

Electronic supplementary information

Molecular design of chiral zirconium metal-organic frameworks for asymmetric transfer hydrogenation of imines

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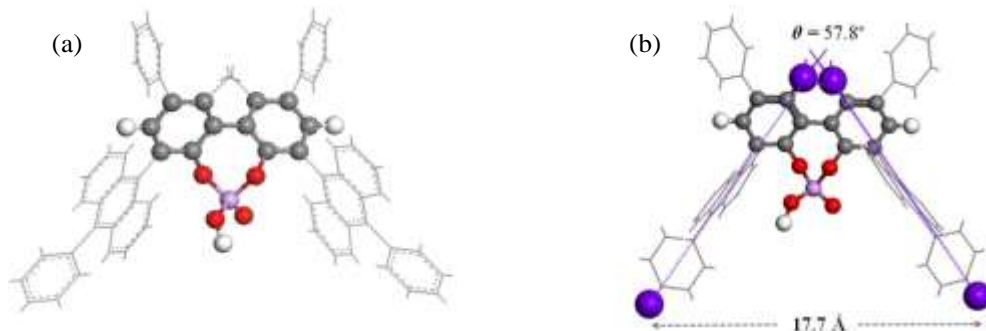


Fig. S1. (a) A chiral phosphoric acid L1A2 (b) Distance and angle between two chiral axes on L1A2. L1 and A2 are represented by the ball-stick and line, respectively.

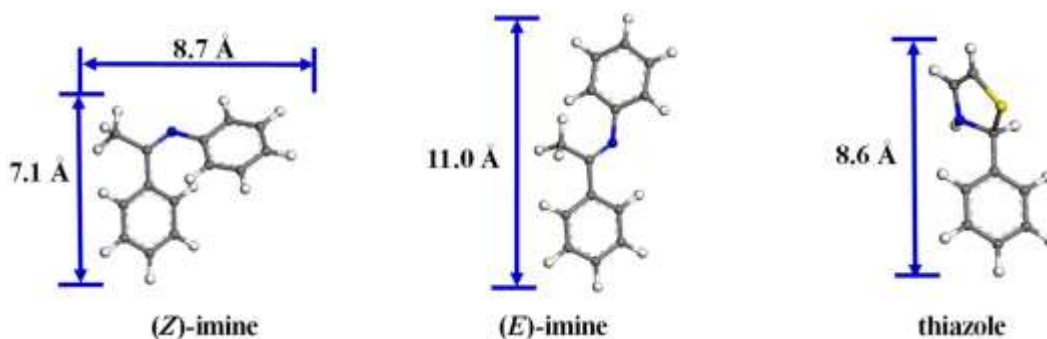


Fig. S2. (Z)- and (E)-imines and thiazole.

Table S1. Electronic energies (E^{ele}) and thermal corrections at 25 °C (G^{therm}) of isolated catalysts in different solvents. The unit is in Hartree.

Isolated catalyst	Dichloromethane		Toluene		Acetonitrile	
	G^{therm}	E^{ele}	G^{therm}	E^{ele}	G^{therm}	E^{ele}
L1A2	0.87922	-1183.65043				
MOF-fcu	3.89931	-1074.49786	3.89931	-1074.49344	3.89931	-1074.49912
MOF-bct	5.80403	-1064.16181	5.80403	-1064.15742	5.80403	-1064.16307

Table S2. Electronic energies (E^{ele}) and thermal corrections at 25 °C (G^{therm}) of intermediates, transition states and products for the ATH on L1A2 in dichloromethane. The unit is in Hartree.

Intermediate/ transition state/product	G^{therm}	E^{ele}
co-ad	1.25003	-2581.38552
(Z)-syn-TS-R	1.25262	-2581.35725
product	1.24967	-2581.41892
co-ad	1.24781	-2581.37635
(Z)-anti-TS-R	1.25161	-2581.34374
product	1.24643	-2581.40837
co-ad	1.25169	-2581.37762
(E)-syn-TS-S	1.24751	-2581.34251
product	1.24569	-2581.40912
co-ad	1.24692	-2581.37982
(E)-anti-TS-S	1.25078	-2581.34286
product	1.25042	-2581.41592

Table S3. Electronic energies (E^{ele}) and thermal corrections at 25 °C (G^{therm}) of intermediates, transition states and products for the ATH on MOFs in different solvents. The unit is in Hartree.

