Hf(6)	37.94(16)
O(10)-Hf(1)-Hf(6)	112.22(16)
O(35)-Hf(1)-Hf(6)	163.13(16)
O(14)-Hf(1)-Hf(6)	87.45(18)
O(13)-Hf(1)-Hf(6)	115.30(18)
C(9)-Hf(1)-Hf(6)	103.7(2)
Hf(5)-Hf(1)-Hf(6)	59.624(11)
Hf(2)-Hf(1)-Hf(6)	90.259(13)
O(6)-Hf(2)-O(2)	90.6(3)
O(6)-Hf(2)-O(34)	84.8(2)
O(2)-Hf(2)-O(34)	142.3(2)
O(6)-Hf(2)-O(18)	142.7(2)
O(2)-Hf(2)-O(18)	82.9(2)
O(34)-Hf(2)-O(18)	78.6(2)
O(6)-Hf(2)-O(38)	144.4(2)
O(2)-Hf(2)-O(38)	91.5(3)
O(34)-Hf(2)-O(38)	113.5(2)
O(18)-Hf(2)-O(38)	72.7(2)
O(6)-Hf(2)-O(24)	81.5(2)
O(2)-Hf(2)-O(24)	142.4(2)
O(34)-Hf(2)-O(24)	73.9(2)
O(18)-Hf(2)-O(24)	124.2(2)
O(38)-Hf(2)-O(24)	75.4(3)
O(6)-Hf(2)-O(4)	72.7(2)
O(2)-Hf(2)-O(4)	68.6(2)
O(34)-Hf(2)-O(4)	142.9(2)

O(18)-Hf(2)-O(4)	135.9(2)
O(38)-Hf(2)-O(4)	75.1(2)
O(24)-Hf(2)-O(4)	73.9(2)
O(6)-Hf(2)-O(1)	69.8(2)
O(2)-Hf(2)-O(1)	70.6(2)
O(34)-Hf(2)-O(1)	72.7(2)
O(18)-Hf(2)-O(1)	73.4(2)
O(38)-Hf(2)-O(1)	143.3(2)
O(24)-Hf(2)-O(1)	137.3(2)
O(4)-Hf(2)-O(1)	123.1(2)
O(6)-Hf(2)-Hf(4)	82.01(18)
O(2)-Hf(2)-Hf(4)	31.83(17)
O(34)-Hf(2)-Hf(4)	110.64(17)
O(18)-Hf(2)-Hf(4)	73.21(16)
O(38)-Hf(2)-Hf(4)	115.90(19)
O(24)-Hf(2)-Hf(4)	162.39(16)
O(4)-Hf(2)-Hf(4)	95.25(16)
O(1)-Hf(2)-Hf(4)	38.96(16)
O(6)-Hf(2)-Hf(1)	31.54(17)
O(2)-Hf(2)-Hf(1)	82.74(18)
O(34)-Hf(2)-Hf(1)	73.92(16)
O(18)-Hf(2)-Hf(1)	111.25(16)
O(38)-Hf(2)-Hf(1)	172.45(17)
O(24)-Hf(2)-Hf(1)	106.30(17)
O(4)-Hf(2)-Hf(1)	98.15(16)
O(1)-Hf(2)-Hf(1)	38.52(15)
Hf(4)-Hf(2)-Hf(1)	60.714(11)
O(6)-Hf(2)-Hf(5)	30.61(17)
O(2)-Hf(2)-Hf(5)	81.75(17)
O(34)-Hf(2)-Hf(5)	109.70(17)
O(18)-Hf(2)-Hf(5)	162.98(16)
O(38)-Hf(2)-Hf(5)	114.99(16)
O(24)-Hf(2)-Hf(5)	72.78(15)
O(4)-Hf(2)-Hf(5)	42.24(17)
O(1)-Hf(2)-Hf(5)	94.47(14)
Hf(4)-Hf(2)-Hf(5)	89.837(12)
Hf(1)-Hf(2)-Hf(5)	59.442(10)
O(6)-Hf(2)-Hf(3)	81.09(18)
O(2)-Hf(2)-Hf(3)	30.76(17)
O(34)-Hf(2)-Hf(3)	163.74(16)
O(18)-Hf(2)-Hf(3)	108.14(17)
O(38)-Hf(2)-Hf(3)	82.77(17)
O(24)-Hf(2)-Hf(3)	111.70(16)
O(4)-Hf(2)-Hf(3)	37.83(17)
O(1)-Hf(2)-Hf(3)	94.71(15)
Hf(4)-Hf(2)-Hf(3)	59.417(11)
Hf(1)-Hf(2)-Hf(3)	89.817(12)
Hf(5)-Hf(2)-Hf(3)	60.026(11)
O(6)-Hf(2)-H(2)	113.5(15)
O(2)-Hf(2)-H(2)	23.7(14)
O(34)-Hf(2)-H(2)	145(3)

