

ARTICLE

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The role of halide ions in the carboxylative cyclization of propargyl alcohol with CO₂ on CuX -deposited UiO-67(bpy) MOFs (X = F, Cl, Br, and I): a DFT study

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Supporting Information

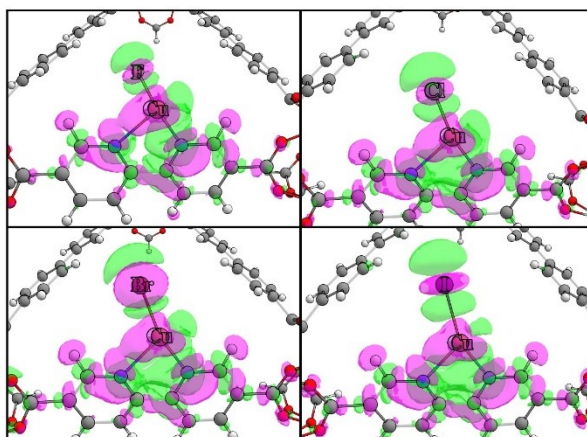


Fig. S1 Illustration of the electron density difference (EDD) (isovalue = 0.001 e a.u.⁻³) of the CuX-deposited UiO-67(bpy) MOF (X = F, Cl, Br, and I). Green and pink regions represent the areas of electron accumulation and electron depletion, respectively.

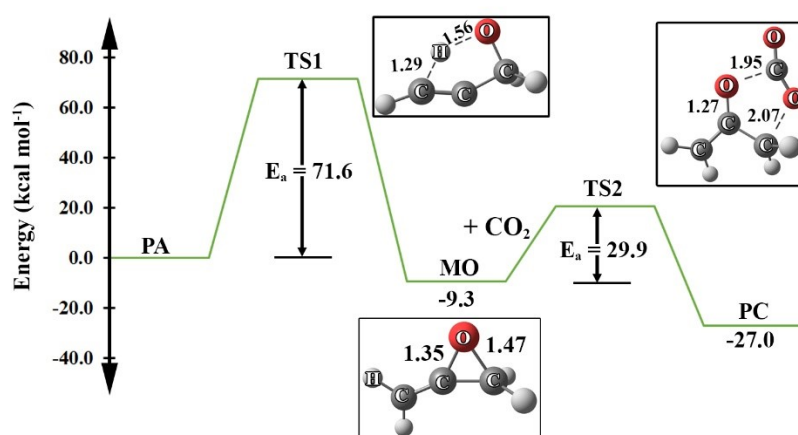


Fig. S2 Energetic profile for the carboxylative cycloaddition of CO₂ with propargyl alcohol through the formation of methyleneoxirane (MO) without a catalyst.

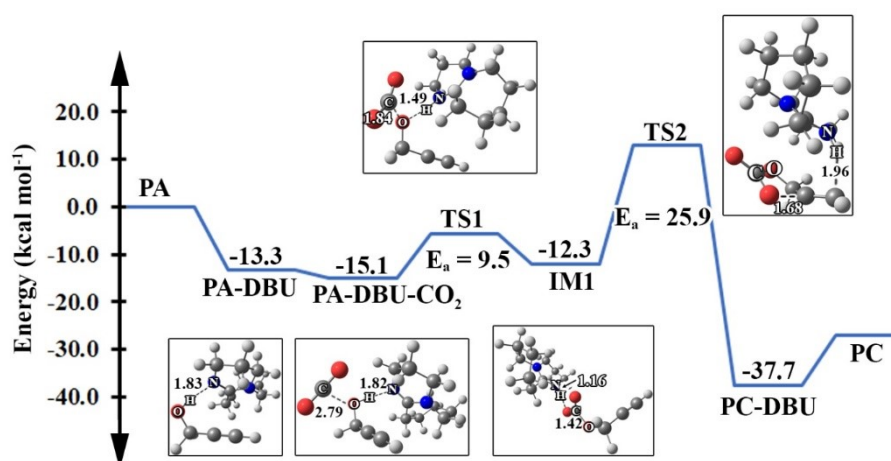


Fig. S3 Energetic profile for the carboxylative cycloaddition of CO₂ with propargyl alcohol catalyzed by the DBU base.

Table S1 Distortion/interaction energy analysis of the propargyl alcohol adsorption on the Cu center of systems in the C-bound configuration (PA complex).
Energies are in kcal mol⁻¹.

Systems	$E_{\text{dist}}(\text{CuX-UiO-67}(\text{bpy}))^{\text{a}}$	$E_{\text{dist}}(\text{PA})^{\text{b}}$	$E_{\text{int}}^{\text{c}}$	E_{ads}
CuF-deposited UiO-67(bpy)	30.7	9.6	-59.2	-18.8
CuCl-deposited UiO-67(bpy)	24.3	7.6	-49.4	-17.5
CuBr-deposited UiO-67(bpy)	23.4	7.7	-47.7	-16.7
CuI-deposited UiO-67(bpy)	18.0	7.6	-42.1	-16.5

$$^{\text{a}}E_{\text{dist}}(\text{CuX-UiO-67}(\text{bpy})) = E_{\text{CuX-UiO-67}(\text{bpy})}^{\text{PA}} - E_{\text{CuX-UiO-67}(\text{bpy})}^{\text{isolated}}$$

$$^{\text{b}}E_{\text{dist}}(\text{PA}) = E_{\text{PA}}^{\text{PA}} - E_{\text{PA}}^{\text{isolated}}$$

$$^{\text{c}}E_{\text{int}} = E_{\text{PA/CuX-UiO-67}(\text{bpy})}^{\text{PA}} - E_{\text{CuX-UiO-67}(\text{bpy})}^{\text{PA}} - E_{\text{PA}}^{\text{PA}}$$

Coordinate all optimized structures.

1. CuF-UiO-67(bpy) system

a. Isolated

N	26.614805000	21.880054000	20.395678000
N	26.745525000	19.944091000	18.425389000
C	26.623720000	20.591445000	20.792807000
C	26.661745000	22.858159000	21.307628000
C	26.774190000	18.999369000	17.450176000
C	26.612416000	19.547714000	19.729491000
C	26.665568000	20.273148000	22.160134000
C	26.705974000	22.634341000	22.694965000
C	26.693320000	17.625985000	17.686423000
C	26.494415000	18.183434000	20.024923000
C	26.701849000	21.292510000	23.101229000
C	26.544296000	17.226312000	19.023073000
C	26.809925000	23.730886000	23.728973000
C	26.809925000	16.592377000	16.590464000
O	26.880885000	24.934153000	23.334955000
O	26.880903000	23.334945000	24.934136000
O	26.880903000	15.387214000	16.986405000
O	26.880885000	16.986395000	15.387197000
Zr	26.878142000	26.881612000	24.237883000
Zr	26.878209000	24.239690000	26.880717000
Zr	26.878209000	13.440633000	16.081660000
Zr	26.878142000	16.083467000	13.439738000
O	24.934203000	26.880849000	23.334882000
O	25.848911000	25.848918000	25.848917000
O	25.849015000	27.912768000	25.849028000
O	27.912782000	25.849032000	25.849031000
O	27.912889000	27.912886000	25.848919000
O	26.880945000	28.827581000	23.334856000
O	28.827591000	26.880922000	23.334870000
O	24.934197000	23.334881000	26.880846000
O	25.849012000	25.849025000	27.912771000
O	27.912892000	25.848913000	27.912887000
O	26.880944000	23.334850000	28.827576000
O	28.827591000	23.334868000	26.880917000
O	25.849012000	12.408579000	14.472325000
O	25.848911000	14.472433000	14.472432000
O	24.934197000	13.440504000	16.986469000
O	26.880944000	11.493774000	16.986500000
O	27.912892000	12.408463000	14.472437000
O	27.912782000	14.472319000	14.472318000
O	28.827591000	13.440433000	16.986482000
O	25.849015000	14.472322000	12.408582000
O	24.934203000	16.986468000	13.440501000
O	27.912889000	14.472431000	12.408464000
O	26.880945000	16.986494000	11.493769000
O	28.827591000	16.986480000	13.440428000
C	23.755332000	26.686089000	23.755213000
Zr	24.236612000	26.881475000	26.880552000
Zr	26.880671000	29.524609000	26.880680000
Zr	29.524440000	26.882357000	26.881381000
C	27.064326000	30.008530000	23.753165000
C	30.008123000	27.066993000	23.753823000
C	23.755714000	23.756676000	26.684338000
Zr	26.880615000	26.881402000	29.524137000
C	27.065914000	23.754135000	30.008060000
C	30.007964000	23.754748000	27.067567000

Zr	24.236612000	13.440798000	13.439875000
Zr	26.880615000	10.797213000	13.439948000
C	23.755714000	13.637012000	16.564674000
C	27.065914000	10.313290000	16.567215000
Zr	29.524440000	13.439969000	13.438993000
C	30.007964000	13.253783000	16.566602000
Zr	26.880671000	13.440670000	10.796741000
C	23.755332000	16.566137000	13.635261000
C	27.064326000	16.568185000	10.312820000
C	30.008123000	16.567527000	13.254357000
O	23.334855000	26.880866000	24.934215000
O	23.334856000	24.934212000	26.880862000
O	25.848909000	27.912895000	27.912897000
O	23.334862000	26.880939000	28.827594000
O	23.334864000	28.827596000	26.880937000
O	24.934210000	30.426941000	26.880925000
O	26.880889000	30.426939000	24.934203000
O	26.880879000	30.426942000	28.827590000
O	27.912786000	27.912776000	27.912777000
O	28.827596000	30.426944000	26.880863000
O	30.426933000	24.934198000	26.880924000
O	30.426936000	26.880929000	24.934199000
O	30.426944000	26.880866000	28.827595000
O	30.426946000	28.827594000	26.880867000
O	24.934211000	26.880924000	30.426942000
O	26.880889000	24.934201000	30.426937000
O	26.880878000	28.827589000	30.426943000
O	28.827598000	26.880862000	30.426940000
O	25.848909000	12.408453000	12.408455000
O	23.334862000	11.493756000	13.440411000
O	23.334855000	15.387135000	13.440484000
O	23.334864000	13.440413000	11.493754000
O	23.334856000	13.440488000	15.387138000
O	24.934211000	9.894408000	13.440426000
O	26.880889000	9.894413000	15.387149000
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O	26.880878000	9.894407000	11.493761000
O	28.827598000	9.894410000	13.440488000
O	30.426944000	11.493755000	13.440484000
O	30.426936000	15.387151000	13.440421000
O	30.426946000	13.440483000	11.493756000
O	30.426933000	13.440426000	15.387152000
O	24.934210000	13.440425000	9.894409000
O	26.880879000	11.493760000	9.894408000
O	26.880889000	15.387147000	9.894411000
O	28.827596000	13.440487000	9.894406000
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C	30.008286000	26.697416000	30.008420000
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C	26.696398000	10.313244000	10.313104000
C	30.008286000	10.312930000	13.623934000
C	30.007968000	13.625768000	10.313113000
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H	30.758179000	27.358190000	23.003211000
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H	30.757581000	23.004153000	27.359935000

H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
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H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
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H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
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H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
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H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
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H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
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C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
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C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
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C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
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C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
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H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000

ARTICLE

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H	15.026933000	28.467383000	15.026933000	C	30.008123000	27.066993000	23.753823000
H	11.853967000	25.294417000	15.026933000	C	23.755714000	23.756676000	26.684338000
H	26.667918000	23.872306000	20.912058000	Zr	26.880615000	26.881402000	29.524137000
H	26.883128000	19.371762000	16.436087000	C	27.065914000	23.754135000	30.008060000
H	26.690551000	19.242247000	22.498070000	C	30.007964000	23.754748000	27.067567000
H	26.363859000	17.864740000	21.053146000	Zr	24.236612000	13.440798000	13.439875000
H	26.744955000	21.065085000	24.161677000	Zr	26.880615000	10.797213000	13.439948000
H	26.474706000	16.168920000	19.255748000	C	23.755714000	13.637012000	16.564674000
Cu	26.887622000	21.783198000	17.976187000	C	27.065914000	10.313290000	16.567215000
F	27.071580000	23.418063000	17.349871000	Zr	29.524440000	13.439969000	13.438993000
b. PA				C	30.007964000	13.253783000	16.566602000
N	26.795872000	21.899425000	20.381593000	Zr	26.880671000	13.440670000	10.796741000
N	26.429501000	19.917235000	18.424116000	C	23.755332000	16.566137000	13.635261000
C	26.611770000	20.621677000	20.771545000	C	27.064326000	16.568185000	10.312820000
C	26.817108000	22.862981000	21.307190000	C	30.008123000	16.567527000	13.254357000
C	26.488826000	18.990906000	17.454235000	O	23.334855000	26.880866000	24.934215000
C	26.631141000	19.559191000	19.717250000	O	23.334856000	24.934212000	26.880862000
C	26.454202000	20.302367000	22.127170000	O	25.848909000	27.912895000	27.912897000
C	26.693073000	22.640604000	22.691334000	O	23.334862000	26.880939000	28.827594000
C	26.718924000	17.627499000	17.686122000	O	23.334864000	28.827596000	26.880937000
C	26.885165000	18.216912000	20.025352000	O	24.934210000	30.426941000	26.880925000
C	26.503020000	21.310099000	23.082209000	O	26.880889000	30.426939000	24.934203000
C	26.908155000	17.256011000	19.022749000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000

Journal Name				ARTICLE			
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H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
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O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
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Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
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O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
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O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
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ARTICLE

Journal Name

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H	9.530447000	22.970897000	13.440450000	O	27.912892000	12.408463000	14.472437000
H	13.440450000	22.970897000	17.350453000	O	27.912782000	14.472319000	14.472318000
H	15.026933000	25.294417000	11.853967000	O	28.827591000	13.440433000	16.986482000
H	11.853967000	28.467383000	11.853967000	O	25.849015000	14.472322000	12.408582000
H	9.530447000	26.880900000	9.530447000	O	24.934203000	16.986468000	13.440501000
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H	26.270644000	19.279365000	22.439945000	Zr	24.236612000	26.881475000	26.880552000
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H	27.095047000	16.212887000	19.257742000	C	27.064326000	30.008530000	23.753165000
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H	23.906188000	24.503246000	18.869185000	Zr	26.880615000	10.797213000	13.439948000
H	22.859957000	23.496224000	17.891160000	C	23.755714000	13.637012000	16.564674000
O	23.521524000	25.303949000	17.053324000	C	27.065914000	10.313290000	16.567215000
H	23.320944000	24.999735000	16.162989000	Zr	29.524440000	13.439969000	13.438993000
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C	26.656993000	20.632897000	20.747721000	C	27.064326000	16.568185000	10.312820000
C	26.378149000	22.853883000	21.339945000	C	30.008123000	16.567527000	13.254357000
C	26.703124000	19.006201000	17.420895000	O	23.334855000	26.880866000	24.934215000
C	26.637034000	19.581367000	19.682991000	O	23.334856000	24.934212000	26.880862000
C	27.025031000	20.322140000	22.068091000	O	25.848909000	27.912895000	27.912897000
C	26.721277000	22.639397000	22.687010000	O	23.334862000	26.880939000	28.827594000
C	26.702275000	17.630622000	17.679021000	O	23.334864000	28.827596000	26.880937000
C	26.577832000	18.218336000	20.015071000	O	24.934210000	30.426941000	26.880925000
C	27.035243000	21.319319000	23.034501000	O	26.880889000	30.426939000	24.934203000
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C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
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O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
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Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
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O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
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Journal Name	ARTICLE						
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C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
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H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
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H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
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H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
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H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000

ARTICLE				Journal Name			
C	13.440450000	30.034298000	10.287052000	H	23.264570000	21.462841000	11.550867000
O	13.440450000	30.426760000	15.387165000	H	24.071575000	19.981621000	11.078812000
O	13.440450000	30.426760000	11.493735000	d. PC/DBU/CO₂			
C	17.333342000	27.201858000	18.960712000	N	26.271672000	21.893237000	20.416812000
C	18.317452000	27.216911000	19.936757000	N	26.523920000	19.942111000	18.379365000
H	16.322082000	27.364756000	19.144577000	C	26.625802000	20.635744000	20.744592000
H	18.007515000	27.477656000	20.830009000	C	26.336833000	22.852823000	21.346739000
H	13.440450000	30.790903000	9.530447000	C	26.576690000	18.988857000	17.424817000
H	17.350453000	26.880900000	9.530447000	C	26.599807000	19.579572000	19.682973000
H	17.350453000	30.790903000	13.440450000	C	27.027680000	20.330409000	22.056922000
H	13.440450000	30.790903000	17.350453000	C	26.712675000	22.641958000	22.686119000
H	9.530447000	30.790903000	13.440450000	C	26.698212000	17.621956000	17.684323000
H	9.530447000	26.880900000	17.350453000	C	26.666800000	18.216833000	20.019755000
H	13.440450000	22.970897000	9.530447000	C	27.048162000	21.325716000	23.024265000
H	9.530447000	22.970897000	13.440450000	C	26.715462000	17.244182000	19.032397000
H	13.440450000	22.970897000	17.350453000	C	26.809925000	23.730886000	23.728973000
H	15.026933000	25.294417000	11.853967000	C	26.809925000	16.592377000	16.590464000
H	11.853967000	28.467383000	11.853967000	O	26.880885000	24.934153000	23.334955000
H	9.530447000	26.880900000	9.530447000	O	26.880903000	23.334945000	24.934136000
H	15.026933000	28.467383000	15.026933000	O	26.880903000	15.387214000	16.986405000
H	11.853967000	25.294417000	15.026933000	O	26.880885000	16.986395000	15.387197000
H	26.121901000	23.856772000	20.998707000	Zr	26.878142000	26.881612000	24.237883000
H	26.699917000	19.380146000	16.401824000	Zr	26.878209000	24.239690000	26.880717000
H	27.326881000	19.315473000	22.339926000	Zr	26.878209000	13.440633000	16.081660000
H	26.478863000	17.916513000	21.052419000	Zr	26.878142000	16.083467000	13.439738000
H	27.310987000	21.095140000	24.060522000	O	24.934203000	26.880849000	23.334882000
H	26.588125000	16.193079000	19.274860000	O	25.848911000	25.848918000	25.848917000
Cu	26.247230000	21.810900000	17.579937000	O	25.849015000	27.912768000	25.849028000
F	25.029583000	20.964395000	16.439088000	O	27.912782000	25.849032000	25.849031000
C	26.267218000	23.704051000	17.122409000	O	27.912889000	27.912886000	25.848919000
C	27.244961000	23.456298000	17.871468000	O	26.880945000	28.827581000	23.334856000
H	28.106066000	23.694577000	18.468566000	O	28.827591000	26.880922000	23.334870000
C	25.308411000	24.343054000	16.189371000	O	24.934197000	23.334881000	26.880846000
H	24.704022000	25.054980000	16.767432000	O	25.849012000	25.849025000	27.912771000
H	24.625983000	23.565292000	15.811979000	O	27.912892000	25.848913000	27.912887000
O	25.942664000	25.043843000	15.156554000	O	26.880944000	23.334850000	28.827576000
H	26.254445000	24.330042000	14.541559000	O	28.827591000	23.334868000	26.880917000
C	25.182228000	23.142502000	10.161624000	O	25.849012000	12.408579000	14.472325000
C	24.333813000	23.974508000	11.122543000	O	25.848911000	14.472433000	14.472432000
C	24.336661000	23.484320000	12.593565000	O	24.934197000	13.440504000	16.986469000
C	24.649239000	21.732579000	9.920101000	O	26.880944000	11.493774000	16.986500000
C	25.377344000	22.438372000	12.897585000	O	27.912892000	12.408463000	14.472437000
C	24.228584000	21.056434000	11.224472000	O	27.912782000	14.472319000	14.472318000
N	25.195230000	21.213999000	12.296258000	O	28.827591000	13.440433000	16.986482000
H	25.273304000	23.667181000	9.204320000	O	25.849015000	14.472322000	12.408582000
H	25.412869000	21.131708000	9.409975000	O	24.934203000	16.986468000	13.440501000
C	27.338140000	21.739500000	14.036068000	O	27.912889000	14.472431000	12.408464000
N	26.356584000	22.753880000	13.682538000	O	26.880945000	16.986494000	11.493769000
C	26.848692000	20.319970000	13.808258000	O	28.827591000	16.986480000	13.440428000
C	26.245910000	20.216383000	12.421855000	C	23.755332000	26.686089000	23.755213000
H	25.806292000	19.231408000	12.243130000	Zr	24.236612000	26.881475000	26.880552000
H	27.591626000	21.883142000	15.096954000	Zr	26.880671000	29.524609000	26.880680000
H	26.202728000	23.078534000	10.563549000	Zr	29.524440000	26.882357000	26.881381000
H	23.780356000	21.761620000	9.249452000	C	27.064326000	30.008530000	23.753165000
H	27.022283000	20.364140000	11.648198000	C	30.008123000	27.066993000	23.753823000
H	28.264904000	21.933159000	13.473259000	C	23.755714000	23.756676000	26.684338000
H	23.302154000	24.021624000	10.750326000	Zr	26.880615000	26.881402000	29.524137000
H	24.705070000	25.003755000	11.099196000	C	27.065914000	23.754135000	30.008060000
H	27.656930000	19.589743000	13.929861000	C	30.007964000	23.754748000	27.067567000
H	26.074767000	20.114586000	14.557509000	Zr	24.236612000	13.440798000	13.439875000
H	24.524047000	24.319260000	13.272543000	Zr	26.880615000	10.797213000	13.439948000
H	23.353735000	23.081159000	12.865476000	C	23.755714000	13.637012000	16.564674000

Journal Name	ARTICLE						
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000
O	26.880879000	30.426942000	28.827590000	H	25.215244000	15.103495000	11.776660000
O	27.912786000	27.912776000	27.912777000	H	25.215244000	28.544690000	25.217855000
O	28.827596000	30.426944000	26.880863000	H	28.555271000	25.223028000	25.222315000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	28.545528000	28.545099000
O	30.426936000	26.880929000	24.934199000	H	25.215026000	25.218505000	28.544917000
O	30.426944000	26.880866000	28.827595000	O	14.472677000	25.848673000	14.472677000
O	30.426946000	28.827594000	26.880867000	O	12.408223000	25.848673000	12.408223000
O	24.934211000	26.880924000	30.426942000	O	14.472677000	25.848673000	12.408223000
O	26.880889000	24.934201000	30.426937000	O	12.408223000	25.848673000	14.472677000
O	26.880878000	28.827589000	30.426943000	Zr	13.440450000	24.397374000	13.440450000
O	28.827598000	26.880862000	30.426940000	O	11.493735000	23.335040000	13.440450000
O	25.848909000	12.408453000	12.408455000	C	10.287052000	23.727502000	13.440450000
O	23.334862000	11.493756000	13.440411000	O	15.387165000	23.335040000	13.440450000
O	23.334855000	15.387135000	13.440484000	C	16.593848000	23.727502000	13.440450000
O	23.334864000	13.440413000	11.493754000	C	17.650268000	22.671082000	13.440450000
O	23.334856000	13.440488000	15.387138000	C	19.634347000	20.687003000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000

ARTICLE

Journal Name

H	23.999268000	19.144577000	13.924306000	H	26.487590000	19.341718000	16.405193000
H	22.313835000	20.830009000	14.037206000	H	27.345679000	19.328556000	22.325647000
Zr	10.956924000	26.880900000	13.440450000	H	26.659815000	17.912654000	21.060486000
O	9.894590000	26.880900000	11.493735000	H	27.347070000	21.102235000	24.043963000
O	12.408223000	27.913127000	14.472677000	H	26.768876000	16.190939000	19.289837000
C	10.287052000	26.880900000	10.287052000	Cu	25.680273000	21.638998000	17.563606000
Zr	15.923976000	26.880900000	13.440450000	F	24.544959000	20.492429000	16.582713000
O	16.986310000	26.880900000	11.493735000	C	25.201040000	23.372548000	16.825495000
C	16.593848000	26.880900000	10.287052000	C	26.193822000	23.523903000	17.579394000
O	16.986310000	26.880900000	15.387165000	H	26.952309000	24.074364000	18.104355000
O	14.472677000	27.913127000	12.408223000	C	24.106853000	23.467495000	15.832267000
C	16.593848000	26.880900000	16.593848000	H	23.183654000	23.719976000	16.369422000
C	17.650268000	26.880900000	17.650268000	H	23.959034000	22.461578000	15.408191000
C	19.634347000	26.880900000	19.634347000	O	24.329041000	24.447087000	14.852091000
O	9.894590000	26.880900000	15.387165000	H	24.892729000	24.009249000	14.162194000
C	10.287052000	26.880900000	16.593848000	C	25.544507000	21.915815000	9.651858000
Zr	13.440450000	26.880900000	15.923976000	C	24.278323000	22.605508000	10.159023000
O	11.493735000	26.880900000	16.986310000	C	24.002132000	22.433767000	11.674614000
O	14.472677000	27.913127000	14.472677000	C	25.522038000	20.391314000	9.742137000
Zr	13.440450000	26.880900000	10.956924000	C	25.191748000	21.933449000	12.448690000
O	11.493735000	26.880900000	9.894590000	C	24.998674000	19.894604000	11.089805000
O	15.387165000	26.880900000	9.894590000	N	25.552704000	20.628804000	12.216546000
O	12.408223000	27.913127000	12.408223000	H	25.731930000	22.215925000	8.615117000
O	15.387165000	26.880900000	16.986310000	H	26.536294000	20.006567000	9.570686000
Zr	13.440450000	29.364426000	13.440450000	C	26.970872000	22.262309000	13.952846000
O	11.493735000	30.426760000	13.440450000	N	25.795996000	22.756592000	13.247927000
C	10.287052000	30.034298000	13.440450000	C	26.879728000	20.774547000	14.238092000
O	15.387165000	30.426760000	13.440450000	C	26.669844000	20.032929000	12.936668000
C	16.593848000	30.034298000	13.440450000	H	26.423287000	18.981733000	13.117994000
O	16.986310000	28.827615000	13.440450000	H	27.074096000	22.831686000	14.884350000
O	9.894590000	28.827615000	13.440450000	H	26.399595000	22.293993000	10.228417000
C	22.671082000	26.880900000	22.671082000	H	24.891460000	19.968194000	8.948701000
C	20.687003000	26.880900000	20.687003000	H	27.582178000	20.041484000	12.315305000
C	21.360638000	27.201858000	22.988008000	H	27.869906000	22.485155000	13.355481000
C	20.384593000	27.216911000	22.003898000	H	23.411226000	22.252344000	9.586613000
H	21.176773000	27.364756000	23.999268000	H	24.365647000	23.674151000	9.940076000
H	19.491341000	27.477656000	22.313835000	H	27.779892000	20.399886000	14.739736000
O	13.440450000	28.827615000	16.986310000	H	26.017952000	20.597372000	14.899175000
C	13.440450000	30.034298000	16.593848000	H	23.711698000	23.387000000	12.120228000
O	13.440450000	28.827615000	9.894590000	H	23.159764000	21.750798000	11.827251000
C	13.440450000	30.034298000	10.287052000	H	23.904586000	19.971833000	11.109004000
O	13.440450000	30.426760000	15.387165000	H	25.238164000	18.838641000	11.241129000
O	13.440450000	30.426760000	11.493735000	C	21.933624000	25.351355000	14.081096000
C	17.333342000	27.201858000	18.960712000	O	21.546049000	25.264647000	15.181102000
C	18.317452000	27.216911000	19.936757000	O	22.241144000	25.461497000	12.957790000
H	16.322082000	27.364756000	19.144577000	e. TS1			
H	18.007515000	27.477656000	20.830009000	N	26.376696000	21.899466000	20.399096000
H	13.440450000	30.790903000	9.530447000	N	26.788826000	19.949514000	18.389092000
H	17.350453000	26.880900000	9.530447000	C	26.670169000	20.633067000	20.748829000
H	17.350453000	30.790903000	13.440450000	C	26.426815000	22.860330000	21.329273000
H	13.440450000	30.790903000	17.350453000	C	26.789935000	19.006210000	17.428482000
H	9.530447000	30.790903000	13.440450000	C	26.654272000	19.580685000	19.684077000
H	9.530447000	26.880900000	17.350453000	C	26.989571000	20.313755000	22.079271000
H	13.440450000	22.970897000	9.530447000	C	26.724044000	22.638769000	22.686542000
H	9.530447000	22.970897000	13.440450000	C	26.704666000	17.631232000	17.678609000
H	13.440450000	22.970897000	17.350453000	C	26.507132000	18.222336000	20.009742000
H	15.026933000	25.294417000	11.853967000	C	26.996914000	21.312484000	23.044672000
H	11.853967000	28.467383000	11.853967000	C	26.549148000	17.252452000	19.018141000
H	9.530447000	26.880900000	9.530447000	C	26.809925000	23.730886000	23.728973000
H	15.026933000	28.467383000	15.026933000	C	26.809925000	16.592377000	16.590464000
H	11.853967000	25.294417000	15.026933000	O	26.880885000	24.934153000	23.334955000
H	26.057043000	23.853043000	21.016129000	O	26.880903000	23.334945000	24.934136000

O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000
O	26.880879000	30.426942000	28.827590000	H	25.215244000	15.103495000	11.776660000
O	27.912786000	27.912776000	27.912777000	H	25.215244000	28.544690000	25.217855000
O	28.827596000	30.426944000	26.880863000	H	28.555271000	25.223028000	25.222315000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	28.545528000	28.545099000
O	30.426936000	26.880929000	24.934199000	H	25.215026000	25.218505000	28.544917000

ARTICLE

Journal Name

O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
C	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.209286000	23.868864000	20.978957000
H	23.999268000	19.144577000	13.924306000	H	26.848316000	19.386996000	16.413255000
H	22.313835000	20.830009000	14.037206000	H	27.257428000	19.299389000	22.359142000
Zr	10.956924000	26.880900000	13.440450000	H	26.342723000	17.926524000	21.040807000
O	9.894590000	26.880900000	11.493735000	H	27.238637000	21.084210000	24.078288000
O	12.408223000	27.913127000	14.472677000	H	26.457016000	16.199165000	19.265209000
C	10.287052000	26.880900000	10.287052000	Cu	26.640264000	21.882203000	17.569478000
Zr	15.923976000	26.880900000	13.440450000	F	25.401520000	21.158109000	16.371355000
O	16.986310000	26.880900000	11.493735000	C	27.113283000	23.788889000	17.318219000
C	16.593848000	26.880900000	10.287052000	C	27.945365000	23.219127000	18.068841000
O	16.986310000	26.880900000	15.387165000	H	28.806241000	23.159008000	18.709487000
O	14.472677000	27.913127000	12.408223000	C	26.378977000	24.825753000	16.531944000
C	16.593848000	26.880900000	16.593848000	H	26.881655000	25.776761000	16.808309000
C	17.650268000	26.880900000	17.650268000	H	25.359944000	24.887669000	16.968678000
C	19.634347000	26.880900000	19.634347000	O	26.365566000	24.649411000	15.180138000
O	9.894590000	26.880900000	15.387165000	H	26.428901000	23.352186000	14.629400000
C	10.287052000	26.880900000	16.593848000	C	25.348277000	23.504834000	10.680130000
Zr	13.440450000	26.880900000	15.923976000	C	24.568988000	24.215658000	11.785737000
O	11.493735000	26.880900000	16.986310000	C	24.415144000	23.412880000	13.100881000
O	14.472677000	27.913127000	14.472677000	C	24.721076000	22.210094000	10.166239000

Journal Name				ARTICLE			
C	25.404399000	22.293974000	13.195154000	O	25.848911000	14.472433000	14.472432000
C	24.279473000	21.278894000	11.297281000	O	24.934197000	13.440504000	16.986469000
N	25.238297000	21.215484000	12.393230000	O	26.880944000	11.493774000	16.986500000
H	25.490795000	24.192159000	9.839886000	O	27.912892000	12.408463000	14.472437000
H	25.438241000	21.695648000	9.514474000	O	27.912782000	14.472319000	14.472318000
C	27.440769000	21.418049000	14.160247000	O	28.827591000	13.440433000	16.986482000
N	26.412624000	22.424553000	14.006080000	O	25.849015000	14.472322000	12.408582000
C	26.923501000	20.064342000	13.718762000	O	24.934203000	16.986468000	13.440501000
C	26.266652000	20.180674000	12.356796000	O	27.912889000	14.472431000	12.408464000
H	25.792034000	19.239975000	12.066182000	O	26.880945000	16.986494000	11.493769000
H	27.724252000	21.405193000	15.220440000	O	28.827591000	16.986480000	13.440428000
H	26.359439000	23.294395000	11.055017000	C	23.755332000	26.686089000	23.755213000
H	23.843600000	22.427470000	9.544161000	Zr	24.236612000	26.881475000	26.880552000
H	27.015077000	20.418749000	11.581682000	Zr	26.880671000	29.524609000	26.880680000
H	28.326843000	21.726466000	13.585778000	Zr	29.524440000	26.882357000	26.881381000
H	23.576038000	24.505037000	11.420260000	C	27.064326000	30.008530000	23.753165000
H	25.100073000	25.142183000	12.021716000	C	30.008123000	27.066993000	23.753823000
H	27.726462000	19.321716000	13.685065000	C	23.755714000	23.756676000	26.684338000
H	26.181757000	19.742319000	14.457061000	Zr	26.880615000	26.881402000	29.524137000
H	24.587479000	24.063574000	13.962229000	C	27.065914000	23.754135000	30.008060000
H	23.407902000	22.995336000	13.195143000	C	30.007964000	23.754748000	27.067567000
H	23.314064000	21.607422000	11.694391000	Zr	24.236612000	13.440798000	13.439875000
H	24.130818000	20.255257000	10.939302000	Zr	26.880615000	10.797213000	13.439948000
C	28.030979000	25.554583000	14.098439000	C	23.755714000	13.637012000	16.564674000
O	28.538766000	26.181746000	14.959501000	C	27.065914000	10.313290000	16.567215000
O	27.805503000	25.074616000	13.040810000	Zr	29.524440000	13.439969000	13.438993000
f. IM1				C	30.007964000	13.253783000	16.566602000
N	26.527769000	21.907811000	20.379973000	Zr	26.880671000	13.440670000	10.796741000
N	26.826763000	19.930001000	18.416861000	C	23.755332000	16.566137000	13.635261000
C	26.666198000	20.623129000	20.762929000	C	27.064326000	16.568185000	10.312820000
C	26.569761000	22.869331000	21.309796000	C	30.008123000	16.567527000	13.254357000
C	26.816705000	18.995817000	17.450885000	O	23.334855000	26.880866000	24.934215000
C	26.646733000	19.564527000	19.705584000	O	23.334856000	24.934212000	26.880862000
C	26.834673000	20.292811000	22.117585000	O	25.848909000	27.912895000	27.912897000
C	26.722002000	22.637390000	22.689219000	O	23.334862000	26.880939000	28.827594000
C	26.693392000	17.623151000	17.685654000	O	23.334864000	28.827596000	26.880937000
C	26.455323000	18.208037000	20.016802000	O	24.934210000	30.426941000	26.880925000
C	26.850126000	21.297953000	23.075468000	O	26.880889000	30.426939000	28.824203000
C	26.503096000	17.242019000	19.020341000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000

ARTICLE

Journal Name

O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000

Journal Name	ARTICLE						
C	13.440450000	30.034298000	16.593848000	H	28.241708000	24.162651000	12.201229000
O	13.440450000	28.827615000	9.894590000	H	26.907510000	24.204982000	13.316337000
C	13.440450000	30.034298000	10.287052000	H	25.323668000	23.071295000	13.871048000
O	13.440450000	30.426760000	15.387165000	H	24.756541000	21.480331000	14.235794000
O	13.440450000	30.426760000	11.493735000	C	30.132389000	24.365335000	14.392622000
C	17.333342000	27.201858000	18.960712000	O	30.568947000	25.314230000	15.026966000
C	18.317452000	27.216911000	19.936757000	O	30.472125000	23.840291000	13.303406000
H	16.322082000	27.364756000	19.144577000	g. TS2			
H	18.007515000	27.477656000	20.830009000	N	26.394432000	21.793768000	20.431161000
H	13.440450000	30.790903000	9.530447000	N	26.744716000	19.905070000	18.498239000
H	17.350453000	26.880900000	9.530447000	C	26.732633000	20.528575000	20.825593000
H	17.350453000	30.790903000	13.440450000	C	26.448516000	22.795450000	21.334855000
H	13.440450000	30.790903000	17.350453000	C	26.707365000	18.991267000	17.507819000
H	9.530447000	30.790903000	13.440450000	C	26.712479000	19.480556000	19.793902000
H	9.530447000	26.880900000	17.350453000	C	27.075765000	20.279817000	22.164802000
H	13.440450000	22.970897000	9.530447000	C	26.746511000	22.621666000	22.696146000
H	9.530447000	22.970897000	13.440450000	C	26.714458000	17.607704000	17.705413000
H	13.440450000	22.970897000	17.350453000	C	26.652735000	18.104674000	20.077819000
H	15.026933000	25.294417000	11.853967000	C	27.052505000	21.303823000	23.095006000
H	11.853967000	28.467383000	11.853967000	C	26.673649000	17.176947000	19.050735000
H	9.530447000	26.880900000	9.530447000	C	26.809925000	23.730886000	23.728973000
H	15.026933000	28.467383000	15.026933000	C	26.809925000	16.592377000	16.590464000
H	11.853967000	25.294417000	15.026933000	O	26.880885000	24.934153000	23.334955000
H	26.475490000	23.890155000	20.942057000	O	26.880903000	23.334945000	24.934136000
H	26.921028000	19.385859000	16.443789000	O	26.880903000	15.387214000	16.986405000
H	26.979511000	19.262434000	22.426846000	O	26.880885000	16.986395000	15.387197000
H	26.262234000	17.905222000	21.040532000	Zr	26.878142000	26.881612000	24.237883000
H	26.982973000	21.062541000	24.126837000	Zr	26.878209000	24.239690000	26.880717000
H	26.389073000	16.189420000	19.261117000	Zr	26.878209000	13.440633000	16.081660000
Cu	27.239565000	21.800914000	17.600965000	Zr	26.878142000	16.083467000	13.439738000
F	25.949852000	21.541714000	16.272707000	O	24.934203000	26.880849000	23.334882000
C	28.453173000	23.301990000	17.242207000	O	25.848911000	25.848918000	25.848917000
C	28.811613000	22.681531000	18.274742000	O	25.849015000	27.912768000	25.849028000
H	29.430451000	22.500767000	19.135142000	O	27.912782000	25.849032000	25.849031000
C	28.408636000	24.233990000	16.103526000	O	27.912889000	27.912886000	25.848919000
H	28.985473000	25.135996000	16.357936000	O	26.880945000	28.827581000	23.334856000
H	27.365058000	24.519007000	15.901872000	O	26.8827591000	26.880922000	23.334870000
O	28.968022000	23.656859000	14.946037000	O	24.934197000	23.334881000	26.880846000
H	29.563397000	22.639503000	12.813438000	O	25.849012000	25.849025000	27.912771000
C	25.491991000	22.490399000	10.977258000	O	27.912892000	25.848913000	27.912887000
C	26.298683000	23.757578000	11.259024000	O	26.880944000	23.334850000	28.827576000
C	27.294709000	23.674438000	12.441301000	O	28.827591000	23.334868000	26.880917000
C	24.574396000	22.041024000	12.112394000	O	25.849012000	12.408579000	14.472325000
C	27.610612000	22.281179000	12.888272000	O	25.848911000	14.472433000	14.472432000
C	25.272503000	22.055358000	13.468380000	O	24.934197000	13.440504000	16.986469000
N	26.633112000	21.526202000	13.385278000	O	26.880944000	11.493774000	16.986500000
H	24.900346000	22.637563000	10.067453000	O	27.912892000	12.408463000	14.472437000
H	24.201262000	21.033823000	11.889243000	O	27.912782000	14.472319000	14.472318000
C	29.290970000	20.594428000	13.355345000	O	28.827591000	13.440433000	16.986482000
N	28.853260000	21.847242000	12.750216000	O	25.849015000	14.472322000	12.408582000
C	28.334999000	20.158357000	14.445498000	O	24.934203000	16.986468000	13.440501000
C	26.916910000	20.192836000	13.915653000	O	27.912889000	14.472431000	12.408464000
H	26.195894000	20.029406000	14.718237000	O	26.880945000	16.986494000	11.493769000
H	30.298013000	20.768565000	13.746268000	O	28.827591000	16.986480000	13.440428000
H	26.190079000	21.674828000	10.743826000	C	23.755332000	26.686089000	23.755213000
H	23.692342000	22.690061000	12.175653000	Zr	24.236612000	26.881475000	26.880552000
H	26.762344000	19.439315000	13.127559000	Zr	26.880671000	29.524609000	26.880680000
H	29.362833000	19.820472000	12.578753000	Zr	29.524440000	26.882357000	26.881381000
H	25.615516000	24.597043000	11.434018000	C	27.064326000	30.008530000	23.753165000
H	26.856224000	24.011096000	10.351943000	C	30.008123000	27.066993000	23.753823000
H	28.579243000	19.150249000	14.789410000	C	23.755714000	23.756676000	26.684338000
H	28.402238000	20.854642000	15.292891000	Zr	26.880615000	26.881402000	29.524137000

ARTICLE

Journal Name

C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000
O	26.880879000	30.426942000	28.827590000	H	25.215244000	15.103495000	11.776660000
O	27.912786000	27.912776000	27.912777000	H	25.215244000	28.544690000	25.217855000
O	28.827596000	30.426944000	26.880863000	H	28.555271000	25.223028000	25.222315000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	28.545528000	28.545099000
O	30.426936000	26.880929000	24.934199000	H	25.215026000	25.218505000	28.544917000
O	30.426944000	26.880866000	28.827595000	O	14.472677000	25.848673000	14.472677000
O	30.426946000	28.827594000	26.880867000	O	12.408223000	25.848673000	12.408223000
O	24.934211000	26.880924000	30.426942000	O	14.472677000	25.848673000	12.408223000
O	26.880889000	24.934201000	30.426937000	O	12.408223000	25.848673000	14.472677000
O	26.880878000	28.827589000	30.426943000	Zr	13.440450000	24.397374000	13.440450000
O	28.827598000	26.880862000	30.426940000	O	11.493735000	23.335040000	13.440450000
O	25.848909000	12.408453000	12.408455000	C	10.287052000	23.727502000	13.440450000
O	23.334862000	11.493756000	13.440411000	O	15.387165000	23.335040000	13.440450000
O	23.334855000	15.387135000	13.440484000	C	16.593848000	23.727502000	13.440450000
O	23.334864000	13.440413000	11.493754000	C	17.650268000	22.671082000	13.440450000
O	23.334856000	13.440488000	15.387138000	C	19.634347000	20.687003000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000