Dichloromethane	Intermediate/ transition state/product	G^{therm}	E^{ele}
MOF-fcu	co-ad	4.27330	-2472.00796
	(Z)-syn-TS-R	4.27249	-2471.98332
	product	4.27769	-2472.03909
	co-ad	4.27003	-2472.00059
	(E)-syn-TS-S product	4.27112 4.27290	-2471.97981 -2472.03277
MOF-bct	co-ad	6.17419	-2461.66024
	(Z)-syn-TS-R	6.17507	-2461.63085
	product	6.16991	-2461.68925
	co-ad	6.17461	-2461.66034
	(E)-syn-TS-S product	6.17345 6.16990	-2461.62520 -2461.68159
Toluene	Intermediate/ transition state/product	G^{therm}	E^{ele}
MOF-fcu	co-ad	4.27330	-2471.99907
	(Z)-syn-TS-R	4.27249	-2471.97592
	product	4.27769	-2472.03288
	co-ad	4.27003	-2472.00059
	(E)-syn-TS-S product	4.27112 4.27290	-2471.97188 -2472.02670
MOF-bct	co-ad	6.17419	-2461.65153
	(Z)-syn-TS-R	6.17507	-2461.62331
	product	6.16991	-2461.68334
	co-ad	6.17461	-2461.65098
	(E)-syn-TS-S product	6.17345 6.16990	-2461.61684 -2461.67577
Acetonitrile	Intermediate/ transition state/product	G^{therm}	E^{ele}
MOF-fcu	co-ad	4.27330	-2472.01057
	(Z)-syn-TS-R	4.27249	-2471.98549
	product	4.27769	-2472.04090
	co-ad	4.27003	-2472.01393
	(E)-syn-TS-S product	4.27112 4.27290	-2471.98218 -2472.03454
MOF-bct	co-ad	6.17419	-2461.66280
	(Z)-syn-TS-R	6.17507	-2461.63307
	product	6.16991	-2461.69097
	co-ad	6.17461	-2461.66313
	(E)-syn-TS-S product	6.17345 6.16990	-2461.62771 -2461.68332

Table S4. Selected bond distances (Å) of optimized transition states on L1A2.

Bond ^a	(Z)-anti-TS-R	(Z)-syn-TS-R	(E)-anti-TS-S	(E)-syn-TS-S
O1-H1	1.73	1.69	1.81	1.77
O2-H2	1.62	1.61	1.60	1.63
C1-H3	1.44	1.50	1.47	1.48
C2-H3	1.35	1.30	1.32	1.31

^aO1 and O2: O atoms of L1A2; C1: C atom of imine; H2, H3 and C2: H and C atoms of thiazole.

Table S5. Selected bond distances (Å) of optimized transition states on MOF-fcu and MOF-bct.

Bond ^a	MOF-fcu		MOF-bct	
	(Z)-syn-TS-R	(E)-syn-TS-S	(Z)-syn-TS-R	(E)-syn-TS-S
O1-H1	1.70	1.83	1.75	1.76
O2-H2	1.59	1.58	1.64	1.63
C1-H3	1.49	1.42	1.50	1.42
C2-H3	1.31	1.34	1.31	1.36

^aO1 and O2: O atoms of chiral phosphoric acid on MOFs;
C1: C atom of imine; H2, H3 and C2: H and C atoms of thiazole.

Table S6. H-bond distances in optimized transition states.

Bond ^a	L1A2		MOF-fcu		MOF-bct	
	O1-H1	O2-H2	O1-H1	O2-H2	O1-H1	O2-H2
(Z)-anti-TS-R	1.73	1.62				
(Z)-syn-TS-R	1.69	1.61	1.70	1.59	1.75	1.64
(E)-anti-TS-S	1.81	1.60				
(E)-syn-TS-S	1.77	1.63	1.83	1.58	1.76	1.63

^aO1 and O2: O atoms of chiral phosphoric acid on MOFs;
C1: C atom of imine; H2, H3 and C2: H and C atoms of thiazole.

Table S7. Close distances (C–H··· O < 3.5 Å) between transition states and frameworks.

MOF-fcu		MOF-bct	
(Z)-syn-TS-R	(E)-syn-TS-S	(Z)-syn-TS-R	(E)-syn-TS-S
2.67	2.83	2.65	2.61
2.68	2.84	2.66	2.75
2.71	2.87	2.76	2.88
2.73	3.04	2.77	2.91
2.78	3.06	2.99	2.93
2.79	3.09	3.30	3.11
2.80	3.21	3.36	3.12
2.88	3.34	3.43	3.43
3.03	3.35	3.45	3.45
3.05	3.50	3.47	
3.15			
3.16			
3.21			
3.24			

Coordinates: Optimized transition states on L1A2 and MOFs.