O(18)-Hf(2)-H(2)	69(2)
O(38)-Hf(2)-H(2)	69.6(16)
O(24)-Hf(2)-H(2)	136(2)
O(4)-Hf(2)-H(2)	72(3)
O(1)-Hf(2)-H(2)	85(2)
Hf(4)-Hf(2)-H(2)	47.8(19)
Hf(1)-Hf(2)-H(2)	105.4(15)
Hf(5)-Hf(2)-H(2)	99(2)
Hf(3)-Hf(2)-H(2)	40(2)
O(8)-Hf(3)-O(2)	89.3(3)
O(8)-Hf(3)-O(29)	146.0(2)
O(2)-Hf(3)-O(29)	97.3(2)
O(8)-Hf(3)-O(36)	85.8(2)
O(2)-Hf(3)-O(36)	142.8(2)
O(29)-Hf(3)-O(36)	107.1(2)
O(8)-Hf(3)-O(25)	141.1(2)
O(2)-Hf(3)-O(25)	82.7(3)
O(29)-Hf(3)-O(25)	72.9(2)
O(36)-Hf(3)-O(25)	78.4(2)
O(8)-Hf(3)-O(4)	71.6(2)
O(2)-Hf(3)-O(4)	68.2(2)
O(29)-Hf(3)-O(4)	80.1(2)
O(36)-Hf(3)-O(4)	142.5(2)
O(25)-Hf(3)-O(4)	137.0(2)
O(8)-Hf(3)-O(12)	79.6(2)
O(2)-Hf(3)-O(12)	141.3(3)
O(29)-Hf(3)-O(12)	74.5(2)
O(36)-Hf(3)-O(12)	73.7(2)
O(25)-Hf(3)-O(12)	127.8(2)
O(4)-Hf(3)-O(12)	73.1(2)
O(8)-Hf(3)-O(5)	69.9(2)
O(2)-Hf(3)-O(5)	70.0(2)
O(29)-Hf(3)-O(5)	143.4(2)
O(36)-Hf(3)-O(5)	73.8(2)
O(25)-Hf(3)-O(5)	71.6(2)
O(4)-Hf(3)-O(5)	122.3(2)
O(12)-Hf(3)-O(5)	136.4(2)
O(8)-Hf(3)-Hf(6)	31.56(17)
O(2)-Hf(3)-Hf(6)	82.35(17)
O(29)-Hf(3)-Hf(6)	177.47(18)
O(36)-Hf(3)-Hf(6)	74.41(17)
O(25)-Hf(3)-Hf(6)	109.56(16)
O(4)-Hf(3)-Hf(6)	97.52(17)
O(12)-Hf(3)-Hf(6)	104.16(16)
O(5)-Hf(3)-Hf(6)	38.74(16)
O(8)-Hf(3)-Hf(4)	81.32(18)
O(2)-Hf(3)-Hf(4)	31.56(17)
O(29)-Hf(3)-Hf(4)	120.04(17)
O(36)-Hf(3)-Hf(4)	111.44(16)
O(25)-Hf(3)-Hf(4)	72.05(17)
O(4)-Hf(3)-Hf(4)	94.67(16)