Journal Name				ARTICLE			
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.215523000	23.784974000	20.945241000
H	23.999268000	19.144577000	13.924306000	H	26.695678000	19.394145000	16.500061000
H	22.313835000	20.830009000	14.037206000	H	27.379832000	19.282384000	22.468969000
Zr	10.956924000	26.880900000	13.440450000	H	26.571647000	17.766506000	21.106929000
O	9.894590000	26.880900000	11.493735000	H	27.303255000	21.114949000	24.133605000
O	12.408223000	27.913127000	14.472677000	H	26.647769000	16.113622000	19.263596000
C	10.287052000	26.880900000	10.287052000	Cu	26.057703000	21.860595000	18.287117000
Zr	15.923976000	26.880900000	13.440450000	F	24.721180000	21.170758000	17.070887000
O	16.986310000	26.880900000	11.493735000	C	25.561858000	24.081948000	16.890196000
C	16.593848000	26.880900000	10.287052000	C	26.547847000	23.690116000	17.590139000
O	16.986310000	26.880900000	15.387165000	H	27.548503000	24.095541000	17.655839000
O	14.472677000	27.913127000	12.408223000	C	24.163756000	23.968564000	16.489330000
C	16.593848000	26.880900000	16.593848000	H	23.568356000	24.792916000	16.905352000
C	17.650268000	26.880900000	17.650268000	H	23.792682000	22.997513000	16.840430000
C	19.634347000	26.880900000	19.634347000	O	24.069918000	23.984257000	15.067565000
O	9.894590000	26.880900000	15.387165000	H	24.677976000	22.472662000	14.364521000
C	10.287052000	26.880900000	16.593848000	C	25.742840000	23.357420000	10.447103000
Zr	13.440450000	26.880900000	15.923976000	C	24.263593000	23.325567000	10.818168000
O	11.493735000	26.880900000	16.986310000	C	23.894986000	22.333135000	11.951103000
O	14.472677000	27.913127000	14.472677000	C	26.224618000	22.098377000	9.728453000
Zr	13.440450000	26.880900000	10.956924000	C	25.066424000	21.642425000	12.579134000
O	11.493735000	26.880900000	9.894590000	C	25.691563000	20.830496000	10.388750000
O	15.387165000	26.880900000	9.894590000	N	25.858494000	20.850624000	11.839041000
O	12.408223000	27.913127000	12.408223000	H	25.939796000	24.231067000	9.818931000
O	15.387165000	26.880900000	16.986310000	H	27.320748000	22.075942000	9.697295000
Zr	13.440450000	29.364426000	13.440450000	C	26.415083000	21.264638000	14.599275000
O	11.493735000	30.426760000	13.440450000	N	25.286601000	21.812228000	13.860721000
C	10.287052000	30.034298000	13.440450000	C	26.972152000	20.055303000	13.876046000
O	15.387165000	30.426760000	13.440450000	C	27.113573000	20.330557000	12.391170000
C	16.593848000	30.034298000	13.440450000	H	27.350580000	19.410377000	11.848655000
O	16.986310000	28.827615000	13.440450000	H	26.017668000	21.042937000	15.599660000
O	9.894590000	28.827615000	13.440450000	H	26.320558000	23.529765000	11.364490000
C	22.671082000	26.880900000	22.671082000	H	25.886620000	22.098425000	8.684676000
C	20.687003000	26.880900000	20.687003000	H	27.916899000	21.058083000	12.200355000
C	21.360638000	27.201858000	22.988008000	H	27.168898000	22.057223000	14.705313000
C	20.384593000	27.216911000	22.003898000	H	23.661898000	23.098508000	9.928821000
H	21.176773000	27.364756000	23.999268000	H	23.983838000	24.321019000	11.163985000
H	19.491341000	27.477656000	22.313835000	H	27.945446000	19.778858000	14.290098000
O	13.440450000	28.827615000	16.986310000	H	26.317043000	19.190843000	14.024292000
C	13.440450000	30.034298000	16.593848000	H	23.378337000	22.871404000	12.748582000
O	13.440450000	28.827615000	9.894590000	H	23.211033000	21.557843000	11.584125000
C	13.440450000	30.034298000	10.287052000	H	24.626322000	20.705145000	10.167438000
O	13.440450000	30.426760000	15.387165000	H	26.192705000	19.930408000	10.020446000
O	13.440450000	30.426760000	11.493735000	C	25.081489000	24.842348000	14.493453000
C	17.333342000	27.201858000	18.960712000	O	25.824324000	25.380732000	15.359196000
C	18.317452000	27.216911000	19.936757000	O	25.076222000	24.865829000	13.268476000
H	16.322082000	27.364756000	19.144577000	h. IM2			
H	18.007515000	27.477656000	20.830009000	N	26.835380000	21.812678000	20.417014000
H	13.440450000	30.790903000	9.530447000	N	26.650536000	19.913728000	18.498532000
H	17.350453000	26.880900000	9.530447000	C	26.642388000	20.526337000	20.835701000
H	17.350453000	30.790903000	13.440450000	C	26.818349000	22.814341000	21.319500000
H	13.440450000	30.790903000	17.350453000	C	26.713946000	18.996026000	17.511641000
H	9.530447000	30.790903000	13.440450000	C	26.677982000	19.487148000	19.799854000
H	9.530447000	26.880900000	17.350453000	C	26.450613000	20.264442000	22.205335000
H	13.440450000	22.970897000	9.530447000	C	26.693877000	22.626456000	22.703010000
H	9.530447000	22.970897000	13.440450000	C	26.738567000	17.611238000	17.704676000
H	13.440450000	22.970897000	17.350453000	C	26.759936000	18.109768000	20.078057000
H	15.026933000	25.294417000	11.853967000	C	26.502872000	21.293059000	23.128275000

ARTICLE

Journal Name

C	26.765990000	17.182305000	19.052683000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	10.3123934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000

H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.937374000	23.813576000	20.905347000
H	23.999268000	19.144577000	13.924306000	H	26.741176000	19.398377000	16.499588000
H	22.313835000	20.830009000	14.037206000	H	26.257523000	19.250700000	22.543939000
Zr	10.956924000	26.880900000	13.440450000	H	26.835161000	17.768203000	21.106410000
O	9.894590000	26.880900000	11.493735000	H	26.389364000	21.091665000	24.188504000
O	12.408223000	27.913127000	14.472677000	H	26.822873000	16.120339000	19.265401000
C	10.287052000	26.880900000	10.287052000	Cu	27.038124000	22.032823000	18.351930000
Zr	15.923976000	26.880900000	13.440450000	F	25.750159000	23.536644000	18.224036000
O	16.986310000	26.880900000	11.493735000	C	28.895207000	23.586415000	16.938962000
C	16.593848000	26.880900000	10.287052000	C	28.388459000	22.353986000	16.982303000
O	16.986310000	26.880900000	15.387165000	H	28.766318000	21.661322000	16.220697000
O	14.472677000	27.913127000	12.408223000	C	28.666415000	24.729609000	17.874649000
C	16.593848000	26.880900000	16.593848000	H	29.264198000	24.648845000	18.794202000
C	17.650268000	26.880900000	17.650268000	H	27.611614000	24.844497000	18.146154000
C	19.634347000	26.880900000	19.634347000	O	29.132469000	25.875227000	17.136668000

ARTICLE

Journal Name

H	26.813169000	23.030804000	15.608406000	O	25.849012000	25.849025000	27.912771000
C	23.757583000	26.089690000	14.609133000	O	27.912892000	25.848913000	27.912887000
C	25.228314000	26.255184000	14.977968000	O	26.880944000	23.334850000	28.827576000
C	25.696918000	25.313787000	16.098140000	O	28.827591000	23.334868000	26.880917000
C	22.800454000	26.048677000	15.795475000	O	25.849012000	12.408579000	14.472325000
C	25.099882000	23.953271000	15.984685000	O	25.848911000	14.472433000	14.472432000
C	23.033961000	24.891003000	16.784250000	O	24.934197000	13.440504000	16.986469000
N	23.799598000	23.771652000	16.233324000	O	26.880944000	11.493774000	16.986500000
H	23.457199000	26.901316000	13.938922000	O	27.912892000	12.408463000	14.472437000
H	21.778366000	25.985902000	15.407252000	O	27.912782000	14.472319000	14.472318000
C	25.231408000	21.667678000	15.231811000	O	28.827591000	13.440433000	16.986482000
N	25.810146000	22.990178000	15.403039000	O	25.849015000	14.472322000	12.408582000
C	24.329808000	21.354601000	16.411835000	O	24.934203000	16.986468000	13.440501000
C	23.282035000	22.435847000	16.567684000	O	27.912889000	14.472431000	12.408464000
H	22.949399000	22.476768000	17.611162000	O	26.880945000	16.986494000	11.493769000
H	26.052519000	20.953118000	15.140522000	O	28.827591000	16.986480000	13.440428000
H	23.632768000	25.166254000	14.029113000	C	23.755332000	26.686089000	23.755213000
H	22.853760000	26.991865000	16.352021000	Zr	24.236612000	26.881475000	26.880552000
H	22.396217000	22.255782000	15.947897000	Zr	26.880671000	29.524609000	26.880680000
H	24.675152000	21.649925000	14.285570000	Zr	29.524440000	26.882357000	26.881381000
H	25.427842000	27.282630000	15.300322000	C	27.064326000	30.008530000	23.753165000
H	25.839705000	26.090652000	14.084408000	C	30.008123000	27.066993000	23.753823000
H	23.848613000	20.379870000	16.294663000	C	23.755714000	23.756676000	26.684338000
H	24.948473000	21.319543000	17.314760000	Zr	26.880615000	26.881402000	29.524137000
H	26.784683000	25.214266000	16.078590000	C	27.065914000	23.754135000	30.008060000
H	25.445973000	25.706754000	17.085585000	C	30.007964000	23.754748000	27.067567000
H	23.538195000	25.219726000	17.700662000	Zr	24.236612000	13.440798000	13.439875000
H	22.076388000	24.467447000	17.094471000	Zr	26.880615000	10.797213000	13.439948000
C	29.869482000	25.444644000	16.081452000	C	23.755714000	13.637012000	16.564674000
O	29.808543000	24.092129000	15.974957000	C	27.065914000	10.313290000	16.567215000
O	30.471304000	26.164539000	15.335656000	Zr	29.524440000	13.439969000	13.438993000
i. TS3				C	30.007964000	13.253783000	16.566602000
N	26.890062000	21.792702000	20.435547000	Zr	26.880671000	13.440670000	10.796741000
N	26.606831000	19.919951000	18.490518000	C	23.755332000	16.566137000	13.635261000
C	26.596606000	20.524932000	20.840111000	C	27.064326000	16.568185000	10.312820000
C	26.858482000	22.807074000	21.320657000	C	30.008123000	16.567527000	13.254357000
C	26.695617000	19.000196000	17.502870000	O	23.334855000	26.880866000	24.934215000
C	26.624943000	19.490811000	19.796679000	O	23.334856000	24.934212000	26.880862000
C	26.301679000	20.281536000	22.193779000	O	25.848909000	27.912895000	27.912897000
C	26.671268000	22.629317000	22.699570000	O	23.334862000	26.880939000	28.827594000
C	26.712262000	17.615241000	17.702101000	O	23.334864000	28.827596000	26.880937000
C	26.677793000	18.114937000	20.073144000	O	24.934210000	30.426941000	26.880925000
C	26.382172000	21.311975000	23.116024000	O	26.880889000	30.426939000	24.934203000
C	26.697014000	17.186195000	19.047837000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000

Journal Name	ARTICLE						
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000

ARTICLE

Journal Name

C	21.360638000	27.201858000	22.988008000	H	24.612490000	21.715204000	14.567503000
C	20.384593000	27.216911000	22.003898000	H	26.357889000	27.383164000	15.068013000
H	21.176773000	27.364756000	23.999268000	H	26.964255000	26.227809000	13.904773000
H	19.491341000	27.477656000	22.313835000	H	23.151196000	21.309510000	16.548434000
O	13.440450000	28.827615000	16.986310000	H	24.303944000	22.184947000	17.578186000
C	13.440450000	30.034298000	16.593848000	H	27.457437000	24.907616000	15.709165000
O	13.440450000	28.827615000	9.894590000	H	26.439293000	25.821973000	16.803154000
C	13.440450000	30.034298000	10.287052000	H	24.482529000	26.413568000	16.943338000
O	13.440450000	30.426760000	15.387165000	H	22.824065000	25.880322000	16.820156000
O	13.440450000	30.426760000	11.493735000	C	31.220338000	23.529213000	17.710276000
C	17.333342000	27.201858000	18.960712000	O	30.444921000	22.519933000	17.199174000
C	18.317452000	27.216911000	19.936757000	O	32.415235000	23.510512000	17.738870000
H	16.322082000	27.364756000	19.144577000	j. PC/DBU			
H	18.007515000	27.477656000	20.830009000	N	26.726074000	21.888948000	20.393148000
H	13.440450000	30.790903000	9.530447000	N	26.505034000	19.932356000	18.435208000
H	17.350453000	26.880900000	9.530447000	C	26.602725000	20.594284000	20.778165000
H	17.350453000	30.790903000	13.440450000	C	26.746502000	22.857747000	21.324387000
H	13.440450000	30.790903000	17.350453000	C	26.558055000	19.009789000	17.465048000
H	9.530447000	30.790903000	13.440450000	C	26.627900000	19.538870000	19.721034000
H	9.530447000	26.880900000	17.350453000	C	26.493244000	20.287084000	22.142368000
H	13.440450000	22.970897000	9.530447000	C	26.685105000	22.629110000	22.702469000
H	9.530447000	22.970897000	13.440450000	C	26.715344000	17.630106000	17.688212000
H	13.440450000	22.970897000	17.350453000	C	26.811376000	18.185700000	20.039665000
H	15.026933000	25.294417000	11.853967000	C	26.553584000	21.291756000	23.098282000
H	11.853967000	28.467383000	11.853967000	C	26.844497000	17.237487000	19.026717000
H	9.530447000	26.880900000	9.530447000	C	26.809932000	23.730853000	23.728958000
H	15.026933000	28.467383000	15.026933000	C	26.809917000	16.592419000	16.590473000
H	11.853967000	25.294417000	15.026933000	O	26.880881000	24.934154000	23.334956000
H	27.011167000	23.794386000	20.888582000	O	26.880908000	23.334959000	24.934140000
H	26.748220000	19.401421000	16.491950000	O	26.880899000	15.387217000	16.986414000
H	26.006216000	19.288393000	22.520062000	O	26.880891000	16.986368000	15.387189000
H	26.731783000	17.777943000	21.104257000	Zr	26.878141000	26.881612000	24.237883000
H	26.205024000	21.123790000	24.170320000	Zr	26.878204000	24.239690000	26.880717000
H	26.736863000	16.123585000	19.261146000	Zr	26.878213000	13.440633000	16.081660000
Cu	26.896651000	21.946819000	18.334846000	Zr	26.878141000	16.083467000	13.439738000
F	26.310272000	23.755477000	18.386032000	O	24.934203000	26.880849000	23.334882000
C	29.099818000	22.883027000	17.235766000	O	25.848911000	25.848918000	25.848917000
C	28.134146000	22.161155000	16.632379000	O	25.849015000	27.912768000	25.849028000
H	28.536075000	21.281086000	16.119825000	O	27.912782000	25.849032000	25.849031000
C	29.058648000	24.133661000	18.068628000	O	27.912889000	27.912886000	25.848919000
H	28.690368000	23.948354000	19.083533000	O	26.880945000	28.827581000	23.334856000
H	28.459634000	24.941725000	17.649348000	O	28.827591000	26.880922000	23.334870000
O	30.437568000	24.533189000	18.148592000	O	24.934197000	23.334881000	26.880846000
H	27.050667000	22.671801000	16.084810000	O	25.849012000	25.849025000	27.912771000
C	24.831906000	26.272235000	14.019880000	O	27.912892000	25.848913000	27.912887000
C	26.205985000	26.367971000	14.681170000	O	26.880944000	23.334850000	28.827576000
C	26.463342000	25.346804000	15.817467000	O	28.827591000	23.334868000	26.880917000
C	23.661311000	26.593018000	14.944449000	O	25.849012000	12.408579000	14.472325000
C	25.493293000	24.204417000	15.846809000	O	25.848911000	14.472433000	14.472432000
C	23.779913000	25.882312000	16.292428000	O	24.934197000	13.440504000	16.986469000
N	24.209121000	24.497086000	16.170720000	O	26.880944000	11.493774000	16.986500000
H	24.799861000	26.934620000	13.148527000	O	27.912892000	12.408463000	14.472437000
H	22.721073000	26.315716000	14.452078000	O	27.912782000	14.472319000	14.472318000
C	25.006758000	21.897852000	15.577073000	O	28.827591000	13.440433000	16.986482000
N	25.934018000	23.015139000	15.534942000	O	25.849015000	14.472322000	12.408582000
C	23.879187000	22.126085000	16.567333000	O	24.934203000	16.986468000	13.440501000
C	23.206705000	23.444629000	16.246531000	O	27.912889000	14.472431000	12.408464000
H	22.486730000	23.721634000	17.025022000	O	26.880945000	16.986494000	11.493769000
H	25.585137000	21.003479000	15.846962000	O	28.827591000	16.986480000	13.440428000
H	24.705182000	25.255788000	13.623007000	C	23.755332000	26.686089000	23.755213000
H	23.605146000	27.672676000	15.131506000	Zr	24.236612000	26.881475000	26.880552000
H	22.648256000	23.383618000	15.298374000	Zr	26.880671000	29.524609000	26.880680000

Journal Name				ARTICLE			
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758588000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000
O	26.880879000	30.426942000	28.827590000	H	25.215244000	15.103495000	11.776660000
O	27.912786000	27.912776000	27.912777000	H	25.215244000	28.544690000	25.217855000
O	28.827596000	30.426944000	26.880863000	H	28.555271000	25.223028000	25.222315000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	28.545528000	28.545099000
O	30.426936000	26.880929000	24.934199000	H	25.215026000	25.218505000	28.544917000
O	30.426944000	26.880866000	28.827595000	O	14.472677000	25.848673000	14.472677000
O	30.426946000	28.827594000	26.880867000	O	12.408223000	25.848673000	12.408223000
O	24.934211000	26.880924000	30.426942000	O	14.472677000	25.848673000	12.408223000
O	26.880889000	24.934201000	30.426937000	O	12.408223000	25.848673000	14.472677000
O	26.880878000	28.827589000	30.426943000	Zr	13.440450000	24.397374000	13.440450000
O	28.827598000	26.880862000	30.426940000	O	11.493735000	23.335040000	13.440450000
O	25.848909000	12.408453000	12.408455000	C	10.287052000	23.727502000	13.440450000
O	23.334862000	11.493756000	13.440411000	O	15.387165000	23.335040000	13.440450000
O	23.334855000	15.387135000	13.440484000	C	16.593848000	23.727502000	13.440450000
O	23.334864000	13.440413000	11.493754000	C	17.650268000	22.671082000	13.440450000
O	23.334856000	13.440488000	15.387138000	C	19.634347000	20.687003000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000

ARTICLE

Journal Name

C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.837234000	23.870273000	20.946632000
H	23.999268000	19.144577000	13.924306000	H	26.466048000	19.386981000	16.447372000
H	22.313835000	20.830009000	14.037206000	H	26.374541000	19.257528000	22.461532000
Zr	10.956924000	26.880900000	13.440450000	H	26.969472000	17.873381000	21.066471000
O	9.894590000	26.880900000	11.493735000	H	26.503997000	21.054382000	24.156230000
O	12.408223000	27.913127000	14.472677000	H	26.993307000	16.187126000	19.255935000
C	10.287052000	26.880900000	10.287052000	Cu	27.166740000	22.329384000	18.382402000
Zr	15.923976000	26.880900000	13.440450000	F	25.750436000	23.367705000	17.807838000
O	16.986310000	26.880900000	11.493735000	C	29.139185000	21.890415000	18.579445000
C	16.593848000	26.880900000	10.287052000	C	28.808631000	22.088746000	17.251296000
O	16.986310000	26.880900000	15.387165000	H	28.688120000	21.231609000	16.595710000
O	14.472677000	27.913127000	12.408223000	C	29.768796000	22.843060000	19.554934000
C	16.593848000	26.880900000	16.593848000	H	29.154738000	23.723241000	19.766173000
C	17.650268000	26.880900000	17.650268000	H	30.763973000	23.184467000	19.242596000
C	19.634347000	26.880900000	19.634347000	O	29.905577000	22.037941000	20.739320000
O	9.894590000	26.880900000	15.387165000	H	29.032232000	23.049337000	16.801780000
C	10.287052000	26.880900000	16.593848000	C	26.537474000	28.455200000	19.318326000
Zr	13.440450000	26.880900000	15.923976000	C	27.016220000	27.386847000	20.292524000
O	11.493735000	26.880900000	16.986310000	C	27.122983000	25.971244000	19.695937000
O	14.472677000	27.913127000	14.472677000	C	25.194647000	28.174556000	18.654595000
Zr	13.440450000	26.880900000	10.956924000	C	27.370483000	25.895611000	18.214883000
O	11.493735000	26.880900000	9.894590000	C	25.098458000	26.788222000	18.007625000
O	15.387165000	26.880900000	9.894590000	N	26.350106000	26.344335000	17.406092000
O	12.408223000	27.913127000	12.408223000	H	26.490270000	29.419918000	19.838270000
O	15.387165000	26.880900000	16.986310000	H	25.018278000	28.944220000	17.893231000
Zr	13.440450000	29.364426000	13.440450000	C	28.671416000	25.495860000	16.355109000
O	11.493735000	30.426760000	13.440450000	N	28.521118000	25.461364000	17.800248000
C	10.287052000	30.034298000	13.440450000	C	27.420287000	24.986759000	15.654109000
O	15.387165000	30.426760000	13.440450000	C	26.249131000	25.871232000	16.023260000
C	16.593848000	30.034298000	13.440450000	H	25.317158000	25.300903000	15.927051000
O	16.986310000	28.827615000	13.440450000	H	29.555664000	24.909052000	16.071415000
O	9.894590000	28.827615000	13.440450000	H	27.293774000	28.572123000	18.531443000
C	22.671082000	26.880900000	22.671082000	H	24.381074000	28.277205000	19.383715000
C	20.687003000	26.880900000	20.687003000	H	26.179525000	26.745975000	15.358423000
C	21.360638000	27.201858000	22.988008000	H	28.881242000	26.528916000	16.026653000
C	20.384593000	27.216911000	22.003898000	H	26.353547000	27.355859000	21.164921000
H	21.176773000	27.364756000	23.999268000	H	27.997169000	27.686945000	20.675106000
H	19.491341000	27.477656000	22.313835000	H	27.540765000	24.956189000	14.566032000
O	13.440450000	28.827615000	16.986310000	H	27.199423000	23.974485000	16.008731000
C	13.440450000	30.034298000	16.593848000	H	27.952697000	25.446303000	20.178946000
O	13.440450000	28.827615000	9.894590000	H	26.208405000	25.405683000	19.911094000
C	13.440450000	30.034298000	10.287052000	H	24.744720000	26.033257000	18.721701000
O	13.440450000	30.426760000	15.387165000	H	24.347792000	26.807617000	17.212370000
O	13.440450000	30.426760000	11.493735000	C	29.697407000	20.741158000	20.433404000
C	17.333342000	27.201858000	18.960712000	O	29.355364000	20.611929000	19.115102000
C	18.317452000	27.216911000	19.936757000	O	29.782293000	19.822150000	21.196552000
H	16.322082000	27.364756000	19.144577000	k. PC			
H	18.007515000	27.477656000	20.830009000	N	26.662566000	21.873041000	20.395749000
H	13.440450000	30.790903000	9.530447000	N	26.532033000	19.917774000	18.454964000
H	17.350453000	26.880900000	9.530447000	C	26.628707000	20.576281000	20.793849000
H	17.350453000	30.790903000	13.440450000	C	26.675585000	22.855944000	21.314280000
H	13.440450000	30.790903000	17.350453000	C	26.575322000	19.006433000	17.475498000
H	9.530447000	30.790903000	13.440450000	C	26.638677000	19.517448000	19.738927000

C	26.616880000	20.274473000	22.162281000	O	25.848909000	27.912895000	27.912897000
C	26.697725000	22.631569000	22.697219000	O	23.334862000	26.880939000	28.827594000
C	26.712480000	17.624432000	17.691783000	O	23.334864000	28.827596000	26.880937000
C	26.787644000	18.158790000	20.049767000	O	24.934210000	30.426941000	26.880925000
C	26.666901000	21.291446000	23.104501000	O	26.880889000	30.426939000	24.934203000
C	26.817935000	17.219648000	19.028655000	O	26.880879000	30.426942000	28.827590000
C	26.809926000	23.730842000	23.728933000	O	27.912786000	27.912776000	27.912777000
C	26.809921000	16.592429000	16.590498000	O	28.827596000	30.426944000	26.880863000
O	26.880884000	24.934158000	23.334969000	O	30.426933000	24.934198000	26.880924000
O	26.880907000	23.334959000	24.934140000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387213000	16.986401000	O	30.426944000	26.880866000	28.827595000
O	26.880889000	16.986370000	15.387189000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878206000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878210000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878141000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000

ARTICLE

Journal Name

H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.677363000	23.870737000	20.920394000
H	23.999268000	19.144577000	13.924306000	H	26.495027000	19.395576000	16.461580000
H	22.313835000	20.830009000	14.037206000	H	26.583370000	19.243605000	22.496477000
Zr	10.956924000	26.880900000	13.440450000	H	26.915141000	17.830087000	21.075479000
O	9.894590000	26.880900000	11.493735000	H	26.687230000	21.064015000	24.165316000
O	12.408223000	27.913127000	14.472677000	H	26.944638000	16.165105000	19.250762000
C	10.287052000	26.880900000	10.287052000	Cu	27.054482000	22.245775000	18.372172000
Zr	15.923976000	26.880900000	13.440450000	F	25.585140000	23.078500000	17.688765000
O	16.986310000	26.880900000	11.493735000	C	29.049607000	21.969159000	18.516758000
C	16.593848000	26.880900000	10.287052000	C	28.672676000	22.342839000	17.233608000

H	28.608502000	21.592549000	16.451353000	C	30.008123000	27.066993000	23.753823000
C	29.674318000	22.786854000	19.611386000	C	23.755714000	23.756676000	26.684338000
H	29.049382000	23.606685000	19.976534000	Zr	26.880615000	26.881402000	29.524137000
H	30.661424000	23.186518000	19.339698000	C	27.065914000	23.754135000	30.008060000
O	29.846132000	21.829552000	20.664849000	C	30.007964000	23.754748000	27.067567000
H	28.782301000	23.376295000	16.920188000	Zr	24.236612000	13.440798000	13.439875000
C	29.731699000	20.580621000	20.154211000	Zr	26.880615000	10.797213000	13.439948000
O	29.386343000	20.638590000	18.835621000	C	23.755714000	13.637012000	16.564674000
O	29.895264000	19.567752000	20.770176000	C	27.065914000	10.313290000	16.567215000
2. CuCl-UiO-67(bpy) system				Zr	29.524440000	13.439969000	13.438993000
a. Isolated				C	30.007964000	13.253783000	16.566602000
N	26.713344000	21.854901000	20.404318000	Zr	26.880671000	13.440670000	10.796741000
N	26.619382000	19.932484000	18.448804000	C	23.755332000	16.566137000	13.635261000
C	26.627280000	20.572081000	20.812619000	C	27.064326000	16.568185000	10.312820000
C	26.734458000	22.844365000	21.306952000	C	30.008123000	16.567527000	13.254357000
C	26.659392000	19.002379000	17.464903000	O	23.334855000	26.880866000	24.934215000
C	26.639316000	19.524707000	19.752156000	O	23.334856000	24.934212000	26.880862000
C	26.542058000	20.270003000	22.179888000	O	25.848909000	27.912895000	27.912897000
C	26.694914000	22.631662000	22.696213000	O	23.334862000	26.880939000	28.827594000
C	26.708010000	17.623366000	17.693446000	O	23.334864000	28.827596000	26.880937000
C	26.680960000	18.157387000	20.048628000	O	24.934210000	30.426941000	26.880925000
C	26.587425000	21.297436000	23.112662000	O	26.880889000	30.426939000	24.934203000
C	26.710815000	17.212017000	19.034135000	O	26.880879000	30.426942000	28.827590000
C	26.809916000	23.730872000	23.728975000	O	27.912786000	27.912776000	27.912777000
C	26.809921000	16.592371000	16.590484000	O	28.827596000	30.426944000	26.880863000
O	26.880884000	24.934148000	23.334939000	O	30.426933000	24.934198000	26.880924000
O	26.880896000	23.334956000	24.934140000	O	30.426936000	26.880929000	24.934199000
O	26.880902000	15.387209000	16.986389000	O	30.426944000	26.880866000	28.827595000
O	26.880882000	16.986414000	15.387203000	O	30.426946000	28.827594000	26.880867000
Zr	26.878150000	26.881612000	24.237884000	O	24.934211000	26.880924000	30.426942000
Zr	26.878217000	24.239691000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878215000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878146000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000

ARTICLE

Journal Name

H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000

H	9.530447000	22.970897000	13.440450000	C	23.755332000	26.686089000	23.755213000
H	13.440450000	22.970897000	17.350453000	Zr	24.236612000	26.881475000	26.880552000
H	15.026933000	25.294417000	11.853967000	Zr	26.880671000	29.524609000	26.880680000
H	11.853967000	28.467383000	11.853967000	Zr	29.524440000	26.882357000	26.881381000
H	9.530447000	26.880900000	9.530447000	C	27.064326000	30.008530000	23.753165000
H	15.026933000	28.467383000	15.026933000	C	30.008123000	27.066993000	23.753823000
H	11.853967000	25.294417000	15.026933000	C	23.755714000	23.756676000	26.684338000
H	26.798487000	23.852230000	20.900248000	Zr	26.880615000	26.881402000	29.524137000
H	26.654633000	19.388008000	16.449416000	C	27.065914000	23.754135000	30.008060000
H	26.443506000	19.245696000	22.524440000	C	30.007964000	23.754748000	27.067567000
H	26.706383000	17.826723000	21.081197000	Zr	24.236612000	13.440798000	13.439875000
H	26.545622000	21.081731000	24.175624000	Zr	26.880615000	10.797213000	13.439948000
H	26.752643000	16.151899000	19.260635000	C	23.755714000	13.637012000	16.564674000
Cu	26.537294000	21.839769000	18.078293000	C	27.065914000	10.313290000	16.567215000
Cl	26.345523000	23.769481000	17.227127000	Zr	29.524440000	13.439969000	13.438993000
b. PA				C	30.007964000	13.253783000	16.566602000
N	26.725991000	21.886355000	20.387893000	Zr	26.880671000	13.440670000	10.796741000
N	26.408433000	19.908302000	18.449230000	C	23.755332000	16.566137000	13.635261000
C	26.655757000	20.601097000	20.789338000	C	27.064326000	16.568185000	10.312820000
C	26.738231000	22.858201000	21.306364000	C	30.008123000	16.567527000	13.254357000
C	26.453933000	18.985354000	17.472300000	O	23.334855000	26.880866000	24.934215000
C	26.669169000	19.544803000	19.731375000	O	23.334856000	24.934212000	26.880862000
C	26.581739000	20.281271000	22.151500000	O	25.848909000	27.912895000	27.912897000
C	26.702986000	22.634735000	22.694238000	O	23.334862000	26.880939000	28.827594000
C	26.724491000	17.626840000	17.689817000	O	23.334864000	28.827596000	26.880937000
C	26.956942000	18.206654000	20.024480000	O	24.934210000	30.426941000	26.880925000
C	26.610702000	21.297468000	23.098008000	O	26.880889000	30.426939000	24.934203000
C	26.965383000	17.251656000	19.016976000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
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ARTICLE

Journal Name

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C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
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Journal Name				ARTICLE			
H	17.350453000	30.790903000	13.440450000	O	28.827591000	23.334868000	26.880917000
H	13.440450000	30.790903000	17.350453000	O	25.849012000	12.408579000	14.472325000
H	9.530447000	30.790903000	13.440450000	O	25.848911000	14.472433000	14.472432000
H	9.530447000	26.880900000	17.350453000	O	24.934197000	13.440504000	16.986469000
H	13.440450000	22.970897000	9.530447000	O	26.880944000	11.493774000	16.986500000
H	9.530447000	22.970897000	13.440450000	O	27.912892000	12.408463000	14.472437000
H	13.440450000	22.970897000	17.350453000	O	27.912782000	14.472319000	14.472318000
H	15.026933000	25.294417000	11.853967000	O	28.827591000	13.440433000	16.986482000
H	11.853967000	28.467383000	11.853967000	O	25.849015000	14.472322000	12.408582000
H	9.530447000	26.880900000	9.530447000	O	24.934203000	16.986468000	13.440501000
H	15.026933000	28.467383000	15.026933000	O	27.912889000	14.472431000	12.408464000
H	11.853967000	25.294417000	15.026933000	O	26.880945000	16.986494000	11.493769000
H	26.787987000	23.876329000	20.922651000	O	28.827591000	16.986480000	13.440428000
H	26.247804000	19.346724000	16.467624000	C	23.755332000	26.686089000	23.755213000
H	26.479045000	19.251346000	22.477714000	Zr	24.236612000	26.881475000	26.880552000
H	27.189478000	17.910814000	21.041820000	Zr	26.880671000	29.524609000	26.880680000
H	26.563539000	21.069692000	24.158245000	Zr	29.524440000	26.882357000	26.881381000
H	27.179381000	16.211104000	19.239193000	C	27.064326000	30.008530000	23.753165000
Cu	25.517728000	21.749016000	18.240722000	C	30.008123000	27.066993000	23.753823000
Cl	23.650858000	21.297688000	19.432920000	C	23.755714000	23.756676000	26.684338000
C	25.170271000	23.500205000	17.451496000	Zr	26.880615000	26.881402000	29.524137000
C	26.217836000	23.047198000	16.932923000	C	27.065914000	23.754135000	30.008060000
H	27.096113000	23.040758000	16.315844000	C	30.007964000	23.754748000	27.067567000
C	23.998193000	24.312324000	17.819178000	Zr	24.236612000	13.440798000	13.439875000
H	24.071947000	24.572449000	18.880040000	Zr	26.880615000	10.797213000	13.439948000
H	23.094839000	23.690250000	17.732648000	C	23.755714000	13.637012000	16.564674000
O	23.911659000	25.525479000	17.101265000	C	27.065914000	10.313290000	16.567215000
H	23.736974000	25.299775000	16.182562000	Zr	29.524440000	13.439969000	13.438993000
c. PA/DBU				C	30.007964000	13.253783000	16.566602000
N	27.036253000	21.818606000	20.447387000	Zr	26.880671000	13.440670000	10.796741000
N	26.820839000	19.930827000	18.457444000	C	23.755332000	16.566137000	13.635261000
C	26.660720000	20.577457000	20.811707000	C	27.064326000	16.568185000	10.312820000
C	27.024937000	22.808301000	21.346243000	C	30.008123000	16.567527000	13.254357000
C	26.828098000	19.010091000	17.475285000	O	23.334855000	26.880866000	24.934215000
C	26.666792000	19.530252000	19.747284000	O	23.334856000	24.934212000	26.880862000
C	26.284313000	20.314613000	22.137580000	O	25.848909000	27.912895000	27.912897000
C	26.701459000	22.631244000	22.699391000	O	23.334862000	26.880939000	26.887594000
C	26.710932000	17.628436000	17.689848000	O	23.334864000	28.827596000	28.8280937000
C	26.533108000	18.166351000	20.039320000	O	24.934210000	30.426941000	26.880925000
C	26.329935000	21.334706000	23.079940000	O	26.880889000	30.426939000	24.934203000
C	26.562999000	17.222406000	19.022690000	O	26.880879000	30.426942000	28.827590000
C	26.810325000	23.730612000	23.728978000	O	27.912786000	27.912776000	27.912777000
C	26.810098000	16.591849000	16.590738000	O	28.827596000	30.426944000	26.880863000
O	26.881204000	24.934112000	23.334886000	O	30.426933000	24.934198000	26.880924000
O	26.880545000	23.335101000	24.934208000	O	30.426936000	26.880929000	24.934199000
O	26.880236000	15.387100000	16.986178000	O	30.426944000	26.880866000	28.827595000
O	26.881598000	16.986586000	15.387301000	O	30.426946000	28.827594000	26.880867000
Zr	26.878045000	26.881615000	24.237876000	O	24.934211000	26.880924000	30.426942000
Zr	26.878157000	24.239686000	26.880719000	O	26.880889000	24.934201000	30.426937000
Zr	26.878194000	13.440632000	16.081661000	O	26.880878000	28.827589000	30.426943000
Zr	26.878031000	16.083475000	13.439734000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000

ARTICLE

Journal Name

O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687041000	19.634387000	13.440265000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988089000	18.960801000	13.761003000
H	27.351814000	17.319223000	9.561837000	C	22.007719000	19.934510000	13.779581000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.309592000	20.832730000	14.034525000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000

Journal Name				ARTICLE			
H	19.491341000	27.477656000	22.313835000	H	26.297852000	21.515121000	14.051677000
O	13.440450000	28.827615000	16.986310000	H	26.372599000	22.125734000	15.714739000
C	13.440450000	30.034298000	16.593848000	H	25.649829000	26.519548000	16.623750000
O	13.440450000	28.827615000	9.894590000	H	24.463483000	25.487997000	17.405124000
C	13.440450000	30.034298000	10.287052000	H	22.889606000	24.310215000	16.844220000
O	13.440450000	30.426760000	15.387165000	H	22.357264000	23.052294000	15.768371000
O	13.440450000	30.426760000	11.493735000	d. PA/DBU/CO₂			
C	17.333342000	27.201858000	18.960712000	N	27.047299000	21.813903000	20.452799000
C	18.317452000	27.216911000	19.936757000	N	26.837070000	19.927216000	18.461409000
H	16.322082000	27.364756000	19.144577000	C	26.666819000	20.573679000	20.815639000
H	18.007515000	27.477656000	20.830009000	C	27.034353000	22.804558000	21.350407000
H	13.440450000	30.790903000	9.530447000	C	26.841263000	19.008025000	17.478090000
H	17.350453000	26.880900000	9.530447000	C	26.672558000	19.527027000	19.750432000
H	17.350453000	30.790903000	13.440450000	C	26.284559000	20.312926000	22.140078000
H	13.440450000	30.790903000	17.350453000	C	26.702739000	22.629700000	22.701308000
H	9.530447000	30.790903000	13.440450000	C	26.712368000	17.627380000	17.690560000
H	9.530447000	26.880900000	17.350453000	C	26.526817000	18.163942000	20.039860000
H	13.440450000	22.970897000	9.530447000	C	26.327275000	21.334247000	23.081501000
H	9.530447000	22.970897000	13.440450000	C	26.555140000	17.220983000	19.022198000
H	13.440450000	22.970897000	17.350453000	C	26.810210000	23.730625000	23.729014000
H	15.026933000	25.294417000	11.853967000	C	26.810074000	16.591978000	16.590624000
H	11.853967000	28.467383000	11.853967000	O	26.881113000	24.934118000	23.334889000
H	9.530447000	26.880900000	9.530447000	O	26.880724000	23.335085000	24.934193000
H	15.026933000	28.467383000	15.026933000	O	26.880549000	15.387139000	16.986241000
H	11.853967000	25.294417000	15.026933000	O	26.881320000	16.986565000	15.387278000
H	27.308099000	23.792391000	20.976983000	Zr	26.878058000	26.881615000	24.237877000
H	26.948582000	19.396504000	16.465270000	Zr	26.878146000	24.239685000	26.880719000
H	25.953340000	19.325927000	22.439529000	Zr	26.878162000	13.440631000	16.081664000
H	26.431923000	17.837332000	21.068167000	Zr	26.878061000	16.083473000	13.439735000
H	26.073061000	21.141661000	24.117160000	O	24.934203000	26.880849000	23.334882000
H	26.486429000	16.162895000	19.245361000	O	25.848911000	25.848918000	25.848917000
Cu	26.991640000	21.986172000	18.164954000	O	25.849015000	27.912768000	25.849028000
Cl	24.812836000	22.696074000	18.295092000	O	27.912782000	25.849032000	25.849031000
C	28.135185000	23.562772000	17.645694000	O	27.912889000	27.912886000	25.848919000
C	28.713987000	22.506173000	17.316289000	O	26.880945000	28.827581000	23.334856000
H	29.484202000	21.869474000	16.925440000	O	28.827591000	26.880922000	23.334870000
C	27.733625000	24.969077000	17.880091000	O	24.934197000	23.334881000	26.880846000
H	28.199754000	25.296607000	18.819439000	O	25.849012000	25.849025000	27.912771000
H	26.643350000	24.987118000	18.047103000	O	27.912892000	25.848913000	27.912887000
O	28.153544000	25.832634000	16.867998000	O	26.880944000	23.334850000	28.827576000
H	27.596820000	25.584649000	16.081241000	O	28.827591000	23.334868000	26.880917000
C	22.841155000	26.330167000	14.717876000	O	25.849012000	12.408579000	14.472325000
C	23.612728000	26.857694000	15.923797000	O	25.848911000	14.472433000	14.472432000
C	24.743647000	25.935992000	16.442506000	O	24.934197000	13.440504000	16.986469000
C	22.042456000	25.058501000	14.987437000	O	26.880944000	11.493774000	16.986500000
C	25.148825000	24.798993000	15.539058000	O	27.912892000	12.408463000	14.472437000
C	22.840828000	24.032615000	15.784020000	O	27.912782000	14.472319000	14.472318000
N	24.189094000	23.866713000	15.262209000	O	28.827591000	13.440433000	16.986482000
H	22.169349000	27.110735000	14.343203000	O	25.849015000	14.472322000	12.408582000
H	21.723253000	24.630004000	14.029576000	O	24.934203000	16.986468000	13.440501000
C	26.731707000	23.642695000	14.254026000	O	27.912889000	14.472431000	12.408464000
N	26.369273000	24.772340000	15.090450000	O	26.880945000	16.986494000	11.493769000
C	26.040755000	22.363881000	14.695379000	O	28.827591000	16.986480000	13.440428000
C	24.541428000	22.565126000	14.709905000	C	23.755332000	26.686089000	23.755213000
H	24.075788000	21.800907000	15.345971000	Zr	24.236612000	26.881475000	26.880552000
H	27.821570000	23.524925000	14.289245000	Zr	26.880671000	29.524609000	26.880680000
H	23.555135000	26.135795000	13.906936000	Zr	29.524440000	26.882357000	26.881381000
H	21.127344000	25.288585000	15.544719000	C	27.064326000	30.008530000	23.753165000
H	24.120113000	22.466320000	13.696629000	C	30.008123000	27.066993000	23.753823000
H	26.477373000	23.862398000	13.203667000	C	23.755714000	23.756676000	26.684338000
H	22.913577000	27.067420000	16.743141000	Zr	26.880615000	26.881402000	29.524137000
H	24.047095000	27.824844000	15.650357000	C	27.065914000	23.754135000	30.008060000