O(12)-Hf(3)-Hf(4)	159.79(17)
O(5)-Hf(3)-Hf(4)	38.64(15)
Hf(6)-Hf(3)-Hf(4)	60.694(10)
O(8)-Hf(3)-Hf(5)	29.98(17)
O(2)-Hf(3)-Hf(5)	80.9(2)
O(29)-Hf(3)-Hf(5)	118.35(18)
O(36)-Hf(3)-Hf(5)	109.89(18)
O(25)-Hf(3)-Hf(5)	161.16(17)
O(4)-Hf(3)-Hf(5)	41.79(16)
O(12)-Hf(3)-Hf(5)	70.99(18)
O(5)-Hf(3)-Hf(5)	94.06(16)
Hf(6)-Hf(3)-Hf(5)	59.117(11)
Hf(4)-Hf(3)-Hf(5)	89.116(13)
O(8)-Hf(3)-Hf(2)	79.74(18)
O(2)-Hf(3)-Hf(2)	30.39(19)
O(29)-Hf(3)-Hf(2)	89.32(18)
O(36)-Hf(3)-Hf(2)	163.57(17)
O(25)-Hf(3)-Hf(2)	108.23(16)
O(4)-Hf(3)-Hf(2)	37.84(15)
O(12)-Hf(3)-Hf(2)	110.92(17)
O(5)-Hf(3)-Hf(2)	93.79(15)
Hf(6)-Hf(3)-Hf(2)	89.173(13)
Hf(4)-Hf(3)-Hf(2)	58.810(11)
Hf(5)-Hf(3)-Hf(2)	59.401(11)
O(8)-Hf(3)-H(2)	113.0(14)
O(2)-Hf(3)-H(2)	24.3(12)
O(29)-Hf(3)-H(2)	74.7(15)
O(36)-Hf(3)-H(2)	144(3)
O(25)-Hf(3)-H(2)	68(2)
O(4)-Hf(3)-H(2)	73(3)
O(12)-Hf(3)-H(2)	138(3)
O(5)-Hf(3)-H(2)	84(2)
Hf(6)-Hf(3)-H(2)	105.3(15)
Hf(4)-Hf(3)-H(2)	47.4(19)
Hf(5)-Hf(3)-H(2)	99(2)
Hf(2)-Hf(3)-H(2)	41(2)
O(2)-Hf(4)-O(3)	96.1(3)
O(2)-Hf(4)-O(26)	84.9(3)
O(3)-Hf(4)-O(26)	143.9(2)
O(2)-Hf(4)-O(1)	75.0(3)
O(3)-Hf(4)-O(1)	70.0(2)
O(26)-Hf(4)-O(1)	143.2(2)
O(2)-Hf(4)-O(5)	74.7(2)
O(3)-Hf(4)-O(5)	69.9(2)
O(26)-Hf(4)-O(5)	75.7(2)
O(1)-Hf(4)-O(5)	125.8(2)
O(2)-Hf(4)-O(17)	85.1(2)
O(3)-Hf(4)-O(17)	142.1(2)
O(26)-Hf(4)-O(17)	74.0(2)
O(1)-Hf(4)-O(17)	73.8(2)
O(5)-Hf(4)-O(17)	144.8(2)

O(2)-Hf(4)-O(16)	150.6(3)
O(3)-Hf(4)-O(16)	87.3(2)
O(26)-Hf(4)-O(16)	75.6(2)
O(1)-Hf(4)-O(16)	132.8(2)
O(5)-Hf(4)-O(16)	79.2(2)
O(17)-Hf(4)-O(16)	109.8(2)
O(2)-Hf(4)-O(15)	152.3(3)
O(3)-Hf(4)-O(15)	84.9(2)
O(26)-Hf(4)-O(15)	110.4(2)
O(1)-Hf(4)-O(15)	79.5(2)
O(5)-Hf(4)-O(15)	130.4(2)
O(17)-Hf(4)-O(15)	77.7(2)
O(16)-Hf(4)-O(15)	57.0(2)
O(2)-Hf(4)-C(13)	178.8(3)
O(3)-Hf(4)-C(13)	83.0(3)
O(26)-Hf(4)-C(13)	95.3(3)
O(1)-Hf(4)-C(13)	105.5(3)
O(5)-Hf(4)-C(13)	104.1(2)
O(17)-Hf(4)-C(13)	96.2(2)
O(16)-Hf(4)-C(13)	28.6(3)
O(15)-Hf(4)-C(13)	28.6(3)
O(2)-Hf(4)-Hf(2)	32.4(2)
O(3)-Hf(4)-Hf(2)	86.30(18)
O(26)-Hf(4)-Hf(2)	110.58(16)
O(1)-Hf(4)-Hf(2)	42.80(16)
O(5)-Hf(4)-Hf(2)	100.07(17)
O(17)-Hf(4)-Hf(2)	74.61(17)
O(16)-Hf(4)-Hf(2)	173.45(17)
O(15)-Hf(4)-Hf(2)	120.71(17)
C(13)-Hf(4)-Hf(2)	148.2(2)
O(2)-Hf(4)-Hf(3)	32.51(18)
O(3)-Hf(4)-Hf(3)	86.23(18)
O(26)-Hf(4)-Hf(3)	75.38(17)
O(1)-Hf(4)-Hf(3)	100.45(16)
O(5)-Hf(4)-Hf(3)	42.45(16)
O(17)-Hf(4)-Hf(3)	111.47(16)
O(16)-Hf(4)-Hf(3)	119.37(16)
O(15)-Hf(4)-Hf(3)	170.56(16)
C(13)-Hf(4)-Hf(3)	146.39(19)
Hf(2)-Hf(4)-Hf(3)	61.773(11)
O(2)-Hf(4)-Hf(1)	82.4(2)
O(3)-Hf(4)-Hf(1)	33.28(18)
O(26)-Hf(4)-Hf(1)	165.97(17)
O(1)-Hf(4)-Hf(1)	36.96(16)
O(5)-Hf(4)-Hf(1)	95.19(17)
O(17)-Hf(4)-Hf(1)	110.58(18)
O(16)-Hf(4)-Hf(1)	113.63(17)
O(15)-Hf(4)-Hf(1)	83.65(17)
C(13)-Hf(4)-Hf(1)	97.3(2)
Hf(2)-Hf(4)-Hf(1)	59.875(11)
Hf(3)-Hf(4)-Hf(1)	90.686(13)