ARTICLE

Journal Name

C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000
O	26.880879000	30.426942000	28.827590000	H	25.215244000	15.103495000	11.776660000
O	27.912786000	27.912776000	27.912777000	H	25.215244000	28.544690000	25.217855000
O	28.827596000	30.426944000	26.880863000	H	28.555271000	25.223028000	25.222315000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	28.545528000	28.545099000
O	30.426936000	26.880929000	24.934199000	H	25.215026000	25.218505000	28.544917000
O	30.426944000	26.880866000	28.827595000	O	14.472677000	25.848673000	14.472677000
O	30.426946000	28.827594000	26.880867000	O	12.408223000	25.848673000	12.408223000
O	24.934211000	26.880924000	30.426942000	O	14.472677000	25.848673000	12.408223000
O	26.880889000	24.934201000	30.426937000	O	12.408223000	25.848673000	14.472677000
O	26.880878000	28.827589000	30.426943000	Zr	13.440450000	24.397374000	13.440450000
O	28.827598000	26.880862000	30.426940000	O	11.493735000	23.335040000	13.440450000
O	25.848909000	12.408453000	12.408455000	C	10.287052000	23.727502000	13.440450000
O	23.334862000	11.493756000	13.440411000	O	15.387165000	23.335040000	13.440450000
O	23.334855000	15.387135000	13.440484000	C	16.593848000	23.727502000	13.440450000
O	23.334864000	13.440413000	11.493754000	C	17.650268000	22.671082000	13.440450000
O	23.334856000	13.440488000	15.387138000	C	19.634347000	20.687003000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687171000	19.634522000	13.439640000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000

Journal Name				ARTICLE			
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H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988074000	18.960785000	13.761074000	H	11.853967000	25.294417000	15.026933000
C	22.006448000	19.934777000	13.780298000	H	27.322808000	23.788032000	20.983522000
H	23.999268000	19.144577000	13.924306000	H	26.969113000	19.394435000	16.469044000
H	22.310760000	20.832199000	14.034408000	H	25.950993000	19.325078000	22.441899000
Zr	10.956924000	26.880900000	13.440450000	H	26.416726000	17.834526000	21.067648000
O	9.894590000	26.880900000	11.493735000	H	26.065324000	21.142738000	24.117734000
O	12.408223000	27.913127000	14.472677000	H	26.469560000	16.161839000	19.243304000
C	10.287052000	26.880900000	10.287052000	Cu	26.991615000	21.979804000	18.181964000
Zr	15.923976000	26.880900000	13.440450000	Cl	24.790660000	22.633579000	18.326637000
O	16.986310000	26.880900000	11.493735000	C	28.100769000	23.597854000	17.718666000
C	16.593848000	26.880900000	10.287052000	C	28.693723000	22.570597000	17.329771000
O	16.986310000	26.880900000	15.387165000	H	29.470624000	21.968846000	16.899024000
O	14.472677000	27.913127000	12.408223000	C	27.660265000	24.966882000	18.056451000
C	16.593848000	26.880900000	16.593848000	H	28.134509000	25.253245000	19.004076000
C	17.650268000	26.880900000	17.650268000	H	26.572536000	24.939293000	18.243150000
C	19.634347000	26.880900000	19.634347000	O	28.025973000	25.918674000	17.096094000
O	9.894590000	26.880900000	15.387165000	H	27.503945000	25.665612000	16.283626000
C	10.287052000	26.880900000	16.593848000	C	22.825987000	26.328675000	14.821353000
Zr	13.440450000	26.880900000	15.923976000	C	23.577546000	26.837914000	16.047838000
O	11.493735000	26.880900000	16.986310000	C	24.669681000	25.889180000	16.594981000
O	14.472677000	27.913127000	14.472677000	C	22.029126000	25.046216000	15.043259000
Zr	13.440450000	26.880900000	10.956924000	C	25.121029000	24.793205000	15.665282000
O	11.493735000	26.880900000	9.894590000	C	22.819472000	23.992462000	15.812208000
O	15.387165000	26.880900000	9.894590000	N	24.182398000	23.863485000	15.318260000
O	12.408223000	27.913127000	12.408223000	H	22.156855000	27.113795000	14.451491000
O	15.387165000	26.880900000	16.986310000	H	21.721364000	24.650007000	14.067783000
Zr	13.440450000	29.364426000	13.440450000	C	26.753951000	23.717181000	14.375090000
O	11.493735000	30.426760000	13.440450000	N	26.354926000	24.801685000	15.253358000
C	10.287052000	30.034298000	13.440450000	C	26.069550000	22.410239000	14.738482000
O	15.387165000	30.426760000	13.440450000	C	24.566789000	22.587859000	14.728085000
C	16.593848000	30.034298000	13.440450000	H	24.101299000	21.793816000	15.326694000
O	16.986310000	28.827615000	13.440450000	H	27.843971000	23.610336000	14.433091000
O	9.894590000	28.827615000	13.440450000	H	23.554349000	26.155202000	14.018498000
C	22.671082000	26.880900000	22.671082000	H	21.106863000	25.253342000	15.597080000
C	20.687003000	26.880900000	20.687003000	H	24.165346000	22.517467000	13.704491000
C	21.360638000	27.201858000	22.988008000	H	26.523178000	23.983313000	13.330080000
C	20.384593000	27.216911000	22.003898000	H	22.865828000	27.067943000	16.850052000
H	21.176773000	27.364756000	23.999268000	H	24.047882000	27.791989000	15.786347000
H	19.491341000	27.477656000	22.313835000	H	26.354840000	21.596198000	14.062711000
O	13.440450000	28.827615000	16.986310000	H	26.381655000	22.129425000	15.753135000
C	13.440450000	30.034298000	16.593848000	H	25.563320000	26.465371000	16.841123000
O	13.440450000	28.827615000	9.894590000	H	24.338693000	25.404837000	17.522822000
C	13.440450000	30.034298000	10.287052000	H	22.838576000	24.219762000	16.885040000
O	13.440450000	30.426760000	15.387165000	H	22.347891000	23.009220000	15.739143000
O	13.440450000	30.426760000	11.493735000	C	27.169625000	28.239656000	18.368206000
C	17.333342000	27.201858000	18.960712000	O	27.568480000	27.808832000	19.379980000
C	18.317452000	27.216911000	19.936757000	O	26.747372000	28.722601000	17.390405000
H	16.322082000	27.364756000	19.144577000	e. TS1			
H	18.007515000	27.477656000	20.830009000	N	26.501017000	21.880040000	20.392192000
H	13.440450000	30.790903000	9.530447000	N	26.798505000	19.929822000	18.432597000
H	17.350453000	26.880900000	9.530447000	C	26.655722000	20.598117000	20.779866000
H	17.350453000	30.790903000	13.440450000	C	26.546951000	22.853577000	21.311155000
H	13.440450000	30.790903000	17.350453000	C	26.801524000	19.000849000	17.459423000
H	9.530447000	30.790903000	13.440450000	C	26.643459000	19.544910000	19.721015000
H	9.530447000	26.880900000	17.350453000	C	26.838776000	20.281294000	22.135280000
H	13.440450000	22.970897000	9.530447000	C	26.716920000	22.633003000	22.690340000
H	9.530447000	22.970897000	13.440450000	C	26.701563000	17.624163000	17.686434000
H	13.440450000	22.970897000	17.350453000	C	26.481694000	18.183980000	20.025846000
H	15.026933000	25.294417000	11.853967000	C	26.855627000	21.295180000	23.083575000
H	11.853967000	28.467383000	11.853967000	C	26.527996000	17.229372000	19.020799000

ARTICLE

Journal Name

C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000
O	26.880879000	30.426942000	28.827590000	H	25.215244000	15.103495000	11.776660000

Journal Name				ARTICLE			
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.439405000	23.868242000	20.930105000
H	23.999268000	19.144577000	13.924306000	H	26.890158000	19.384688000	16.445695000
H	22.313835000	20.830009000	14.037206000	H	26.993434000	19.254371000	22.451437000
Zr	10.956924000	26.880900000	13.440450000	H	26.306019000	17.871762000	21.049969000
O	9.894590000	26.880900000	11.493735000	H	26.998910000	21.068383000	24.135411000
O	12.408223000	27.913127000	14.472677000	H	26.425304000	16.173623000	19.251183000
C	10.287052000	26.880900000	10.287052000	Cu	26.577718000	21.912421000	17.840948000
Zr	15.923976000	26.880900000	13.440450000	Cl	24.608597000	21.469714000	16.814724000
O	16.986310000	26.880900000	11.493735000	C	27.225417000	23.761895000	17.367753000
C	16.593848000	26.880900000	10.287052000	C	28.160306000	23.091360000	17.860382000
O	16.986310000	26.880900000	15.387165000	H	29.143367000	22.883862000	18.237458000
O	14.472677000	27.913127000	12.408223000	C	26.414190000	24.798146000	16.668236000
C	16.593848000	26.880900000	16.593848000	H	26.899742000	25.758569000	16.934510000
C	17.650268000	26.880900000	17.650268000	H	25.407170000	24.813115000	17.123911000
C	19.634347000	26.880900000	19.634347000	O	26.368080000	24.624315000	15.310906000
O	9.894590000	26.880900000	15.387165000	H	26.401342000	23.237970000	14.762386000

ARTICLE

Journal Name

C	25.373558000	23.625189000	10.895970000	O	27.912892000	25.848913000	27.912887000
C	24.574566000	24.263486000	12.030916000	O	26.880944000	23.334850000	28.827576000
C	24.384510000	23.369146000	13.279575000	O	28.827591000	23.334868000	26.880917000
C	24.758621000	22.366693000	10.285607000	O	25.849012000	12.408579000	14.472325000
C	25.377636000	22.252934000	13.317232000	O	25.848911000	14.472433000	14.472432000
C	24.300914000	21.356120000	11.339866000	O	24.934197000	13.440504000	16.986469000
N	25.239334000	21.226066000	12.450587000	O	26.880944000	11.493774000	16.986500000
H	25.530363000	24.365488000	10.104904000	O	27.912892000	12.408463000	14.472437000
H	25.487215000	21.900665000	9.610536000	O	27.912782000	14.472319000	14.472318000
C	27.416722000	21.342741000	14.268061000	O	28.827591000	13.440433000	16.986482000
N	26.372062000	22.336376000	14.155128000	O	25.849015000	14.472322000	12.408582000
C	26.950494000	20.015285000	13.700256000	O	24.934203000	16.986468000	13.440501000
C	26.296530000	20.224447000	12.347179000	O	27.912889000	14.472431000	12.408464000
H	25.849447000	19.295513000	11.984004000	O	26.880945000	16.986494000	11.493769000
H	27.670330000	21.256138000	15.333916000	O	28.827591000	16.986480000	13.440428000
H	26.378618000	23.395039000	11.275091000	C	23.755332000	26.686089000	23.755213000
H	23.889891000	22.623290000	9.666451000	Zr	24.236612000	26.881475000	26.880552000
H	27.042589000	20.543576000	11.600404000	Zr	26.880671000	29.524609000	26.880680000
H	28.315221000	21.714397000	13.754945000	Zr	29.524440000	26.882357000	26.881381000
H	23.592301000	24.589059000	11.667657000	C	27.064326000	30.008530000	23.753165000
H	25.111174000	25.162119000	12.347648000	C	30.008123000	27.066993000	23.753823000
H	27.783703000	19.312303000	13.606480000	C	23.755714000	23.756676000	26.684338000
H	26.221837000	19.570289000	14.386664000	Zr	26.880615000	26.881402000	29.524137000
H	24.523581000	23.956284000	14.190100000	C	27.065914000	23.754135000	30.008060000
H	23.379546000	22.939185000	13.317215000	C	30.007964000	23.754748000	27.067567000
H	23.326561000	21.648797000	11.741439000	Zr	24.236612000	13.440798000	13.439875000
H	24.169525000	20.357839000	10.911198000	Zr	26.880615000	10.797213000	13.439948000
C	27.979900000	25.364015000	14.330712000	C	23.755714000	13.637012000	16.564674000
O	28.547077000	26.004294000	15.154346000	C	27.065914000	10.313290000	16.567215000
O	27.804889000	24.893120000	13.250344000	Zr	29.524440000	13.439969000	13.438993000
f. IM1				C	30.007964000	13.253783000	16.566602000
N	26.666747000	21.878604000	20.384984000	Zr	26.880671000	13.440670000	10.796741000
N	26.885593000	19.909896000	18.460041000	C	23.755332000	16.566137000	13.635261000
C	26.659874000	20.592084000	20.790654000	C	27.064326000	16.568185000	10.312820000
C	26.701220000	22.852978000	21.303438000	C	30.008123000	16.567527000	13.254357000
C	26.868074000	18.991635000	17.478751000	O	23.334855000	26.880866000	24.934215000
C	26.644556000	19.534056000	19.736322000	O	23.334856000	24.934212000	26.880862000
C	26.681306000	20.274176000	22.157466000	O	25.848909000	27.912895000	27.912897000
C	26.717004000	22.631861000	22.692714000	O	23.334862000	26.880939000	28.827594000
C	26.691635000	17.620606000	17.690519000	O	23.334864000	28.827596000	26.880937000
C	26.398237000	18.181935000	20.023442000	O	24.934210000	30.426941000	26.880925000
C	26.704811000	21.292138000	23.101196000	O	26.880889000	30.426939000	24.934203000
C	26.450082000	17.229080000	19.015125000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000

O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000

ARTICLE

Journal Name

C	20.384593000	27.216911000	22.003898000	H	25.824787000	24.649039000	11.331944000
H	21.176773000	27.364756000	23.99268000	H	27.272898000	24.265961000	10.431285000
H	19.491341000	27.477656000	22.313835000	H	28.589668000	19.217242000	14.835203000
O	13.440450000	28.827615000	16.986310000	H	28.304243000	20.893112000	15.382404000
C	13.440450000	30.034298000	16.593848000	H	28.356823000	24.334795000	12.472673000
O	13.440450000	28.827615000	9.894590000	H	26.867013000	24.251119000	13.367607000
C	13.440450000	30.034298000	10.287052000	H	25.250446000	23.014506000	13.536353000
O	13.440450000	30.426760000	15.387165000	H	24.728875000	21.379097000	13.737458000
O	13.440450000	30.426760000	11.493735000	C	30.256370000	24.354927000	14.847397000
C	17.333342000	27.201858000	18.960712000	O	30.817891000	25.044065000	15.685093000
C	18.317452000	27.216911000	19.936757000	O	30.602876000	23.939788000	13.711018000
H	16.322082000	27.364756000	19.144577000	g. TS2			
H	18.007515000	27.477656000	20.830009000	N	26.389759000	21.812509000	20.426083000
H	13.440450000	30.790903000	9.530447000	N	26.662346000	19.910226000	18.484964000
H	17.350453000	26.880900000	9.530447000	C	26.700849000	20.544621000	20.816551000
H	17.350453000	30.790903000	13.440450000	C	26.444651000	22.808392000	21.334175000
H	13.440450000	30.790903000	17.350453000	C	26.640720000	18.994342000	17.497505000
H	9.530447000	30.790903000	13.440450000	C	26.679136000	19.492863000	19.778052000
H	9.530447000	26.880900000	17.350453000	C	27.029244000	20.281437000	22.155371000
H	13.440450000	22.970897000	9.530447000	C	26.735788000	22.623360000	22.695079000
H	9.530447000	22.970897000	13.440450000	C	26.705812000	17.611863000	17.701473000
H	13.440450000	22.970897000	17.350453000	C	26.667445000	18.118295000	20.070369000
H	15.026933000	25.294417000	11.853967000	C	27.020076000	21.303271000	23.090357000
H	11.853967000	28.467383000	11.853967000	C	26.701375000	17.187334000	19.045588000
H	9.530447000	26.880900000	9.530447000	C	26.809925000	23.730886000	23.728973000
H	15.026933000	28.467383000	15.026933000	C	26.809925000	16.592377000	16.590464000
H	11.853967000	25.294417000	15.026933000	O	26.880885000	24.934153000	23.334955000
H	26.722677000	23.870140000	20.915575000	O	26.880903000	23.334945000	24.934136000
H	27.016250000	19.384078000	16.476612000	O	26.880903000	15.387214000	16.986405000
H	26.705026000	19.241095000	22.489703000	O	26.880885000	16.986395000	15.387197000
H	26.164298000	17.871030000	21.036165000	Zr	26.878142000	26.881612000	24.237883000
H	26.732924000	21.065396000	24.162313000	Zr	26.878209000	24.239690000	26.880717000
H	26.297679000	16.177343000	19.237104000	Zr	26.878209000	13.440633000	16.081660000
Cu	27.286120000	21.857227000	17.875704000	Zr	26.878142000	16.083467000	13.439738000
Cl	25.578255000	22.050470000	16.409868000	O	24.934203000	26.880849000	23.334882000
C	28.595497000	23.309038000	17.436778000	O	25.848911000	25.848918000	25.848917000
C	29.084080000	22.542144000	18.294630000	O	25.849015000	27.912768000	25.849028000
H	29.806955000	22.172172000	18.996448000	O	27.912782000	25.849032000	25.849031000
C	28.387417000	24.324977000	16.388222000	O	27.912889000	27.912886000	25.848919000
H	28.908235000	25.240144000	16.702418000	O	26.880945000	28.827581000	23.334856000
H	27.315866000	24.517291000	16.264461000	O	28.827591000	26.880922000	23.334870000
O	28.899357000	23.894004000	15.149344000	O	24.934197000	23.334881000	26.880846000
H	29.686490000	22.829301000	13.135971000	O	25.849012000	25.849025000	27.912771000
C	25.983501000	22.585020000	10.720258000	O	27.912892000	25.848913000	27.912887000
C	26.607542000	23.890345000	11.214609000	O	26.880944000	23.334850000	28.827576000
C	27.411044000	23.792048000	12.535640000	O	28.827591000	23.334868000	26.880917000
C	24.918292000	21.997390000	11.644188000	O	25.849012000	12.408579000	14.472325000
C	27.732408000	22.393245000	12.958007000	O	25.848911000	14.472433000	14.472432000
C	25.348504000	22.013660000	13.106124000	O	24.934197000	13.440504000	16.986469000
N	26.731439000	21.569840000	13.275728000	O	26.880944000	11.493774000	16.986500000
H	25.555623000	22.744548000	9.724958000	O	27.912892000	12.408463000	14.472437000
H	24.687646000	20.971545000	11.330109000	O	27.912782000	14.472319000	14.472318000
C	29.406309000	20.746975000	13.549505000	O	28.827591000	13.440433000	16.986482000
N	28.998811000	22.021400000	12.977007000	O	25.849015000	14.472322000	12.408582000
C	28.350753000	20.231461000	14.504947000	O	24.934203000	16.986468000	13.440501000
C	26.996451000	20.240736000	13.826269000	O	27.912889000	14.472431000	12.408464000
H	26.200274000	20.037343000	14.549616000	O	26.880945000	16.986494000	11.493769000
H	30.361221000	20.917952000	14.055214000	O	28.827591000	16.986480000	13.440428000
H	26.782916000	21.844364000	10.580382000	C	23.755332000	26.686089000	23.755213000
H	23.983079000	22.564485000	11.561528000	Zr	24.236612000	26.881475000	26.880552000
H	26.939223000	19.486672000	13.025638000	Zr	26.880671000	29.524609000	26.880680000
H	29.583329000	20.021766000	12.742703000	Zr	29.524440000	26.882357000	26.881381000

Journal Name				ARTICLE			
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000
O	26.880879000	30.426942000	28.827590000	H	25.215244000	15.103495000	11.776660000
O	27.912786000	27.912776000	27.912777000	H	25.215244000	28.544690000	25.217855000
O	28.827596000	30.426944000	26.880863000	H	28.555271000	25.223028000	25.222315000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	28.545528000	28.545099000
O	30.426936000	26.880929000	24.934199000	H	25.215026000	25.218505000	28.544917000
O	30.426944000	26.880866000	28.827595000	O	14.472677000	25.848673000	14.472677000
O	30.426946000	28.827594000	26.880867000	O	12.408223000	25.848673000	12.408223000
O	24.934211000	26.880924000	30.426942000	O	14.472677000	25.848673000	12.408223000
O	26.880889000	24.934201000	30.426937000	O	12.408223000	25.848673000	14.472677000
O	26.880878000	28.827589000	30.426943000	Zr	13.440450000	24.397374000	13.440450000
O	28.827598000	26.880862000	30.426940000	O	11.493735000	23.335040000	13.440450000
O	25.848909000	12.408453000	12.408455000	C	10.287052000	23.727502000	13.440450000
O	23.334862000	11.493756000	13.440411000	O	15.387165000	23.335040000	13.440450000
O	23.334855000	15.387135000	13.440484000	C	16.593848000	23.727502000	13.440450000
O	23.334864000	13.440413000	11.493754000	C	17.650268000	22.671082000	13.440450000
O	23.334856000	13.440488000	15.387138000	C	19.634347000	20.687003000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000

ARTICLE

Journal Name

C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.227248000	23.803218000	20.949955000
H	23.999268000	19.144577000	13.924306000	H	26.565366000	19.396364000	16.490741000
H	22.313835000	20.830009000	14.037206000	H	27.308989000	19.277698000	22.460618000
Zr	10.956924000	26.880900000	13.440450000	H	26.617707000	17.779188000	21.100610000
O	9.894590000	26.880900000	11.493735000	H	27.260516000	21.106443000	24.129982000
O	12.408223000	27.913127000	14.472677000	H	26.715190000	16.124469000	19.262450000
C	10.287052000	26.880900000	10.287052000	Cu	26.099828000	21.930408000	18.267951000
Zr	15.923976000	26.880900000	13.440450000	Cl	24.227354000	21.326287000	16.994943000
O	16.986310000	26.880900000	11.493735000	C	26.213462000	24.228663000	16.846477000
C	16.593848000	26.880900000	10.287052000	C	27.041275000	23.526707000	17.505668000
O	16.986310000	26.880900000	15.387165000	H	28.122773000	23.574154000	17.502676000
O	14.472677000	27.913127000	12.408223000	C	24.868439000	24.626184000	16.450480000
C	16.593848000	26.880900000	16.593848000	H	24.650998000	25.648182000	16.790164000
C	17.650268000	26.880900000	17.650268000	H	24.142075000	23.927016000	16.883045000
C	19.634347000	26.880900000	19.634347000	O	24.750877000	24.549313000	15.035227000
O	9.894590000	26.880900000	15.387165000	H	25.126584000	22.749144000	14.590517000
C	10.287052000	26.880900000	16.593848000	C	25.728821000	23.281044000	10.481502000
Zr	13.440450000	26.880900000	15.923976000	C	24.352079000	23.503804000	11.099585000
O	11.493735000	26.880900000	16.986310000	C	24.018084000	22.598896000	12.315251000
O	14.472677000	27.913127000	14.472677000	C	25.900302000	21.929081000	9.792785000
Zr	13.440450000	26.880900000	10.956924000	C	25.183302000	21.811962000	12.826388000
O	11.493735000	26.880900000	9.894590000	C	25.357385000	20.782847000	10.642045000
O	15.387165000	26.880900000	9.894590000	N	25.761467000	20.889686000	12.041743000
O	12.408223000	27.913127000	12.408223000	H	25.932151000	24.080902000	9.763252000
O	15.387165000	26.880900000	16.986310000	H	26.959123000	21.758583000	9.562231000
Zr	13.440450000	29.364426000	13.440450000	C	26.820984000	21.448475000	14.609570000
O	11.493735000	30.426760000	13.440450000	N	25.621909000	22.039749000	14.042194000
C	10.287052000	30.034298000	13.440450000	C	27.079938000	20.109030000	13.954152000
O	15.387165000	30.426760000	13.440450000	C	27.010495000	20.238375000	12.445517000
C	16.593848000	30.034298000	13.440450000	H	27.038984000	19.255224000	11.966709000
O	16.986310000	28.827615000	13.440450000	H	26.652022000	21.365299000	15.688681000
O	9.894590000	28.827615000	13.440450000	H	26.478613000	23.411483000	11.272215000
C	22.671082000	26.880900000	22.671082000	H	25.369977000	21.913689000	8.832460000
C	20.687003000	26.880900000	20.687003000	H	27.859441000	20.825808000	12.063514000
C	21.360638000	27.201858000	22.988008000	H	27.654789000	22.148471000	14.460100000
C	20.384593000	27.216911000	22.003898000	H	23.572936000	23.374560000	10.337693000
H	21.176773000	27.364756000	23.999268000	H	24.313078000	24.535851000	11.449011000
H	19.491341000	27.477656000	22.313835000	H	28.057627000	19.717183000	14.245736000
O	13.440450000	28.827615000	16.986310000	H	26.333211000	19.382450000	14.292693000
C	13.440450000	30.034298000	16.593848000	H	23.649318000	23.209282000	13.142631000
O	13.440450000	28.827615000	9.894590000	H	23.222814000	21.892074000	12.055072000
C	13.440450000	30.034298000	10.287052000	H	24.263421000	20.762836000	10.601802000
O	13.440450000	30.426760000	15.387165000	H	25.697267000	19.805447000	10.285991000
O	13.440450000	30.426760000	11.493735000	C	25.966488000	25.011963000	14.402885000
C	17.333342000	27.201858000	18.960712000	O	26.871443000	25.312931000	15.229455000
C	18.317452000	27.216911000	19.936757000	O	25.936163000	24.985897000	13.178729000
H	16.322082000	27.364756000	19.144577000	h. IM2			
H	18.007515000	27.477656000	20.830009000	N	26.853458000	21.845423000	20.409941000
H	13.440450000	30.790903000	9.530447000	N	26.618835000	19.927368000	18.471018000
H	17.350453000	26.880900000	9.530447000	C	26.653712000	20.560236000	20.811080000
H	17.350453000	30.790903000	13.440450000	C	26.833825000	22.839368000	21.323831000
H	13.440450000	30.790903000	17.350453000	C	26.676444000	19.006013000	17.493814000
H	9.530447000	30.790903000	13.440450000	C	26.683120000	19.515350000	19.766496000
H	9.530447000	26.880900000	17.350453000	C	26.448323000	20.280506000	22.173393000

C	26.699286000	22.629930000	22.700353000	O	23.334862000	26.880939000	28.827594000
C	26.737844000	17.619961000	17.698212000	O	23.334864000	28.827596000	26.880937000
C	26.792430000	18.144725000	20.062506000	O	24.934210000	30.426941000	26.880925000
C	26.497864000	21.297880000	23.111207000	O	26.880889000	30.426939000	24.934203000
C	26.797209000	17.206511000	19.043735000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000

ARTICLE

Journal Name

H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.939569000	23.843525000	20.920128000
H	23.999268000	19.144577000	13.924306000	H	26.667105000	19.395017000	16.475952000
H	22.313835000	20.830009000	14.037206000	H	26.242196000	19.264504000	22.495791000
Zr	10.956924000	26.880900000	13.440450000	H	26.892044000	17.814070000	21.091968000
O	9.894590000	26.880900000	11.493735000	H	26.372257000	21.085702000	24.168098000
O	12.408223000	27.913127000	14.472677000	H	26.875283000	16.147292000	19.265683000
C	10.287052000	26.880900000	10.287052000	Cu	27.020468000	22.233915000	18.420551000
Zr	15.923976000	26.880900000	13.440450000	Cl	25.119943000	23.887952000	18.691245000
O	16.986310000	26.880900000	11.493735000	C	28.482411000	23.905318000	16.621236000
C	16.593848000	26.880900000	10.287052000	C	28.108302000	22.650733000	16.884802000
O	16.986310000	26.880900000	15.387165000	H	28.468338000	21.916438000	16.152195000

C	28.261195000	25.159572000	17.404407000	O	27.912889000	27.912886000	25.848919000
H	28.950222000	25.256566000	18.255008000	O	26.880945000	28.827581000	23.334856000
H	27.235445000	25.260220000	17.777639000	O	28.827591000	26.880922000	23.334870000
O	28.556516000	26.209802000	16.463710000	O	24.934197000	23.334881000	26.880846000
H	26.498610000	23.251477000	15.526109000	O	25.849012000	25.849025000	27.912771000
C	23.093387000	25.731688000	14.084722000	O	27.912892000	25.848913000	27.912887000
C	24.498360000	26.167279000	14.485727000	O	26.880944000	23.334850000	28.827576000
C	25.057202000	25.410150000	15.702735000	O	28.827591000	23.334868000	26.880917000
C	22.088996000	25.671486000	15.230033000	O	25.849012000	12.408579000	14.472325000
C	24.644907000	23.977217000	15.720056000	O	25.848911000	14.472433000	14.472432000
C	22.446808000	24.701399000	16.369158000	O	24.934197000	13.440504000	16.986469000
N	23.380398000	23.638949000	15.985960000	O	26.880944000	11.493774000	16.986500000
H	22.710726000	26.406884000	13.312857000	O	27.912892000	12.408463000	14.472437000
H	21.116108000	25.390898000	14.814027000	O	27.912782000	14.472319000	14.472318000
C	25.118230000	21.658881000	15.283013000	O	28.827591000	13.440433000	16.986482000
N	25.511809000	23.054022000	15.330294000	O	25.849015000	14.472322000	12.408582000
C	24.224837000	21.339663000	16.468345000	O	24.934203000	16.986468000	13.440501000
C	23.066040000	22.314804000	16.557057000	O	27.912889000	14.472431000	12.408464000
H	22.832538000	22.495143000	17.613868000	O	26.880945000	16.986494000	11.493769000
H	26.031841000	21.060417000	15.290556000	O	28.827591000	16.986480000	13.440428000
H	23.143919000	24.742274000	13.611689000	C	23.755332000	26.686089000	23.755213000
H	21.955310000	26.670458000	15.661199000	Zr	24.236612000	26.881475000	26.880552000
H	22.157812000	21.951496000	16.066038000	Zr	26.880671000	29.524609000	26.880680000
H	24.613354000	21.482733000	14.325885000	Zr	29.524440000	26.882357000	26.881381000
H	24.514981000	27.236715000	14.720106000	C	27.064326000	30.008530000	23.753165000
H	25.171224000	26.029526000	13.633034000	C	30.008123000	27.066993000	23.753823000
H	23.851802000	20.313356000	16.407746000	C	23.755714000	23.756676000	26.684338000
H	24.830337000	21.423979000	17.377096000	Zr	26.880615000	26.881402000	29.524137000
H	26.149535000	25.459818000	15.709970000	C	27.065914000	23.754135000	30.008060000
H	24.727208000	25.859479000	16.644034000	C	30.007964000	23.754748000	27.067567000
H	22.873365000	25.209241000	17.244325000	Zr	24.236612000	13.440798000	13.439875000
H	21.545251000	24.194928000	16.721508000	Zr	26.880615000	10.797213000	13.439948000
C	29.189511000	25.675687000	15.389749000	C	23.755714000	13.637012000	16.564674000
O	29.220954000	24.321479000	15.479438000	C	27.065914000	10.313290000	16.567215000
O	29.636241000	26.313124000	14.478161000	Zr	29.524440000	13.439969000	13.438993000
i. TS3				C	30.007964000	13.253783000	16.566602000
N	26.852584000	21.841482000	20.415762000	Zr	26.880671000	13.440670000	10.796741000
N	26.618616000	19.930163000	18.476720000	C	23.755332000	16.566137000	13.635261000
C	26.694098000	20.554613000	20.821387000	C	27.064326000	16.568185000	10.312820000
C	26.816181000	22.834790000	21.327248000	C	30.008123000	16.567527000	13.254357000
C	26.663790000	19.008263000	17.495716000	O	23.334855000	26.880866000	24.934215000
C	26.724129000	19.515018000	19.770736000	O	23.334856000	24.934212000	26.880862000
C	26.506839000	20.269092000	22.184582000	O	25.848909000	27.912895000	27.912897000
C	26.708628000	22.624825000	22.705071000	O	23.334862000	26.880939000	28.827594000
C	26.748344000	17.623035000	17.699549000	O	23.334864000	28.827596000	26.880937000
C	26.855896000	18.146788000	20.060410000	O	24.934210000	30.426941000	26.880925000
C	26.541814000	21.290076000	23.120247000	O	26.880889000	30.426939000	24.934203000
C	26.845085000	17.208863000	19.041178000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000

ARTICLE

Journal Name

O	23.334856000	13.440488000	15.387138000	C	19.634347000	20.687003000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000

Journal Name				ARTICLE			
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O	9.894590000	28.827615000	13.440450000	H	23.213325000	24.634770000	13.597612000
C	22.671082000	26.880900000	22.671082000	H	22.016007000	26.650993000	15.555160000
C	20.687003000	26.880900000	20.687003000	H	22.016919000	21.947345000	16.094175000
C	21.360638000	27.201858000	22.988008000	H	24.545261000	21.465984000	14.419258000
C	20.384593000	27.216911000	22.003898000	H	24.623783000	27.111162000	14.688964000
H	21.176773000	27.364756000	23.999268000	H	25.281289000	25.839290000	13.674975000
H	19.491341000	27.477656000	22.313835000	H	23.628841000	20.248841000	16.419191000
O	13.440450000	28.827615000	16.986310000	H	24.600609000	21.276662000	17.472671000
C	13.440450000	30.034298000	16.593848000	H	26.144685000	25.307128000	15.804933000
O	13.440450000	28.827615000	9.894590000	H	24.685461000	25.785473000	16.661949000
C	13.440450000	30.034298000	10.287052000	H	22.795614000	25.184576000	17.194496000
O	13.440450000	30.426760000	15.387165000	H	21.465044000	24.202072000	16.621228000
O	13.440450000	30.426760000	11.493735000	C	30.234636000	25.360686000	17.280955000
C	17.333342000	27.201858000	18.960712000	O	29.854552000	24.117912000	16.843878000
C	18.317452000	27.216911000	19.936757000	O	31.309347000	25.844482000	17.083519000
H	16.322082000	27.364756000	19.144577000	j. PC/DBU			
H	18.007515000	27.477656000	20.830009000	N	26.670244000	21.871067000	20.401032000
H	13.440450000	30.790903000	9.530447000	N	26.468016000	19.915478000	18.459264000
H	17.350453000	26.880900000	9.530447000	C	26.632894000	20.574618000	20.796446000
H	17.350453000	30.790903000	13.440450000	C	26.681314000	22.849924000	21.323279000
H	13.440450000	30.790903000	17.350453000	C	26.513088000	19.000925000	17.480530000
H	9.530447000	30.790903000	13.440450000	C	26.650491000	19.521521000	19.738685000
H	9.530447000	26.880900000	17.350453000	C	26.605978000	20.270017000	22.164619000
H	13.440450000	22.970897000	9.530447000	C	26.697369000	22.625170000	22.703716000
H	9.530447000	22.970897000	13.440450000	C	26.719578000	17.626649000	17.692030000
H	13.440450000	22.970897000	17.350453000	C	26.880790000	18.172971000	20.042389000
H	15.026933000	25.294417000	11.853967000	C	26.654553000	21.284584000	23.110152000
H	11.853967000	28.467383000	11.853967000	C	26.903943000	17.231505000	19.023421000
H	9.530447000	26.880900000	9.530447000	C	26.809925000	23.730886000	23.728973000
H	15.026933000	28.467383000	15.026933000	C	26.809925000	16.592377000	16.590464000
H	11.853967000	25.294417000	15.026933000	O	26.880885000	24.934153000	23.334955000
H	26.875637000	23.843373000	20.925941000	O	26.880903000	23.334945000	24.934136000
H	26.622371000	19.397256000	16.479768000	O	26.880903000	15.387214000	16.986405000
H	26.323581000	19.249749000	22.510212000	O	26.880885000	16.986395000	15.387197000
H	26.983400000	17.818193000	21.087218000	Zr	26.878142000	26.881612000	24.237883000
H	26.429919000	21.077866000	24.178603000	Zr	26.878209000	24.239690000	26.880717000
H	26.939449000	16.150334000	19.259933000	Zr	26.878209000	13.440633000	16.808166000
Cu	26.707811000	22.174618000	18.379399000	Zr	26.878142000	16.083467000	13.439738000
Cl	24.995075000	23.826302000	18.795497000	O	24.934203000	26.880849000	23.334882000
C	28.530790000	23.867621000	17.192786000	O	25.848911000	25.848918000	25.848917000
C	27.845984000	22.771948000	16.816781000	O	25.849015000	27.912768000	25.849028000
H	28.450566000	22.084239000	16.215358000	O	27.912782000	25.849032000	25.849031000
C	28.117098000	25.034968000	18.043530000	O	27.912889000	27.912886000	25.848919000
H	27.973214000	24.765200000	19.096758000	O	26.880945000	28.827581000	23.334856000
H	27.197979000	25.526116000	17.712139000	O	28.827591000	26.880922000	23.334870000
O	29.220522000	25.946184000	17.948493000	O	24.934197000	23.334881000	26.880846000
H	26.581431000	22.977210000	16.137015000	O	25.849012000	25.849025000	27.912771000
C	23.177085000	25.638342000	14.040254000	O	27.912892000	25.848913000	27.912887000
C	24.578590000	26.033901000	14.492456000	O	26.880944000	23.334850000	28.827576000
C	25.052893000	25.295126000	15.754660000	O	28.827591000	23.334868000	26.880917000
C	22.126026000	25.640281000	15.143765000	O	25.849012000	12.408579000	14.472325000
C	24.621215000	23.863872000	15.779395000	O	25.848911000	14.472433000	14.472432000
C	22.401048000	24.671373000	16.307115000	O	24.934197000	13.440504000	16.986469000
N	23.314236000	23.575402000	15.980104000	O	26.880944000	11.493774000	16.986500000
H	22.851672000	26.306346000	13.235894000	O	27.912892000	12.408463000	14.472437000
H	21.159163000	25.393791000	14.692710000	O	27.912782000	14.472319000	14.472318000
C	25.016891000	21.577651000	15.403341000	O	28.827591000	13.440433000	16.986482000
N	25.509473000	22.935120000	15.505650000	O	25.849015000	14.472322000	12.408582000
C	24.045444000	21.255383000	16.528313000	O	24.934203000	16.986468000	13.440501000
C	22.933916000	22.287605000	16.586926000	O	27.912889000	14.472431000	12.408464000
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ARTICLE

Journal Name

O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000
O	26.880879000	30.426942000	28.827590000	H	25.215244000	15.103495000	11.776660000
O	27.912786000	27.912776000	27.912777000	H	25.215244000	28.544690000	25.217855000
O	28.827596000	30.426944000	26.880863000	H	28.555271000	25.223028000	25.222315000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	28.545528000	28.545099000
O	30.426936000	26.880929000	24.934199000	H	25.215026000	25.218505000	28.544917000
O	30.426944000	26.880866000	28.827595000	O	14.472677000	25.848673000	14.472677000
O	30.426946000	28.827594000	26.880867000	O	12.408223000	25.848673000	12.408223000
O	24.934211000	26.880924000	30.426942000	O	14.472677000	25.848673000	12.408223000
O	26.880889000	24.934201000	30.426937000	O	12.408223000	25.848673000	14.472677000
O	26.880878000	28.827589000	30.426943000	Zr	13.440450000	24.397374000	13.440450000
O	28.827598000	26.880862000	30.426940000	O	11.493735000	23.335040000	13.440450000
O	25.848909000	12.408453000	12.408455000	C	10.287052000	23.727502000	13.440450000
O	23.334862000	11.493756000	13.440411000	O	15.387165000	23.335040000	13.440450000
O	23.334855000	15.387135000	13.440484000	C	16.593848000	23.727502000	13.440450000
O	23.334864000	13.440413000	11.493754000	C	17.650268000	22.671082000	13.440450000
O	23.334856000	13.440488000	15.387138000	C	19.634347000	20.687003000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000

Journal Name	ARTICLE						
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.690969000	23.862789000	20.932591000
H	23.999268000	19.144577000	13.924306000	H	26.370309000	19.380620000	16.469804000
H	22.313835000	20.830009000	14.037206000	H	26.555546000	19.238160000	22.494315000
Zr	10.956924000	26.880900000	13.440450000	H	27.078758000	17.859421000	21.061809000
O	9.894590000	26.880900000	11.493735000	H	26.663064000	21.054304000	24.170609000
O	12.408223000	27.913127000	14.472677000	H	27.087579000	16.184304000	19.240838000
C	10.287052000	26.880900000	10.287052000	Cu	26.875695000	22.267551000	18.363904000
Zr	15.923976000	26.880900000	13.440450000	Cl	25.120209000	23.492976000	17.734713000
O	16.986310000	26.880900000	11.493735000	C	28.961705000	22.025657000	18.335588000
C	16.593848000	26.880900000	10.287052000	C	28.453001000	22.236391000	17.075683000
O	16.986310000	26.880900000	15.387165000	H	28.318272000	21.399601000	16.397681000
O	14.472677000	27.913127000	12.408223000	C	29.605488000	22.982264000	19.294203000
C	16.593848000	26.880900000	16.593848000	H	28.974340000	23.826010000	19.580162000
C	17.650268000	26.880900000	17.650268000	H	30.553228000	23.386214000	18.916069000
C	19.634347000	26.880900000	19.634347000	O	29.879387000	22.148501000	20.435417000
O	9.894590000	26.880900000	15.387165000	H	28.491413000	23.237733000	16.664087000
C	10.287052000	26.880900000	16.593848000	C	26.557743000	28.564333000	19.554364000
Zr	13.440450000	26.880900000	15.923976000	C	26.962360000	27.378016000	20.420873000
O	11.493735000	26.880900000	16.986310000	C	27.043112000	26.025992000	19.688289000
O	14.472677000	27.913127000	14.472677000	C	25.233911000	28.411233000	18.814927000
Zr	13.440450000	26.880900000	10.956924000	C	27.355790000	26.092282000	18.218384000
O	11.493735000	26.880900000	9.894590000	C	25.126463000	27.102776000	18.023768000
O	15.387165000	26.880900000	9.894590000	N	26.390917000	26.677286000	17.433206000
O	12.408223000	27.913127000	12.408223000	H	26.523545000	29.464854000	20.179528000
O	15.387165000	26.880900000	16.986310000	H	25.113113000	29.265469000	18.137026000
Zr	13.440450000	29.364426000	13.440450000	C	28.747515000	25.749633000	16.386301000
O	11.493735000	30.426760000	13.440450000	N	28.498891000	25.627373000	17.813043000
C	10.287052000	30.034298000	13.440450000	C	27.485592000	25.540333000	15.563280000
O	15.387165000	30.426760000	13.440450000	C	26.446149000	26.558403000	15.979840000
C	16.593848000	30.034298000	13.440450000	H	25.455259000	26.247450000	15.626669000
O	16.986310000	28.827615000	13.440450000	H	29.526241000	25.027771000	16.101389000
O	9.894590000	28.827615000	13.440450000	H	27.348605000	28.740592000	18.813594000
C	22.671082000	26.880900000	22.671082000	H	24.394487000	28.461135000	19.520141000
C	20.687003000	26.880900000	20.687003000	H	26.657353000	27.543226000	15.532712000
C	21.360638000	27.201858000	22.988008000	H	29.173405000	26.742768000	16.164603000
C	20.384593000	27.216911000	22.003898000	H	26.266280000	27.282823000	21.261327000
H	21.176773000	27.364756000	23.999268000	H	27.937944000	27.599466000	20.864107000
H	19.491341000	27.477656000	22.313835000	H	27.677946000	25.618791000	14.488332000
O	13.440450000	28.827615000	16.986310000	H	27.082376000	24.539254000	15.762958000
C	13.440450000	30.034298000	16.593848000	H	27.833404000	25.425817000	20.148062000
O	13.440450000	28.827615000	9.894590000	H	26.105101000	25.468008000	19.805045000
C	13.440450000	30.034298000	10.287052000	H	24.728231000	26.290732000	18.643980000
O	13.440450000	30.426760000	15.387165000	H	24.409098000	27.216074000	17.206046000
O	13.440450000	30.426760000	11.493735000	C	29.730153000	20.854430000	20.097108000
C	17.333342000	27.201858000	18.960712000	O	29.294115000	20.750580000	18.799932000
C	18.317452000	27.216911000	19.936757000	O	29.928704000	19.914434000	20.810886000
H	16.322082000	27.364756000	19.144577000	k. PC			
H	18.007515000	27.477656000	20.830009000	N	26.670403000	21.857746000	20.402816000
H	13.440450000	30.790903000	9.530447000	N	26.513102000	19.914349000	18.466663000

ARTICLE

Journal Name

C	26.628261000	20.564081000	20.807109000	C	27.064326000	16.568185000	10.312820000
C	26.677955000	22.848297000	21.313613000	C	30.008123000	16.567527000	13.254357000
C	26.557037000	19.003320000	17.482988000	O	23.334855000	26.880866000	24.934215000
C	26.643038000	19.510001000	19.750745000	O	23.334856000	24.934212000	26.880862000
C	26.602377000	20.267287000	22.176000000	O	25.848909000	27.912895000	27.912897000
C	26.695462000	22.629132000	22.697819000	O	23.334862000	26.880939000	28.827594000
C	26.715743000	17.623874000	17.694680000	O	23.334864000	28.827596000	26.880937000
C	26.819133000	18.153511000	20.052865000	O	24.934210000	30.426941000	26.880925000
C	26.654308000	21.290541000	23.111592000	O	26.880889000	30.426939000	24.934203000
C	26.847078000	17.217257000	19.029331000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000

Journal Name				ARTICLE			
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.676961000	23.859568000	20.909974000
H	23.999268000	19.144577000	13.924306000	H	26.456869000	19.392888000	16.471164000
H	22.313835000	20.830009000	14.037206000	H	26.554203000	19.238251000	22.514767000
Zr	10.956924000	26.880900000	13.440450000	H	26.970028000	17.827714000	21.076430000
O	9.894590000	26.880900000	11.493735000	H	26.665891000	21.069518000	24.173887000
O	12.408223000	27.913127000	14.472677000	H	26.992251000	16.164067000	19.246212000

Cu	26.957638000	22.159661000	18.353341000	Zr	24.236612000	26.881475000	26.880552000
Cl	25.416470000	23.554747000	17.600763000	Zr	26.880671000	29.524609000	26.880680000
C	29.046854000	21.925172000	18.435733000	Zr	29.524440000	26.882357000	26.881381000
C	28.609955000	22.210661000	17.163346000	C	27.064326000	30.008530000	23.753165000
H	28.526769000	21.416205000	16.428746000	C	30.008123000	27.066993000	23.753823000
C	29.621618000	22.823061000	19.492360000	C	23.755714000	23.756676000	26.684338000
H	28.955684000	23.631309000	19.807462000	Zr	26.880615000	26.881402000	29.524137000
H	30.591083000	23.252354000	19.205379000	C	27.065914000	23.754135000	30.008060000
O	29.828974000	21.928556000	20.593639000	C	30.007964000	23.754748000	27.067567000
H	28.635522000	23.232123000	16.800366000	Zr	24.236612000	13.440798000	13.439875000
C	29.728993000	20.651804000	20.161662000	Zr	26.880615000	10.797213000	13.439948000
O	29.377670000	20.627485000	18.838056000	C	23.755714000	13.637012000	16.564674000
O	29.905756000	19.676262000	20.829671000	C	27.065914000	10.313290000	16.567215000
3. CuBr-UiO-67(bpy) system							
a. Isolated							
N	26.706241000	21.848241000	20.406162000	Zr	29.524440000	13.439969000	13.438993000
N	26.609182000	19.928424000	18.458099000	C	30.007964000	13.253783000	16.566602000
C	26.629413000	20.564982000	20.818309000	Zr	26.880671000	13.440670000	10.796741000
C	26.725952000	22.840130000	21.307492000	C	23.755332000	16.566137000	13.635261000
C	26.649925000	19.002752000	17.471156000	C	27.064326000	16.568185000	10.312820000
C	26.642836000	19.517322000	19.759255000	C	30.008123000	16.567527000	13.254357000
C	26.550976000	20.266194000	22.186340000	O	23.334855000	26.880866000	24.934215000
C	26.694996000	22.629873000	22.697140000	O	23.334856000	24.934212000	26.880862000
C	26.709655000	17.622766000	17.695070000	O	25.848909000	27.912895000	27.912897000
C	26.697383000	18.149949000	20.053089000	O	23.334862000	26.880939000	28.827594000
C	26.595364000	21.295668000	23.116784000	O	23.334864000	28.827596000	26.880937000
C	26.725204000	17.208244000	19.035041000	O	24.934210000	30.426941000	26.880925000
C	26.809925000	23.730886000	23.728973000	O	26.880889000	30.426939000	24.934203000
C	26.809925000	16.592377000	16.590464000	O	26.880879000	30.426942000	28.827590000
O	26.880885000	24.934153000	23.334955000	O	27.912786000	27.912776000	27.912777000
O	26.880903000	23.334945000	24.934136000	O	28.827596000	30.426944000	26.880863000
O	26.880903000	15.387214000	16.986405000	O	30.426933000	24.934198000	26.880924000
O	26.880885000	16.986395000	15.387197000	O	30.426936000	26.880929000	24.934199000
Zr	26.878142000	26.881612000	24.237883000	O	30.426944000	26.880866000	28.827595000
Zr	26.878209000	24.239690000	26.880717000	O	30.426946000	28.827594000	26.880867000
Zr	26.878209000	13.440633000	16.081660000	O	24.934211000	26.880924000	30.426942000
Zr	26.878142000	16.083467000	13.439738000	O	26.880889000	24.934201000	30.426937000
O	24.934203000	26.880849000	23.334882000	O	26.880878000	28.827589000	30.426943000
O	25.848911000	25.848918000	25.848917000	O	28.827598000	26.880862000	30.426940000
O	25.849015000	27.912768000	25.849028000	O	25.848909000	12.408453000	12.408455000
O	27.912782000	25.849032000	25.849031000	O	23.334862000	11.493756000	13.440411000
O	27.912889000	27.912886000	25.848919000	O	23.334855000	15.387135000	13.440484000
O	26.880945000	28.827581000	23.334856000	O	23.334864000	13.440413000	11.493754000
O	28.827591000	26.880922000	23.334870000	O	23.334856000	13.440488000	15.387138000
O	24.934197000	23.334881000	26.880846000	O	24.934211000	9.894408000	13.440426000
O	25.849012000	25.849025000	27.912771000	O	26.880889000	9.894413000	15.387149000
O	27.912892000	25.848913000	27.912887000	O	27.912786000	12.408573000	12.408574000
O	26.880944000	23.334850000	28.827576000	O	26.880878000	9.894407000	11.493761000
O	28.827591000	23.334868000	26.880917000	O	28.827598000	9.894410000	13.440488000
O	25.849012000	12.408579000	14.472325000	O	30.426944000	11.493755000	13.440484000
O	25.848911000	14.472433000	14.472432000	O	30.426936000	15.387151000	13.440421000
O	24.934197000	13.440504000	16.986469000	O	30.426946000	13.440483000	11.493756000
O	26.880944000	11.493774000	16.986500000	O	30.426933000	13.440426000	15.387152000
O	27.912892000	12.408463000	14.472437000	O	24.934210000	13.440425000	9.894409000
O	27.912782000	14.472319000	14.472318000	O	26.880879000	11.493760000	9.894408000
O	28.827591000	13.440433000	16.986482000	O	26.880889000	15.387147000	9.894411000
O	25.849015000	14.472322000	12.408582000	O	28.827596000	13.440487000	9.894406000
O	24.934203000	16.986468000	13.440501000	C	23.753697000	27.066116000	30.007949000
O	27.912889000	14.472431000	12.408464000	C	23.753135000	30.008630000	27.063604000
O	26.880945000	16.986494000	11.493769000	C	26.696398000	30.008246000	30.008106000
O	28.827591000	16.986480000	13.440428000	C	30.007968000	30.008237000	26.695581000
C	23.755332000	26.686089000	23.755213000	C	30.008286000	26.697416000	30.008420000
				C	23.753697000	10.313401000	13.255234000
				C	23.753135000	13.257746000	10.312720000

C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000

ARTICLE

Journal Name

H	13.440450000	30.790903000	17.350453000	O	24.934203000	16.986468000	13.440501000
H	9.530447000	30.790903000	13.440450000	O	27.912889000	14.472431000	12.408464000
H	9.530447000	26.880900000	17.350453000	O	26.880945000	16.986494000	11.493769000
H	13.440450000	22.970897000	9.530447000	O	28.827591000	16.986480000	13.440428000
H	9.530447000	22.970897000	13.440450000	C	23.755332000	26.686089000	23.755213000
H	13.440450000	22.970897000	17.350453000	Zr	24.236612000	26.881475000	26.880552000
H	15.026933000	25.294417000	11.853967000	Zr	26.880671000	29.524609000	26.880680000
H	11.853967000	28.467383000	11.853967000	Zr	29.524440000	26.882357000	26.881381000
H	9.530447000	26.880900000	9.530447000	C	27.064326000	30.008530000	23.753165000
H	15.026933000	28.467383000	15.026933000	C	30.008123000	27.066993000	23.753823000
H	11.853967000	25.294417000	15.026933000	C	23.755714000	23.756676000	26.684338000
H	26.781175000	23.847605000	20.898484000	Zr	26.880615000	26.881402000	29.524137000
H	26.634880000	19.392510000	16.457154000	C	27.065914000	23.754135000	30.008060000
H	26.457962000	19.241865000	22.532511000	C	30.007964000	23.754748000	27.067567000
H	26.734082000	17.816722000	21.084622000	Zr	24.236612000	13.440798000	13.439875000
H	26.558693000	21.081992000	24.180288000	Zr	26.880615000	10.797213000	13.439948000
H	26.775575000	16.147803000	19.258199000	C	23.755714000	13.637012000	16.564674000
Cu	26.497338000	21.856866000	18.117508000	C	27.065914000	10.313290000	16.567215000
Br	26.230162000	23.863041000	17.170980000	Zr	29.524440000	13.439969000	13.438993000
b. PA				C	30.007964000	13.253783000	16.566602000
N	26.712602000	21.883909000	20.389258000	Zr	26.880671000	13.440670000	10.796741000
N	26.396711000	19.905339000	18.454258000	C	23.755332000	16.566137000	13.635261000
C	26.661087000	20.598091000	20.791799000	C	27.064326000	16.568185000	10.312820000
C	26.725047000	22.856937000	21.306744000	C	30.008123000	16.567527000	13.254357000
C	26.441243000	18.983088000	17.476126000	O	23.334855000	26.880866000	24.934215000
C	26.674521000	19.542817000	19.733384000	O	23.334856000	24.934212000	26.880862000
C	26.603925000	20.278421000	22.154861000	O	25.848909000	27.912895000	27.912897000
C	26.704986000	22.633847000	22.694774000	O	23.334862000	26.880939000	28.827594000
C	26.725572000	17.626831000	17.690333000	O	23.334864000	28.827596000	26.880937000
C	26.976191000	18.207098000	20.022872000	O	24.934210000	30.426941000	26.880925000
C	26.629798000	21.295784000	23.100118000	O	26.880889000	30.426939000	24.934203000
C	26.982150000	17.252628000	19.014879000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	26.8827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	28.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000

Journal Name				ARTICLE			
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
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H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
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ARTICLE

Journal Name

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H	13.440450000	30.790903000	9.530447000	O	27.912892000	25.848913000	27.912887000
H	17.350453000	26.880900000	9.530447000	O	26.880944000	23.334850000	28.827576000
H	17.350453000	30.790903000	13.440450000	O	28.827591000	23.334868000	26.880917000
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H	9.530447000	30.790903000	13.440450000	O	25.848911000	14.472433000	14.472432000
H	9.530447000	26.880900000	17.350453000	O	24.934197000	13.440504000	16.986469000
H	13.440450000	22.970897000	9.530447000	O	26.880944000	11.493774000	16.986500000
H	9.530447000	22.970897000	13.440450000	O	27.912892000	12.408463000	14.472437000
H	13.440450000	22.970897000	17.350453000	O	27.912782000	14.472319000	14.472318000
H	15.026933000	25.294417000	11.853967000	O	28.827591000	13.440433000	16.986482000
H	11.853967000	28.467383000	11.853967000	O	25.849015000	14.472322000	12.408582000
H	9.530447000	26.880900000	9.530447000	O	24.934203000	16.986468000	13.440501000
H	15.026933000	28.467383000	15.026933000	O	27.912889000	14.472431000	12.408464000
H	11.853967000	25.294417000	15.026933000	O	26.880945000	16.986494000	11.493769000
H	26.759894000	23.875048000	20.921326000	O	28.827591000	16.986480000	13.440428000
H	26.221498000	19.343203000	16.473871000	C	23.755332000	26.686089000	23.755213000
H	26.516072000	19.247657000	22.482829000	Zr	24.236612000	26.881475000	26.880552000
H	27.221273000	17.912869000	21.037746000	Zr	26.880671000	29.524609000	26.880680000
H	26.593979000	21.068587000	24.160886000	Zr	29.524440000	26.882357000	26.881381000
H	27.206286000	16.213652000	19.234360000	C	27.064326000	30.008530000	23.753165000
Cu	25.509789000	21.749682000	18.245533000	C	30.008123000	27.066993000	23.753823000
Br	23.490342000	21.306729000	19.444586000	C	23.755714000	23.756676000	26.684338000
C	25.224744000	23.516198000	17.447110000	Zr	26.880615000	26.881402000	29.524137000
C	26.271472000	23.036464000	16.952881000	C	27.065914000	23.754135000	30.008060000
H	27.165025000	23.000509000	16.359587000	C	30.007964000	23.754748000	27.067567000
C	24.072493000	24.372614000	17.777526000	Zr	24.236612000	13.440798000	13.439875000
H	24.128496000	24.641090000	18.837473000	Zr	26.880615000	10.797213000	13.439948000
H	23.150001000	23.781948000	17.673200000	C	23.755714000	13.637012000	16.564674000
O	24.048667000	25.580730000	17.046969000	C	27.065914000	10.313290000	16.567215000
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c. PA/DBU				C	30.007964000	13.253783000	16.566602000
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N	26.806249000	19.930819000	18.460742000	C	23.755332000	16.566137000	13.635261000
C	26.669204000	20.572713000	20.816333000	C	27.064326000	16.568185000	10.312820000
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C	26.812689000	19.011294000	17.477095000	O	23.334855000	26.880866000	23.934215000
C	26.674149000	19.526425000	19.752061000	O	23.334856000	24.934212000	26.880862000
C	26.304006000	20.308518000	22.144914000	O	25.848909000	27.912895000	27.912897000
C	26.703878000	22.629893000	22.700670000	O	23.334862000	26.880939000	28.827594000
C	26.712771000	17.628223000	17.691048000	O	23.334864000	28.827596000	26.880937000
C	26.558251000	18.160930000	20.043712000	O	24.934210000	30.426941000	26.880925000
C	26.345355000	21.330519000	23.085180000	O	26.880889000	30.426939000	24.934203000
C	26.584356000	17.219026000	19.025204000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
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Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
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Journal Name	ARTICLE						
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O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
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C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
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C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
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H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
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H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
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H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
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H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000

ARTICLE

Journal Name

C	20.687003000	26.880900000	20.687003000	H	24.054667000	22.535431000	13.664766000
C	21.360638000	27.201858000	22.988008000	H	26.436390000	23.909462000	13.169253000
C	20.384593000	27.216911000	22.003898000	H	22.859863000	27.163153000	16.629053000
H	21.176773000	27.364756000	23.999268000	H	24.016937000	27.924366000	15.563445000
H	19.491341000	27.477656000	22.313835000	H	26.224473000	21.571391000	14.036243000
O	13.440450000	28.827615000	16.986310000	H	26.296170000	22.195065000	15.693961000
C	13.440450000	30.034298000	16.593848000	H	25.608557000	26.613307000	16.550832000
O	13.440450000	28.827615000	9.894590000	H	24.406353000	25.600965000	17.333460000
C	13.440450000	30.034298000	10.287052000	H	22.812066000	24.458504000	16.754021000
O	13.440450000	30.426760000	15.387165000	H	22.287069000	23.177551000	15.704924000
O	13.440450000	30.426760000	11.493735000	d. PA/DBU/CO₂			
C	17.333342000	27.201858000	18.960712000	N	27.040767000	21.812901000	20.452588000
C	18.317452000	27.216911000	19.936757000	N	26.820609000	19.927391000	18.464578000
H	16.322082000	27.364756000	19.144577000	C	26.676229000	20.568850000	20.820429000
H	18.007515000	27.477656000	20.830009000	C	27.026946000	22.804490000	21.350005000
H	13.440450000	30.790903000	9.530447000	C	26.823982000	19.009446000	17.479743000
H	17.350453000	26.880900000	9.530447000	C	26.680624000	19.523066000	19.755383000
H	17.350453000	30.790903000	13.440450000	C	26.306107000	20.306420000	22.147805000
H	13.440450000	30.790903000	17.350453000	C	26.705779000	22.628237000	22.702649000
H	9.530447000	30.790903000	13.440450000	C	26.714516000	17.627080000	17.691877000
H	9.530447000	26.880900000	17.350453000	C	26.554883000	18.158114000	20.044740000
H	13.440450000	22.970897000	9.530447000	C	26.344123000	21.329757000	23.087029000
H	9.530447000	22.970897000	13.440450000	C	26.579111000	17.217271000	19.025122000
H	13.440450000	22.970897000	17.350453000	C	26.809925000	23.730886000	23.728973000
H	15.026933000	25.294417000	11.853967000	C	26.809925000	16.592377000	16.590464000
H	11.853967000	28.467383000	11.853967000	O	26.880885000	24.934153000	23.334955000
H	9.530447000	26.880900000	9.530447000	O	26.880903000	23.334945000	24.934136000
H	15.026933000	28.467383000	15.026933000	O	26.880903000	15.387214000	16.986405000
H	11.853967000	25.294417000	15.026933000	O	26.880885000	16.986395000	15.387197000
H	27.288074000	23.794373000	20.973111000	Zr	26.878142000	26.881612000	24.237883000
H	26.915800000	19.400415000	16.466202000	Zr	26.878209000	24.239690000	26.880717000
H	25.983313000	19.317317000	22.449713000	Zr	26.878209000	13.440633000	16.081660000
H	26.473692000	17.829707000	21.073389000	Zr	26.878142000	16.083467000	13.439738000
H	26.095351000	21.137230000	24.123960000	O	24.934203000	26.880849000	23.334882000
H	26.520484000	16.158525000	19.246905000	O	25.848911000	25.848918000	25.848917000
Cu	26.932343000	21.992269000	18.176725000	O	25.849015000	27.912768000	25.849028000
Br	24.619058000	22.711229000	18.343228000	O	27.912782000	25.849032000	25.849031000
C	28.053117000	23.582232000	17.623044000	O	27.912889000	27.912886000	25.848919000
C	28.631540000	22.529862000	17.282042000	O	26.880945000	28.827581000	23.334856000
H	29.391247000	21.890547000	16.875771000	O	28.827591000	26.880922000	23.334870000
C	27.654451000	24.990232000	17.855321000	O	24.934197000	23.334881000	26.880846000
H	28.097420000	25.310486000	18.808183000	O	25.849012000	25.849025000	27.912771000
H	26.560465000	25.014766000	17.994263000	O	27.912892000	25.848913000	27.912887000
O	28.106675000	25.854014000	16.857734000	O	26.880944000	23.334850000	28.827576000
H	27.559142000	25.622496000	16.060030000	O	28.827591000	23.334868000	26.880917000
C	22.832498000	26.428879000	14.601968000	O	25.849012000	12.408579000	14.472325000
C	23.578041000	26.956210000	15.825393000	O	25.848911000	14.472433000	14.472432000
C	24.699283000	26.035120000	16.367784000	O	24.934197000	13.440504000	16.986469000
C	22.013310000	25.168047000	14.863535000	O	26.880944000	11.493774000	16.986500000
C	25.103144000	24.883345000	15.482825000	O	27.912892000	12.408463000	14.472437000
C	22.780626000	24.152692000	15.701006000	O	27.912782000	14.472319000	14.472318000
N	24.135864000	23.958423000	15.208643000	O	28.827591000	13.440433000	16.986482000
H	22.179180000	27.214083000	14.205205000	O	25.849015000	14.472322000	12.408582000
H	21.718256000	24.723703000	13.904881000	O	24.934203000	16.986468000	13.440501000
C	26.681627000	23.695555000	14.222915000	O	27.912889000	14.472431000	12.408464000
N	26.327467000	24.837410000	15.046770000	O	26.880945000	16.986494000	11.493769000
C	25.973205000	22.428547000	14.670913000	O	28.827591000	16.986480000	13.440428000
C	24.476002000	22.645359000	14.676764000	C	23.755332000	26.686089000	23.755213000
H	24.002228000	21.897663000	15.326608000	Zr	24.236612000	26.881475000	26.880552000
H	27.769745000	23.565198000	14.266043000	Zr	26.880671000	29.524609000	26.880680000
H	23.564857000	26.221169000	13.811010000	Zr	29.524440000	26.882357000	26.881381000
H	21.084830000	25.415524000	15.389776000	C	27.064326000	30.008530000	23.753165000

C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000
O	26.880879000	30.426942000	28.827590000	H	25.215244000	15.103495000	11.776660000
O	27.912786000	27.912776000	27.912777000	H	25.215244000	28.544690000	25.217855000
O	28.827596000	30.426944000	26.880863000	H	28.555271000	25.223028000	25.222315000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	28.545528000	28.545099000
O	30.426936000	26.880929000	24.934199000	H	25.215026000	25.218505000	28.544917000
O	30.426944000	26.880866000	28.827595000	O	14.472677000	25.848673000	14.472677000
O	30.426946000	28.827594000	26.880867000	O	12.408223000	25.848673000	12.408223000
O	24.934211000	26.880924000	30.426942000	O	14.472677000	25.848673000	12.408223000
O	26.880889000	24.934201000	30.426937000	O	12.408223000	25.848673000	14.472677000
O	26.880878000	28.827589000	30.426943000	Zr	13.440450000	24.397374000	13.440450000
O	28.827598000	26.880862000	30.426940000	O	11.493735000	23.335040000	13.440450000
O	25.848909000	12.408453000	12.408455000	C	10.287052000	23.727502000	13.440450000
O	23.334862000	11.493756000	13.440411000	O	15.387165000	23.335040000	13.440450000
O	23.334855000	15.387135000	13.440484000	C	16.593848000	23.727502000	13.440450000
O	23.334864000	13.440413000	11.493754000	C	17.650268000	22.671082000	13.440450000
O	23.334856000	13.440488000	15.387138000	C	19.634347000	20.687003000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000

ARTICLE

Journal Name

H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	27.302981000	23.790136000	20.979638000
H	23.999268000	19.144577000	13.924306000	H	26.932405000	19.398980000	16.469630000
H	22.313835000	20.830009000	14.037206000	H	25.983790000	19.315801000	22.452758000
Zr	10.956924000	26.880900000	13.440450000	H	26.463252000	17.826194000	21.073571000
O	9.894590000	26.880900000	11.493735000	H	26.089370000	21.137934000	24.124920000
O	12.408223000	27.913127000	14.472677000	H	26.507853000	16.156970000	19.245461000
C	10.287052000	26.880900000	10.287052000	Cu	26.928268000	21.985433000	18.192015000
Zr	15.923976000	26.880900000	13.440450000	Br	24.592483000	22.642639000	18.375525000
O	16.986310000	26.880900000	11.493735000	C	28.014551000	23.616018000	17.691466000
C	16.593848000	26.880900000	10.287052000	C	28.608473000	22.592242000	17.297016000
O	16.986310000	26.880900000	15.387165000	H	29.374018000	21.986688000	16.852036000
O	14.472677000	27.913127000	12.408223000	C	27.579316000	24.988444000	18.023642000
C	16.593848000	26.880900000	16.593848000	H	28.029688000	25.266684000	18.985067000
C	17.650268000	26.880900000	17.650268000	H	26.486741000	24.972669000	18.180190000
C	19.634347000	26.880900000	19.634347000	O	27.982903000	25.938044000	17.076603000
O	9.894590000	26.880900000	15.387165000	H	27.471126000	25.701068000	16.253374000
C	10.287052000	26.880900000	16.593848000	C	22.821906000	26.430584000	14.704285000
Zr	13.440450000	26.880900000	15.923976000	C	23.541676000	26.936736000	15.951973000
O	11.493735000	26.880900000	16.986310000	C	24.633490000	25.994862000	16.514663000
O	14.472677000	27.913127000	14.472677000	C	22.004949000	25.158430000	14.915845000
Zr	13.440450000	26.880900000	10.956924000	C	25.077880000	24.878190000	15.606405000
O	11.493735000	26.880900000	9.894590000	C	22.760712000	24.119243000	15.734969000
O	15.387165000	26.880900000	9.894590000	N	24.129746000	23.954685000	15.270836000
O	12.408223000	27.913127000	12.408223000	H	22.172272000	27.220919000	14.311779000
O	15.387165000	26.880900000	16.986310000	H	21.728781000	24.742310000	13.938969000
Zr	13.440450000	29.364426000	13.440450000	C	26.701662000	23.759899000	14.341655000
O	11.493735000	30.426760000	13.440450000	N	26.314769000	24.862273000	15.203695000
C	10.287052000	30.034298000	13.440450000	C	25.996759000	22.467174000	14.717045000
O	15.387165000	30.426760000	13.440450000	C	24.496682000	22.665213000	14.701068000
C	16.593848000	30.034298000	13.440450000	H	24.021019000	21.889218000	15.315393000
O	16.986310000	28.827615000	13.440450000	H	27.789664000	23.637818000	14.406114000
O	9.894590000	28.827615000	13.440450000	H	23.571143000	26.245052000	13.923664000
C	22.671082000	26.880900000	22.671082000	H	21.065929000	25.384355000	15.432177000
C	20.687003000	26.880900000	20.687003000	H	24.093675000	22.583796000	13.678981000
C	21.360638000	27.201858000	22.988008000	H	26.479764000	24.016843000	13.292475000
C	20.384593000	27.216911000	22.003898000	H	22.807712000	27.149395000	16.739143000
H	21.176773000	27.364756000	23.999268000	H	24.006270000	27.899003000	15.711795000
H	19.491341000	27.477656000	22.313835000	H	26.272395000	21.641762000	14.051197000
O	13.440450000	28.827615000	16.986310000	H	26.300921000	22.192018000	15.735444000
C	13.440450000	30.034298000	16.593848000	H	25.530541000	26.570300000	16.750026000
O	13.440450000	28.827615000	9.894590000	H	24.300707000	25.528280000	17.451521000
C	13.440450000	30.034298000	10.287052000	H	22.762859000	24.385322000	16.798989000
O	13.440450000	30.426760000	15.387165000	H	22.277472000	23.140232000	15.691046000
O	13.440450000	30.426760000	11.493735000	C	27.177617000	28.264605000	18.374264000
C	17.333342000	27.201858000	18.960712000	O	27.589848000	27.823529000	19.376165000
C	18.317452000	27.216911000	19.936757000	O	26.743873000	28.757656000	17.406568000
H	16.322082000	27.364756000	19.144577000	e. TS1			
H	18.007515000	27.477656000	20.830009000	N	26.516182000	21.876816000	20.391322000
H	13.440450000	30.790903000	9.530447000	N	26.805017000	19.926708000	18.438493000
H	17.350453000	26.880900000	9.530447000	C	26.653045000	20.593593000	20.783136000
H	17.350453000	30.790903000	13.440450000	C	26.561198000	22.851882000	21.309281000
H	13.440450000	30.790903000	17.350453000	C	26.809759000	18.999110000	17.463652000
H	9.530447000	30.790903000	13.440450000	C	26.641787000	19.540198000	19.725385000
H	9.530447000	26.880900000	17.350453000	C	26.817358000	20.278009000	22.141055000
H	13.440450000	22.970897000	9.530447000	C	26.715165000	22.632242000	22.690535000

Journal Name				ARTICLE			
C	26.701338000	17.622947000	17.687478000	O	23.334864000	28.827596000	26.880937000
C	26.470846000	18.179560000	20.027035000	O	24.934210000	30.426941000	26.880925000
C	26.835997000	21.293608000	23.087357000	O	26.880889000	30.426939000	24.934203000
C	26.517282000	17.226795000	19.020475000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000

ARTICLE

Journal Name

H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.467029000	23.866686000	20.925171000
H	23.999268000	19.144577000	13.924306000	H	26.907903000	19.383185000	16.450835000
H	22.313835000	20.830009000	14.037206000	H	26.956318000	19.249979000	22.460803000
Zr	10.956924000	26.880900000	13.440450000	H	26.287817000	17.866393000	21.049580000
O	9.894590000	26.880900000	11.493735000	H	26.966392000	21.067317000	24.140946000
O	12.408223000	27.913127000	14.472677000	H	26.406793000	16.171295000	19.248247000
C	10.287052000	26.880900000	10.287052000	Cu	26.565872000	21.916197000	17.874328000
Zr	15.923976000	26.880900000	13.440450000	Br	24.441635000	21.481325000	16.855140000
O	16.986310000	26.880900000	11.493735000	C	27.246045000	23.756120000	17.369967000
C	16.593848000	26.880900000	10.287052000	C	28.176687000	23.065424000	17.839830000
O	16.986310000	26.880900000	15.387165000	H	29.161051000	22.829578000	18.195564000
O	14.472677000	27.913127000	12.408223000	C	26.448950000	24.811034000	16.684968000

Journal Name				ARTICLE			
H	26.967331000	25.759064000	16.928035000	O	26.880945000	28.827581000	23.334856000
H	25.451113000	24.856730000	17.155400000	O	28.827591000	26.880922000	23.334870000
O	26.368299000	24.628451000	15.327375000	O	24.934197000	23.334881000	26.880846000
H	26.404966000	23.217043000	14.765431000	O	25.849012000	25.849025000	27.912771000
C	25.382066000	23.622795000	10.899903000	O	27.912892000	25.848913000	27.912887000
C	24.585391000	24.262034000	12.035685000	O	26.880944000	23.334850000	28.827576000
C	24.391360000	23.365436000	13.282247000	O	28.827591000	23.334868000	26.880917000
C	24.764783000	22.366363000	10.287817000	O	25.849012000	12.408579000	14.472325000
C	25.381969000	22.247458000	13.319248000	O	25.848911000	14.472433000	14.472432000
C	24.306797000	21.354249000	11.340371000	O	24.934197000	13.440504000	16.986469000
N	25.245675000	21.223258000	12.451158000	O	26.880944000	11.493774000	16.986500000
H	25.540426000	24.363820000	10.109905000	O	27.912892000	12.408463000	14.472437000
H	25.491932000	21.900492000	9.611080000	O	27.912782000	14.472319000	14.472318000
C	27.421049000	21.332842000	14.272740000	O	28.827591000	13.440433000	16.986482000
N	26.374671000	22.324829000	14.161196000	O	25.849015000	14.472322000	12.408582000
C	26.955030000	20.007277000	13.700475000	O	24.934203000	16.986468000	13.440501000
C	26.301756000	20.219996000	12.347639000	O	27.912889000	14.472431000	12.408464000
H	25.853441000	19.292224000	11.983237000	O	26.880945000	16.986494000	11.493769000
H	27.673613000	21.243998000	15.338641000	O	28.827591000	16.986480000	13.440428000
H	26.386597000	23.391219000	11.279154000	C	23.755332000	26.686089000	23.755213000
H	23.895537000	22.624822000	9.670217000	Zr	24.236612000	26.881475000	26.880552000
H	27.047982000	20.539422000	11.601416000	Zr	26.880671000	29.524609000	26.880680000
H	28.319064000	21.707897000	13.761409000	Zr	29.524440000	26.882357000	26.881381000
H	23.604064000	24.591892000	11.673816000	C	27.064326000	30.008530000	23.753165000
H	25.127983000	25.156092000	12.354587000	C	30.008123000	27.066993000	23.753823000
H	27.788271000	19.304623000	13.605198000	C	23.755714000	23.756676000	26.684338000
H	26.226105000	19.559823000	14.385229000	Zr	26.880615000	26.881402000	29.524137000
H	24.527027000	23.950191000	14.194683000	C	27.065914000	23.754135000	30.008060000
H	23.385888000	22.936115000	13.316780000	C	30.007964000	23.754748000	27.067567000
H	23.332602000	21.645987000	11.742856000	Zr	24.236612000	13.440798000	13.439875000
H	24.175946000	20.356252000	10.911031000	Zr	26.880615000	10.797213000	13.439948000
C	27.890814000	25.350968000	14.334010000	C	23.755714000	13.637012000	16.564674000
O	28.507210000	25.996996000	15.122476000	C	27.065914000	10.313290000	16.567215000
O	27.699630000	24.894374000	13.245442000	Zr	29.524440000	13.439969000	13.438993000
f. IM1				C	30.007964000	13.253783000	16.566602000
N	26.631685000	21.878151000	20.385536000	Zr	26.880671000	13.440670000	10.796741000
N	26.838967000	19.914414000	18.454526000	C	23.755332000	16.566137000	13.635261000
C	26.654299000	20.591355000	20.790446000	C	27.064326000	16.568185000	10.312820000
C	26.670310000	22.852903000	21.303849000	C	30.008123000	16.567527000	13.254357000
C	26.822481000	18.995485000	17.473330000	O	23.334855000	26.880866000	24.934215000
C	26.637854000	19.533387000	19.736329000	O	23.334856000	24.934212000	26.880862000
C	26.706089000	20.273852000	22.156527000	O	25.848909000	27.912895000	27.912897000
C	26.715568000	22.631702000	22.692492000	O	23.334862000	26.880939000	28.827594000
C	26.689665000	17.620355000	17.690323000	O	23.334864000	28.827596000	26.880937000
C	26.430326000	18.175876000	20.028895000	O	24.934210000	30.426941000	26.880925000
C	26.730141000	21.291713000	23.100223000	O	26.880889000	30.426939000	24.934203000
C	26.484756000	17.224238000	19.019939000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000

ARTICLE

Journal Name

O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	12.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.223150000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000

O	9.894590000	28.827615000	13.440450000	H	27.154524000	21.839379000	10.486952000
C	22.671082000	26.880900000	22.671082000	H	24.253018000	22.457655000	11.204680000
C	20.687003000	26.880900000	20.687003000	H	27.077666000	19.431132000	12.979345000
C	21.360638000	27.201858000	22.988008000	H	29.728378000	20.019060000	12.849696000
C	20.384593000	27.216911000	22.003898000	H	26.037126000	24.594913000	11.198732000
H	21.176773000	27.364756000	23.999268000	H	27.569034000	24.284815000	10.416409000
H	19.491341000	27.477656000	22.313835000	H	28.610765000	19.199477000	14.885031000
O	13.440450000	28.827615000	16.986310000	H	28.275833000	20.874477000	15.403084000
C	13.440450000	30.034298000	16.593848000	H	28.489029000	24.318457000	12.534717000
O	13.440450000	28.827615000	9.894590000	H	26.933129000	24.205728000	13.304540000
C	13.440450000	30.034298000	10.287052000	H	25.315729000	22.933715000	13.293734000
O	13.440450000	30.426760000	15.387165000	H	24.809338000	21.283470000	13.430265000
O	13.440450000	30.426760000	11.493735000	C	30.282622000	24.353189000	14.980259000
C	17.333342000	27.201858000	18.960712000	O	30.823155000	25.001638000	15.863022000
C	18.317452000	27.216911000	19.936757000	O	30.678125000	23.941247000	13.858325000
H	16.322082000	27.364756000	19.144577000	g. TS2			
H	18.007515000	27.477656000	20.830009000	N	26.389579000	21.813822000	20.425811000
H	13.440450000	30.790903000	9.530447000	N	26.675599000	19.912140000	18.482348000
H	17.350453000	26.880900000	9.530447000	C	26.700310000	20.546271000	20.815112000
H	17.350453000	30.790903000	13.440450000	C	26.442046000	22.809004000	21.334252000
H	13.440450000	30.790903000	17.350453000	C	26.657815000	18.994434000	17.495744000
H	9.530447000	30.790903000	13.440450000	C	26.681548000	19.494867000	19.775035000
H	9.530447000	26.880900000	17.350453000	C	27.025122000	20.281377000	22.154337000
H	13.440450000	22.970897000	9.530447000	C	26.733991000	22.623427000	22.695077000
H	9.530447000	22.970897000	13.440450000	C	26.708113000	17.612095000	17.701220000
H	13.440450000	22.970897000	17.350453000	C	26.657514000	18.120631000	20.068760000
H	15.026933000	25.294417000	11.853967000	C	27.016668000	21.303182000	23.089705000
H	11.853967000	28.467383000	11.853967000	C	26.689046000	17.188242000	19.045256000
H	9.530447000	26.880900000	9.530447000	C	26.809925000	23.730886000	23.728973000
H	15.026933000	28.467383000	15.026933000	C	26.809925000	16.592377000	16.590464000
H	11.853967000	25.294417000	15.026933000	O	26.880885000	24.934153000	23.334955000
H	26.668824000	23.870264000	20.915934000	O	26.880903000	23.334945000	24.934136000
H	26.929512000	19.392908000	16.467379000	O	26.880903000	15.387214000	16.986405000
H	26.752081000	19.241310000	22.487943000	O	26.880885000	16.986395000	15.387197000
H	26.225250000	17.859771000	21.046217000	Zr	26.878142000	26.881612000	24.237883000
H	26.779713000	21.064929000	24.160507000	Zr	26.878209000	24.239690000	26.880717000
H	26.362626000	16.169279000	19.244897000	Zr	26.878209000	13.440633000	16.081660000
Cu	27.201470000	21.872659000	17.876917000	Zr	26.878142000	16.083467000	16.439738000
Br	25.400200000	22.081032000	16.321723000	O	24.934203000	26.880849000	23.334882000
C	28.522902000	23.329818000	17.458330000	O	25.848911000	25.848918000	25.848917000
C	29.008019000	22.548023000	18.303341000	O	25.849015000	27.912768000	25.849028000
H	29.721135000	22.159600000	19.004773000	O	27.912782000	25.849032000	25.849031000
C	28.339082000	24.361333000	16.419742000	O	27.912889000	27.912886000	25.848919000
H	28.843415000	25.273754000	16.766430000	O	26.880945000	28.827581000	23.334856000
H	27.271578000	24.549340000	16.262920000	O	28.827591000	26.880922000	23.334870000
O	28.891871000	23.949942000	15.192043000	O	24.934197000	23.334881000	26.880846000
H	29.793275000	22.826690000	13.261583000	O	25.849012000	25.849025000	27.912771000
C	26.322552000	22.553050000	10.561957000	O	27.912892000	25.848913000	27.912887000
C	26.854752000	23.867403000	11.132447000	O	26.880944000	23.334850000	28.827576000
C	27.548440000	23.763565000	12.513680000	O	28.827591000	23.334868000	26.880917000
C	25.194169000	21.920523000	11.374540000	O	25.849012000	12.408579000	14.472325000
C	27.855622000	22.364952000	12.947822000	O	25.848911000	14.472433000	14.472432000
C	25.477447000	21.937171000	12.871698000	O	24.934197000	13.440504000	16.986469000
N	26.845798000	21.520706000	13.175884000	O	26.880944000	11.493774000	16.986500000
H	25.983973000	22.715955000	9.533389000	O	27.912892000	12.408463000	14.472437000
H	25.029775000	20.890402000	11.034246000	O	27.912782000	14.472319000	14.472318000
C	29.499141000	20.735397000	13.651321000	O	28.827591000	13.440433000	16.986482000
N	29.120676000	22.012403000	13.067777000	O	25.849015000	14.472322000	12.408582000
C	28.386513000	20.209776000	14.533578000	O	24.934203000	16.986468000	13.440501000
C	27.080767000	20.201836000	13.765919000	O	27.912889000	14.472431000	12.408464000
H	26.240763000	20.008976000	14.441842000	O	26.880945000	16.986494000	11.493769000
H	30.420205000	20.904586000	14.216735000	O	28.827591000	16.986480000	13.440428000

ARTICLE

Journal Name

C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000
O	26.880879000	30.426942000	28.827590000	H	25.215244000	15.103495000	11.776660000
O	27.912786000	27.912776000	27.912777000	H	25.215244000	28.544690000	25.217855000
O	28.827596000	30.426944000	26.880863000	H	28.555271000	25.223028000	25.222315000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	28.545528000	28.545099000
O	30.426936000	26.880929000	24.934199000	H	25.215026000	25.218505000	28.544917000
O	30.426944000	26.880866000	28.827595000	O	14.472677000	25.848673000	14.472677000
O	30.426946000	28.827594000	26.880867000	O	12.408223000	25.848673000	12.408223000
O	24.934211000	26.880924000	30.426942000	O	14.472677000	25.848673000	12.408223000
O	26.880889000	24.934201000	30.426937000	O	12.408223000	25.848673000	14.472677000
O	26.880878000	28.827589000	30.426943000	Zr	13.440450000	24.397374000	13.440450000
O	28.827598000	26.880862000	30.426940000	O	11.493735000	23.335040000	13.440450000
O	25.848909000	12.408453000	12.408455000	C	10.287052000	23.727502000	13.440450000
O	23.334862000	11.493756000	13.440411000	O	15.387165000	23.335040000	13.440450000
O	23.334855000	15.387135000	13.440484000	C	16.593848000	23.727502000	13.440450000
O	23.334864000	13.440413000	11.493754000	C	17.650268000	22.671082000	13.440450000
O	23.334856000	13.440488000	15.387138000	C	19.634347000	20.687003000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000