O(8)-Hf(5)-O(6)	89.6(3)
O(8)-Hf(5)-O(23)	141.2(2)
O(6)-Hf(5)-O(23)	83.4(2)
O(8)-Hf(5)-O(11)	85.4(3)
O(6)-Hf(5)-O(11)	141.8(2)
O(23)-Hf(5)-O(11)	77.4(2)
O(8)-Hf(5)-O(21)	85.3(2)
O(6)-Hf(5)-O(21)	143.1(2)
O(23)-Hf(5)-O(21)	121.7(2)
O(11)-Hf(5)-O(21)	74.2(2)
O(8)-Hf(5)-O(9)	143.1(2)
O(6)-Hf(5)-O(9)	84.0(2)
O(23)-Hf(5)-O(9)	74.1(2)
O(11)-Hf(5)-O(9)	120.9(3)
O(21)-Hf(5)-O(9)	78.7(2)
O(8)-Hf(5)-O(7)	70.8(2)
O(6)-Hf(5)-O(7)	70.4(2)
O(23)-Hf(5)-O(7)	139.4(2)
O(11)-Hf(5)-O(7)	141.0(2)
O(21)-Hf(5)-O(7)	73.5(2)
O(9)-Hf(5)-O(7)	72.8(2)
O(8)-Hf(5)-O(4)	69.1(2)
O(6)-Hf(5)-O(4)	69.5(2)
O(23)-Hf(5)-O(4)	72.7(2)
O(11)-Hf(5)-O(4)	73.4(2)
O(21)-Hf(5)-O(4)	139.8(2)
O(9)-Hf(5)-O(4)	139.3(2)
O(7)-Hf(5)-O(4)	122.2(2)
O(8)-Hf(5)-Hf(6)	31.65(18)
O(6)-Hf(5)-Hf(6)	82.22(17)
O(23)-Hf(5)-Hf(6)	163.82(17)
O(11)-Hf(5)-Hf(6)	110.14(18)
O(21)-Hf(5)-Hf(6)	74.44(17)
O(9)-Hf(5)-Hf(6)	111.53(17)
O(7)-Hf(5)-Hf(6)	39.47(15)
O(4)-Hf(5)-Hf(6)	95.26(16)
O(8)-Hf(5)-Hf(1)	81.88(18)
O(6)-Hf(5)-Hf(1)	31.98(16)
O(23)-Hf(5)-Hf(1)	108.81(17)
O(11)-Hf(5)-Hf(1)	165.55(19)
O(21)-Hf(5)-Hf(1)	111.26(17)
O(9)-Hf(5)-Hf(1)	73.59(17)
O(7)-Hf(5)-Hf(1)	38.61(14)
O(4)-Hf(5)-Hf(1)	95.64(15)
Hf(6)-Hf(5)-Hf(1)	60.654(11)
O(8)-Hf(5)-Hf(2)	81.07(16)
O(6)-Hf(5)-Hf(2)	30.29(17)
O(23)-Hf(5)-Hf(2)	73.73(17)
O(11)-Hf(5)-Hf(2)	111.70(17)
O(21)-Hf(5)-Hf(2)	164.54(18)
O(9)-Hf(5)-Hf(2)	108.24(16)