Journal Name	ARTICLE						
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.222677000	23.803714000	20.950803000
H	23.999268000	19.144577000	13.924306000	H	26.598983000	19.394083000	16.487101000
H	22.313835000	20.830009000	14.037206000	H	27.302401000	19.276974000	22.459591000
Zr	10.956924000	26.880900000	13.440450000	H	26.598025000	17.783425000	21.099085000
O	9.894590000	26.880900000	11.493735000	H	27.256079000	21.105638000	24.129466000
O	12.408223000	27.913127000	14.472677000	H	26.690468000	16.125439000	19.262915000
C	10.287052000	26.880900000	10.287052000	Cu	26.068226000	21.926668000	18.267512000
Zr	15.923976000	26.880900000	13.440450000	Br	24.052617000	21.223229000	17.015108000
O	16.986310000	26.880900000	11.493735000	C	26.155241000	24.230650000	16.820933000
C	16.593848000	26.880900000	10.287052000	C	26.981045000	23.526686000	17.481377000
O	16.986310000	26.880900000	15.387165000	H	28.062767000	23.577099000	17.472783000
O	14.472677000	27.913127000	12.408223000	C	24.812260000	24.630115000	16.421163000
C	16.593848000	26.880900000	16.593848000	H	24.594786000	25.653064000	16.757672000
C	17.650268000	26.880900000	17.650268000	H	24.082116000	23.934034000	16.853126000
C	19.634347000	26.880900000	19.634347000	O	24.698601000	24.549136000	15.005633000
O	9.894590000	26.880900000	15.387165000	H	25.089120000	22.752727000	14.561961000
C	10.287052000	26.880900000	16.593848000	C	25.708743000	23.268348000	10.456910000
Zr	13.440450000	26.880900000	15.923976000	C	24.327424000	23.485549000	11.066695000
O	11.493735000	26.880900000	16.986310000	C	23.993138000	22.584239000	12.284876000
O	14.472677000	27.913127000	14.472677000	C	25.891935000	21.914228000	9.775377000
Zr	13.440450000	26.880900000	10.956924000	C	25.160372000	21.806076000	12.804640000
O	11.493735000	26.880900000	9.894590000	C	25.350807000	20.768546000	10.626505000
O	15.387165000	26.880900000	9.894590000	N	25.747284000	20.883274000	12.027799000
O	12.408223000	27.913127000	12.408223000	H	25.910983000	24.065999000	9.735915000
O	15.387165000	26.880900000	16.986310000	H	26.952983000	21.748813000	9.551508000
Zr	13.440450000	29.364426000	13.440450000	C	26.787488000	21.457239000	14.601903000
O	11.493735000	30.426760000	13.440450000	N	25.591381000	22.042034000	14.021736000
C	10.287052000	30.034298000	13.440450000	C	27.061870000	20.119008000	13.950305000
O	15.387165000	30.426760000	13.440450000	C	26.998941000	20.242677000	12.440774000
C	16.593848000	30.034298000	13.440450000	H	27.037026000	19.258032000	11.965702000
O	16.986310000	28.827615000	13.440450000	H	26.605388000	21.371098000	15.679055000
O	9.894590000	28.827615000	13.440450000	H	26.453624000	23.407124000	11.250871000
C	22.671082000	26.880900000	22.671082000	H	25.367135000	21.891506000	8.812183000
C	20.687003000	26.880900000	20.687003000	H	27.845320000	20.835181000	12.060975000
C	21.360638000	27.201858000	22.988008000	H	27.618943000	22.162141000	14.463620000
C	20.384593000	27.216911000	22.003898000	H	23.553090000	23.347845000	10.301432000
H	21.176773000	27.364756000	23.999268000	H	24.280031000	24.518970000	11.410980000
H	19.491341000	27.477656000	22.313835000	H	28.042093000	19.737893000	14.247820000
O	13.440450000	28.827615000	16.986310000	H	26.321010000	19.386402000	14.288322000
C	13.440450000	30.034298000	16.593848000	H	23.617094000	23.196196000	13.107915000
O	13.440450000	28.827615000	9.894590000	H	23.202985000	21.871558000	12.024821000
C	13.440450000	30.034298000	10.287052000	H	24.257185000	20.742659000	10.581162000
O	13.440450000	30.426760000	15.387165000	H	25.697412000	19.791632000	10.276005000
O	13.440450000	30.426760000	11.493735000	C	25.916203000	25.011772000	14.376321000
C	17.333342000	27.201858000	18.960712000	O	26.819056000	25.311464000	15.205770000
C	18.317452000	27.216911000	19.936757000	O	25.889183000	24.985768000	13.152249000
H	16.322082000	27.364756000	19.144577000	h. IM2			
H	18.007515000	27.477656000	20.830009000	N	26.651727000	21.838119000	20.413268000
H	13.440450000	30.790903000	9.530447000	N	26.501923000	19.924445000	18.482354000
H	17.350453000	26.880900000	9.530447000	C	26.654700000	20.545220000	20.826167000

ARTICLE

Journal Name

C	26.634899000	22.827579000	21.325744000	C	30.008123000	16.567527000	13.254357000
C	26.551603000	19.005049000	17.496071000	O	23.334855000	26.880866000	24.934215000
C	26.677771000	19.510866000	19.771161000	O	23.334856000	24.934212000	26.880862000
C	26.643067000	20.252883000	22.201831000	O	25.848909000	27.912895000	27.912897000
C	26.697119000	22.622111000	22.708571000	O	23.334862000	26.880939000	28.827594000
C	26.728100000	17.626372000	17.695017000	O	23.334864000	28.827596000	26.880937000
C	26.885686000	18.150471000	20.051826000	O	24.934210000	30.426941000	26.880925000
C	26.685650000	21.277698000	23.131782000	O	26.880889000	30.426939000	24.934203000
C	26.891330000	17.215264000	19.031798000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758588000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000

Journal Name				ARTICLE			
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.567262000	23.835577000	20.920775000
H	23.999268000	19.144577000	13.924306000	H	26.437468000	19.396672000	16.486679000
H	22.313835000	20.830009000	14.037206000	H	26.595635000	19.224130000	22.545257000
Zr	10.956924000	26.880900000	13.440450000	H	27.057994000	17.824887000	21.072963000
O	9.894590000	26.880900000	11.493735000	H	26.704809000	21.061020000	24.194702000
O	12.408223000	27.913127000	14.472677000	H	27.046437000	16.162718000	19.244032000
C	10.287052000	26.880900000	10.287052000	Cu	26.562106000	22.125428000	18.325843000

ARTICLE

Journal Name

Br	24.398571000	23.484048000	18.620640000	O	24.934203000	26.880849000	23.334882000
C	28.353794000	24.137105000	17.476355000	O	25.848911000	25.848918000	25.848917000
C	27.797554000	22.985619000	17.095036000	O	25.849015000	27.912768000	25.849028000
H	28.071947000	22.670150000	16.080555000	O	27.912782000	25.849032000	25.849031000
C	28.253978000	24.856349000	18.783298000	O	27.912889000	27.912886000	25.848919000
H	28.897098000	24.433986000	19.567719000	O	26.880945000	28.827581000	23.334856000
H	27.223028000	24.896324000	19.162239000	O	28.827591000	26.880922000	23.334870000
O	28.711798000	26.188483000	18.487527000	O	24.934197000	23.334881000	26.880846000
H	26.408738000	24.424830000	16.345137000	O	25.849012000	25.849025000	27.912771000
C	25.154288000	28.451988000	15.513399000	O	27.912892000	25.848913000	27.912887000
C	25.760772000	28.063455000	16.859346000	O	26.880944000	23.334850000	28.827576000
C	25.503141000	26.600879000	17.299321000	O	28.827591000	23.334868000	26.880917000
C	23.627579000	28.472581000	15.498247000	O	25.849012000	12.408579000	14.472325000
C	24.895398000	25.721519000	16.256255000	O	25.848911000	14.472433000	14.472432000
C	23.022338000	27.251587000	16.184320000	O	24.934197000	13.440504000	16.986469000
N	23.677542000	26.005256000	15.790045000	O	26.880944000	11.493774000	16.986500000
H	25.532401000	29.433907000	15.213943000	O	27.912892000	12.408463000	14.472437000
H	23.268176000	28.540349000	14.464570000	O	27.912782000	14.472319000	14.472318000
C	25.025432000	23.633412000	14.977027000	O	28.827591000	13.440433000	16.986482000
N	25.595606000	24.707755000	15.782095000	O	25.849015000	14.472322000	12.408582000
C	23.513844000	23.715967000	14.985753000	O	24.934203000	16.986468000	13.440501000
C	23.060354000	25.147556000	14.781023000	O	27.912889000	14.472431000	12.408464000
H	21.975894000	25.236612000	14.894393000	O	26.880945000	16.986494000	11.493769000
H	25.368267000	22.695064000	15.429149000	O	28.827591000	16.986480000	13.440428000
H	25.516434000	27.755160000	14.744990000	C	23.755332000	26.686089000	23.755213000
H	23.252006000	29.363759000	16.015002000	Zr	24.236612000	26.881475000	26.880552000
H	23.317624000	25.515406000	13.776096000	Zr	26.880671000	29.524609000	26.880680000
H	25.435324000	23.692544000	13.961241000	Zr	29.524440000	26.882357000	26.881381000
H	25.391126000	28.738964000	17.639356000	C	27.064326000	30.008530000	23.753165000
H	26.842384000	28.220298000	16.815345000	C	30.008123000	27.066993000	23.753823000
H	23.103477000	23.084031000	14.197760000	C	23.755714000	23.756676000	26.684338000
H	23.151291000	23.361611000	15.956948000	Zr	26.880615000	26.881402000	29.524137000
H	26.435605000	26.135590000	17.616390000	C	27.065914000	23.754135000	30.008060000
H	24.846561000	26.536036000	18.174316000	C	30.007964000	23.754748000	27.067567000
H	23.093934000	27.346562000	17.272640000	Zr	24.236612000	13.440798000	13.439875000
H	21.960670000	27.147084000	15.948826000	Zr	26.880615000	10.797213000	13.439948000
C	29.282822000	26.197674000	17.253770000	C	23.755714000	13.637012000	16.564674000
O	29.172722000	24.985261000	16.665905000	C	27.065914000	10.313290000	16.567215000
O	29.785836000	27.167009000	16.755914000	Zr	29.524440000	13.439969000	13.438993000
i. TS3				C	30.007964000	13.253783000	16.566602000
N	26.886316000	21.844394000	20.416933000	Zr	26.880671000	13.440670000	10.796741000
N	26.625729000	19.934988000	18.469953000	C	23.755332000	16.566137000	13.635261000
C	26.685016000	20.561922000	20.815924000	C	27.064326000	16.568185000	10.312820000
C	26.861996000	22.834927000	21.333128000	C	30.008123000	16.567527000	13.254357000
C	26.672870000	19.010863000	17.491648000	O	23.334855000	26.880866000	24.934215000
C	26.711581000	19.521160000	19.764892000	O	23.334856000	24.934212000	26.880862000
C	26.458872000	20.278109000	22.173886000	O	25.848909000	27.912895000	27.912897000
C	26.709406000	22.625507000	22.705444000	O	23.334862000	26.880939000	28.827594000
C	26.743205000	17.624623000	17.698357000	O	23.334864000	28.827596000	26.880937000
C	26.824410000	18.152159000	20.059163000	O	24.934210000	30.426941000	26.880925000
C	26.494684000	21.295566000	23.113360000	O	26.880889000	30.426939000	24.934203000
C	26.818845000	17.212325000	19.041253000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000

O	25.848909000	12.408453000	12.408455000	C	10.287052000	23.727502000	13.440450000
O	23.334862000	11.493756000	13.440411000	O	15.387165000	23.335040000	13.440450000
O	23.334855000	15.387135000	13.440484000	C	16.593848000	23.727502000	13.440450000
O	23.334864000	13.440413000	11.493754000	C	17.650268000	22.671082000	13.440450000
O	23.334856000	13.440488000	15.387138000	C	19.634347000	20.687003000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	30.008630000	27.063604000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	30.008246000	30.008106000	C	20.687003000	19.634347000	13.440450000
C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000

ARTICLE	Journal Name						
O	11.493735000	30.426760000	13.440450000	N	25.478730000	22.935571000	15.508853000
C	10.287052000	30.034298000	13.440450000	C	24.025508000	21.253537000	16.543138000
O	15.387165000	30.426760000	13.440450000	C	22.901475000	22.273584000	16.576441000
C	16.593848000	30.034298000	13.440450000	H	22.651524000	22.500704000	17.621258000
O	16.986310000	28.827615000	13.440450000	H	25.881792000	20.914325000	15.463331000
O	9.894590000	28.827615000	13.440450000	H	23.125659000	24.578714000	13.559589000
C	22.671082000	26.880900000	22.671082000	H	22.032594000	26.644633000	15.526375000
C	20.687003000	26.880900000	20.687003000	H	21.989043000	21.913537000	16.090135000
C	21.360638000	27.201858000	22.988008000	H	24.549955000	21.435056000	14.436535000
C	20.384593000	27.216911000	22.003898000	H	24.594484000	27.062743000	14.548961000
H	21.176773000	27.364756000	23.999268000	H	25.221810000	25.730020000	13.594205000
H	19.491341000	27.477656000	22.313835000	H	23.622240000	20.240539000	16.444425000
O	13.440450000	28.827615000	16.986310000	H	24.570995000	21.295918000	17.492832000
C	13.440450000	30.034298000	16.593848000	H	26.076945000	25.324917000	15.771123000
O	13.440450000	28.827615000	9.894590000	H	24.591806000	25.808834000	16.579760000
C	13.440450000	30.034298000	10.287052000	H	22.717141000	25.140417000	17.168365000
O	13.440450000	30.426760000	15.387165000	H	21.401880000	24.163907000	16.547678000
O	13.440450000	30.426760000	11.493735000	C	30.210855000	25.407667000	17.183612000
C	17.333342000	27.201858000	18.960712000	O	29.825301000	24.155878000	16.776430000
C	18.317452000	27.216911000	19.936757000	O	31.281349000	25.888516000	16.959174000
H	16.322082000	27.364756000	19.144577000	j. PC/DBU			
H	18.007515000	27.477656000	20.830009000	N	26.671414000	21.866639000	20.402508000
H	13.440450000	30.790903000	9.530447000	N	26.490087000	19.914921000	18.462769000
H	17.350453000	26.880900000	9.530447000	C	26.639050000	20.570616000	20.800373000
H	17.350453000	30.790903000	13.440450000	C	26.680659000	22.847315000	21.323171000
H	13.440450000	30.790903000	17.350453000	C	26.530830000	19.002444000	17.482041000
H	9.530447000	30.790903000	13.440450000	C	26.655426000	19.517264000	19.743376000
H	9.530447000	26.880900000	17.350453000	C	26.615881000	20.268034000	22.168935000
H	13.440450000	22.970897000	9.530447000	C	26.699488000	22.624563000	22.703947000
H	9.530447000	22.970897000	13.440450000	C	26.719197000	17.625646000	17.692842000
H	13.440450000	22.970897000	17.350453000	C	26.862391000	18.164868000	20.046441000
H	15.026933000	25.294417000	11.853967000	C	26.662101000	21.284332000	23.112509000
H	11.853967000	28.467383000	11.853967000	C	26.884725000	17.225702000	19.025394000
H	9.530447000	26.880900000	9.530447000	C	26.809925000	23.730886000	23.728973000
H	15.026933000	28.467383000	15.026933000	C	26.809925000	16.592377000	16.590464000
H	11.853967000	25.294417000	15.026933000	O	26.880885000	24.934153000	23.334955000
H	26.969492000	23.842950000	20.941926000	O	26.880903000	23.334945000	24.934136000
H	26.646956000	19.397257000	16.474217000	O	26.880903000	15.387214000	16.986405000
H	26.241225000	19.262887000	22.491018000	O	26.880885000	16.986395000	15.387197000
H	26.935390000	17.824478000	21.088157000	Zr	26.878142000	26.881612000	24.237883000
H	26.347357000	21.084245000	24.167626000	Zr	26.878209000	24.239690000	26.880717000
H	26.900893000	16.153338000	19.263169000	Zr	26.878209000	13.440633000	16.081660000
Cu	26.721065000	22.204390000	18.390151000	Zr	26.878142000	16.083467000	13.439738000
Br	24.877874000	23.925724000	18.913072000	O	24.934203000	26.880849000	23.334882000
C	28.509106000	23.910365000	17.152362000	O	25.848911000	25.848918000	25.848917000
C	27.820945000	22.806098000	16.807437000	O	25.849015000	27.912768000	25.849028000
H	28.418854000	22.111607000	16.206880000	O	27.912782000	25.849032000	25.849031000
C	28.106287000	25.093939000	17.985627000	O	27.912889000	27.912886000	25.848919000
H	27.976758000	24.845689000	19.046071000	O	26.880945000	28.827581000	23.334856000
H	27.181939000	25.577521000	17.656630000	O	28.827591000	26.880922000	23.334870000
O	29.206795000	26.003968000	17.856454000	O	24.934197000	23.334881000	26.880846000
H	26.554263000	22.998774000	16.140957000	O	25.849012000	25.849025000	27.912771000
C	23.112630000	25.591233000	13.982295000	O	27.912892000	25.848913000	27.912887000
C	24.526352000	25.978637000	14.403303000	O	26.880944000	23.334850000	28.827576000
C	24.986691000	25.293099000	15.698375000	O	28.827591000	23.334868000	26.880917000
C	22.087353000	25.631724000	15.109241000	O	25.849012000	12.408579000	14.472325000
C	24.575364000	23.856668000	15.756206000	O	25.848911000	14.472433000	14.472432000
C	22.342129000	24.643364000	16.262660000	O	24.934197000	13.440504000	16.986469000
N	23.268836000	23.554378000	15.945615000	O	26.880944000	11.493774000	16.986500000
H	22.779987000	26.248260000	13.171960000	O	27.912892000	12.408463000	14.472437000
H	21.100492000	25.432519000	14.679594000	O	27.912782000	14.472319000	14.472318000
C	25.006187000	21.570233000	15.424662000	O	28.827591000	13.440433000	16.986482000

Journal Name	ARTICLE						
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000
Zr	29.524440000	13.439969000	13.438993000	H	23.003255000	27.356162000	30.758555000
C	30.007964000	13.253783000	16.566602000	H	23.001913000	30.759916000	27.349810000
Zr	26.880671000	13.440670000	10.796741000	H	26.407446000	30.758917000	30.758911000
C	23.755332000	16.566137000	13.635261000	H	30.758582000	30.758568000	26.405278000
C	27.064326000	16.568185000	10.312820000	H	30.759373000	26.409850000	30.759355000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	9.562795000	12.965188000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	12.971540000	9.561434000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	9.562439000	9.562434000
O	25.848909000	27.912895000	27.912897000	H	30.759373000	9.561995000	13.911500000
O	23.334862000	26.880939000	28.827594000	H	30.758582000	13.916071000	9.562782000
O	23.334864000	28.827596000	26.880937000	H	25.215026000	11.776433000	15.102845000
O	24.934210000	30.426941000	26.880925000	H	28.544134000	11.776251000	11.775822000
O	26.880889000	30.426939000	24.934203000	H	28.555271000	15.099035000	15.098322000
O	26.880879000	30.426942000	28.827590000	H	25.215244000	15.103495000	11.776660000
O	27.912786000	27.912776000	27.912777000	H	25.215244000	28.544690000	25.217855000
O	28.827596000	30.426944000	26.880863000	H	28.555271000	25.223028000	25.222315000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	28.545528000	28.545099000
O	30.426936000	26.880929000	24.934199000	H	25.215026000	25.218505000	28.544917000
O	30.426944000	26.880866000	28.827595000	O	14.472677000	25.848673000	12.472677000
O	30.426946000	28.827594000	26.880867000	O	12.408223000	25.848673000	12.408223000
O	24.934211000	26.880924000	30.426942000	O	14.472677000	25.848673000	12.408223000
O	26.880889000	24.934201000	30.426937000	O	12.408223000	25.848673000	14.472677000
O	26.880878000	28.827589000	30.426943000	Zr	13.440450000	24.397374000	13.440450000
O	28.827598000	26.880862000	30.426940000	O	11.493735000	23.335040000	13.440450000
O	25.848909000	12.408453000	12.408455000	C	10.287052000	23.727502000	13.440450000
O	23.334862000	11.493756000	13.440411000	O	15.387165000	23.335040000	13.440450000
O	23.334855000	15.387135000	13.440484000	C	16.593848000	23.727502000	13.440450000
O	23.334864000	13.440413000	11.493754000	C	17.650268000	22.671082000	13.440450000
O	23.334856000	13.440488000	15.387138000	C	19.634347000	20.687003000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	18.960712000	22.988008000	13.761408000
O	26.880889000	9.894413000	15.387149000	C	19.936757000	22.003898000	13.776461000
O	27.912786000	12.408573000	12.408574000	H	19.144577000	23.999268000	13.924306000
O	26.880878000	9.894407000	11.493761000	H	20.830009000	22.313835000	14.037206000
O	28.827598000	9.894410000	13.440488000	O	9.894590000	24.934185000	13.440450000
O	30.426944000	11.493755000	13.440484000	O	16.986310000	24.934185000	13.440450000
O	30.426936000	15.387151000	13.440421000	C	17.333342000	21.360638000	13.119492000
O	30.426946000	13.440483000	11.493756000	C	18.317452000	20.384593000	13.104439000
O	30.426933000	13.440426000	15.387152000	H	16.322082000	21.176773000	12.956594000
O	24.934210000	13.440425000	9.894409000	H	18.007515000	19.491341000	12.843694000
O	26.880879000	11.493760000	9.894408000	C	22.988008000	26.559942000	21.360638000
O	26.880889000	15.387147000	9.894411000	C	22.003898000	26.544889000	20.384593000
O	28.827596000	13.440487000	9.894406000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	27.066116000	30.007949000	H	22.313835000	26.284144000	19.491341000

ARTICLE

Journal Name

C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.685278000	23.859979000	20.930859000
H	23.999268000	19.144577000	13.924306000	H	26.400014000	19.386734000	16.471398000
H	22.313835000	20.830009000	14.037206000	H	26.571045000	19.236666000	22.500861000
Zr	10.956924000	26.880900000	13.440450000	H	27.040058000	17.844924000	21.067587000
O	9.894590000	26.880900000	11.493735000	H	26.673220000	21.055918000	24.173301000
O	12.408223000	27.913127000	14.472677000	H	27.051961000	16.175706000	19.242402000
C	10.287052000	26.880900000	10.287052000	Cu	26.852495000	22.244582000	18.359252000
Zr	15.923976000	26.880900000	13.440450000	Br	24.963116000	23.470025000	17.656786000
O	16.986310000	26.880900000	11.493735000	C	28.958922000	22.055933000	18.333120000
C	16.593848000	26.880900000	10.287052000	C	28.444246000	22.257480000	17.075722000
O	16.986310000	26.880900000	15.387165000	H	28.324832000	21.419901000	16.395906000
O	14.472677000	27.913127000	12.408223000	C	29.579242000	23.024441000	19.294523000
C	16.593848000	26.880900000	16.593848000	H	28.927760000	23.851496000	19.582832000
C	17.650268000	26.880900000	17.650268000	H	30.516708000	23.453031000	18.918417000
C	19.634347000	26.880900000	19.634347000	O	29.871650000	22.195314000	20.434255000
O	9.894590000	26.880900000	15.387165000	H	28.460313000	23.260975000	16.667715000
C	10.287052000	26.880900000	16.593848000	C	26.558126000	28.586242000	19.560530000
Zr	13.440450000	26.880900000	15.923976000	C	26.955214000	27.393774000	20.421611000
O	11.493735000	26.880900000	16.986310000	C	27.021428000	26.044693000	19.682496000
O	14.472677000	27.913127000	14.472677000	C	25.229241000	28.446887000	18.827922000
Zr	13.440450000	26.880900000	10.956924000	C	27.326310000	26.115635000	18.211011000
O	11.493735000	26.880900000	9.894590000	C	25.104106000	27.143721000	18.031398000
O	15.387165000	26.880900000	9.894590000	N	26.360401000	26.707029000	17.430566000
O	12.408223000	27.913127000	12.408223000	H	26.535018000	29.485476000	20.188028000
O	15.387165000	26.880900000	16.986310000	H	25.111383000	29.305003000	18.154570000
Zr	13.440450000	29.364426000	13.440450000	C	28.702815000	25.788128000	16.369225000
O	11.493735000	30.426760000	13.440450000	N	28.465792000	25.650498000	17.796467000
C	10.287052000	30.034298000	13.440450000	C	27.439267000	25.551950000	15.555848000
O	15.387165000	30.426760000	13.440450000	C	26.376489000	26.542979000	15.979092000
C	16.593848000	30.034298000	13.440450000	H	25.388212000	26.179647000	15.668927000
O	16.986310000	28.827615000	13.440450000	H	29.496503000	25.087290000	16.074188000
O	9.894590000	28.827615000	13.440450000	H	27.346818000	28.757105000	18.816237000
C	22.671082000	26.880900000	22.671082000	H	24.394506000	28.500150000	19.538543000
C	20.687003000	26.880900000	20.687003000	H	26.532502000	27.522268000	15.499457000
C	21.360638000	27.201858000	22.988008000	H	29.100338000	26.793929000	16.151365000
C	20.384593000	27.216911000	22.003898000	H	26.261384000	27.301638000	21.264044000
H	21.176773000	27.364756000	23.999268000	H	27.934398000	27.604520000	20.862173000
H	19.491341000	27.477656000	22.313835000	H	27.620521000	25.633671000	14.479267000
O	13.440450000	28.827615000	16.986310000	H	27.061469000	24.541745000	15.758357000
C	13.440450000	30.034298000	16.593848000	H	27.810775000	25.437786000	20.134606000
O	13.440450000	28.827615000	9.894590000	H	26.080799000	25.491127000	19.802937000
C	13.440450000	30.034298000	10.287052000	H	24.699065000	26.332526000	18.648888000
O	13.440450000	30.426760000	15.387165000	H	24.383991000	27.270176000	17.217969000
O	13.440450000	30.426760000	11.493735000	C	29.743149000	20.898853000	20.097159000
C	17.333342000	27.201858000	18.960712000	O	29.308131000	20.787410000	18.799835000

O	29.957651000	19.962642000	20.810946000	Zr	29.524440000	13.439969000	13.438993000
k. PC				C	30.007964000	13.253783000	16.566602000
N	26.639011000	21.856523000	20.404758000	Zr	26.880671000	13.440670000	10.796741000
N	26.484100000	19.910263000	18.471583000	C	23.755332000	16.566137000	13.635261000
C	26.639224000	20.562396000	20.809239000	C	27.064326000	16.568185000	10.312820000
C	26.643437000	22.846784000	21.315969000	C	30.008123000	16.567527000	13.254357000
C	26.526765000	18.999285000	17.487021000	O	23.334855000	26.880866000	24.934215000
C	26.657638000	19.510218000	19.752648000	O	23.334856000	24.934212000	26.880862000
C	26.645608000	20.264619000	22.178195000	O	25.848909000	27.912895000	27.912897000
C	26.697275000	22.628034000	22.698855000	O	23.334862000	26.880939000	28.827594000
C	26.720686000	17.624074000	17.695101000	O	23.334864000	28.827596000	26.880937000
C	26.871591000	18.158032000	20.049595000	O	24.934210000	30.426941000	26.880925000
C	26.691868000	21.288573000	23.112906000	O	26.880889000	30.426939000	24.934203000
C	26.892295000	17.221287000	19.026533000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000
O	27.912889000	14.472431000	12.408464000	C	30.007968000	30.008237000	26.695581000
O	26.880945000	16.986494000	11.493769000	C	30.008286000	26.697416000	30.008420000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	10.313401000	13.255234000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	13.257746000	10.312720000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	10.313244000	10.313104000
Zr	26.880671000	29.524609000	26.880680000	C	30.008286000	10.312930000	13.623934000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	13.625768000	10.313113000
C	27.064326000	30.008530000	23.753165000	H	27.351814000	30.759513000	23.002127000
C	30.008123000	27.066993000	23.753823000	H	30.758179000	27.358190000	23.003211000
C	23.755714000	23.756676000	26.684338000	H	23.008991000	23.009158000	26.377462000
Zr	26.880615000	26.881402000	29.524137000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	23.754135000	30.008060000	H	30.757581000	23.004153000	27.359935000
C	30.007964000	23.754748000	27.067567000	H	23.008991000	13.943888000	17.312192000
Zr	24.236612000	13.440798000	13.439875000	H	27.355985000	9.562959000	17.317948000
Zr	26.880615000	10.797213000	13.439948000	H	30.757582000	12.961415000	17.317197000
C	23.755714000	13.637012000	16.564674000	H	27.351814000	17.319223000	9.561837000
C	27.065914000	10.313290000	16.567215000	H	30.758179000	17.318139000	12.963160000

ARTICLE

Journal Name

H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	24.934185000	9.894590000	H	18.007515000	27.477656000	20.830009000
C	13.440450000	23.727502000	10.287052000	H	13.440450000	30.790903000	9.530447000
O	13.440450000	24.934185000	16.986310000	H	17.350453000	26.880900000	9.530447000
C	13.440450000	23.727502000	16.593848000	H	17.350453000	30.790903000	13.440450000
O	13.440450000	23.335040000	15.387165000	H	13.440450000	30.790903000	17.350453000
O	13.440450000	23.335040000	11.493735000	H	9.530447000	30.790903000	13.440450000
C	18.960712000	26.559942000	17.333342000	H	9.530447000	26.880900000	17.350453000
C	19.936757000	26.544889000	18.317452000	H	13.440450000	22.970897000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	9.530447000	22.970897000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	22.970897000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	15.026933000	25.294417000	11.853967000
C	20.384593000	18.317452000	13.104439000	H	11.853967000	28.467383000	11.853967000
H	21.176773000	16.322082000	12.956594000	H	9.530447000	26.880900000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	15.026933000	28.467383000	15.026933000
C	22.988008000	18.960712000	13.761408000	H	11.853967000	25.294417000	15.026933000
C	22.003898000	19.936757000	13.776461000	H	26.606085000	23.857706000	20.913070000
H	23.999268000	19.144577000	13.924306000	H	26.390881000	19.385127000	16.477931000

H	26.62510000	19.234783000	22.517383000	O	27.912889000	14.472431000	12.408464000
H	27.052215000	17.836369000	21.069655000	O	26.880945000	16.986494000	11.493769000
H	26.726690000	21.067916000	24.174703000	O	28.827591000	16.986480000	11.440428000
H	27.062474000	16.171175000	19.240211000	C	23.755332000	26.686089000	23.755213000
Cu	26.774522000	22.158613000	18.338062000	Zr	24.236612000	26.881475000	26.880552000
Br	25.067740000	23.608416000	17.672151000	Zr	26.880671000	29.524609000	26.880680000
C	28.894967000	22.075747000	18.310770000	Zr	29.524440000	26.882357000	26.881381000
C	28.375610000	22.271652000	17.055320000	C	27.064326000	30.008530000	23.753165000
H	28.307698000	21.440409000	16.361156000	C	30.008123000	27.066993000	23.753823000
C	29.440616000	23.060755000	19.302590000	C	23.755714000	23.756676000	26.684338000
H	28.723791000	23.826530000	19.613337000	Zr	26.880615000	26.881402000	29.524137000
H	30.357978000	23.553573000	18.953900000	C	27.065914000	23.754135000	30.008060000
O	29.767637000	22.235372000	20.428066000	C	30.007964000	23.754748000	27.067567000
H	28.311795000	23.275256000	16.650539000	Zr	24.236612000	13.440798000	13.439875000
C	29.725012000	20.935187000	20.063732000	Zr	26.880615000	10.797213000	13.439948000
O	29.318996000	20.823650000	18.759150000	C	23.755714000	13.637012000	16.564674000
O	29.989565000	20.006050000	20.767408000	C	27.065914000	10.313290000	16.567215000
4. CuI-UiO-67(bpy) system				Zr	29.524440000	13.439969000	13.438993000
a. Isolated				C	30.007964000	13.253783000	16.566602000
N	26.673404000	21.843107000	20.407035000	Zr	26.880671000	13.440670000	10.796741000
N	26.548494000	19.917228000	18.473356000	C	23.755332000	16.566137000	13.635261000
C	26.634605000	20.556559000	20.824339000	C	27.064326000	16.568185000	10.312820000
C	26.690278000	22.837395000	21.309520000	C	30.008123000	16.567527000	13.254357000
C	26.593839000	19.001415000	17.481257000	O	23.334855000	26.880866000	24.934215000
C	26.652823000	19.506913000	19.768327000	O	23.334856000	24.934212000	26.880862000
C	26.585990000	20.260904000	22.193424000	O	25.848909000	27.912895000	27.912897000
C	26.694847000	22.627307000	22.698587000	O	23.334862000	26.880939000	28.827594000
C	26.715414000	17.622345000	17.697145000	O	23.334864000	28.827596000	26.880937000
C	26.777350000	18.143350000	20.058111000	O	24.934210000	30.426941000	26.880925000
C	26.627510000	21.291889000	23.122047000	O	26.880889000	30.426939000	24.934203000
C	26.798116000	17.207120000	19.034409000	O	26.880879000	30.426942000	28.827590000
C	26.809925000	23.730886000	23.728973000	O	27.912786000	27.912776000	27.912777000
C	26.809925000	16.592377000	16.590464000	O	28.827596000	30.426944000	26.880863000
O	26.880885000	24.934153000	23.334955000	O	30.426933000	24.934198000	26.880924000
O	26.880903000	23.334945000	24.934136000	O	30.426936000	26.880929000	24.934199000
O	26.880903000	15.387214000	16.986405000	O	30.426944000	26.880866000	28.827595000
O	26.880885000	16.986395000	15.387197000	O	30.426946000	28.827594000	26.880867000
Zr	26.878142000	26.881612000	24.237883000	O	24.934211000	26.880924000	30.426942000
Zr	26.878209000	24.239690000	26.880717000	O	26.880889000	24.934201000	30.426937000
Zr	26.878209000	13.440633000	16.081660000	O	26.880878000	28.827589000	30.426943000
Zr	26.878142000	16.083467000	13.439738000	O	28.827598000	26.880862000	30.426940000
O	24.934203000	26.880849000	23.334882000	O	25.848909000	12.408453000	12.408455000
O	25.848911000	25.848918000	25.848917000	O	23.334862000	11.493756000	13.440411000
O	25.849015000	27.912768000	25.849028000	O	23.334855000	15.387135000	13.440484000
O	27.912782000	25.849032000	25.849031000	O	23.334864000	13.440413000	11.493754000
O	27.912889000	27.912886000	25.848919000	O	23.334856000	13.440488000	15.387138000
O	26.880945000	28.827581000	23.334856000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	26.880922000	23.334870000	O	26.880889000	9.894413000	15.387149000
O	24.934197000	23.334881000	26.880846000	O	27.912786000	12.408573000	12.408574000
O	25.849012000	25.849025000	27.912771000	O	26.880878000	9.894407000	11.493761000
O	27.912892000	25.848913000	27.912887000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	23.334850000	28.827576000	O	30.426944000	11.493755000	13.440484000
O	28.827591000	23.334868000	26.880917000	O	30.426936000	15.387151000	13.440421000
O	25.849012000	12.408579000	14.472325000	O	30.426946000	13.440483000	11.493756000
O	25.848911000	14.472433000	14.472432000	O	30.426933000	13.440426000	15.387152000
O	24.934197000	13.440504000	16.986469000	O	24.934210000	13.440425000	9.894409000
O	26.880944000	11.493774000	16.986500000	O	26.880879000	11.493760000	9.894408000
O	27.912892000	12.408463000	14.472437000	O	26.880889000	15.387147000	9.894411000
O	27.912782000	14.472319000	14.472318000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	13.440433000	16.986482000	C	23.753697000	27.066116000	30.007949000
O	25.849015000	14.472322000	12.408582000	C	23.753135000	30.008630000	27.063604000
O	24.934203000	16.986468000	13.440501000	C	26.696398000	30.008246000	30.008106000

ARTICLE

Journal Name

C	30.007968000	30.008237000	26.695581000	O	13.440450000	24.934185000	9.894590000
C	30.008286000	26.697416000	30.008420000	C	13.440450000	23.727502000	10.287052000
C	23.753697000	10.313401000	13.255234000	O	13.440450000	24.934185000	16.986310000
C	23.753135000	13.257746000	10.312720000	C	13.440450000	23.727502000	16.593848000
C	26.696398000	10.313244000	10.313104000	O	13.440450000	23.335040000	15.387165000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	23.335040000	11.493735000
C	30.007968000	13.625768000	10.313113000	C	18.960712000	26.559942000	17.333342000
H	27.351814000	30.759513000	23.002127000	C	19.936757000	26.544889000	18.317452000
H	30.758179000	27.358190000	23.003211000	H	19.144577000	26.397044000	16.322082000
H	23.008991000	23.009158000	26.377462000	H	20.830009000	26.284144000	18.007515000
H	27.355985000	23.003402000	30.758391000	C	21.360638000	17.333342000	13.119492000
H	30.757581000	23.004153000	27.359935000	C	20.384593000	18.317452000	13.104439000
H	23.008991000	13.943888000	17.312192000	H	21.176773000	16.322082000	12.956594000
H	27.355985000	9.562959000	17.317948000	H	19.491341000	18.007515000	12.843694000
H	30.757582000	12.961415000	17.317197000	C	22.988008000	18.960712000	13.761408000
H	27.351814000	17.319223000	9.561837000	C	22.003898000	19.936757000	13.776461000
H	30.758179000	17.318139000	12.963160000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	27.356162000	30.758555000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	30.759916000	27.349810000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	30.758917000	30.758911000	O	9.894590000	26.880900000	11.493735000
H	30.758582000	30.758568000	26.405278000	O	12.408223000	27.913127000	14.472677000
H	30.759373000	26.409850000	30.759355000	C	10.287052000	26.880900000	10.287052000
H	23.003255000	9.562795000	12.965188000	Zr	15.923976000	26.880900000	13.440450000
H	23.001913000	12.971540000	9.561434000	O	16.986310000	26.880900000	11.493735000
H	26.407446000	9.562439000	9.562434000	C	16.593848000	26.880900000	10.287052000
H	30.759373000	9.561995000	13.911500000	O	16.986310000	26.880900000	15.387165000
H	30.758582000	13.916071000	9.562782000	O	14.472677000	27.913127000	12.408223000
H	25.215026000	11.776433000	15.102845000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	11.776251000	11.775822000	C	17.650268000	26.880900000	17.650268000
H	28.555271000	15.099035000	15.098322000	C	19.634347000	26.880900000	19.634347000
H	25.215244000	15.103495000	11.776660000	O	9.894590000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	C	10.287052000	26.880900000	16.593848000
H	28.555271000	25.223028000	25.222315000	Zr	13.440450000	26.880900000	15.923976000
H	28.544134000	28.545528000	28.545099000	O	11.493735000	26.880900000	16.986310000
H	25.215026000	25.218505000	28.544917000	O	14.472677000	27.913127000	14.472677000
O	14.472677000	25.848673000	14.472677000	Zr	13.440450000	26.880900000	10.956924000
O	12.408223000	25.848673000	12.408223000	O	11.493735000	26.880900000	9.894590000
O	14.472677000	25.848673000	12.408223000	O	15.387165000	26.880900000	9.894590000
O	12.408223000	25.848673000	14.472677000	O	12.408223000	27.913127000	12.408223000
Zr	13.440450000	24.397374000	13.440450000	O	15.387165000	26.880900000	16.986310000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	30.426760000	13.440450000
O	15.387165000	23.335040000	13.440450000	C	10.287052000	30.034298000	13.440450000
C	16.593848000	23.727502000	13.440450000	O	15.387165000	30.426760000	13.440450000
C	17.650268000	22.671082000	13.440450000	C	16.593848000	30.034298000	13.440450000
C	19.634347000	20.687003000	13.440450000	O	16.986310000	28.827615000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	9.894590000	28.827615000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	22.671082000	26.880900000	22.671082000
H	19.144577000	23.999268000	13.924306000	C	20.687003000	26.880900000	20.687003000
H	20.830009000	22.313835000	14.037206000	C	21.360638000	27.201858000	22.988008000
O	9.894590000	24.934185000	13.440450000	C	20.384593000	27.216911000	22.003898000
O	16.986310000	24.934185000	13.440450000	H	21.176773000	27.364756000	23.999268000
C	17.333342000	21.360638000	13.119492000	H	19.491341000	27.477656000	22.313835000
C	18.317452000	20.384593000	13.104439000	O	13.440450000	28.827615000	16.986310000
H	16.322082000	21.176773000	12.956594000	C	13.440450000	30.034298000	16.593848000
H	18.007515000	19.491341000	12.843694000	O	13.440450000	28.827615000	9.894590000
C	22.988008000	26.559942000	21.360638000	C	13.440450000	30.034298000	10.287052000
C	22.003898000	26.544889000	20.384593000	O	13.440450000	30.426760000	15.387165000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	30.426760000	11.493735000
H	22.313835000	26.284144000	19.491341000	C	17.333342000	27.201858000	18.960712000
C	22.671082000	17.650268000	13.440450000	C	18.317452000	27.216911000	19.936757000
C	20.687003000	19.634347000	13.440450000	H	16.322082000	27.364756000	19.144577000