O(7)-Hf(5)-Hf(2)	95.03(14)
O(4)-Hf(5)-Hf(2)	39.33(15)
Hf(6)-Hf(5)-Hf(2)	90.102(12)
Hf(1)-Hf(5)-Hf(2)	59.628(10)
O(8)-Hf(5)-Hf(3)	30.34(17)
O(6)-Hf(5)-Hf(3)	81.36(19)
O(23)-Hf(5)-Hf(3)	110.91(17)
O(11)-Hf(5)-Hf(3)	75.31(19)
O(21)-Hf(5)-Hf(3)	109.39(18)
O(9)-Hf(5)-Hf(3)	163.76(17)
O(7)-Hf(5)-Hf(3)	95.55(15)
O(4)-Hf(5)-Hf(3)	38.92(16)
Hf(6)-Hf(5)-Hf(3)	59.538(11)
Hf(1)-Hf(5)-Hf(3)	90.244(13)
Hf(2)-Hf(5)-Hf(3)	60.573(11)
O(8)-Hf(6)-O(3)	94.5(2)
O(8)-Hf(6)-O(22)	83.2(2)
O(3)-Hf(6)-O(22)	143.9(3)
O(8)-Hf(6)-O(5)	74.1(2)
O(3)-Hf(6)-O(5)	69.6(2)
O(22)-Hf(6)-O(5)	141.7(2)
O(8)-Hf(6)-O(7)	73.6(2)
O(3)-Hf(6)-O(7)	70.7(2)
O(22)-Hf(6)-O(7)	74.2(2)
O(5)-Hf(6)-O(7)	125.6(2)
O(8)-Hf(6)-O(37)	83.1(2)
O(3)-Hf(6)-O(37)	143.0(2)
O(22)-Hf(6)-O(37)	72.7(2)
O(5)-Hf(6)-O(37)	74.3(2)
O(7)-Hf(6)-O(37)	141.4(2)
O(8)-Hf(6)-O(19)	151.4(3)
O(3)-Hf(6)-O(19)	92.1(2)
O(22)-Hf(6)-O(19)	107.0(2)
O(5)-Hf(6)-O(19)	82.3(2)
O(7)-Hf(6)-O(19)	134.5(2)
O(37)-Hf(6)-O(19)	75.0(2)
O(8)-Hf(6)-O(20)	149.5(3)
O(3)-Hf(6)-O(20)	89.1(2)
O(22)-Hf(6)-O(20)	76.4(2)
O(5)-Hf(6)-O(20)	134.8(2)
O(7)-Hf(6)-O(20)	79.1(2)
O(37)-Hf(6)-O(20)	111.4(2)
O(19)-Hf(6)-O(20)	58.3(3)
O(8)-Hf(6)-C(21)	172.5(3)
O(3)-Hf(6)-C(21)	92.9(3)
O(22)-Hf(6)-C(21)	90.0(3)
O(5)-Hf(6)-C(21)	110.0(3)
O(7)-Hf(6)-C(21)	107.7(3)
O(37)-Hf(6)-C(21)	91.8(3)
O(19)-Hf(6)-C(21)	29.2(3)
O(20)-Hf(6)-C(21)	29.2(3)

O(8)-Hf(6)-Hf(5)	31.71(19)
O(3)-Hf(6)-Hf(5)	86.03(18)
O(22)-Hf(6)-Hf(5)	73.17(17)
O(5)-Hf(6)-Hf(5)	99.57(16)
O(7)-Hf(6)-Hf(5)	42.20(16)
O(37)-Hf(6)-Hf(5)	108.07(16)
O(19)-Hf(6)-Hf(5)	176.69(17)
O(20)-Hf(6)-Hf(5)	118.87(18)
C(21)-Hf(6)-Hf(5)	148.1(2)
O(8)-Hf(6)-Hf(3)	32.00(18)
O(3)-Hf(6)-Hf(3)	86.06(17)
O(22)-Hf(6)-Hf(3)	107.94(17)
O(5)-Hf(6)-Hf(3)	42.47(16)
O(7)-Hf(6)-Hf(3)	99.78(16)
O(37)-Hf(6)-Hf(3)	72.44(16)
O(19)-Hf(6)-Hf(3)	121.31(17)
O(20)-Hf(6)-Hf(3)	175.14(17)
C(21)-Hf(6)-Hf(3)	150.5(2)
Hf(5)-Hf(6)-Hf(3)	61.346(11)
O(8)-Hf(6)-Hf(1)	81.08(19)
O(3)-Hf(6)-Hf(1)	33.51(19)
O(22)-Hf(6)-Hf(1)	111.42(18)
O(5)-Hf(6)-Hf(1)	95.22(16)
O(7)-Hf(6)-Hf(1)	37.30(15)
O(37)-Hf(6)-Hf(1)	162.99(16)
O(19)-Hf(6)-Hf(1)	117.52(16)
O(20)-Hf(6)-Hf(1)	85.50(18)
C(21)-Hf(6)-Hf(1)	104.5(2)
Hf(5)-Hf(6)-Hf(1)	59.722(11)
Hf(3)-Hf(6)-Hf(1)	90.751(12)
Hf(1)-O(1)-Hf(4)	106.0(2)
Hf(1)-O(1)-Hf(2)	99.0(2)
Hf(4)-O(1)-Hf(2)	98.2(2)
Hf(4)-O(2)-Hf(2)	115.8(3)
Hf(4)-O(2)-Hf(3)	115.9(3)
Hf(2)-O(2)-Hf(3)	118.9(3)
Hf(4)-O(2)-H(2)	114(6)
Hf(2)-O(2)-H(2)	96(7)
Hf(3)-O(2)-H(2)	91(7)
Hf(4)-O(3)-Hf(1)	113.6(3)
Hf(4)-O(3)-Hf(6)	114.0(3)
Hf(1)-O(3)-Hf(6)	112.9(3)
Hf(2)-O(4)-Hf(3)	104.3(2)
Hf(2)-O(4)-Hf(5)	98.4(3)
Hf(3)-O(4)-Hf(5)	99.3(2)
Hf(2)-O(4)-H(4)	105(7)
Hf(3)-O(4)-H(4)	135(8)
Hf(5)-O(4)-H(4)	109(7)
Hf(4)-O(5)-Hf(6)	106.0(3)
Hf(4)-O(5)-Hf(3)	98.9(2)
Hf(6)-O(5)-Hf(3)	98.8(3)

Hf(4)-O(5)-H(5)	123(7)
Hf(6)-O(5)-H(5)	114(7)
Hf(3)-O(5)-H(5)	113(7)
Hf(2)-O(6)-Hf(1)	117.1(3)
Hf(2)-O(6)-Hf(5)	119.1(3)
Hf(1)-O(6)-Hf(5)	115.9(3)
Hf(1)-O(7)-Hf(6)	104.8(2)
Hf(1)-O(7)-Hf(5)	99.4(2)
Hf(6)-O(7)-Hf(5)	98.3(2)
Hf(1)-O(7)-H(7)	121(3)
Hf(6)-O(7)-H(7)	118(3)
Hf(5)-O(7)-H(7)	111(3)
Hf(6)-O(8)-Hf(5)	116.6(3)
Hf(6)-O(8)-Hf(3)	116.4(3)
Hf(5)-O(8)-Hf(3)	119.7(3)
O(10)-C(1)-O(9)	124.9(9)
O(10)-C(1)-C(2)	117.0(9)
O(9)-C(1)-C(2)	118.1(9)
C(1)-O(9)-Hf(5)	133.7(6)
C(1)-O(10)-Hf(1)	133.0(6)
C(4)-C(2)-C(3)	111.9(13)
C(4)-C(2)-C(1)	108.6(11)
C(3)-C(2)-C(1)	114.0(10)
C(4)-C(2)-H(2A)	107.3
C(3)-C(2)-H(2A)	107.3
C(1)-C(2)-H(2A)	107.3
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
O(12)-C(5)-O(11)	126.0(9)
O(12)-C(5)-C(6)	119.1(9)
O(11)-C(5)-C(6)	114.9(9)
C(5)-O(11)-Hf(5)	132.4(6)
C(5)-O(12)-Hf(3)	134.7(7)
C(7)-C(6)-C(8)	111.8(10)
C(7)-C(6)-C(5)	112.9(9)
C(8)-C(6)-C(5)	108.6(8)
C(7)-C(6)-H(6A)	107.8
C(8)-C(6)-H(6A)	107.8
C(5)-C(6)-H(6A)	107.8
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5

H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
O(14)-C(9)-O(13)	117.5(9)
O(14)-C(9)-C(10)	119.9(10)
O(13)-C(9)-C(10)	122.5(10)
O(14)-C(9)-Hf(1)	58.7(5)
O(13)-C(9)-Hf(1)	59.0(5)
C(10)-C(9)-Hf(1)	172.0(9)
C(9)-O(13)-Hf(1)	92.4(6)
C(9)-O(14)-Hf(1)	92.8(6)
C(11)-C(10)-C(12)	113.8(12)
C(11)-C(10)-C(9)	112.2(11)
C(12)-C(10)-C(9)	113.2(10)
C(11)-C(10)-H(10A)	105.6
C(12)-C(10)-H(10A)	105.6
C(9)-C(10)-H(10A)	105.6
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
O(15)-C(13)-O(16)	115.9(8)
O(15)-C(13)-C(14)	124.5(8)
O(16)-C(13)-C(14)	119.5(8)
O(15)-C(13)-Hf(4)	59.9(5)
O(16)-C(13)-Hf(4)	56.7(4)
C(14)-C(13)-Hf(4)	169.4(6)
C(13)-O(15)-Hf(4)	91.5(5)
C(13)-O(16)-Hf(4)	94.7(5)
C(13)-C(14)-C(15)	111.9(8)
C(13)-C(14)-C(16)	107.9(8)
C(15)-C(14)-C(16)	110.9(9)
C(13)-C(14)-H(14A)	108.7
C(15)-C(14)-H(14A)	108.7
C(16)-C(14)-H(14A)	108.7
C(14)-C(15)-H(15A)	109.5