H	18.007515000	27.477656000	20.830009000	O	25.848911000	14.472433000	14.472432000
H	13.440450000	30.790903000	9.530447000	O	24.934197000	13.440504000	16.986469000
H	17.350453000	26.880900000	9.530447000	O	26.880944000	11.493774000	16.986500000
H	17.350453000	30.790903000	13.440450000	O	27.912892000	12.408463000	14.472437000
H	13.440450000	30.790903000	17.350453000	O	27.912782000	14.472319000	14.472318000
H	9.530447000	30.790903000	13.440450000	O	28.827591000	13.440433000	16.986482000
H	9.530447000	26.880900000	17.350453000	O	25.849015000	14.472322000	12.408582000
H	13.440450000	22.970897000	9.530447000	O	24.934203000	16.986468000	13.440501000
H	9.530447000	22.970897000	13.440450000	O	27.912889000	14.472431000	12.408464000
H	13.440450000	22.970897000	17.350453000	O	26.880945000	16.986494000	11.493769000
H	15.026933000	25.294417000	11.853967000	O	28.827591000	16.986480000	13.440428000
H	11.853967000	28.467383000	11.853967000	O	23.755332000	26.686089000	23.755213000
H	9.530447000	26.880900000	9.530447000	C	24.236612000	26.881475000	26.880552000
H	15.026933000	28.467383000	15.026933000	Zr	26.880671000	29.524609000	26.880680000
H	11.853967000	25.294417000	15.026933000	Zr	29.524440000	26.882357000	26.881381000
H	26.711019000	23.845681000	20.900209000	Zr	27.064326000	30.008530000	23.753165000
H	26.523458000	19.395445000	16.470802000	C	30.008123000	27.066993000	23.753823000
H	26.514856000	19.234945000	22.540008000	C	23.755714000	23.756676000	26.684338000
H	26.873662000	17.809869000	21.085882000	C	Zr	26.880615000	26.881402000
H	26.612401000	21.079631000	24.186201000	C	27.065914000	23.754135000	30.008060000
H	26.896304000	16.148647000	19.251114000	Zr	C	30.007964000	23.754748000
Cu	26.287256000	21.892984000	18.227258000	C	Zr	24.236612000	13.440798000
I	25.620748000	23.949076000	17.074077000	Zr	Zr	26.880615000	10.797213000
b. PA				C	C	23.755714000	13.637012000
N	26.513792000	21.866411000	20.406325000	C	C	27.065914000	10.313290000
N	26.599793000	19.929708000	18.436610000	Zr	Zr	29.524440000	13.439969000
C	26.686713000	20.586554000	20.793804000	C	C	30.007964000	13.253783000
C	26.541832000	22.844356000	21.319963000	Zr	Zr	26.880671000	13.440670000
C	26.602244000	19.002490000	17.460110000	C	C	23.755332000	16.566137000
C	26.681256000	19.537355000	19.733306000	C	C	27.064326000	16.568185000
C	26.856810000	20.277045000	22.152419000	C	C	30.008123000	16.567527000
C	26.719119000	22.630540000	22.697640000	O	O	23.334855000	26.880866000
C	26.713680000	17.624532000	17.688760000	O	O	23.334856000	24.934212000
C	26.745470000	18.170681000	20.041224000	O	O	25.848909000	27.912895000
C	26.865744000	21.294427000	23.094738000	O	O	23.334862000	26.880939000
C	26.771855000	17.223937000	19.029878000	O	O	23.334864000	28.827596000
C	26.809925000	23.730886000	23.728973000	O	O	24.934210000	30.426941000
C	26.809925000	16.592377000	16.590464000	O	O	26.880889000	30.426939000
O	26.880885000	24.934153000	23.334955000	O	O	26.880879000	30.426942000
O	26.880903000	23.334945000	24.934136000	O	O	27.912786000	27.912776000
O	26.880903000	15.387214000	16.986405000	O	O	28.827596000	30.426944000
O	26.880885000	16.986395000	15.387197000	O	O	30.426933000	24.934198000
Zr	26.878142000	26.881612000	24.237883000	O	O	30.426936000	26.880929000
Zr	26.878209000	24.239690000	26.880717000	O	O	30.426944000	26.880866000
Zr	26.878209000	13.440633000	16.081660000	O	O	30.426946000	28.827594000
Zr	26.878142000	16.083467000	13.439738000	O	O	24.934211000	26.880924000
O	24.934203000	26.880849000	23.334882000	O	O	26.880889000	24.934201000
O	25.848911000	25.848918000	25.848917000	O	O	28.827598000	26.880862000
O	25.849015000	27.912768000	25.849028000	O	O	25.848909000	12.408453000
O	27.912782000	25.849032000	25.849031000	O	O	23.334862000	11.493756000
O	27.912889000	27.912886000	25.848919000	O	O	24.934211000	9.894408000
O	26.880945000	28.827581000	23.334856000	O	O	26.880889000	9.894413000
O	28.827591000	26.880922000	23.334870000	O	O	27.912786000	12.408573000
O	24.934197000	23.334881000	26.880846000	O	O	14.472325000	
O	25.849012000	25.849025000	27.912771000				
O	27.912892000	25.848913000	27.912887000				
O	26.880944000	23.334850000	28.827576000				
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ARTICLE

Journal Name

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O	30.426944000	11.493755000	13.440484000	C	18.960712000	22.988008000	13.761408000
O	30.426936000	15.387151000	13.440421000	C	19.936757000	22.003898000	13.776461000
O	30.426946000	13.440483000	11.493756000	H	19.144577000	23.999268000	13.924306000
O	30.426933000	13.440426000	15.387152000	H	20.830009000	22.313835000	14.037206000
O	24.934210000	13.440425000	9.894409000	O	9.894590000	24.934185000	13.440450000
O	26.880879000	11.493760000	9.894408000	O	16.986310000	24.934185000	13.440450000
O	26.880889000	15.387147000	9.894411000	C	17.333342000	21.360638000	13.119492000
O	28.827596000	13.440487000	9.894406000	C	18.317452000	20.384593000	13.104439000
C	23.753697000	27.066116000	30.007949000	H	16.322082000	21.176773000	12.956594000
C	23.753135000	30.008630000	27.063604000	H	18.007515000	19.491341000	12.843694000
C	26.696398000	30.008246000	30.008106000	C	22.988008000	26.559942000	21.360638000
C	30.007968000	30.008237000	26.695581000	C	22.003898000	26.544889000	20.384593000
C	30.008286000	26.697416000	30.008420000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	10.313401000	13.255234000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	13.257746000	10.312720000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	10.313244000	10.313104000	C	20.687003000	19.634347000	13.440450000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	24.934185000	9.894590000
C	30.007968000	13.625768000	10.313113000	C	13.440450000	23.727502000	10.287052000
H	27.351814000	30.759513000	23.002127000	O	13.440450000	24.934185000	16.986310000
H	30.758179000	27.358190000	23.003211000	C	13.440450000	23.727502000	16.593848000
H	23.008991000	23.009158000	26.377462000	O	13.440450000	23.335040000	15.387165000
H	27.355985000	23.003402000	30.758391000	O	13.440450000	23.335040000	11.493735000
H	30.757581000	23.004153000	27.359935000	C	18.960712000	26.559942000	17.333342000
H	23.008991000	13.943888000	17.312192000	C	19.936757000	26.544889000	18.317452000
H	27.355985000	9.562959000	17.317948000	H	19.144577000	26.397044000	16.322082000
H	30.757582000	12.961415000	17.317197000	H	20.830009000	26.284144000	18.007515000
H	27.351814000	17.319223000	9.561837000	C	21.360638000	17.333342000	13.119492000
H	30.758179000	17.318139000	12.963160000	C	20.384593000	18.317452000	13.104439000
H	23.003255000	27.356162000	30.758555000	H	21.176773000	16.322082000	12.956594000
H	23.001913000	30.759916000	27.349810000	H	19.491341000	18.007515000	12.843694000
H	26.407446000	30.758917000	30.758911000	C	22.988008000	18.960712000	13.761408000
H	30.758582000	30.758568000	26.405278000	C	22.003898000	19.936757000	13.776461000
H	30.759373000	26.409850000	30.759355000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	9.562795000	12.965188000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	12.971540000	9.561434000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	9.562439000	9.562434000	O	9.894590000	26.880900000	11.493735000
H	30.759373000	9.561995000	13.911500000	O	12.408223000	27.913127000	14.472677000
H	30.758582000	13.916071000	9.562782000	C	10.287052000	26.880900000	10.287052000
H	25.215026000	11.776433000	15.102845000	Zr	15.923976000	26.880900000	13.440450000
H	28.544134000	11.776251000	11.775822000	O	16.986310000	26.880900000	11.493735000
H	28.555271000	15.099035000	15.098322000	C	16.593848000	26.880900000	10.287052000
H	25.215244000	15.103495000	11.776660000	O	16.986310000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	O	14.472677000	27.913127000	12.408223000
H	28.555271000	25.223028000	25.222315000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	28.545528000	28.545099000	C	17.650268000	26.880900000	17.650268000
H	25.215026000	25.218505000	28.544917000	C	19.634347000	26.880900000	19.634347000
O	14.472677000	25.848673000	14.472677000	O	9.894590000	26.880900000	15.387165000
O	12.408223000	25.848673000	12.408223000	C	10.287052000	26.880900000	16.593848000
O	14.472677000	25.848673000	12.408223000	Zr	13.440450000	26.880900000	15.923976000
O	12.408223000	25.848673000	14.472677000	O	11.493735000	26.880900000	16.986310000
Zr	13.440450000	24.397374000	13.440450000	O	14.472677000	27.913127000	14.472677000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	26.880900000	10.956924000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	26.880900000	9.894590000
O	15.387165000	23.335040000	13.440450000	O	15.387165000	26.880900000	9.894590000
C	16.593848000	23.727502000	13.440450000	O	12.408223000	27.913127000	12.408223000

Journal Name				ARTICLE			
O	15.387165000	26.880900000	16.986310000	C	26.651869000	20.598321000	20.777256000
Zr	13.440450000	29.364426000	13.440450000	C	26.582311000	22.857133000	21.304991000
O	11.493735000	30.426760000	13.440450000	C	26.731675000	18.995649000	17.453943000
C	10.287052000	30.034298000	13.440450000	C	26.634864000	19.542065000	19.722018000
O	15.387165000	30.426760000	13.440450000	C	26.795229000	20.280885000	22.137326000
C	16.593848000	30.034298000	13.440450000	C	26.715262000	22.634408000	22.688213000
O	16.986310000	28.827615000	13.440450000	C	26.692569000	17.619007000	17.689125000
O	9.894590000	28.827615000	13.440450000	C	26.520054000	18.177310000	20.032033000
C	22.671082000	26.880900000	22.671082000	C	26.815392000	21.294619000	23.084975000
C	20.687003000	26.880900000	20.687003000	C	26.570963000	17.221841000	19.028140000
C	21.360638000	27.201858000	22.988008000	C	26.809925000	23.730886000	23.728973000
C	20.384593000	27.216911000	22.003898000	C	26.809925000	16.592377000	16.590464000
H	21.176773000	27.364756000	23.999268000	O	26.880885000	24.934153000	23.334955000
H	19.491341000	27.477656000	22.313835000	O	26.880903000	23.334945000	24.934136000
O	13.440450000	28.827615000	16.986310000	O	26.880903000	15.387214000	16.986405000
C	13.440450000	30.034298000	16.593848000	O	26.880885000	16.986395000	15.387197000
O	13.440450000	28.827615000	9.894590000	Zr	26.878142000	26.881612000	24.237883000
C	13.440450000	30.034298000	10.287052000	Zr	26.878209000	24.239690000	26.880717000
O	13.440450000	30.426760000	15.387165000	Zr	26.878209000	13.440633000	16.081660000
O	13.440450000	30.426760000	11.493735000	Zr	26.878142000	16.083467000	13.439738000
C	17.333342000	27.201858000	18.960712000	O	24.934203000	26.880849000	23.334882000
C	18.317452000	27.216911000	19.936757000	O	25.848911000	25.848918000	25.848917000
H	16.322082000	27.364756000	19.144577000	O	25.849015000	27.912768000	25.849028000
H	18.007515000	27.477656000	20.830009000	O	27.912782000	25.849032000	25.849031000
H	13.440450000	30.790903000	9.530447000	O	27.912889000	27.912886000	25.848919000
H	17.350453000	26.880900000	9.530447000	O	26.880945000	28.827581000	23.334856000
H	17.350453000	30.790903000	13.440450000	O	28.827591000	26.880922000	23.334870000
H	13.440450000	30.790903000	17.350453000	O	24.934197000	23.334881000	26.880846000
H	9.530447000	30.790903000	13.440450000	O	25.849012000	25.849025000	27.912771000
H	9.530447000	26.880900000	17.350453000	O	27.912892000	25.848913000	27.912887000
H	13.440450000	22.970897000	9.530447000	O	26.880944000	23.334850000	28.827576000
H	9.530447000	22.970897000	13.440450000	O	28.827591000	23.334868000	26.880917000
H	13.440450000	22.970897000	17.350453000	O	25.849012000	12.408579000	14.472325000
H	15.026933000	25.294417000	11.853967000	O	25.848911000	14.472433000	14.472432000
H	11.853967000	28.467383000	11.853967000	O	24.934197000	13.440504000	16.986469000
H	9.530447000	26.880900000	9.530447000	O	26.880944000	11.493774000	16.986500000
H	15.026933000	28.467383000	15.026933000	O	27.912892000	12.408463000	14.472437000
H	11.853967000	25.294417000	15.026933000	O	27.912782000	14.472319000	14.472318000
H	26.409890000	23.854924000	20.937766000	O	28.827591000	13.440433000	16.986482000
H	26.502764000	19.382346000	16.447256000	O	25.849015000	14.472322000	12.408582000
H	26.993833000	19.252248000	22.480586000	O	24.934203000	16.986468000	13.440501000
H	26.766452000	17.841560000	21.074118000	O	27.912889000	14.472431000	12.408464000
H	27.002633000	21.074185000	24.147107000	O	26.880945000	16.986494000	11.493769000
H	26.837052000	16.166489000	19.258506000	O	28.827591000	16.986480000	13.440428000
Cu	26.128402000	21.902047000	18.029104000	C	23.755332000	26.686089000	23.755213000
I	23.557889000	21.697913000	17.851415000	Zr	24.236612000	26.881475000	26.880552000
C	26.621752000	23.690026000	17.300085000	Zr	26.880671000	29.524609000	26.880680000
C	27.656820000	22.991730000	17.359901000	Zr	29.524440000	26.882357000	26.881381000
H	28.689995000	22.710795000	17.297758000	C	27.064326000	30.008530000	23.753165000
C	25.689569000	24.800771000	17.028005000	C	30.008123000	27.066993000	23.753823000
H	25.566777000	25.383601000	17.947551000	C	23.755714000	23.756676000	26.684338000
H	24.698887000	24.393920000	16.781187000	Zr	26.880615000	26.881402000	29.524137000
O	26.178247000	25.703498000	16.056783000	C	27.065914000	23.754135000	30.008060000
H	26.163339000	25.253052000	15.215790000	C	30.007964000	23.754748000	27.067567000
c. PA/DBU				Zr	24.236612000	13.440798000	13.439875000
N	26.538138000	21.884132000	20.384017000	Zr	26.880615000	10.797213000	13.439948000
N	26.736835000	19.926164000	18.427497000	C	23.755714000	13.637012000	16.564674000

ARTICLE

Journal Name

C	27.065914000	10.313290000	16.567215000	H	30.757581000	23.004153000	27.359935000
Zr	29.524440000	13.439969000	13.438993000	H	23.008991000	13.943888000	17.312192000
C	30.007964000	13.253783000	16.566602000	H	27.355985000	9.562959000	17.317948000
Zr	26.880671000	13.440670000	10.796741000	H	30.757582000	12.961415000	17.317197000
C	23.755332000	16.566137000	13.635261000	H	27.351814000	17.319223000	9.561837000
C	27.064326000	16.568185000	10.312820000	H	30.758179000	17.318139000	12.963160000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	27.356162000	30.758555000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	30.759916000	27.349810000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	30.758917000	30.758911000
O	25.848909000	27.912895000	27.912897000	H	30.758582000	30.758568000	26.405278000
O	23.334862000	26.880939000	28.827594000	H	30.759373000	26.409850000	30.759355000
O	23.334864000	28.827596000	26.880937000	H	23.003255000	9.562795000	12.965188000
O	24.934210000	30.426941000	26.880925000	H	23.001913000	12.971540000	9.561434000
O	26.880889000	30.426939000	24.934203000	H	26.407446000	9.562439000	9.562434000
O	26.880879000	30.426942000	28.827590000	H	30.759373000	9.561995000	13.911500000
O	27.912786000	27.912776000	27.912777000	H	30.758582000	13.916071000	9.562782000
O	28.827596000	30.426944000	26.880863000	H	25.215026000	11.776433000	15.102845000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	11.776251000	11.775822000
O	30.426936000	26.880929000	24.934199000	H	28.555271000	15.099035000	15.098322000
O	30.426944000	26.880866000	28.827595000	H	25.215244000	15.103495000	11.776660000
O	30.426946000	28.827594000	26.880867000	H	25.215244000	28.544690000	25.217855000
O	24.934211000	26.880924000	30.426942000	H	28.555271000	25.223028000	25.222315000
O	26.880889000	24.934201000	30.426937000	H	28.544134000	28.545528000	28.545099000
O	26.880878000	28.827589000	30.426943000	H	25.215026000	25.218505000	28.544917000
O	28.827598000	26.880862000	30.426940000	O	14.472677000	25.848673000	14.472677000
O	25.848909000	12.408453000	12.408455000	O	12.408223000	25.848673000	12.408223000
O	23.334862000	11.493756000	13.440411000	O	14.472677000	25.848673000	12.408223000
O	23.334855000	15.387135000	13.440484000	O	12.408223000	25.848673000	14.472677000
O	23.334864000	13.440413000	11.493754000	Zr	13.440450000	24.397374000	13.440450000
O	23.334856000	13.440488000	15.387138000	O	11.493735000	23.335040000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	10.287052000	23.727502000	13.440450000
O	26.880889000	9.894413000	15.387149000	O	15.387165000	23.335040000	13.440450000
O	27.912786000	12.408573000	12.408574000	C	16.593848000	23.727502000	13.440450000
O	26.880878000	9.894407000	11.493761000	C	17.650268000	22.671082000	13.440450000
O	28.827598000	9.894410000	13.440488000	C	19.634347000	20.687003000	13.440450000
O	30.426944000	11.493755000	13.440484000	C	18.960712000	22.988008000	13.761408000
O	30.426936000	15.387151000	13.440421000	C	19.936757000	22.003898000	13.776461000
O	30.426946000	13.440483000	11.493756000	H	19.144577000	23.999268000	13.924306000
O	30.426933000	13.440426000	15.387152000	H	20.830009000	22.313835000	14.037206000
O	24.934210000	13.440425000	9.894409000	O	9.894590000	24.934185000	13.440450000
O	26.880879000	11.493760000	9.894408000	O	16.986310000	24.934185000	13.440450000
O	26.880889000	15.387147000	9.894411000	C	17.333342000	21.360638000	13.119492000
O	28.827596000	13.440487000	9.894406000	C	18.317452000	20.384593000	13.104439000
C	23.753697000	27.066116000	30.007949000	H	16.322082000	21.176773000	12.956594000
C	23.753135000	30.008630000	27.063604000	H	18.007515000	19.491341000	12.843694000
C	26.696398000	30.008246000	30.008106000	C	22.988008000	26.559942000	21.360638000
C	30.007968000	30.008237000	26.695581000	C	22.003898000	26.544889000	20.384593000
C	30.008286000	26.697416000	30.008420000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	10.313401000	13.255234000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	13.257746000	10.312720000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	10.313244000	10.313104000	C	20.687003000	19.634347000	13.440450000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	24.934185000	9.894590000
C	30.007968000	13.625768000	10.313113000	C	13.440450000	23.727502000	10.287052000
H	27.351814000	30.759513000	23.002127000	O	13.440450000	24.934185000	16.986310000
H	30.758179000	27.358190000	23.003211000	C	13.440450000	23.727502000	16.593848000
H	23.008991000	23.009158000	26.377462000	O	13.440450000	23.335040000	15.387165000
H	27.355985000	23.003402000	30.758391000	O	13.440450000	23.335040000	11.493735000

Journal Name				ARTICLE			
C	18.960712000	26.559942000	17.333342000	H	13.440450000	30.790903000	9.530447000
C	19.936757000	26.544889000	18.317452000	H	17.350453000	26.880900000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	17.350453000	30.790903000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	30.790903000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	9.530447000	30.790903000	13.440450000
C	20.384593000	18.317452000	13.104439000	H	9.530447000	26.880900000	17.350453000
H	21.176773000	16.322082000	12.956594000	H	13.440450000	22.970897000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	9.530447000	22.970897000	13.440450000
C	22.988008000	18.960712000	13.761408000	H	13.440450000	22.970897000	17.350453000
C	22.003898000	19.936757000	13.776461000	H	15.026933000	25.294417000	11.853967000
H	23.999268000	19.144577000	13.924306000	H	11.853967000	28.467383000	11.853967000
H	22.313835000	20.830009000	14.037206000	H	9.530447000	26.880900000	9.530447000
Zr	10.956924000	26.880900000	13.440450000	H	15.026933000	28.467383000	15.026933000
O	9.894590000	26.880900000	11.493735000	H	11.853967000	25.294417000	15.026933000
O	12.408223000	27.913127000	14.472677000	H	26.506281000	23.873943000	20.922641000
C	10.287052000	26.880900000	10.287052000	H	26.756339000	19.376896000	16.436005000
Zr	15.923976000	26.880900000	13.440450000	H	26.913176000	19.251643000	22.460256000
O	16.986310000	26.880900000	11.493735000	H	26.385073000	17.859983000	21.060344000
C	16.593848000	26.880900000	10.287052000	H	26.929122000	21.065489000	24.139864000
O	16.986310000	26.880900000	15.387165000	H	26.511769000	16.163760000	19.262837000
O	14.472677000	27.913127000	12.408223000	Cu	26.722708000	21.905801000	17.852488000
C	16.593848000	26.880900000	16.593848000	I	24.519574000	21.797035000	16.462344000
C	17.650268000	26.880900000	17.650268000	C	27.680515000	23.580548000	17.308274000
C	19.634347000	26.880900000	19.634347000	C	28.479754000	22.835741000	17.916035000
O	9.894590000	26.880900000	15.387165000	H	29.381871000	22.490848000	18.382378000
C	10.287052000	26.880900000	16.593848000	C	27.126103000	24.679863000	16.482378000
Zr	13.440450000	26.880900000	15.923976000	H	26.716533000	25.441192000	17.157967000
O	11.493735000	26.880900000	16.986310000	H	26.272120000	24.280562000	15.911012000
O	14.472677000	27.913127000	14.472677000	O	28.096093000	25.280311000	15.676741000
Zr	13.440450000	26.880900000	10.956924000	H	28.342752000	24.578411000	15.020677000
O	11.493735000	26.880900000	9.894590000	C	26.601592000	22.873433000	10.761235000
O	15.387165000	26.880900000	9.894590000	C	26.019796000	23.952018000	11.670908000
O	12.408223000	27.913127000	12.408223000	C	26.233430000	23.716936000	13.186970000
O	15.387165000	26.880900000	16.986310000	C	25.932670000	21.510047000	10.902653000
Zr	13.440450000	29.364426000	13.440450000	C	27.238890000	22.649792000	13.531690000
O	11.493735000	30.426760000	13.440450000	C	25.735631000	21.098847000	12.361245000
C	10.287052000	30.034298000	13.440450000	N	26.900719000	21.367193000	13.189513000
O	15.387165000	30.426760000	13.440450000	H	26.542248000	23.202365000	9.717783000
C	16.593848000	30.034298000	13.440450000	H	26.534417000	20.754017000	10.381178000
O	16.986310000	28.827615000	13.440450000	C	29.296025000	21.961921000	14.437287000
O	9.894590000	28.827615000	13.440450000	N	28.342295000	23.009330000	14.116410000
C	22.671082000	26.880900000	22.671082000	C	28.608846000	20.647470000	14.762638000
C	20.687003000	26.880900000	20.687003000	C	27.716006000	20.239298000	13.609821000
C	21.360638000	27.201858000	22.988008000	H	27.041848000	19.424338000	13.911709000
C	20.384593000	27.216911000	22.003898000	H	29.900885000	22.300003000	15.287684000
H	21.176773000	27.364756000	23.999268000	H	27.673104000	22.771666000	10.980425000
H	19.491341000	27.477656000	22.313835000	H	24.949832000	21.514586000	10.413469000
O	13.440450000	28.827615000	16.986310000	H	28.313528000	19.854189000	12.767066000
C	13.440450000	30.034298000	16.593848000	H	29.994659000	21.827942000	13.594990000
O	13.440450000	28.827615000	9.894590000	H	24.947251000	24.062779000	11.467284000
C	13.440450000	30.034298000	10.287052000	H	26.475497000	24.909072000	11.397759000
O	13.440450000	30.426760000	15.387165000	H	29.318174000	19.842991000	14.988472000
O	13.440450000	30.426760000	11.493735000	H	27.993143000	20.814891000	15.657646000
C	17.333342000	27.201858000	18.960712000	H	26.586363000	24.635854000	13.661387000
C	18.317452000	27.216911000	19.936757000	H	25.287326000	23.457011000	13.679168000
H	16.322082000	27.364756000	19.144577000	H	24.860692000	21.602997000	12.790908000
H	18.007515000	27.477656000	20.830009000	H	25.533541000	20.026817000	12.423162000

d. PA/DBU/CO ₂							
N	26.501713000	21.872616000	20.394452000	Zr	24.236612000	13.440798000	13.439875000
N	26.731379000	19.927277000	18.436371000	Zr	26.880615000	10.797213000	13.439948000
C	26.642125000	20.589156000	20.786885000	C	23.755714000	13.637012000	16.564674000
C	26.549906000	22.849850000	21.310902000	C	27.065914000	10.313290000	16.567215000
C	26.736246000	18.999630000	17.459531000	Zr	29.524440000	13.439969000	13.438993000
C	26.628901000	19.535989000	19.729729000	C	30.007964000	13.253783000	16.566602000
C	26.812355000	20.276836000	22.144616000	Zr	26.880671000	13.440670000	10.796741000
C	26.711674000	22.631836000	22.691032000	C	23.755332000	16.566137000	13.635261000
C	26.694162000	17.621092000	17.689801000	C	27.064326000	16.568185000	10.312820000
C	26.518731000	18.170594000	20.035234000	C	30.008123000	16.567527000	13.254357000
C	26.834773000	21.293792000	23.088962000	O	23.334855000	26.880866000	24.934215000
C	26.569455000	17.219409000	19.027313000	O	23.334856000	24.934212000	26.880862000
C	26.809925000	23.730886000	23.728973000	O	25.848909000	27.912895000	27.912897000
C	26.809925000	16.592377000	16.590464000	O	23.334862000	26.880939000	28.827594000
O	26.880885000	24.934153000	23.334955000	O	23.334864000	28.827596000	26.880937000
O	26.880903000	23.334945000	24.934136000	O	24.934210000	30.426941000	26.880925000
O	26.880903000	15.387214000	16.986405000	O	26.880889000	30.426939000	24.934203000
O	26.880885000	16.986395000	15.387197000	O	26.880879000	30.426942000	28.827590000
Zr	26.878142000	26.881612000	24.237883000	O	27.912786000	27.912776000	27.912777000
Zr	26.878209000	24.239690000	26.880717000	O	28.827596000	30.426944000	26.880863000
Zr	26.878209000	13.440633000	16.081660000	O	30.426933000	24.934198000	26.880924000
Zr	26.878142000	16.083467000	13.439738000	O	30.426936000	26.880929000	24.934199000
O	24.934203000	26.880849000	23.334882000	O	30.426944000	26.880866000	28.827595000
O	25.848911000	25.848918000	25.848917000	O	30.426946000	28.827594000	26.880867000
O	25.849015000	27.912768000	25.849028000	O	24.934211000	26.880924000	30.426942000
O	27.912782000	25.849032000	25.849031000	O	26.880889000	24.934201000	30.426937000
O	27.912889000	27.912886000	25.848919000	O	26.880878000	28.827589000	30.426943000
O	26.880945000	28.827581000	23.334856000	O	28.827598000	26.880862000	30.426940000
O	28.827591000	26.880922000	23.334870000	O	25.848909000	12.408453000	12.408455000
O	24.934197000	23.334881000	26.880846000	O	23.334862000	11.493756000	13.440411000
O	25.849012000	25.849025000	27.912771000	O	23.334855000	15.387135000	13.440484000
O	27.912892000	25.848913000	27.912887000	O	23.334864000	13.440413000	11.493754000
O	26.880944000	23.334850000	28.827576000	O	23.334856000	13.440488000	15.387138000
O	28.827591000	23.334868000	26.880917000	O	24.934211000	9.894408000	13.440426000
O	25.849012000	12.408579000	14.472325000	O	26.880889000	9.894413000	15.387149000
O	25.848911000	14.472433000	14.472432000	O	27.912786000	12.408573000	12.408574000
O	24.934197000	13.440504000	16.986469000	O	26.880878000	9.894407000	11.493761000
O	26.880944000	11.493774000	16.986500000	O	28.827598000	9.894410000	13.440488000
O	27.912892000	12.408463000	14.472437000	O	30.426944000	11.493755000	13.440484000
O	27.912782000	14.472319000	14.472318000	O	30.426936000	15.387151000	13.440421000
O	28.827591000	13.440433000	16.986482000	O	30.426946000	13.440483000	11.493756000
O	25.849015000	14.472322000	12.408582000	O	30.426933000	13.440426000	15.387152000
O	24.934203000	16.986468000	13.440501000	O	24.934210000	13.440425000	9.894409000
O	27.912889000	14.472431000	12.408464000	O	26.880879000	11.493760000	9.894408000
O	26.880945000	16.986494000	11.493769000	O	26.880889000	15.387147000	9.894411000
O	28.827591000	16.986480000	13.440428000	O	28.827596000	13.440487000	9.894406000
C	23.755332000	26.686089000	23.755213000	C	23.753697000	27.066116000	30.007949000
Zr	24.236612000	26.881475000	26.880552000	C	23.753135000	30.008630000	27.063604000
Zr	26.880671000	29.524609000	26.880680000	C	26.696398000	30.008246000	30.008106000
Zr	29.524440000	26.882357000	26.881381000	C	30.007968000	30.008237000	26.695581000
C	27.064326000	30.008530000	23.753165000	C	30.008286000	26.697416000	30.008420000
C	30.008123000	27.066993000	23.753823000	C	23.753697000	10.313401000	13.255234000
C	23.755714000	23.756676000	26.684338000	C	23.753135000	13.257746000	10.312720000
Zr	26.880615000	26.881402000	29.524137000	C	26.696398000	10.313244000	10.313104000
C	27.065914000	23.754135000	30.008060000	C	30.008286000	10.312930000	13.623934000
C	30.007964000	23.754748000	27.067567000	C	30.007968000	13.625768000	10.313113000
				H	27.351814000	30.759513000	23.002127000

Journal Name				ARTICLE			
H	30.758179000	27.358190000	23.003211000	C	13.440450000	23.727502000	16.593848000
H	23.008991000	23.009158000	26.377462000	O	13.440450000	23.335040000	15.387165000
H	27.355985000	23.003402000	30.758391000	O	13.440450000	23.335040000	11.493735000
H	30.757581000	23.004153000	27.359935000	C	18.960712000	26.559942000	17.333342000
H	23.008991000	13.943888000	17.312192000	C	19.936757000	26.544889000	18.317452000
H	27.355985000	9.562959000	17.317948000	H	19.144577000	26.397044000	16.322082000
H	30.757582000	12.961415000	17.317197000	H	20.830009000	26.284144000	18.007515000
H	27.351814000	17.319223000	9.561837000	C	21.360638000	17.333342000	13.119492000
H	30.758179000	17.318139000	12.963160000	C	20.384593000	18.317452000	13.104439000
H	23.003255000	27.356162000	30.758555000	H	21.176773000	16.322082000	12.956594000
H	23.001913000	30.759916000	27.349810000	H	19.491341000	18.007515000	12.843694000
H	26.407446000	30.758917000	30.758911000	C	22.988008000	18.960712000	13.761408000
H	30.758582000	30.758568000	26.405278000	C	22.003898000	19.936757000	13.776461000
H	30.759373000	26.409850000	30.759355000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	9.562795000	12.965188000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	12.971540000	9.561434000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	9.562439000	9.562434000	O	9.894590000	26.880900000	11.493735000
H	30.759373000	9.561995000	13.911500000	O	12.408223000	27.913127000	14.472677000
H	30.758582000	13.916071000	9.562782000	C	10.287052000	26.880900000	10.287052000
H	25.215026000	11.776433000	15.102845000	Zr	15.923976000	26.880900000	13.440450000
H	28.544134000	11.776251000	11.775822000	O	16.986310000	26.880900000	11.493735000
H	28.555271000	15.099035000	15.098322000	C	16.593848000	26.880900000	10.287052000
H	25.215244000	15.103495000	11.776660000	O	16.986310000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	O	14.472677000	27.913127000	12.408223000
H	28.555271000	25.223028000	25.222315000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	28.545528000	28.545099000	C	17.650268000	26.880900000	17.650268000
H	25.215026000	25.218505000	28.544917000	C	19.634347000	26.880900000	19.634347000
O	14.472677000	25.848673000	14.472677000	O	9.894590000	26.880900000	15.387165000
O	12.408223000	25.848673000	12.408223000	C	10.287052000	26.880900000	16.593848000
O	14.472677000	25.848673000	12.408223000	Zr	13.440450000	26.880900000	15.923976000
O	12.408223000	25.848673000	14.472677000	O	11.493735000	26.880900000	16.986310000
Zr	13.440450000	24.397374000	13.440450000	O	14.472677000	27.913127000	14.472677000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	26.880900000	10.956924000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	26.880900000	9.894590000
O	15.387165000	23.335040000	13.440450000	O	15.387165000	26.880900000	9.894590000
C	16.593848000	23.727502000	13.440450000	O	12.408223000	27.913127000	12.408223000
C	17.650268000	22.671082000	13.440450000	O	15.387165000	26.880900000	16.986310000
C	19.634347000	20.687003000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	11.493735000	30.426760000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	10.287052000	30.034298000	13.440450000
H	19.144577000	23.999268000	13.924306000	O	15.387165000	30.426760000	13.440450000
H	20.830009000	22.313835000	14.037206000	C	16.593848000	30.034298000	13.440450000
O	9.894590000	24.934185000	13.440450000	O	16.986310000	28.827615000	13.440450000
O	16.986310000	24.934185000	13.440450000	O	9.894590000	28.827615000	13.440450000
C	17.333342000	21.360638000	13.119492000	C	22.671082000	26.880900000	22.671082000
C	18.317452000	20.384593000	13.104439000	C	20.687003000	26.880900000	20.687003000
H	16.322082000	21.176773000	12.956594000	C	21.360638000	27.201858000	22.988008000
H	18.007515000	19.491341000	12.843694000	C	20.384593000	27.216911000	22.003898000
C	22.988008000	26.559942000	21.360638000	H	21.176773000	27.364756000	23.999268000
C	22.003898000	26.544889000	20.384593000	H	19.491341000	27.477656000	22.313835000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	28.827615000	16.986310000
H	22.313835000	26.284144000	19.491341000	C	13.440450000	30.034298000	16.593848000
C	22.671082000	17.650268000	13.440450000	O	13.440450000	28.827615000	9.894590000
C	20.687003000	19.634347000	13.440450000	C	13.440450000	30.034298000	10.287052000
O	13.440450000	24.934185000	9.894590000	O	13.440450000	30.426760000	15.387165000
C	13.440450000	23.727502000	10.287052000	O	13.440450000	30.426760000	11.493735000
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ARTICLE

Journal Name

C	18.317452000	27.216911000	19.936757000	H	24.659700000	23.738914000	13.956016000
H	16.322082000	27.364756000	19.144577000	H	24.284721000	21.988815000	12.898311000
H	18.007515000	27.477656000	20.830009000	H	25.012793000	20.514605000	12.291113000
H	13.440450000	30.790903000	9.530447000	C	26.046840000	27.666202000	15.085129000
H	17.350453000	26.880900000	9.530447000	O	25.609402000	27.796295000	16.161824000
H	17.350453000	30.790903000	13.440450000	O	26.440043000	27.586992000	13.986105000
H	13.440450000	30.790903000	17.350453000	e. TS1			
H	9.530447000	30.790903000	13.440450000	N	26.541802000	21.872171000	20.392432000
H	9.530447000	26.880900000	17.350453000	N	26.779211000	19.926658000	18.443875000
H	13.440450000	22.970897000	9.530447000	C	26.645586000	20.586867000	20.789699000
H	9.530447000	22.970897000	13.440450000	C	26.584125000	22.850101000	21.307787000
H	13.440450000	22.970897000	17.350453000	C	26.792977000	18.999427000	17.467977000
H	15.026933000	25.294417000	11.853967000	C	26.634955000	19.534349000	19.732705000
H	11.853967000	28.467383000	11.853967000	C	26.777368000	20.273471000	22.151392000
H	9.530447000	26.880900000	9.530447000	C	26.711304000	22.631477000	22.691683000
H	15.026933000	28.467383000	15.026933000	C	26.700022000	17.621883000	17.689111000
H	11.853967000	25.294417000	15.026933000	C	26.482213000	18.171374000	20.031817000
H	26.451947000	23.864015000	20.926150000	C	26.800528000	21.291910000	23.094165000
H	26.774890000	19.383322000	16.442911000	C	26.528452000	17.221457000	19.022830000
H	26.950734000	19.249823000	22.466925000	C	26.809925000	23.730886000	23.728973000
H	26.384470000	17.850399000	21.062897000	C	26.809925000	16.592377000	16.590464000
H	26.969039000	21.069162000	24.142361000	O	26.880885000	24.934153000	23.334955000
H	26.508962000	16.160445000	19.257417000	O	26.880903000	23.334945000	24.934136000
Cu	26.593042000	21.925664000	17.934374000	O	26.880903000	15.387214000	16.986405000
I	24.319263000	21.747494000	16.663210000	O	26.880885000	16.986395000	15.387197000
C	27.401642000	23.700340000	17.448005000	Zr	26.878142000	26.881612000	24.237883000
C	28.297788000	22.960691000	17.906361000	Zr	26.878209000	24.239690000	26.880717000
H	29.256647000	22.632310000	18.256487000	Zr	26.878209000	13.440633000	16.081660000
C	26.697387000	24.826773000	16.797244000	Zr	26.878142000	16.083467000	13.439738000
H	26.337188000	25.510099000	17.576102000	O	24.934203000	26.880849000	23.334882000
H	25.801775000	24.430063000	16.290660000	O	25.848911000	25.848918000	25.848917000
O	27.535710000	25.548615000	15.936696000	O	25.849015000	27.912768000	25.849028000
H	27.753464000	24.906005000	15.207775000	O	27.912782000	25.849032000	25.849031000
C	25.842096000	23.599730000	10.945332000	O	27.912889000	27.912886000	25.848919000
C	25.278405000	24.538191000	12.007694000	O	26.880945000	28.827581000	23.334856000
C	25.567506000	24.115335000	13.467462000	O	28.827591000	26.880922000	23.334870000
C	25.237094000	22.199823000	10.957498000	O	24.934197000	23.334881000	26.880846000
C	26.640725000	23.073049000	13.635413000	O	25.849012000	25.849025000	27.912771000
C	25.156498000	21.595779000	12.359726000	O	27.912892000	25.848913000	27.912887000
N	26.357059000	21.824364000	13.149032000	O	26.880944000	23.334850000	28.827576000
H	25.707078000	24.044987000	9.953413000	O	28.827591000	23.334868000	26.880917000
H	25.828898000	21.545192000	10.305025000	O	25.849012000	12.408579000	14.472325000
C	28.752603000	22.379360000	14.379717000	O	25.848911000	14.472433000	14.472432000
N	27.749613000	23.416656000	14.219334000	O	24.934197000	13.440504000	16.986469000
C	28.114129000	21.025109000	14.634655000	O	26.880944000	11.493774000	16.986500000
C	27.186567000	20.676077000	13.489925000	O	27.912892000	12.408463000	14.472437000
H	26.521246000	19.846732000	13.770236000	O	27.912782000	14.472319000	14.472318000
H	29.407023000	22.661642000	15.213199000	O	28.827591000	13.440433000	16.986482000
H	26.927784000	23.521019000	11.090184000	O	25.849015000	14.472322000	12.408582000
H	24.222817000	22.219468000	10.537945000	O	24.934203000	16.986468000	13.440501000
H	27.757498000	20.340381000	12.608924000	O	27.912889000	14.472431000	12.408464000
H	29.391051000	22.334682000	13.481889000	O	26.880945000	16.986494000	11.493769000
H	24.195227000	24.644280000	11.867856000	O	28.827591000	16.986480000	13.440428000
H	25.701810000	25.534591000	11.845368000	C	23.755332000	26.686089000	23.755213000
H	28.853826000	20.228954000	14.773718000	Zr	24.236612000	26.881475000	26.880552000
H	27.527190000	21.109535000	15.560988000	Zr	26.880671000	29.524609000	26.880680000
H	25.893755000	24.983441000	14.043691000	Zr	29.524440000	26.882357000	26.881381000

Journal Name				ARTICLE			
C	27.064326000	30.008530000	23.753165000	C	23.753697000	10.313401000	13.255234000
C	30.008123000	27.066993000	23.753823000	C	23.753135000	13.257746000	10.312720000
C	23.755714000	23.756676000	26.684338000	C	26.696398000	10.313244000	10.313104000
Zr	26.880615000	26.881402000	29.524137000	C	30.008286000	10.312930000	13.623934000
C	27.065914000	23.754135000	30.008060000	C	30.007968000	13.625768000	10.313113000
C	30.007964000	23.754748000	27.067567000	H	27.351814000	30.759513000	23.002127000
Zr	24.236612000	13.440798000	13.439875000	H	30.758179000	27.358190000	23.003211000
Zr	26.880615000	10.797213000	13.439948000	H	23.008991000	23.009158000	26.377462000
C	23.755714000	13.637012000	16.564674000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	10.313290000	16.567215000	H	30.757581000	23.004153000	27.359935000
Zr	29.524440000	13.439969000	13.438993000	H	23.008991000	13.943888000	17.312192000
C	30.007964000	13.253783000	16.566602000	H	27.355985000	9.562959000	17.317948000
Zr	26.880671000	13.440670000	10.796741000	H	30.757582000	12.961415000	17.317197000
C	23.755332000	16.566137000	13.635261000	H	27.351814000	17.319223000	9.561837000
C	27.064326000	16.568185000	10.312820000	H	30.758179000	17.318139000	12.963160000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	27.356162000	30.758555000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	30.759916000	27.349810000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	30.758917000	30.758911000
O	25.848909000	27.912895000	27.912897000	H	30.758582000	30.758568000	26.405278000
O	23.334862000	26.880939000	28.827594000	H	30.759373000	26.409850000	30.759355000
O	23.334864000	28.827596000	26.880937000	H	23.003255000	9.562795000	12.965188000
O	24.934210000	30.426941000	26.880925000	H	23.001913000	12.971540000	9.561434000
O	26.880889000	30.426939000	24.934203000	H	26.407446000	9.562439000	9.562434000
O	26.880879000	30.426942000	28.827590000	H	30.759373000	9.561995000	13.911500000
O	27.912786000	27.912776000	27.912777000	H	30.758582000	13.916071000	9.562782000
O	28.827596000	30.426944000	26.880863000	H	25.215026000	11.776433000	15.102845000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	11.776251000	11.775822000
O	30.426936000	26.880929000	24.934199000	H	28.555271000	15.099035000	15.098322000
O	30.426944000	26.880866000	28.827595000	H	25.215244000	15.103495000	11.776660000
O	30.426946000	28.827594000	26.880867000	H	25.215244000	28.544690000	25.217855000
O	24.934211000	26.880924000	30.426942000	H	28.555271000	25.223028000	25.222315000
O	26.880889000	24.934201000	30.426937000	H	28.544134000	28.545528000	28.545099000
O	26.880878000	28.827589000	30.426943000	H	25.215026000	25.218505000	28.544917000
O	28.827598000	26.880862000	30.426940000	O	14.472677000	25.848673000	14.472677000
O	25.848909000	12.408453000	12.408455000	O	12.408223000	25.848673000	12.408223000
O	23.334862000	11.493756000	13.440411000	O	14.472677000	25.848673000	12.408223000
O	23.334855000	15.387135000	13.440484000	O	12.408223000	25.848673000	14.472677000
O	23.334864000	13.440413000	11.493754000	Zr	13.440450000	24.397374000	13.440450000
O	23.334856000	13.440488000	15.387138000	O	11.493735000	23.335040000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	10.287052000	23.727502000	13.440450000
O	26.880889000	9.894413000	15.387149000	O	15.387165000	23.335040000	13.440450000
O	27.912786000	12.408573000	12.408574000	C	16.593848000	23.727502000	13.440450000
O	26.880878000	9.894407000	11.493761000	C	17.650268000	22.671082000	13.440450000
O	28.827598000	9.894410000	13.440488000	C	19.634347000	20.687003000	13.440450000
O	30.426944000	11.493755000	13.440484000	C	18.960712000	22.988008000	13.761408000
O	30.426936000	15.387151000	13.440421000	C	19.936757000	22.003898000	13.776461000
O	30.426946000	13.440483000	11.493756000	H	19.144577000	23.999268000	13.924306000
O	30.426933000	13.440426000	15.387152000	H	20.830009000	22.313835000	14.037206000
O	24.934210000	13.440425000	9.894409000	O	9.894590000	24.934185000	13.440450000
O	26.880879000	11.493760000	9.894408000	O	16.986310000	24.934185000	13.440450000
O	26.880889000	15.387147000	9.894411000	C	17.333342000	21.360638000	13.119492000
O	28.827596000	13.440487000	9.894406000	C	18.317452000	20.384593000	13.104439000
C	23.753697000	27.066116000	30.007949000	H	16.322082000	21.176773000	12.956594000
C	23.753135000	30.008630000	27.063604000	H	18.007515000	19.491341000	12.843694000
C	26.696398000	30.008246000	30.008106000	C	22.988008000	26.559942000	21.360638000
C	30.007968000	30.008237000	26.695581000	C	22.003898000	26.544889000	20.384593000
C	30.008286000	26.697416000	30.008420000	H	23.999268000	26.397044000	21.176773000