C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
O(18)-C(17)-O(17)	124.6(8)
O(18)-C(17)-C(18)	117.8(8)
O(17)-C(17)-C(18)	117.5(8)
C(17)-O(17)-Hf(4)	131.9(6)
C(17)-O(18)-Hf(2)	135.5(6)
C(17)-C(18)-C(19)	111.4(8)
C(17)-C(18)-C(20)	108.1(8)
C(19)-C(18)-C(20)	110.6(9)
C(17)-C(18)-H(18A)	108.9
C(19)-C(18)-H(18A)	108.9
C(20)-C(18)-H(18A)	108.9
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
O(20)-C(21)-O(19)	119.3(9)
O(20)-C(21)-C(22)	119.9(9)
O(19)-C(21)-C(22)	120.6(9)
O(20)-C(21)-Hf(6)	60.1(5)
O(19)-C(21)-Hf(6)	59.6(5)
C(22)-C(21)-Hf(6)	168.3(7)
C(21)-O(19)-Hf(6)	91.1(6)
C(21)-O(20)-Hf(6)	90.7(6)
C(21)-C(22)-C(24)	110.6(9)
C(21)-C(22)-C(23)	105.7(8)
C(24)-C(22)-C(23)	113.2(9)
C(21)-C(22)-H(22A)	109.1
C(24)-C(22)-H(22A)	109.1
C(23)-C(22)-H(22A)	109.1
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5

C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
O(21)-C(25)-O(22)	125.4(9)
O(21)-C(25)-C(26)	117.8(9)
O(22)-C(25)-C(26)	116.8(9)
C(25)-O(21)-Hf(5)	132.9(6)
C(25)-O(22)-Hf(6)	133.6(6)
C(27)-C(26)-C(25)	112.2(9)
C(27)-C(26)-C(28)	112.0(10)
C(25)-C(26)-C(28)	106.6(9)
C(27)-C(26)-H(26A)	108.6
C(25)-C(26)-H(26A)	108.6
C(28)-C(26)-H(26A)	108.6
C(26)-C(27)-H(27A)	109.5
C(26)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(26)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(26)-C(28)-H(28A)	109.5
C(26)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(26)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
O(23)-C(29)-O(24)	124.5(8)
O(23)-C(29)-C(30)	116.1(8)
O(24)-C(29)-C(30)	119.4(8)
C(29)-O(23)-Hf(5)	135.0(6)
C(29)-O(24)-Hf(2)	133.7(6)
C(29)-C(30)-C(31)	108.9(9)
C(29)-C(30)-C(32)	112.8(8)
C(31)-C(30)-C(32)	111.9(9)
C(29)-C(30)-H(30A)	107.7
C(31)-C(30)-H(30A)	107.7
C(32)-C(30)-H(30A)	107.7
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5

H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
O(25)-C(33)-O(26)	125.4(10)
O(25)-C(33)-C(34)	117.3(8)
O(26)-C(33)-C(34)	117.3(9)
C(33)-O(25)-Hf(3)	135.8(6)
C(33)-O(26)-Hf(4)	131.2(6)
C(36)-C(34)-C(33)	110.4(8)
C(36)-C(34)-C(35)	110.9(9)
C(33)-C(34)-C(35)	107.8(9)
C(36)-C(34)-H(34A)	109.3
C(33)-C(34)-H(34A)	109.3
C(35)-C(34)-H(34A)	109.3
C(34)-C(35)-H(35A)	109.5
C(34)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(34)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(34)-C(36)-H(36A)	109.5
C(34)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(34)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
O(27)-C(37)-O(28)	123.7(9)
O(27)-C(37)-C(38)	124.8(9)
O(28)-C(37)-C(38)	111.5(9)
C(37)-O(28)-H(28)	109.5
C(37)-C(38)-C(39)	110.1(9)
C(37)-C(38)-C(40)	109.5(9)
C(39)-C(38)-C(40)	111.0(10)
C(37)-C(38)-H(38A)	108.7
C(39)-C(38)-H(38A)	108.7
C(40)-C(38)-H(38A)	108.7
C(38)-C(39)-H(39A)	109.5
C(38)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(38)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(38)-C(40)-H(40A)	109.5
C(38)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	109.5
C(38)-C(40)-H(40C)	109.5
H(40A)-C(40)-H(40C)	109.5
H(40B)-C(40)-H(40C)	109.5
O(42)-C(41)-O(29)	123.5(9)
O(42)-C(41)-C(43)	119.1(8)