ARTICLE

Journal Name

H	22.313835000	26.284144000	19.491341000	C	13.440450000	30.034298000	16.593848000
C	22.671082000	17.650268000	13.440450000	O	13.440450000	28.827615000	9.894590000
C	20.687003000	19.634347000	13.440450000	C	13.440450000	30.034298000	10.287052000
O	13.440450000	24.934185000	9.894590000	O	13.440450000	30.426760000	15.387165000
C	13.440450000	23.727502000	10.287052000	O	13.440450000	30.426760000	11.493735000
O	13.440450000	24.934185000	16.986310000	C	17.333342000	27.201858000	18.960712000
C	13.440450000	23.727502000	16.593848000	C	18.317452000	27.216911000	19.936757000
O	13.440450000	23.335040000	15.387165000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	23.335040000	11.493735000	H	18.007515000	27.477656000	20.830009000
C	18.960712000	26.559942000	17.333342000	H	13.440450000	30.790903000	9.530447000
C	19.936757000	26.544889000	18.317452000	H	17.350453000	26.880900000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	17.350453000	30.790903000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	30.790903000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	9.530447000	30.790903000	13.440450000
C	20.384593000	18.317452000	13.104439000	H	9.530447000	26.880900000	17.350453000
H	21.176773000	16.322082000	12.956594000	H	13.440450000	22.970897000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	9.530447000	22.970897000	13.440450000
C	22.988008000	18.960712000	13.761408000	H	13.440450000	22.970897000	17.350453000
C	22.003898000	19.936757000	13.776461000	H	15.026933000	25.294417000	11.853967000
H	23.999268000	19.144577000	13.924306000	H	11.853967000	28.467383000	11.853967000
H	22.313835000	20.830009000	14.037206000	H	9.530447000	26.880900000	9.530447000
Zr	10.956924000	26.880900000	13.440450000	H	15.026933000	28.467383000	15.026933000
O	9.894590000	26.880900000	11.493735000	H	11.853967000	25.294417000	15.026933000
O	12.408223000	27.913127000	14.472677000	H	26.512695000	23.864718000	20.918629000
C	10.287052000	26.880900000	10.287052000	H	26.884105000	19.384736000	16.454877000
Zr	15.923976000	26.880900000	13.440450000	H	26.886256000	19.244211000	22.478211000
O	16.986310000	26.880900000	11.493735000	H	26.315402000	17.852667000	21.055289000
C	16.593848000	26.880900000	10.287052000	H	26.908119000	21.066697000	24.150475000
O	16.986310000	26.880900000	15.387165000	H	26.429630000	16.164601000	19.249060000
O	14.472677000	27.913127000	12.408223000	Cu	26.495015000	21.924644000	17.943102000
C	16.593848000	26.880900000	16.593848000	I	24.053834000	21.551584000	17.078834000
C	17.650268000	26.880900000	17.650268000	C	27.149856000	23.751245000	17.320135000
C	19.634347000	26.880900000	19.634347000	C	28.113697000	23.060891000	17.715447000
O	9.894590000	26.880900000	15.387165000	H	29.119114000	22.805203000	17.987840000
C	10.287052000	26.880900000	16.593848000	C	26.314912000	24.792898000	16.655589000
Zr	13.440450000	26.880900000	15.923976000	H	26.804069000	25.751883000	16.918275000
O	11.493735000	26.880900000	16.986310000	H	25.317311000	24.798682000	17.129298000
O	14.472677000	27.913127000	14.472677000	O	26.246040000	24.624509000	15.297154000
Zr	13.440450000	26.880900000	10.956924000	H	26.298989000	23.233621000	14.764378000
O	11.493735000	26.880900000	9.894590000	C	25.396282000	23.567386000	10.850567000
O	15.387165000	26.880900000	9.894590000	C	24.564918000	24.209584000	11.959361000
O	12.408223000	27.913127000	12.408223000	C	24.335810000	23.320975000	13.205546000
O	15.387165000	26.880900000	16.986310000	C	24.808630000	22.298225000	10.236058000
Zr	13.440450000	29.364426000	13.440450000	C	25.341095000	22.218100000	13.291468000
O	11.493735000	30.426760000	13.440450000	C	24.346724000	21.285764000	11.287056000
C	10.287052000	30.034298000	13.440450000	N	25.259208000	21.188112000	12.423039000
O	15.387165000	30.426760000	13.440450000	H	25.565873000	24.302314000	10.057163000
C	16.593848000	30.034298000	13.440450000	H	25.555777000	21.838991000	9.576786000
O	16.986310000	28.827615000	13.440450000	C	27.365655000	21.353929000	14.317669000
O	9.894590000	28.827615000	13.440450000	N	26.294013000	22.315970000	14.177996000
C	22.671082000	26.880900000	22.671082000	C	26.966681000	20.017660000	13.720023000
C	20.687003000	26.880900000	20.687003000	C	26.348260000	20.217440000	12.349302000
C	21.360638000	27.201858000	22.988008000	H	25.942637000	19.277342000	11.966593000
C	20.384593000	27.216911000	22.003898000	H	27.587300000	21.265725000	15.390348000
H	21.176773000	27.364756000	23.999268000	H	26.393870000	23.349574000	11.255623000
H	19.491341000	27.477656000	22.313835000	H	23.948123000	22.539638000	9.599793000
O	13.440450000	28.827615000	16.986310000	H	27.106682000	20.564876000	11.628412000

Journal Name				ARTICLE			
H	28.268426000	21.760559000	13.839632000	O	26.880945000	16.986494000	11.493769000
H	23.593288000	24.533101000	11.567227000	O	28.827591000	16.986480000	13.440428000
H	25.092674000	25.109056000	12.288053000	C	23.755332000	26.686089000	23.755213000
H	27.829060000	19.348644000	13.644887000	Zr	24.236612000	26.881475000	26.880552000
H	26.236621000	19.530015000	14.375245000	Zr	26.880671000	29.524609000	26.880680000
H	24.426952000	23.917047000	14.116461000	Zr	29.524440000	26.882357000	26.881381000
H	23.334813000	22.880709000	13.203940000	C	27.064326000	30.008530000	23.753165000
H	23.355681000	21.555928000	11.662317000	C	30.008123000	27.066993000	23.753823000
H	24.251656000	20.280768000	10.864714000	C	23.755714000	23.756676000	26.684338000
C	27.853939000	25.345836000	14.310251000	Zr	26.880615000	26.881402000	29.524137000
O	28.431906000	25.985536000	15.127064000	C	27.065914000	23.754135000	30.008060000
O	27.673667000	24.871928000	13.231425000	C	30.007964000	23.754748000	27.067567000
f. IM1				Zr	24.236612000	13.440798000	13.439875000
N	26.604122000	21.873207000	20.387501000	Zr	26.880615000	10.797213000	13.439948000
N	26.762945000	19.916655000	18.451256000	C	23.755714000	13.637012000	16.564674000
C	26.648153000	20.586669000	20.793301000	C	27.065914000	10.313290000	16.567215000
C	26.645219000	22.850550000	21.303854000	Zr	29.524440000	13.439969000	13.438993000
C	26.748598000	18.995859000	17.471325000	C	30.007964000	13.253783000	16.566602000
C	26.631537000	19.528196000	19.740462000	Zr	26.880671000	13.440670000	10.796741000
C	26.721216000	20.272604000	22.159025000	C	23.755332000	16.566137000	13.635261000
C	26.713274000	22.631336000	22.692037000	C	27.064326000	16.568185000	10.312820000
C	26.687406000	17.616984000	17.692704000	C	30.008123000	16.567527000	13.254357000
C	26.491954000	18.163289000	20.039569000	O	23.334855000	26.880866000	24.934215000
C	26.746428000	21.291976000	23.100719000	O	23.334856000	24.934212000	26.880862000
C	26.547625000	17.214099000	19.029022000	O	25.848909000	27.912895000	27.912897000
C	26.809925000	23.730886000	23.728973000	O	23.334862000	26.880939000	28.827594000
C	26.809925000	16.592377000	16.590464000	O	23.334864000	28.827596000	26.880937000
O	26.880885000	24.934153000	23.334955000	O	24.934210000	30.426941000	26.880925000
O	26.880903000	23.334945000	24.934136000	O	26.880889000	30.426939000	24.934203000
O	26.880903000	15.387214000	16.986405000	O	26.880879000	30.426942000	28.827590000
O	26.880885000	16.986395000	15.387197000	O	27.912786000	27.912776000	27.912777000
Zr	26.878142000	26.881612000	24.237883000	O	28.827596000	30.426944000	26.880863000
Zr	26.878209000	24.239690000	26.880717000	O	30.426933000	24.934198000	26.880924000
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Zr	26.878142000	16.083467000	13.439738000	O	30.426944000	26.880866000	28.827595000
O	24.934203000	26.880849000	23.334882000	O	30.426946000	28.827594000	26.880867000
O	25.848911000	25.848918000	25.848917000	O	24.934211000	26.880924000	30.426942000
O	25.849015000	27.912768000	25.849028000	O	26.880889000	24.934201000	30.426937000
O	27.912782000	25.849032000	25.849031000	O	26.880878000	28.827589000	30.426943000
O	27.912889000	27.912886000	25.848919000	O	28.827598000	26.880862000	30.426940000
O	26.880945000	28.827581000	23.334856000	O	25.848909000	12.408453000	12.408455000
O	28.827591000	26.880922000	23.334870000	O	23.334862000	11.493756000	13.440411000
O	24.934197000	23.334881000	26.880846000	O	23.334855000	15.387135000	13.440484000
O	25.849012000	25.849025000	27.912771000	O	23.334864000	13.440413000	11.493754000
O	27.912892000	25.848913000	27.912887000	O	23.334856000	13.440488000	15.387138000
O	26.880944000	23.334850000	28.827576000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	23.334868000	26.880917000	O	26.880889000	9.894413000	15.387149000
O	25.849012000	12.408579000	14.472325000	O	27.912786000	12.408573000	12.408574000
O	25.848911000	14.472433000	14.472432000	O	26.880878000	9.894407000	11.493761000
O	24.934197000	13.440504000	16.986469000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	11.493774000	16.986500000	O	30.426944000	11.493755000	13.440484000
O	27.912892000	12.408463000	14.472437000	O	30.426936000	15.387151000	13.440421000
O	27.912782000	14.472319000	14.472318000	O	30.426946000	13.440483000	11.493756000
O	28.827591000	13.440433000	16.986482000	O	30.426933000	13.440426000	15.387152000
O	25.849015000	14.472322000	12.408582000	O	24.934210000	13.440425000	9.894409000
O	24.934203000	16.986468000	13.440501000	O	26.880879000	11.493760000	9.894408000
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ARTICLE

Journal Name

O	28.827596000	13.440487000	9.894406000	C	18.317452000	20.384593000	13.104439000
C	23.753697000	27.066116000	30.007949000	H	16.322082000	21.176773000	12.956594000
C	23.753135000	30.008630000	27.063604000	H	18.007515000	19.491341000	12.843694000
C	26.696398000	30.008246000	30.008106000	C	22.988008000	26.559942000	21.360638000
C	30.007968000	30.008237000	26.695581000	C	22.003898000	26.544889000	20.384593000
C	30.008286000	26.697416000	30.008420000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	10.313401000	13.255234000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	13.257746000	10.312720000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	10.313244000	10.313104000	C	20.687003000	19.634347000	13.440450000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	24.934185000	9.894590000
C	30.007968000	13.625768000	10.313113000	C	13.440450000	23.727502000	10.287052000
H	27.351814000	30.759513000	23.002127000	O	13.440450000	24.934185000	16.986310000
H	30.758179000	27.358190000	23.003211000	C	13.440450000	23.727502000	16.593848000
H	23.008991000	23.009158000	26.377462000	O	13.440450000	23.335040000	15.387165000
H	27.355985000	23.003402000	30.758391000	O	13.440450000	23.335040000	11.493735000
H	30.757581000	23.004153000	27.359935000	C	18.960712000	26.559942000	17.333342000
H	23.008991000	13.943888000	17.312192000	C	19.936757000	26.544889000	18.317452000
H	27.355985000	9.562959000	17.317948000	H	19.144577000	26.397044000	16.322082000
H	30.757582000	12.961415000	17.317197000	H	20.830009000	26.284144000	18.007515000
H	27.351814000	17.319223000	9.561837000	C	21.360638000	17.333342000	13.119492000
H	30.758179000	17.318139000	12.963160000	C	20.384593000	18.317452000	13.104439000
H	23.003255000	27.356162000	30.758555000	H	21.176773000	16.322082000	12.956594000
H	23.001913000	30.759916000	27.349810000	H	19.491341000	18.007515000	12.843694000
H	26.407446000	30.758917000	30.758911000	C	22.988008000	18.960712000	13.761408000
H	30.758582000	30.758568000	26.405278000	C	22.003898000	19.936757000	13.776461000
H	30.759373000	26.409850000	30.759355000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	9.562795000	12.965188000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	12.971540000	9.561434000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	9.562439000	9.562434000	O	9.894590000	26.880900000	11.493735000
H	30.759373000	9.561995000	13.911500000	O	12.408223000	27.913127000	14.472677000
H	30.758582000	13.916071000	9.562782000	C	10.287052000	26.880900000	10.287052000
H	25.215026000	11.776433000	15.102845000	Zr	15.923976000	26.880900000	13.440450000
H	28.544134000	11.776251000	11.775822000	O	16.986310000	26.880900000	11.493735000
H	28.555271000	15.099035000	15.098322000	C	16.593848000	26.880900000	10.287052000
H	25.215244000	15.103495000	11.776660000	O	16.986310000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	O	14.472677000	27.913127000	12.408223000
H	28.555271000	25.223028000	25.222315000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	28.545528000	28.545099000	C	17.650268000	26.880900000	17.650268000
H	25.215026000	25.218505000	28.544917000	C	19.634347000	26.880900000	19.634347000
O	14.472677000	25.848673000	14.472677000	O	9.894590000	26.880900000	15.387165000
O	12.408223000	25.848673000	12.408223000	C	10.287052000	26.880900000	16.593848000
O	14.472677000	25.848673000	12.408223000	Zr	13.440450000	26.880900000	15.923976000
O	12.408223000	25.848673000	14.472677000	O	11.493735000	26.880900000	16.986310000
Zr	13.440450000	24.397374000	13.440450000	O	14.472677000	27.913127000	14.472677000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	26.880900000	10.956924000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	26.880900000	9.894590000
O	15.387165000	23.335040000	13.440450000	O	15.387165000	26.880900000	9.894590000
C	16.593848000	23.727502000	13.440450000	O	12.408223000	27.913127000	12.408223000
C	17.650268000	22.671082000	13.440450000	O	15.387165000	26.880900000	16.986310000
C	19.634347000	20.687003000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	11.493735000	30.426760000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	10.287052000	30.034298000	13.440450000
H	19.144577000	23.999268000	13.924306000	O	15.387165000	30.426760000	13.440450000
H	20.830009000	22.313835000	14.037206000	C	16.593848000	30.034298000	13.440450000
O	9.894590000	24.934185000	13.440450000	O	16.986310000	28.827615000	13.440450000
O	16.986310000	24.934185000	13.440450000	O	9.894590000	28.827615000	13.440450000
C	17.333342000	21.360638000	13.119492000	C	22.671082000	26.880900000	22.671082000

C	20.687003000	26.880900000	20.687003000	C	27.214267000	20.138269000	13.739391000
C	21.360638000	27.201858000	22.988008000	H	26.305813000	19.885874000	14.298799000
C	20.384593000	27.216911000	22.003898000	H	30.421012000	21.034192000	14.609897000
H	21.176773000	27.364756000	23.999268000	H	27.670076000	21.654510000	10.474973000
H	19.491341000	27.477656000	22.313835000	H	24.666866000	22.133995000	10.737335000
O	13.440450000	28.827615000	16.986310000	H	27.362818000	19.370003000	12.965405000
C	13.440450000	30.034298000	16.593848000	H	29.982907000	20.065324000	13.196108000
O	13.440450000	28.827615000	9.894590000	H	26.316074000	24.365128000	10.885940000
C	13.440450000	30.034298000	10.287052000	H	27.955565000	24.120251000	10.331704000
O	13.440450000	30.426760000	15.387165000	H	28.632454000	19.229917000	15.066673000
O	13.440450000	30.426760000	11.493735000	H	28.156322000	20.888577000	15.506799000
C	17.333342000	27.201858000	18.960712000	H	28.586727000	24.277713000	12.547443000
C	18.317452000	27.216911000	19.936757000	H	26.946255000	24.128937000	13.108400000
H	16.322082000	27.364756000	19.144577000	H	25.385289000	22.766610000	12.927353000
H	18.007515000	27.477656000	20.830009000	H	24.946943000	21.092197000	13.071798000
H	13.440450000	30.790903000	9.530447000	C	30.191269000	24.465077000	15.113067000
H	17.350453000	26.880900000	9.530447000	O	30.677671000	25.090509000	16.042447000
H	17.350453000	30.790903000	13.440450000	O	30.659979000	24.057432000	14.017448000
H	13.440450000	30.790903000	17.350453000	g. TS2			
H	9.530447000	30.790903000	13.440450000	N	26.417585000	21.825219000	20.419236000
H	9.530447000	26.880900000	17.350453000	N	26.685816000	19.916740000	18.475528000
H	13.440450000	22.970897000	9.530447000	C	26.692346000	20.551901000	20.811660000
H	9.530447000	22.970897000	13.440450000	C	26.464522000	22.817455000	21.330221000
H	13.440450000	22.970897000	17.350453000	C	26.677169000	18.996230000	17.491703000
H	15.026933000	25.294417000	11.853967000	C	26.675969000	19.500975000	19.768008000
H	11.853967000	28.467383000	11.853967000	C	26.981239000	20.277596000	22.156775000
H	9.530447000	26.880900000	9.530447000	C	26.729162000	22.624197000	22.695332000
H	15.026933000	28.467383000	15.026933000	C	26.707526000	17.613621000	17.699731000
H	11.853967000	25.294417000	15.026933000	C	26.634258000	18.128031000	20.063980000
H	26.625770000	23.866896000	20.913915000	C	26.978232000	21.299197000	23.093088000
H	26.788590000	19.393991000	16.460624000	C	26.665596000	17.192634000	19.042752000
H	26.780003000	19.241548000	22.492450000	C	26.809925000	23.730886000	23.728973000
H	26.341370000	17.838820000	21.063584000	C	26.809925000	16.592377000	16.590464000
H	26.810704000	21.067038000	24.160564000	O	26.880885000	24.934153000	23.334955000
H	26.477508000	16.155250000	19.257200000	O	26.880903000	23.334945000	24.934136000
Cu	27.037445000	21.897844000	17.903507000	O	26.880903000	15.387214000	16.986405000
I	24.997799000	22.137545000	16.301149000	O	26.880885000	16.986395000	15.387197000
C	28.356637000	23.363251000	17.437082000	Zr	26.878142000	26.881612000	24.237883000
C	28.884305000	22.550899000	18.224203000	Zr	26.878209000	24.239690000	26.880717000
H	29.616771000	22.120879000	18.879328000	Zr	26.878209000	13.440633000	16.081660000
C	28.168886000	24.431531000	16.434587000	Zr	26.878142000	16.083467000	13.439738000
H	28.625588000	25.344641000	16.840116000	O	24.934203000	26.880849000	23.334882000
H	27.103278000	24.593035000	16.243194000	O	25.848911000	25.848918000	25.848917000
O	28.782217000	24.086280000	15.216161000	O	25.849015000	27.912768000	25.849028000
H	29.863850000	22.872216000	13.443930000	O	27.912782000	25.849032000	25.849031000
C	26.800031000	22.320871000	10.393347000	O	27.912889000	27.912886000	25.848919000
C	27.174849000	23.688095000	10.964606000	O	26.880945000	28.827581000	23.334856000
C	27.679675000	23.680520000	12.429574000	O	28.827591000	26.880922000	23.334870000
C	25.599286000	21.661070000	11.068785000	O	24.934197000	23.334881000	26.880846000
C	27.982915000	22.316533000	12.964760000	O	25.849012000	25.849025000	27.912771000
C	25.657762000	21.761986000	12.588943000	O	27.912892000	25.848913000	27.912887000
N	26.984169000	21.439680000	13.112449000	O	26.880944000	23.334850000	28.827576000
H	26.605900000	22.417092000	9.320016000	O	28.827591000	23.334868000	26.880917000
H	25.538851000	20.608416000	10.764823000	O	25.849012000	12.408579000	14.472325000
C	29.600452000	20.790936000	13.927943000	O	25.848911000	14.472433000	14.472432000
N	29.235588000	22.022871000	13.247895000	O	24.934197000	13.440504000	16.986469000
C	28.408414000	20.222830000	14.667954000	O	26.880944000	11.493774000	16.986500000

ARTICLE

Journal Name

O	27.912892000	12.408463000	14.472437000	O	30.426936000	15.387151000	13.440421000
O	27.912782000	14.472319000	14.472318000	O	30.426946000	13.440483000	11.493756000
O	28.827591000	13.440433000	16.986482000	O	30.426933000	13.440426000	15.387152000
O	25.849015000	14.472322000	12.408582000	O	24.934210000	13.440425000	9.894409000
O	24.934203000	16.986468000	13.440501000	O	26.880879000	11.493760000	9.894408000
O	27.912889000	14.472431000	12.408464000	O	26.880889000	15.387147000	9.894411000
O	26.880945000	16.986494000	11.493769000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	27.066116000	30.007949000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	30.008630000	27.063604000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	30.008246000	30.008106000
Zr	26.880671000	29.524609000	26.880680000	C	30.007968000	30.008237000	26.695581000
Zr	29.524440000	26.882357000	26.881381000	C	30.008286000	26.697416000	30.008420000
C	27.064326000	30.008530000	23.753165000	C	23.753697000	10.313401000	13.255234000
C	30.008123000	27.066993000	23.753823000	C	23.753135000	13.257746000	10.312720000
C	23.755714000	23.756676000	26.684338000	C	26.696398000	10.313244000	10.313104000
Zr	26.880615000	26.881402000	29.524137000	C	30.008286000	10.312930000	13.623934000
C	27.065914000	23.754135000	30.008060000	C	30.007968000	13.625768000	10.313113000
C	30.007964000	23.754748000	27.067567000	H	27.351814000	30.759513000	23.002127000
Zr	24.236612000	13.440798000	13.439875000	H	30.758179000	27.358190000	23.003211000
Zr	26.880615000	10.797213000	13.439948000	H	23.008991000	23.009158000	26.377462000
C	23.755714000	13.637012000	16.564674000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	10.313290000	16.567215000	H	30.757581000	23.004153000	27.359935000
Zr	29.524440000	13.439969000	13.438993000	H	23.008991000	13.943888000	17.312192000
C	30.007964000	13.253783000	16.566602000	H	27.355985000	9.562959000	17.317948000
Zr	26.880671000	13.440670000	10.796741000	H	30.757582000	12.961415000	17.317197000
C	23.755332000	16.566137000	13.635261000	H	27.351814000	17.319223000	9.561837000
C	27.064326000	16.568185000	10.312820000	H	30.758179000	17.318139000	12.963160000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	27.356162000	30.758555000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	30.759916000	27.349810000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	30.758917000	30.758911000
O	25.848909000	27.912895000	27.912897000	H	30.758582000	30.758568000	26.405278000
O	23.334862000	26.880939000	28.827594000	H	30.759373000	26.409850000	30.759355000
O	23.334864000	28.827596000	26.880937000	H	23.003255000	9.562795000	12.965188000
O	24.934210000	30.426941000	26.880925000	H	23.001913000	12.971540000	9.561434000
O	26.880889000	30.426939000	24.934203000	H	26.407446000	9.562439000	9.562434000
O	26.880879000	30.426942000	28.827590000	H	30.759373000	9.561995000	13.911500000
O	27.912786000	27.912776000	27.912777000	H	30.758582000	13.916071000	9.562782000
O	28.827596000	30.426944000	26.880863000	H	25.215026000	11.776433000	15.102845000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	11.776251000	11.775822000
O	30.426936000	26.880929000	24.934199000	H	28.555271000	15.099035000	15.098322000
O	30.426944000	26.880866000	28.827595000	H	25.215244000	15.103495000	11.776660000
O	30.426946000	28.827594000	26.880867000	H	25.215244000	28.544690000	25.217855000
O	24.934211000	26.880924000	30.426942000	H	28.555271000	25.223028000	25.222315000
O	26.880889000	24.934201000	30.426937000	H	28.544134000	28.545528000	28.545099000
O	26.880878000	28.827589000	30.426943000	H	25.215026000	25.218505000	28.544917000
O	28.827598000	26.880862000	30.426940000	O	14.472677000	25.848673000	14.472677000
O	25.848909000	12.408453000	12.408455000	O	12.408223000	25.848673000	12.408223000
O	23.334862000	11.493756000	13.440411000	O	14.472677000	25.848673000	12.408223000
O	23.334855000	15.387135000	13.440484000	O	12.408223000	25.848673000	14.472677000
O	23.334864000	13.440413000	11.493754000	Zr	13.440450000	24.397374000	13.440450000
O	23.334856000	13.440488000	15.387138000	O	11.493735000	23.335040000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	10.287052000	23.727502000	13.440450000
O	26.880889000	9.894413000	15.387149000	O	15.387165000	23.335040000	13.440450000
O	27.912786000	12.408573000	12.408574000	C	16.593848000	23.727502000	13.440450000
O	26.880878000	9.894407000	11.493761000	C	17.650268000	22.671082000	13.440450000
O	28.827598000	9.894410000	13.440488000	C	19.634347000	20.687003000	13.440450000
O	30.426944000	11.493755000	13.440484000	C	18.960712000	22.988008000	13.761408000

C	19.936757000	22.003898000	13.776461000	C	10.287052000	30.034298000	13.440450000
H	19.144577000	23.999268000	13.924306000	O	15.387165000	30.426760000	13.440450000
H	20.830009000	22.313835000	14.037206000	C	16.593848000	30.034298000	13.440450000
O	9.894590000	24.934185000	13.440450000	O	16.986310000	28.827615000	13.440450000
O	16.986310000	24.934185000	13.440450000	O	9.894590000	28.827615000	13.440450000
C	17.333342000	21.360638000	13.119492000	C	22.671082000	26.880900000	22.671082000
C	18.317452000	20.384593000	13.104439000	C	20.687003000	26.880900000	20.687003000
H	16.322082000	21.176773000	12.956594000	C	21.360638000	27.201858000	22.988008000
H	18.007515000	19.491341000	12.843694000	C	20.384593000	27.216911000	22.003898000
C	22.988008000	26.559942000	21.360638000	H	21.176773000	27.364756000	23.999268000
C	22.003898000	26.544889000	20.384593000	H	19.491341000	27.477656000	22.313835000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	28.827615000	16.986310000
H	22.313835000	26.284144000	19.491341000	C	13.440450000	30.034298000	16.593848000
C	22.671082000	17.650268000	13.440450000	O	13.440450000	28.827615000	9.894590000
C	20.687003000	19.634347000	13.440450000	C	13.440450000	30.034298000	10.287052000
O	13.440450000	24.934185000	9.894590000	O	13.440450000	30.426760000	15.387165000
C	13.440450000	23.727502000	10.287052000	O	13.440450000	30.426760000	11.493735000
O	13.440450000	24.934185000	16.986310000	C	17.333342000	27.201858000	18.960712000
C	13.440450000	23.727502000	16.593848000	C	18.317452000	27.216911000	19.936757000
O	13.440450000	23.335040000	15.387165000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	23.335040000	11.493735000	H	18.007515000	27.477656000	20.830009000
C	18.960712000	26.559942000	17.333342000	H	13.440450000	30.790903000	9.530447000
C	19.936757000	26.544889000	18.317452000	H	17.350453000	26.880900000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	17.350453000	30.790903000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	30.790903000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	9.530447000	30.790903000	13.440450000
C	20.384593000	18.317452000	13.104439000	H	9.530447000	26.880900000	17.350453000
H	21.176773000	16.322082000	12.956594000	H	13.440450000	22.970897000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	9.530447000	22.970897000	13.440450000
C	22.988008000	18.960712000	13.761408000	H	13.440450000	22.970897000	17.350453000
C	22.003898000	19.936757000	13.776461000	H	15.026933000	25.294417000	11.853967000
H	23.999268000	19.144577000	13.924306000	H	11.853967000	28.467383000	11.853967000
H	22.313835000	20.830009000	14.037206000	H	9.530447000	26.880900000	9.530447000
Zr	10.956924000	26.880900000	13.440450000	H	15.026933000	28.467383000	15.026933000
O	9.894590000	26.880900000	11.493735000	H	11.853967000	25.294417000	15.026933000
O	12.408223000	27.913127000	14.472677000	H	26.268186000	23.816261000	20.945410000
C	10.287052000	26.880900000	10.287052000	H	26.642922000	19.391539000	16.479901000
Zr	15.923976000	26.880900000	13.440450000	H	27.227126000	19.267051000	22.467964000
O	16.986310000	26.880900000	11.493735000	H	26.561684000	17.792954000	21.093951000
C	16.593848000	26.880900000	10.287052000	H	27.193969000	21.095968000	24.136916000
O	16.986310000	26.880900000	15.387165000	H	26.651663000	16.130282000	19.262364000
O	14.472677000	27.913127000	12.408223000	Cu	26.094176000	21.955409000	18.272621000
C	16.593848000	26.880900000	16.593848000	I	23.759574000	21.227541000	17.146963000
C	17.650268000	26.880900000	17.650268000	C	26.295999000	24.237309000	16.755456000
C	19.634347000	26.880900000	19.634347000	C	27.066882000	23.466506000	17.408502000
O	9.894590000	26.880900000	15.387165000	H	28.149561000	23.432062000	17.375435000
C	10.287052000	26.880900000	16.593848000	C	24.993375000	24.750183000	16.354280000
Zr	13.440450000	26.880900000	15.923976000	H	24.870436000	25.794039000	16.673098000
O	11.493735000	26.880900000	16.986310000	H	24.201093000	24.137341000	16.804427000
O	14.472677000	27.913127000	14.472677000	O	24.866896000	24.653692000	14.940722000
Zr	13.440450000	26.880900000	10.956924000	H	25.198985000	22.829982000	14.543056000
O	11.493735000	26.880900000	9.894590000	C	25.695467000	23.211839000	10.419206000
O	15.387165000	26.880900000	9.894590000	C	24.353073000	23.504961000	11.082204000
O	12.408223000	27.913127000	12.408223000	C	24.020569000	22.631199000	12.320485000
O	15.387165000	26.880900000	16.986310000	C	25.796660000	21.836590000	9.763161000
Zr	13.440450000	29.364426000	13.440450000	C	25.177123000	21.826737000	12.821621000
O	11.493735000	30.426760000	13.440450000	C	25.260157000	20.728949000	10.666700000

ARTICLE

Journal Name

N	25.713202000	20.871836000	12.048249000	O	26.880944000	23.334850000	28.827576000
H	25.899258000	23.983823000	9.671171000	O	28.827591000	23.334868000	26.880917000
H	26.839499000	21.629677000	9.492847000	O	25.849012000	12.408579000	14.472325000
C	26.832005000	21.450864000	14.593606000	O	25.848911000	14.472433000	14.472432000
N	25.651755000	22.074535000	14.021112000	O	24.934197000	13.440504000	16.986469000
C	27.064443000	20.105329000	13.940039000	O	26.880944000	11.493774000	16.986500000
C	26.971542000	20.226929000	12.431979000	O	27.912892000	12.408463000	14.472437000
H	26.997765000	19.242200000	11.957181000	O	27.912782000	14.472319000	14.472318000
H	26.657693000	21.368490000	15.673593000	O	28.827591000	13.440433000	16.986482000
H	26.479851000	23.336645000	11.176638000	O	25.849015000	14.472322000	12.408582000
H	25.225542000	21.810629000	8.826887000	O	24.934203000	16.986468000	13.440501000
H	27.811224000	20.817391000	12.034480000	O	27.912889000	14.472431000	12.408464000
H	27.684056000	22.130346000	14.454666000	O	26.880945000	16.986494000	11.493769000
H	23.541147000	23.404308000	10.351201000	O	28.827591000	16.986480000	13.440428000
H	24.376231000	24.541799000	11.419547000	C	23.755332000	26.686089000	23.755213000
H	28.043095000	19.706110000	14.218185000	Zr	24.236612000	26.881475000	26.880552000
H	26.317148000	19.386664000	14.293212000	Zr	26.880671000	29.524609000	26.880680000
H	23.678140000	23.262818000	13.143482000	Zr	29.524440000	26.882357000	26.881381000
H	23.205021000	21.937681000	12.089668000	C	27.064326000	30.008530000	23.753165000
H	24.165482000	20.730654000	10.665046000	C	30.008123000	27.066993000	23.753823000
H	25.568096000	19.733779000	10.331593000	C	23.755714000	23.756676000	26.684338000
C	26.115627000	25.014700000	14.300837000	Zr	26.880615000	26.881402000	29.524137000
O	27.042460000	25.247418000	15.125445000	C	27.065914000	23.754135000	30.008060000
O	26.081212000	24.977818000	13.077839000	C	30.007964000	23.754748000	27.067567000
h. IM2				Zr	24.236612000	13.440798000	13.439875000
N	26.662625000	21.842198000	20.409511000	Zr	26.880615000	10.797213000	13.439948000
N	26.539854000	19.925829000	18.479127000	C	23.755714000	13.637012000	16.564674000
C	26.660192000	20.549449000	20.823044000	C	27.065914000	10.313290000	16.567215000
C	26.652010000	22.829145000	21.325412000	Zr	29.524440000	13.439969000	13.438993000
C	26.578214000	19.007578000	17.493029000	C	30.007964000	13.253783000	16.566602000
C	26.677570000	19.510630000	19.769374000	Zr	26.880671000	13.440670000	10.796741000
C	26.643018000	20.255739000	22.197552000	C	23.755332000	16.566137000	13.635261000
C	26.700346000	22.621978000	22.708041000	C	27.064326000	16.568185000	10.312820000
C	26.723720000	17.625602000	17.695077000	C	30.008123000	16.567527000	13.254357000
C	26.840838000	18.145685000	20.055309000	O	23.334855000	26.880866000	24.934215000
C	26.680786000	21.278612000	23.130125000	O	23.334856000	24.934212000	26.880862000
C	26.849796000	17.211409000	19.033685000	O	25.848909000	27.912895000	27.912897000
C	26.809925000	23.730886000	23.728973000	O	23.334862000	26.880939000	28.827594000
C	26.809925000	16.592377000	16.590464000	O	23.334864000	28.827596000	26.880937000
O	26.880885000	24.934153000	23.334955000	O	24.934210000	30.426941000	26.880925000
O	26.880903000	23.334945000	24.934136000	O	26.880889000	30.426939000	24.934203000
O	26.880903000	15.387214000	16.986405000	O	26.880879000	30.426942000	28.827590000
O	26.880885000	16.986395000	15.387197000	O	27.912786000	27.912776000	27.912777000
Zr	26.878142000	26.881612000	24.237883000	O	28.827596000	30.426944000	26.880863000
Zr	26.878209000	24.239690000	26.880717000	O	30.426933000	24.934198000	26.880924000
Zr	26.878209000	13.440633000	16.081660000	O	30.426936000	26.880929000	24.934199000
Zr	26.878142000	16.083467000	13.439738000	O	30.426944000	26.880866000	28.827595000
O	24.934203000	26.880849000	23.334882000	O	30.426946000	28.827594000	26.880867000
O	25.848911000	25.848918000	25.848917000	O	24.934211000	26.880924000	30.426942000
O	25.849015000	27.912768000	25.849028000	O	26.880889000	24.934201000	30.426937000
O	27.912782000	25.849032000	25.849031000	O	26.880878000	28.827589000	30.426943000
O	27.912889000	27.912886000	25.848919000	O	28.827598000	26.880862000	30.426940000
O	26.880945000	28.827581000	23.334856000	O	25.848909000	12.408453000	12.408455000
O	28.827591000	26.880922000	23.334870000	O	23.334862000	11.493756000	13.440411000
O	24.934197000	23.334881000	26.880846000	O	23.334855000	15.387135000	13.440484000
O	25.849012000	25.849025000	27.912771000	O	23.334864000	13.440413000	11.493754000
O	27.912892000	25.848913000	27.912887000	O	23.334856000	13.440488000	15.387138000

Journal Name				ARTICLE			
O	24.934211000	9.894408000	13.440426000	C	10.287052000	23.727502000	13.440450000
O	26.880889000	9.894413000	15.387149000	O	15.387165000	23.335040000	13.440450000
O	27.912786000	12.408573000	12.408574000	C	16.593848000	23.727502000	13.440450000
O	26.880878000	9.894407000	11.493761000	C	17.650268000	22.671082000	13.440450000
O	28.827598000	9.894410000	13.440488000	C	19.634347000	20.687003000	13.440450000
O	30.426944000	11.493755000	13.440484000	C	18.960712000	22.988008000	13.761408000
O	30.426936000	15.387151000	13.440421000	C	19.936757000	22.003898000	13.776461000
O	30.426946000	13.440483000	11.493756000	H	19.144577000	23.999268000	13.924306000
O	30.426933000	13.440426000	15.387152000	H	20.830009000	22.313835000	14.037206000
O	24.934210000	13.440425000	9.894409000	O	9.894590000	24.934185000	13.440450000
O	26.880879000	11.493760000	9.894408000	O	16.986310000	24.934185000	13.440450000
O	26.880889000	15.387147000	9.894411000	C	17.333342000	21.360638000	13.119492000
O	28.827596000	13.440487000	9.894406000	C	18.317452000	20.384593000	13.104439000
C	23.753697000	27.066116000	30.007949000	H	16.322082000	21.176773000	12.956594000
C	23.753135000	30.008630000	27.063604000	H	18.007515000	19.491341000	12.843694000
C	26.696398000	30.008246000	30.008106000	C	22.988008000	26.559942000	21.360638000
C	30.007968000	30.008237000	26.695581000	C	22.003898000	26.544889000	20.384593000
C	30.008286000	26.697416000	30.008420000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	10.313401000	13.255234000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	13.257746000	10.312720000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	10.313244000	10.313104000	C	20.687003000	19.634347000	13.440450000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	24.934185000	9.894590000
C	30.007968000	13.625768000	10.313113000	C	13.440450000	23.727502000	10.287052000
H	27.351814000	30.759513000	23.002127000	O	13.440450000	24.934185000	16.986310000
H	30.758179000	27.358190000	23.003211000	C	13.440450000	23.727502000	16.593848000
H	23.008991000	23.009158000	26.377462000	O	13.440450000	23.335040000	15.387165000
H	27.355985000	23.003402000	30.758391000	O	13.440450000	23.335040000	11.493735000
H	30.757581000	23.004153000	27.359935000	C	18.960712000	26.559942000	17.333342000
H	23.008991000	13.943888000	17.312192000	C	19.936757000	26.544889000	18.317452000
H	27.355985000	9.562959000	17.317948000	H	19.144577000	26.397044000	16.322082000
H	30.757582000	12.961415000	17.317197000	H	20.830009000	26.284144000	18.007515000
H	27.351814000	17.319223000	9.561837000	C	21.360638000	17.333342000	13.119492000
H	30.758179000	17.318139000	12.963160000	C	20.384593000	18.317452000	13.104439000
H	23.003255000	27.356162000	30.758555000	H	21.176773000	16.322082000	12.956594000
H	23.001913000	30.759916000	27.349810000	H	19.491341000	18.007515000	12.843694000
H	26.407446000	30.758917000	30.758911000	C	22.988008000	18.960712000	13.761408000
H	30.758582000	30.758568000	26.405278000	C	22.003898000	19.936757000	13.776461000
H	30.759373000	26.409850000	30.759355000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	9.562795000	12.965188000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	12.971540000	9.561434000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	9.562439000	9.562434000	O	9.894590000	26.880900000	11.493735000
H	30.759373000	9.561995000	13.911500000	O	12.408223000	27.913127000	14.472677000
H	30.758582000	13.916071000	9.562782000	C	10.287052000	26.880900000	10.287052000
H	25.215026000	11.776433000	15.102845000	Zr	15.923976000	26.880900000	13.440450000
H	28.544134000	11.776251000	11.775822000	O	16.986310000	26.880900000	11.493735000
H	28.555271000	15.099035000	15.098322000	C	16.593848000	26.880900000	10.287052000
H	25.215244000	15.103495000	11.776660000	O	16.986310000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	O	14.472677000	27.913127000	12.408223000
H	28.555271000	25.223028000	25.222315000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	28.545528000	28.545099000	C	17.650268000	26.880900000	17.650268000
H	25.215026000	25.218505000	28.544917000	C	19.634347000	26.880900000	19.634347000
O	14.472677000	25.848673000	14.472677000	O	9.894590000	26.880900000	15.387165000
O	12.408223000	25.848673000	12.408223000	C	10.287052000	26.880900000	16.593848000
O	14.472677000	25.848673000	12.408223000	Zr	13.440450000	26.880900000	15.923976000
O	12.408223000	25.848673000	14.472677000	O	11.493735000	26.880900000	16.986310000
Zr	13.440450000	24.397374000	13.440450000	O	14.472677000	27.913127000	14.472677000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	26.880900000	10.956924000

ARTICLE

Journal Name

O	11.493735000	26.880900000	9.894590000	C	24.979470000	28.483567000	15.447690000
O	15.387165000	26.880900000	9.894590000	C	25.459683000	28.082727000	16.840704000
O	12.408223000	27.913127000	12.408223000	C	25.128213000	26.626746000	17.256887000
O	15.387165000	26.880900000	16.986310000	C	23.460390000	28.535431000	15.295582000
Zr	13.440450000	29.364426000	13.440450000	C	24.605768000	25.764233000	16.155155000
O	11.493735000	30.426760000	13.440450000	C	22.774288000	27.327056000	15.925261000
C	10.287052000	30.034298000	13.440450000	N	23.437415000	26.068287000	15.584805000
O	15.387165000	30.426760000	13.440450000	H	25.403212000	29.457406000	15.186057000
C	16.593848000	30.034298000	13.440450000	H	23.195604000	28.610424000	14.234186000
O	16.986310000	28.827615000	13.440450000	C	24.845135000	23.703860000	14.839676000
O	9.894590000	28.827615000	13.440450000	N	25.327794000	24.740810000	15.742670000
C	22.671082000	26.880900000	22.671082000	C	23.344901000	23.813162000	14.664640000
C	20.687003000	26.880900000	20.687003000	C	22.929888000	25.259677000	14.478680000
C	21.360638000	27.201858000	22.988008000	H	21.840351000	25.357170000	14.474205000
C	20.384593000	27.216911000	22.003898000	H	25.115522000	22.744057000	15.295386000
H	21.176773000	27.364756000	23.999268000	H	25.396517000	27.781521000	14.712391000
H	19.491341000	27.477656000	22.313835000	H	23.058035000	29.433954000	15.778243000
O	13.440450000	28.827615000	16.986310000	H	23.301018000	25.667067000	13.525939000
C	13.440450000	30.034298000	16.593848000	H	25.378367000	23.788719000	13.884892000
O	13.440450000	28.827615000	9.894590000	H	25.040576000	28.766850000	17.587407000
C	13.440450000	30.034298000	10.287052000	H	26.544557000	28.214578000	16.885575000
O	13.440450000	30.426760000	15.387165000	H	23.031016000	23.226953000	13.799275000
O	13.440450000	30.426760000	11.493735000	H	22.853410000	23.409889000	15.557232000
C	17.333342000	27.201858000	18.960712000	H	26.010856000	26.137028000	17.667515000
C	18.317452000	27.216911000	19.936757000	H	24.388621000	26.587845000	18.064008000
H	16.322082000	27.364756000	19.144577000	H	22.763544000	27.421410000	17.015317000
H	18.007515000	27.477656000	20.830009000	H	21.731586000	27.240251000	15.610033000
H	13.440450000	30.790903000	9.530447000	C	28.767952000	26.484069000	17.109771000
H	17.350453000	26.880900000	9.530447000	O	28.741595000	25.262428000	16.535831000
H	17.350453000	30.790903000	13.440450000	O	29.106360000	27.500115000	16.565490000
H	13.440450000	30.790903000	17.350453000	i. TS3			
H	9.530447000	30.790903000	13.440450000	N	26.970328000	21.843053000	20.419471000
H	9.530447000	26.880900000	17.350453000	N	26.667235000	19.941622000	18.454273000
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H	9.530447000	22.970897000	13.440450000	C	26.972518000	22.826936000	21.345653000
H	13.440450000	22.970897000	17.350453000	C	26.720078000	19.013219000	17.481992000
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H	11.853967000	28.467383000	11.853967000	C	26.340925000	20.305112000	22.141974000
H	9.530447000	26.880900000	9.530447000	C	26.712010000	22.627882000	22.702674000
H	15.026933000	28.467383000	15.026933000	C	26.732342000	17.625874000	17.695415000
H	11.853967000	25.294417000	15.026933000	C	26.729524000	18.160789000	20.055433000
H	26.602859000	23.840851000	20.927908000	C	26.382525000	21.316160000	23.088697000
H	26.486238000	19.401934000	16.482726000	C	26.736115000	17.217021000	19.040457000
H	26.596206000	19.226697000	22.539461000	C	26.809925000	23.730886000	23.728973000
H	26.974956000	17.813460000	21.079809000	C	26.809925000	16.592377000	16.590464000
H	26.692856000	21.060537000	24.192813000	O	26.880885000	24.934153000	23.334955000
H	26.975676000	16.155480000	19.248589000	O	26.880903000	23.334945000	24.934136000
Cu	26.554366000	22.120403000	18.321509000	O	26.880903000	15.387214000	16.986405000
I	23.951480000	23.206995000	18.631943000	O	26.880885000	16.986395000	15.387197000
C	28.087108000	24.338705000	17.414018000	Zr	26.878142000	26.881612000	24.237883000
C	27.619220000	23.138183000	17.067031000	Zr	26.878209000	24.239690000	26.880717000
H	27.847999000	22.861498000	16.029558000	Zr	26.878209000	13.440633000	16.081660000
C	28.018962000	25.057880000	18.723171000	Zr	26.878142000	16.083467000	13.439738000
H	28.756343000	24.709235000	19.458981000	O	24.934203000	26.880849000	23.334882000
H	27.020836000	25.005404000	19.181054000	O	25.848911000	25.848918000	25.848917000
O	28.318909000	26.425733000	18.390838000	O	25.849015000	27.912768000	25.849028000
H	26.108734000	24.456893000	16.349187000	O	27.912782000	25.849032000	25.849031000

O	27.912889000	27.912886000	25.848919000	O	28.827598000	26.880862000	30.426940000
O	26.880945000	28.827581000	23.334856000	O	25.848909000	12.408453000	12.408455000
O	28.827591000	26.880922000	23.334870000	O	23.334862000	11.493756000	13.440411000
O	24.934197000	23.334881000	26.880846000	O	23.334855000	15.387135000	13.440484000
O	25.849012000	25.849025000	27.912771000	O	23.334864000	13.440413000	11.493754000
O	27.912892000	25.848913000	27.912887000	O	23.334856000	13.440488000	15.387138000
O	26.880944000	23.334850000	28.827576000	O	24.934211000	9.894408000	13.440426000
O	28.827591000	23.334868000	26.880917000	O	26.880889000	9.894413000	15.387149000
O	25.849012000	12.408579000	14.472325000	O	27.912786000	12.408573000	12.408574000
O	25.848911000	14.472433000	14.472432000	O	26.880878000	9.894407000	11.493761000
O	24.934197000	13.440504000	16.986469000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	11.493774000	16.986500000	O	30.426944000	11.493755000	13.440484000
O	27.912892000	12.408463000	14.472437000	O	30.426936000	15.387151000	13.440421000
O	27.912782000	14.472319000	14.472318000	O	30.426946000	13.440483000	11.493756000
O	28.827591000	13.440433000	16.986482000	O	30.426933000	13.440426000	15.387152000
O	25.849015000	14.472322000	12.408582000	O	24.934210000	13.440425000	9.894409000
O	24.934203000	16.986468000	13.440501000	O	26.880879000	11.493760000	9.894408000
O	27.912889000	14.472431000	12.408464000	O	26.880889000	15.387147000	9.894411000
O	26.880945000	16.986494000	11.493769000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	27.066116000	30.007949000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	30.008630000	27.063604000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	30.008246000	30.008106000
Zr	26.880671000	29.524609000	26.880680000	C	30.007968000	30.008237000	26.695581000
Zr	29.524440000	26.882357000	26.881381000	C	30.008286000	26.697416000	30.008420000
C	27.064326000	30.008530000	23.753165000	C	23.753697000	10.313401000	13.255234000
C	30.008123000	27.066993000	23.753823000	C	23.753135000	13.257746000	10.312720000
C	23.755714000	23.756676000	26.684338000	C	26.696398000	10.313244000	10.313104000
Zr	26.880615000	26.881402000	29.524137000	C	30.008286000	10.312930000	13.623934000
C	27.065914000	23.754135000	30.008060000	C	30.007968000	13.625768000	10.313113000
C	30.007964000	23.754748000	27.067567000	H	27.351814000	30.759513000	23.002127000
Zr	24.236612000	13.440798000	13.439875000	H	30.758179000	27.358190000	23.003211000
Zr	26.880615000	10.797213000	13.439948000	H	23.008991000	23.009158000	26.377462000
C	23.755714000	13.637012000	16.564674000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	10.313290000	16.567215000	H	30.757581000	23.004153000	27.359935000
Zr	29.524440000	13.439969000	13.438993000	H	23.008991000	13.943888000	17.312192000
C	30.007964000	13.253783000	16.566602000	H	27.355985000	9.562959000	17.317948000
Zr	26.880671000	13.440670000	10.796741000	H	30.757582000	12.961415000	17.317197000
C	23.755332000	16.566137000	13.635261000	H	27.351814000	17.319223000	9.561837000
C	27.064326000	16.568185000	10.312820000	H	30.758179000	17.318139000	12.963160000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	27.356162000	30.758555000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	30.759916000	27.349810000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	30.758917000	30.758911000
O	25.848909000	27.912895000	27.912897000	H	30.758582000	30.758568000	26.405278000
O	23.334862000	26.880939000	28.827594000	H	30.759373000	26.409850000	30.759355000
O	23.334864000	28.827596000	26.880937000	H	23.003255000	9.562795000	12.965188000
O	24.934210000	30.426941000	26.880925000	H	23.001913000	12.971540000	9.561434000
O	26.880889000	30.426939000	24.934203000	H	26.407446000	9.562439000	9.562434000
O	26.880879000	30.426942000	28.827590000	H	30.759373000	9.561995000	13.911500000
O	27.912786000	27.912776000	27.912777000	H	30.758582000	13.916071000	9.562782000
O	28.827596000	30.426944000	26.880863000	H	25.215026000	11.776433000	15.102845000
O	30.426933000	24.934198000	26.880924000	H	28.544134000	11.776251000	11.775822000
O	30.426936000	26.880929000	24.934199000	H	28.555271000	15.099035000	15.098322000
O	30.426944000	26.880866000	28.827595000	H	25.215244000	15.103495000	11.776660000
O	30.426946000	28.827594000	26.880867000	H	25.215244000	28.544690000	25.217855000
O	24.934211000	26.880924000	30.426942000	H	28.555271000	25.223028000	25.222315000
O	26.880889000	24.934201000	30.426937000	H	28.544134000	28.545528000	28.545099000
O	26.880878000	28.827589000	30.426943000	H	25.215026000	25.218505000	28.544917000

ARTICLE

Journal Name

O	14.472677000	25.848673000	14.472677000	O	9.894590000	26.880900000	15.387165000
O	12.408223000	25.848673000	12.408223000	C	10.287052000	26.880900000	16.593848000
O	14.472677000	25.848673000	12.408223000	Zr	13.440450000	26.880900000	15.923976000
O	12.408223000	25.848673000	14.472677000	O	11.493735000	26.880900000	16.986310000
Zr	13.440450000	24.397374000	13.440450000	O	14.472677000	27.913127000	14.472677000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	26.880900000	10.956924000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	26.880900000	9.894590000
O	15.387165000	23.335040000	13.440450000	O	15.387165000	26.880900000	9.894590000
C	16.593848000	23.727502000	13.440450000	O	12.408223000	27.913127000	12.408223000
C	17.650268000	22.671082000	13.440450000	O	15.387165000	26.880900000	16.986310000
C	19.634347000	20.687003000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	11.493735000	30.426760000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	10.287052000	30.034298000	13.440450000
H	19.144577000	23.999268000	13.924306000	O	15.387165000	30.426760000	13.440450000
H	20.830009000	22.313835000	14.037206000	C	16.593848000	30.034298000	13.440450000
O	9.894590000	24.934185000	13.440450000	O	16.986310000	28.827615000	13.440450000
O	16.986310000	24.934185000	13.440450000	O	9.894590000	28.827615000	13.440450000
C	17.333342000	21.360638000	13.119492000	C	22.671082000	26.880900000	22.671082000
C	18.317452000	20.384593000	13.104439000	C	20.687003000	26.880900000	20.687003000
H	16.322082000	21.176773000	12.956594000	C	21.360638000	27.201858000	22.988008000
H	18.007515000	19.491341000	12.843694000	C	20.384593000	27.216911000	22.003898000
C	22.988008000	26.559942000	21.360638000	H	21.176773000	27.364756000	23.999268000
C	22.003898000	26.544889000	20.384593000	H	19.491341000	27.477656000	22.313835000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	28.827615000	16.986310000
H	22.313835000	26.284144000	19.491341000	C	13.440450000	30.034298000	16.593848000
C	22.671082000	17.650268000	13.440450000	O	13.440450000	28.827615000	9.894590000
C	20.687003000	19.634347000	13.440450000	C	13.440450000	30.034298000	10.287052000
O	13.440450000	24.934185000	9.894590000	O	13.440450000	30.426760000	15.387165000
C	13.440450000	23.727502000	10.287052000	O	13.440450000	30.426760000	11.493735000
O	13.440450000	24.934185000	16.986310000	C	17.333342000	27.201858000	18.960712000
C	13.440450000	23.727502000	16.593848000	C	18.317452000	27.216911000	19.936757000
O	13.440450000	23.335040000	15.387165000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	23.335040000	11.493735000	H	18.007515000	27.477656000	20.830009000
C	18.960712000	26.559942000	17.333342000	H	13.440450000	30.790903000	9.530447000
C	19.936757000	26.544889000	18.317452000	H	17.350453000	26.880900000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	17.350453000	30.790903000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	30.790903000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	9.530447000	30.790903000	13.440450000
C	20.384593000	18.317452000	13.104439000	H	9.530447000	26.880900000	17.350453000
H	21.176773000	16.322082000	12.956594000	H	13.440450000	22.970897000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	9.530447000	22.970897000	13.440450000
C	22.988008000	18.960712000	13.761408000	H	13.440450000	22.970897000	17.350453000
C	22.003898000	19.936757000	13.776461000	H	15.026933000	25.294417000	11.853967000
H	23.999268000	19.144577000	13.924306000	H	11.853967000	28.467383000	11.853967000
H	22.313835000	20.830009000	14.037206000	H	9.530447000	26.880900000	9.530447000
Zr	10.956924000	26.880900000	13.440450000	H	15.026933000	28.467383000	15.026933000
O	9.894590000	26.880900000	11.493735000	H	11.853967000	25.294417000	15.026933000
O	12.408223000	27.913127000	14.472677000	H	27.196851000	23.823774000	20.978195000
C	10.287052000	26.880900000	10.287052000	H	26.755225000	19.393869000	16.462693000
Zr	15.923976000	26.880900000	13.440450000	H	26.040540000	19.304835000	22.437926000
O	16.986310000	26.880900000	11.493735000	H	26.784431000	17.834276000	21.089280000
C	16.593848000	26.880900000	10.287052000	H	26.152879000	21.112757000	24.129992000
O	16.986310000	26.880900000	15.387165000	H	26.772503000	16.156580000	19.268328000
O	14.472677000	27.913127000	12.408223000	Cu	26.837893000	22.239079000	18.401343000
C	16.593848000	26.880900000	16.593848000	I	24.817433000	24.130128000	19.072183000
C	17.650268000	26.880900000	17.650268000	C	28.568791000	23.904714000	16.989562000
C	19.634347000	26.880900000	19.634347000	C	27.830176000	22.803679000	16.750191000

Journal Name				ARTICLE			
H	28.379824000	22.061509000	16.159628000	Zr	26.878209000	13.440633000	16.081660000
C	28.242937000	25.159156000	17.749467000	Zr	26.878142000	16.083467000	13.439738000
H	28.123849000	24.993095000	18.826655000	O	24.934203000	26.880849000	23.334882000
H	27.335839000	25.664099000	17.401445000	O	25.848911000	25.848918000	25.848917000
O	29.378605000	26.006157000	17.532921000	O	25.849015000	27.912768000	25.849028000
H	26.553033000	23.008699000	16.124254000	O	27.912782000	25.849032000	25.849031000
C	23.105265000	25.446982000	13.772805000	O	27.912889000	27.912886000	25.848919000
C	24.520529000	25.853044000	14.172945000	O	26.880945000	28.827581000	23.334856000
C	24.949988000	25.285673000	15.533895000	O	28.827591000	26.880922000	23.334870000
C	22.079711000	25.584595000	14.892140000	O	24.934197000	23.334881000	26.880846000
C	24.551053000	23.852707000	15.688518000	O	25.849012000	25.849025000	27.912771000
C	22.296326000	24.652463000	16.100830000	O	27.912892000	25.848913000	27.912887000
N	23.243180000	23.556076000	15.878495000	O	26.880944000	23.334850000	28.827576000
H	22.782353000	26.045620000	12.914835000	O	28.827591000	23.334868000	26.880917000
H	21.086442000	25.400568000	14.472292000	O	25.849012000	12.408579000	14.472325000
C	24.996413000	21.554560000	15.484740000	O	25.848911000	14.472433000	14.472432000
N	25.462203000	22.923995000	15.508347000	O	24.934197000	13.440504000	16.986469000
C	23.994463000	21.287672000	16.596349000	O	26.880944000	11.493774000	16.986500000
C	22.865108000	22.302410000	16.555665000	O	27.912892000	12.408463000	14.472437000
H	22.581197000	22.572695000	17.582164000	O	27.912782000	14.472319000	14.472318000
H	25.873160000	20.906338000	15.576339000	O	28.827591000	13.440433000	16.986482000
H	23.108747000	24.405672000	13.426810000	O	25.849015000	14.472322000	12.408582000
H	22.062535000	26.620524000	15.252107000	O	24.934203000	16.986468000	13.440501000
H	21.967510000	21.914324000	16.064600000	O	27.912889000	14.472431000	12.408464000
H	24.562134000	21.369391000	14.495242000	O	26.880945000	16.986494000	11.493769000
H	24.601749000	26.944946000	14.219543000	O	28.827591000	16.986480000	13.440428000
H	25.224275000	25.520544000	13.402064000	C	23.755332000	26.686089000	23.755213000
H	23.596418000	20.269690000	16.535076000	Zr	24.236612000	26.881475000	26.880552000
H	24.522132000	21.374506000	17.553862000	Zr	26.880671000	29.524609000	26.880680000
H	26.036885000	25.340044000	15.637951000	Zr	29.524440000	26.882357000	26.881381000
H	24.519902000	25.870921000	16.353517000	C	27.064326000	30.008530000	23.753165000
H	22.630576000	25.202773000	16.991515000	C	30.008123000	27.066993000	23.753823000
H	21.350101000	24.178659000	16.374918000	C	23.755714000	23.756676000	26.684338000
C	30.323492000	25.332921000	16.847645000	Zr	26.880615000	26.881402000	29.524137000
O	29.867380000	24.077233000	16.530541000	C	27.065914000	23.754135000	30.008060000
O	31.399964000	25.753531000	16.546675000	C	30.007964000	23.754748000	27.067567000
j. PC/DBU				Zr	24.236612000	13.440798000	13.439875000
N	26.614526000	21.852629000	20.408920000	Zr	26.880615000	10.797213000	13.439948000
N	26.468302000	19.903019000	18.478376000	C	23.755714000	13.637012000	16.564674000
C	26.652148000	20.557815000	20.811656000	C	27.065914000	10.313290000	16.567215000
C	26.622686000	22.838466000	21.324899000	Zr	29.524440000	13.439969000	13.438993000
C	26.505453000	18.996019000	17.491960000	C	30.007964000	13.253783000	16.566602000
C	26.663834000	19.504830000	19.755158000	Zr	26.880671000	13.440670000	10.796741000
C	26.699563000	20.260402000	22.180272000	C	23.755332000	16.566137000	13.635261000
C	26.705586000	22.622100000	22.704834000	C	27.064326000	16.568185000	10.312820000
C	26.720123000	17.622698000	17.695417000	C	30.008123000	16.567527000	13.254357000
C	26.893419000	18.154525000	20.049138000	O	23.334855000	26.880866000	24.934215000
C	26.738970000	21.282578000	23.117500000	O	23.334856000	24.934212000	26.880862000
C	26.911916000	17.220231000	19.023945000	O	25.848909000	27.912895000	27.912897000
C	26.809925000	23.730886000	23.728973000	O	23.334862000	26.880939000	28.827594000
C	26.809925000	16.592377000	16.590464000	O	23.334864000	28.827596000	26.880937000
O	26.880885000	24.934153000	23.334955000	O	24.934210000	30.426941000	26.880925000
O	26.880903000	23.334945000	24.934136000	O	26.880889000	30.426939000	24.934203000
O	26.880903000	15.387214000	16.986405000	O	26.880879000	30.426942000	28.827590000
O	26.880885000	16.986395000	15.387197000	O	27.912786000	27.912776000	27.912777000
Zr	26.878142000	26.881612000	24.237883000	O	28.827596000	30.426944000	26.880863000
Zr	26.878209000	24.239690000	26.880717000	O	30.426933000	24.934198000	26.880924000

ARTICLE

Journal Name

O	30.426936000	26.880929000	24.934199000	H	28.555271000	15.099035000	15.098322000
O	30.426944000	26.880866000	28.827595000	H	25.215244000	15.103495000	11.776660000
O	30.426946000	28.827594000	26.880867000	H	25.215244000	28.544690000	25.217855000
O	24.934211000	26.880924000	30.426942000	H	28.555271000	25.223028000	25.222315000
O	26.880889000	24.934201000	30.426937000	H	28.544134000	28.545528000	28.545099000
O	26.880878000	28.827589000	30.426943000	H	25.215026000	25.218505000	28.544917000
O	28.827598000	26.880862000	30.426940000	O	14.472677000	25.848673000	14.472677000
O	25.848909000	12.408453000	12.408455000	O	12.408223000	25.848673000	12.408223000
O	23.334862000	11.493756000	13.440411000	O	14.472677000	25.848673000	12.408223000
O	23.334855000	15.387135000	13.440484000	O	12.408223000	25.848673000	14.472677000
O	23.334864000	13.440413000	11.493754000	Zr	13.440450000	24.397374000	13.440450000
O	23.334856000	13.440488000	15.387138000	O	11.493735000	23.335040000	13.440450000
O	24.934211000	9.894408000	13.440426000	C	10.287052000	23.727502000	13.440450000
O	26.880889000	9.894413000	15.387149000	O	15.387165000	23.335040000	13.440450000
O	27.912786000	12.408573000	12.408574000	C	16.593848000	23.727502000	13.440450000
O	26.880878000	9.894407000	11.493761000	C	17.650268000	22.671082000	13.440450000
O	28.827598000	9.894410000	13.440488000	C	19.634347000	20.687003000	13.440450000
O	30.426944000	11.493755000	13.440484000	C	18.960712000	22.988008000	13.761408000
O	30.426936000	15.387151000	13.440421000	C	19.936757000	22.003898000	13.776461000
O	30.426946000	13.440483000	11.493756000	H	19.144577000	23.999268000	13.924306000
O	30.426933000	13.440426000	15.387152000	H	20.830009000	22.313835000	14.037206000
O	24.934210000	13.440425000	9.894409000	O	9.894590000	24.934185000	13.440450000
O	26.880879000	11.493760000	9.894408000	O	16.986310000	24.934185000	13.440450000
O	26.880889000	15.387147000	9.894411000	C	17.333342000	21.360638000	13.119492000
O	28.827596000	13.440487000	9.894406000	C	18.317452000	20.384593000	13.104439000
C	23.753697000	27.066116000	30.007949000	H	16.322082000	21.176773000	12.956594000
C	23.753135000	30.008630000	27.063604000	H	18.007515000	19.491341000	12.843694000
C	26.696398000	30.008246000	30.008106000	C	22.988008000	26.559942000	21.360638000
C	30.007968000	30.008237000	26.695581000	C	22.003898000	26.544889000	20.384593000
C	30.008286000	26.697416000	30.008420000	H	23.999268000	26.397044000	21.176773000
C	23.753697000	10.313401000	13.255234000	H	22.313835000	26.284144000	19.491341000
C	23.753135000	13.257746000	10.312720000	C	22.671082000	17.650268000	13.440450000
C	26.696398000	10.313244000	10.313104000	C	20.687003000	19.634347000	13.440450000
C	30.008286000	10.312930000	13.623934000	O	13.440450000	24.934185000	9.894590000
C	30.007968000	13.625768000	10.313113000	C	13.440450000	23.727502000	10.287052000
H	27.351814000	30.759513000	23.002127000	O	13.440450000	24.934185000	16.986310000
H	30.758179000	27.358190000	23.003211000	C	13.440450000	23.727502000	16.593848000
H	23.008991000	23.009158000	26.377462000	O	13.440450000	23.335040000	15.387165000
H	27.355985000	23.003402000	30.758391000	O	13.440450000	23.335040000	11.493735000
H	30.757581000	23.004153000	27.359935000	C	18.960712000	26.559942000	17.333342000
H	23.008991000	13.943888000	17.312192000	C	19.936757000	26.544889000	18.317452000
H	27.355985000	9.562959000	17.317948000	H	19.144577000	26.397044000	16.322082000
H	30.757582000	12.961415000	17.317197000	H	20.830009000	26.284144000	18.007515000
H	27.351814000	17.319223000	9.561837000	C	21.360638000	17.333342000	13.119492000
H	30.758179000	17.318139000	12.963160000	C	20.384593000	18.317452000	13.104439000
H	23.003255000	27.356162000	30.758555000	H	21.176773000	16.322082000	12.956594000
H	23.001913000	30.759916000	27.349810000	H	19.491341000	18.007515000	12.843694000
H	26.407446000	30.758917000	30.758911000	C	22.988008000	18.960712000	13.761408000
H	30.758582000	30.758568000	26.405278000	C	22.003898000	19.936757000	13.776461000
H	30.759373000	26.409850000	30.759355000	H	23.999268000	19.144577000	13.924306000
H	23.003255000	9.562795000	12.965188000	H	22.313835000	20.830009000	14.037206000
H	23.001913000	12.971540000	9.561434000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	9.562439000	9.562434000	O	9.894590000	26.880900000	11.493735000
H	30.759373000	9.561995000	13.911500000	O	12.408223000	27.913127000	14.472677000
H	30.758582000	13.916071000	9.562782000	C	10.287052000	26.880900000	10.287052000
H	25.215026000	11.776433000	15.102845000	Zr	15.923976000	26.880900000	13.440450000
H	28.544134000	11.776251000	11.775822000	O	16.986310000	26.880900000	11.493735000

Journal Name				ARTICLE			
C	16.593848000	26.880900000	10.287052000	H	26.800133000	21.059499000	24.177555000
O	16.986310000	26.880900000	15.387165000	H	27.095927000	16.171706000	19.233862000
O	14.472677000	27.913127000	12.408223000	Cu	26.708097000	22.183752000	18.354436000
C	16.593848000	26.880900000	16.593848000	I	24.611516000	23.426157000	17.541170000
C	17.650268000	26.880900000	17.650268000	C	28.854494000	22.112366000	18.272510000
C	19.634347000	26.880900000	19.634347000	C	28.285666000	22.341464000	17.046311000
O	9.894590000	26.880900000	15.387165000	H	28.183760000	21.530941000	16.331816000
C	10.287052000	26.880900000	16.593848000	C	29.447085000	23.059961000	19.270988000
Zr	13.440450000	26.880900000	15.923976000	H	28.761886000	23.833900000	19.619926000
O	11.493735000	26.880900000	16.986310000	H	30.351444000	23.558083000	18.901157000
O	14.472677000	27.913127000	14.472677000	O	29.804003000	22.189163000	20.360877000
Zr	13.440450000	26.880900000	10.956924000	H	28.223013000	23.362721000	16.690948000
O	11.493735000	26.880900000	9.894590000	C	26.619197000	28.647691000	19.601653000
O	15.387165000	26.880900000	9.894590000	C	26.948408000	27.425197000	20.451127000
O	12.408223000	27.913127000	12.408223000	C	26.983411000	26.083002000	19.694535000
O	15.387165000	26.880900000	16.986310000	C	25.293868000	28.582483000	18.852193000
Zr	13.440450000	29.364426000	13.440450000	C	27.310654000	26.176499000	18.228750000
O	11.493735000	30.426760000	13.440450000	C	25.125238000	27.290127000	18.046413000
C	10.287052000	30.034298000	13.440450000	N	26.366206000	26.805897000	17.454744000
O	15.387165000	30.426760000	13.440450000	H	26.632279000	29.538088000	20.241526000
C	16.593848000	30.034298000	13.440450000	H	25.222990000	29.451602000	18.186187000
O	16.986310000	28.827615000	13.440450000	C	28.729413000	25.852832000	16.404122000
O	9.894590000	28.827615000	13.440450000	N	28.445407000	25.693182000	17.821370000
C	22.671082000	26.880900000	22.671082000	C	27.478606000	25.778280000	15.542421000
C	20.687003000	26.880900000	20.687003000	C	26.490598000	26.828791000	16.003820000
C	21.360638000	27.201858000	22.988008000	H	25.499998000	26.633148000	15.574914000
C	20.384593000	27.216911000	22.003898000	H	29.454036000	25.082530000	16.103988000
H	21.176773000	27.364756000	23.999268000	H	27.424846000	28.791790000	18.869396000
H	19.491341000	27.477656000	22.313835000	H	24.453298000	28.663769000	19.553587000
O	13.440450000	28.827615000	16.986310000	H	26.797597000	27.832012000	15.664740000
C	13.440450000	30.034298000	16.593848000	H	29.239418000	26.815791000	16.235752000
O	13.440450000	28.827615000	9.894590000	H	26.232512000	27.348368000	21.275827000
C	13.440450000	30.034298000	10.287052000	H	27.924027000	27.591166000	20.917486000
O	13.440450000	30.426760000	15.387165000	H	27.704843000	25.914989000	14.480155000
O	13.440450000	30.426760000	11.493735000	H	27.010441000	24.791467000	15.659295000
C	17.333342000	27.201858000	18.960712000	H	27.749328000	25.447710000	20.147011000
C	18.317452000	27.216911000	19.936757000	H	26.026483000	25.554614000	19.800301000
H	16.322082000	27.364756000	19.144577000	H	24.692338000	26.496302000	18.665832000
H	18.007515000	27.477656000	20.830009000	H	24.411171000	27.436862000	17.230773000
H	13.440450000	30.790903000	9.530447000	C	29.720113000	20.906447000	19.964790000
H	17.350453000	26.880900000	9.530447000	O	29.260845000	20.840181000	18.672104000
H	17.350453000	30.790903000	13.440450000	O	29.986719000	19.946488000	20.627284000
H	13.440450000	30.790903000	17.350453000	k. PC			
H	9.530447000	30.790903000	13.440450000	N	26.613142000	21.857671000	20.407249000
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H	9.530447000	26.880900000	9.530447000	C	26.688282000	22.628205000	22.701489000
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H	26.568024000	23.848657000	20.927715000	C	26.704731000	21.289719000	23.116611000
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H	26.715692000	19.229978000	22.517614000	C	26.809924000	23.730866000	23.728960000
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ARTICLE

Journal Name

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O	26.880901000	15.387210000	16.986393000	O	26.880879000	30.426942000	28.827590000
O	26.880886000	16.986407000	15.387201000	O	27.912786000	27.912776000	27.912777000
Zr	26.878143000	26.881612000	24.237883000	O	28.827596000	30.426944000	26.880863000
Zr	26.878211000	24.239690000	26.880717000	O	30.426933000	24.934198000	26.880924000
Zr	26.878210000	13.440633000	16.081660000	O	30.426936000	26.880929000	24.934199000
Zr	26.878143000	16.083467000	13.439738000	O	30.426944000	26.880866000	28.827595000
O	24.934203000	26.880849000	23.334882000	O	30.426946000	28.827594000	26.880867000
O	25.848911000	25.848918000	25.848917000	O	24.934211000	26.880924000	30.426942000
O	25.849015000	27.912768000	25.849028000	O	26.880889000	24.934201000	30.426937000
O	27.912782000	25.849032000	25.849031000	O	26.880878000	28.827589000	30.426943000
O	27.912889000	27.912886000	25.848919000	O	28.827598000	26.880862000	30.426940000
O	26.880945000	28.827581000	23.334856000	O	25.848909000	12.408453000	12.408455000
O	28.827591000	26.880922000	23.334870000	O	23.334862000	11.493756000	13.440411000
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O	28.827591000	23.334868000	26.880917000	O	26.880889000	9.894413000	15.387149000
O	25.849012000	12.408579000	14.472325000	O	27.912786000	12.408573000	12.408574000
O	25.848911000	14.472433000	14.472432000	O	26.880878000	9.894407000	11.493761000
O	24.934197000	13.440504000	16.986469000	O	28.827598000	9.894410000	13.440488000
O	26.880944000	11.493774000	16.986500000	O	30.426944000	11.493755000	13.440484000
O	27.912892000	12.408463000	14.472437000	O	30.426936000	15.387151000	13.440421000
O	27.912782000	14.472319000	14.472318000	O	30.426946000	13.440483000	11.493756000
O	28.827591000	13.440433000	16.986482000	O	30.426933000	13.440426000	15.387152000
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O	24.934203000	16.986468000	13.440501000	O	26.880879000	11.493760000	9.894408000
O	27.912889000	14.472431000	12.408464000	O	26.880889000	15.387147000	9.894411000
O	26.880945000	16.986494000	11.493769000	O	28.827596000	13.440487000	9.894406000
O	28.827591000	16.986480000	13.440428000	C	23.753697000	27.066116000	30.007949000
C	23.755332000	26.686089000	23.755213000	C	23.753135000	30.008630000	27.063604000
Zr	24.236612000	26.881475000	26.880552000	C	26.696398000	30.008246000	30.008106000
Zr	26.880671000	29.524609000	26.880680000	C	30.007968000	30.008237000	26.695581000
Zr	29.524440000	26.882357000	26.881381000	C	30.008286000	26.697416000	30.008420000
C	27.064326000	30.008530000	23.753165000	C	23.753697000	10.313401000	13.255234000
C	30.008123000	27.066993000	23.753823000	C	23.753135000	13.257746000	10.312720000
C	23.755714000	23.756676000	26.684338000	C	26.696398000	10.313244000	10.313104000
Zr	26.880615000	26.881402000	29.524137000	C	30.008286000	10.312930000	13.623934000
C	27.065914000	23.754135000	30.008060000	C	30.007968000	13.625768000	10.313113000
C	30.007964000	23.754748000	27.067567000	H	27.351814000	30.759513000	23.002127000
Zr	24.236612000	13.440798000	13.439875000	H	30.758179000	27.358190000	23.003211000
Zr	26.880615000	10.797213000	13.439948000	H	23.008991000	23.009158000	26.377462000
C	23.755714000	13.637012000	16.564674000	H	27.355985000	23.003402000	30.758391000
C	27.065914000	10.313290000	16.567215000	H	30.757581000	23.004153000	27.359935000
Zr	29.524440000	13.439969000	13.438993000	H	23.008991000	13.943888000	17.312192000
C	30.007964000	13.253783000	16.566602000	H	27.355985000	9.562959000	17.317948000
Zr	26.880671000	13.440670000	10.796741000	H	30.757582000	12.961415000	17.317197000
C	23.755332000	16.566137000	13.635261000	H	27.351814000	17.319223000	9.561837000
C	27.064326000	16.568185000	10.312820000	H	30.758179000	17.318139000	12.963160000
C	30.008123000	16.567527000	13.254357000	H	23.003255000	27.356162000	30.758555000
O	23.334855000	26.880866000	24.934215000	H	23.001913000	30.759916000	27.349810000
O	23.334856000	24.934212000	26.880862000	H	26.407446000	30.758917000	30.758911000
O	25.848909000	27.912895000	27.912897000	H	30.758582000	30.758568000	26.405278000
O	23.334862000	26.880939000	28.827594000	H	30.759373000	26.409850000	30.759355000
O	23.334864000	28.827596000	26.880937000	H	23.003255000	9.562795000	12.965188000

Journal Name				ARTICLE			
H	23.001913000	12.971540000	9.561434000	Zr	10.956924000	26.880900000	13.440450000
H	26.407446000	9.562439000	9.562434000	O	9.894590000	26.880900000	11.493735000
H	30.759373000	9.561995000	13.911500000	O	12.408223000	27.913127000	14.472677000
H	30.758582000	13.916071000	9.562782000	C	10.287052000	26.880900000	10.287052000
H	25.215026000	11.776433000	15.102845000	Zr	15.923976000	26.880900000	13.440450000
H	28.544134000	11.776251000	11.775822000	O	16.986310000	26.880900000	11.493735000
H	28.555271000	15.099035000	15.098322000	C	16.593848000	26.880900000	10.287052000
H	25.215244000	15.103495000	11.776660000	O	16.986310000	26.880900000	15.387165000
H	25.215244000	28.544690000	25.217855000	O	14.472677000	27.913127000	12.408223000
H	28.555271000	25.223028000	25.222315000	C	16.593848000	26.880900000	16.593848000
H	28.544134000	28.545528000	28.545099000	C	17.650268000	26.880900000	17.650268000
H	25.215026000	25.218505000	28.544917000	C	19.634347000	26.880900000	19.634347000
O	14.472677000	25.848673000	14.472677000	O	9.894590000	26.880900000	15.387165000
O	12.408223000	25.848673000	12.408223000	C	10.287052000	26.880900000	16.593848000
O	14.472677000	25.848673000	12.408223000	Zr	13.440450000	26.880900000	15.923976000
O	12.408223000	25.848673000	14.472677000	O	11.493735000	26.880900000	16.986310000
Zr	13.440450000	24.397374000	13.440450000	O	14.472677000	27.913127000	14.472677000
O	11.493735000	23.335040000	13.440450000	Zr	13.440450000	26.880900000	10.956924000
C	10.287052000	23.727502000	13.440450000	O	11.493735000	26.880900000	9.894590000
O	15.387165000	23.335040000	13.440450000	O	15.387165000	26.880900000	9.894590000
C	16.593848000	23.727502000	13.440450000	O	12.408223000	27.913127000	12.408223000
C	17.650268000	22.671082000	13.440450000	O	15.387165000	26.880900000	16.986310000
C	19.634347000	20.687003000	13.440450000	Zr	13.440450000	29.364426000	13.440450000
C	18.960712000	22.988008000	13.761408000	O	11.493735000	30.426760000	13.440450000
C	19.936757000	22.003898000	13.776461000	C	10.287052000	30.034298000	13.440450000
H	19.144577000	23.999268000	13.924306000	O	15.387165000	30.426760000	13.440450000
H	20.830009000	22.313835000	14.037206000	C	16.593848000	30.034298000	13.440450000
O	9.894590000	24.934185000	13.440450000	O	16.986310000	28.827615000	13.440450000
O	16.986310000	24.934185000	13.440450000	O	9.894590000	28.827615000	13.440450000
C	17.333342000	21.360638000	13.119492000	C	22.671082000	26.880900000	22.671082000
C	18.317452000	20.384593000	13.104439000	C	20.687003000	26.880900000	20.687003000
H	16.322082000	21.176773000	12.956594000	C	21.360638000	27.201858000	22.988008000
H	18.007515000	19.491341000	12.843694000	C	20.384593000	27.216911000	22.003898000
C	22.988008000	26.559942000	21.360638000	H	21.176773000	27.364756000	23.999268000
C	22.003898000	26.544889000	20.384593000	H	19.491341000	27.477656000	22.313835000
H	23.999268000	26.397044000	21.176773000	O	13.440450000	28.827615000	16.986310000
H	22.313835000	26.284144000	19.491341000	C	13.440450000	30.034298000	16.593848000
C	22.671082000	17.650268000	13.440450000	O	13.440450000	28.827615000	9.894590000
C	20.687003000	19.634347000	13.440450000	C	13.440450000	30.034298000	10.287052000
O	13.440450000	24.934185000	9.894590000	O	13.440450000	30.426760000	15.387165000
C	13.440450000	23.727502000	10.287052000	O	13.440450000	30.426760000	11.493735000
O	13.440450000	24.934185000	16.986310000	C	17.333342000	27.201858000	18.960712000
C	13.440450000	23.727502000	16.593848000	C	18.317452000	27.216911000	19.936757000
O	13.440450000	23.335040000	15.387165000	H	16.322082000	27.364756000	19.144577000
O	13.440450000	23.335040000	11.493735000	H	18.007515000	27.477656000	20.830009000
C	18.960712000	26.559942000	17.333342000	H	13.440450000	30.790903000	9.530447000
C	19.936757000	26.544889000	18.317452000	H	17.350453000	26.880900000	9.530447000
H	19.144577000	26.397044000	16.322082000	H	17.350453000	30.790903000	13.440450000
H	20.830009000	26.284144000	18.007515000	H	13.440450000	30.790903000	17.350453000
C	21.360638000	17.333342000	13.119492000	H	9.530447000	30.790903000	13.440450000
C	20.384593000	18.317452000	13.104439000	H	9.530447000	26.880900000	17.350453000
H	21.176773000	16.322082000	12.956594000	H	13.440450000	22.970897000	9.530447000
H	19.491341000	18.007515000	12.843694000	H	9.530447000	22.970897000	13.440450000
C	22.988008000	18.960712000	13.761408000	H	13.440450000	22.970897000	17.350453000
C	22.003898000	19.936757000	13.776461000	H	15.026933000	25.294417000	11.853967000
H	23.999268000	19.144577000	13.924306000	H	11.853967000	28.467383000	11.853967000
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ARTICLE

Journal Name

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H	26.362486000	19.372789000	16.474842000
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H	27.112026000	17.855084000	21.062260000
H	26.752752000	21.071228000	24.178282000
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Cu	26.230616000	21.902625000	18.217618000
I	25.244169000	24.052080000	17.444700000
C	29.012851000	22.461054000	18.330723000
C	28.652592000	22.089051000	17.101846000
H	28.765768000	21.063705000	16.771859000
C	28.960484000	23.801280000	18.992142000
H	27.943112000	24.220275000	19.000033000
H	29.642325000	24.535772000	18.553166000
O	29.383858000	23.525130000	20.334363000
H	28.296312000	22.831940000	16.399444000
C	29.633563000	22.210224000	20.476317000
O	29.476122000	21.565657000	19.272504000
O	29.942436000	21.660948000	21.491635000