O(29)-C(41)-C(43)	117.3(9)
C(41)-O(29)-Hf(3)	144.4(6)
C(41)-C(43)-C(45)	110.4(8)
C(41)-C(43)-C(44)	112.4(8)
C(45)-C(43)-C(44)	110.2(9)
C(41)-C(43)-H(43A)	107.9
C(45)-C(43)-H(43A)	107.9
C(44)-C(43)-H(43A)	107.9
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(43)-C(45)-H(45A)	109.5
C(43)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(43)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
O(30)-C(46)-O(31)	123.3(10)
O(30)-C(46)-C(47)	124.4(11)
O(31)-C(46)-C(47)	112.3(11)
C(46)-C(47)-C(48)	112.5(11)
C(46)-C(47)-C(49)	110.4(11)
C(48)-C(47)-C(49)	111.6(12)
C(46)-C(47)-H(47A)	107.3
C(48)-C(47)-H(47A)	107.3
C(49)-C(47)-H(47A)	107.3
C(46)-O(31)-H(31)	109.5
C(47)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(47)-C(49)-H(49A)	109.5
C(47)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(47)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
O(32)-C(50)-O(33)	124.7(10)
O(32)-C(50)-C(51)	122.7(11)
O(33)-C(50)-C(51)	112.6(10)
C(50)-O(32)-H(32)	109.5
C(50)-O(33)-H(33)	109.5
C(53)-C(51)-C(52)	115.7(13)
C(53)-C(51)-C(50)	112.4(12)
C(52)-C(51)-C(50)	112.8(11)
C(53)-C(51)-H(51A)	104.9

C(52)-C(51)-H(51A)	104.9
C(50)-C(51)-H(51A)	104.9
C(51)-C(52)-H(52A)	109.5
C(51)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(51)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(51)-C(53)-H(53A)	109.5
C(51)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(51)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
O(35)-C(54)-O(34)	124.3(9)
O(35)-C(54)-C(55)	119.6(9)
O(34)-C(54)-C(55)	116.1(8)
C(54)-O(34)-Hf(2)	134.3(6)
C(54)-O(35)-Hf(1)	134.4(7)
C(54)-C(55)-C(57)	111.4(9)
C(54)-C(55)-C(56)	112.5(8)
C(57)-C(55)-C(56)	111.1(10)
C(54)-C(55)-H(55A)	107.2
C(57)-C(55)-H(55A)	107.2
C(56)-C(55)-H(55A)	107.2
C(55)-C(56)-H(56A)	109.5
C(55)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5
C(55)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
C(55)-C(57)-H(57A)	109.5
C(55)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(55)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
O(37)-C(58)-O(36)	125.5(9)
O(37)-C(58)-C(59)	116.9(8)
O(36)-C(58)-C(59)	117.6(9)
C(60)-C(59)-C(61)	111.5(9)
C(60)-C(59)-C(58)	108.3(9)
C(61)-C(59)-C(58)	113.3(8)
C(60)-C(59)-H(59A)	107.9
C(61)-C(59)-H(59A)	107.9
C(58)-C(59)-H(59A)	107.9
C(58)-O(36)-Hf(3)	134.0(6)
C(58)-O(37)-Hf(6)	133.5(6)
Hf(2)-O(38)-H(38C)	135(5)
Hf(2)-O(38)-H(38D)	126(5)
H(38C)-O(38)-H(38D)	99(2)

C(59)-C(60)-H(60A)	109.5
C(59)-C(60)-H(60B)	109.5
H(60A)-C(60)-H(60B)	109.5
C(59)-C(60)-H(60C)	109.5
H(60A)-C(60)-H(60C)	109.5
H(60B)-C(60)-H(60C)	109.5
C(59)-C(61)-H(61A)	109.5
C(59)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(59)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5