On L1A2:			H 4.32660000	-4.17640000	-2.84920000
(Z)-syn-TS-R			H 4.95930000	-4.62760000	-1.26620000
C -7.41730000	-2.12750000	1.70300000	H 0.09990000	8.30510000	-0.85810000
C -8.31140000	-3.14170000	1.34720000	H 4.31790000	9.09320000	-1.06720000
C -7.84760000	-4.28400000	0.68690000	H 4.79310000	6.70020000	-0.66220000
C -6.48900000	-4.41350000	0.38100000	H 0.56020000	5.91510000	-0.44800000
C -5.58920000	-3.39650000	0.73430000	H 5.87950000	-0.24640000	3.92070000
C -6.05970000	-2.25420000	1.39740000	H 7.39950000	-2.81970000	0.80760000
C -0.87650000	-4.36230000	2.21530000	H 9.39880000	-3.28230000	2.18000000
C -1.35850000	-4.57390000	3.44770000	H 9.65320000	-2.22880000	4.40950000
C -2.72080000	-4.45010000	3.75010000	H 7.89540000	-0.70780000	5.27090000
C -3.63120000	-4.11370000	2.82610000	H 4.52400000	0.62440000	-2.15310000
C -4.60290000	-2.95570000	-2.01680000	H 3.45360000	5.43080000	-2.97440000
C -4.11720000	-2.69450000	-3.23830000	H 2.16720000	5.99300000	2.05860000
C -2.74670000	-2.74220000	-3.52420000	H 1.75570000	4.93760000	4.15310000
C -1.83320000	-3.06510000	-2.59860000	H 2.08870000	2.54340000	4.49860000
C 1.12250000	7.95330000	-0.81480000	H 2.87270000	1.10270000	2.77180000
C 2.17940000	8.85120000	-0.98970000	H 0.96130000	-5.65160000	-4.13460000
C 3.50040000	8.39680000	-0.93260000	H 1.65740000	-7.54140000	-5.56440000
C 3.76660000	7.04330000	-0.70300000	H 3.46050000	-9.07130000	-4.82020000
C 2.70890000	6.13670000	-0.53150000	H 4.56290000	-8.71640000	-2.62840000
C 1.38520000	6.60020000	-0.58400000	H 3.86940000	-6.84360000	-1.17710000
C 4.27010000	1.67070000	-2.26280000	H -0.67370000	-4.85510000	4.23800000
C 4.44510000	2.24890000	-3.45900000	H -3.04760000	-4.63540000	4.76560000
C 4.14800000	3.59880000	-3.68840000	H 4.82780000	1.65390000	-4.27870000
C 3.67660000	4.40200000	-2.72460000	H 4.30140000	4.00390000	-4.68070000
C 2.33330000	4.92710000	2.14270000	H 4.89900000	-3.73860000	2.51890000
C 2.10470000	4.33570000	3.32340000	H 3.67050000	-4.26180000	1.36570000
C 2.30090000	2.96290000	3.52320000	H 5.36780000	-4.23500000	0.89300000
C 2.74710000	2.15500000	2.55170000	C 3.39110000	-6.97710000	-2.13950000
C -2.24400000	-3.39310000	-1.21040000	C 3.78100000	-8.04330000	-2.95550000
C -3.69240000	-3.30940000	-0.89950000	C 3.15820000	-8.24480000	-4.19030000
C -4.15140000	-3.52530000	0.41400000	C 2.14140000	-7.38240000	-4.60950000
C -3.22450000	-3.84830000	1.42380000	C 1.74860000	-6.31470000	-3.79670000
C -1.78040000	-3.97020000	1.10520000	C 4.29180000	-3.92670000	-1.78260000
C 3.74210000	2.44960000	-1.11550000	C 4.60030000	-3.69930000	1.46520000
C 3.45270000	3.88640000	-1.35100000	C 7.49000000	-2.36610000	1.78670000
C 2.98740000	4.70130000	-0.29980000	C 8.62720000	-2.62420000	2.55810000
C 2.79170000	4.13400000	0.97460000	C 8.77170000	-2.02880000	3.81420000
C 3.04500000	2.68940000	1.19970000	C 7.78080000	-1.17100000	4.29950000
H -7.77530000	-1.24420000	2.21600000	C 6.64180000	-0.91040000	3.53160000
H -8.54060000	-5.06870000	0.41280000	C 4.99230000	0.10350000	1.13520000
H -6.13790000	-5.30150000	-0.13010000	C 5.27920000	-1.22760000	1.45360000
H -5.37300000	-1.46850000	1.67740000	C 4.42200000	-2.25930000	1.00690000
H 0.18510000	-4.48920000	2.04830000	C 3.31620000	-1.92410000	0.18750000
H -4.66850000	-4.04300000	3.12580000	C 3.02730000	-0.56770000	-0.05410000
H -5.67120000	-2.88430000	-1.86070000	C 2.40550000	-2.96140000	-0.39060000
H -4.80520000	-2.42800000	-4.03090000	C 2.86360000	-3.98050000	-1.26060000
H -2.41620000	-2.50700000	-4.52820000	C 1.95180000	-4.97180000	-1.69170000
H -0.78960000	-3.06880000	-2.88450000	C 0.60820000	-4.89940000	-1.30870000
H 4.71610000	-2.92840000	-1.66330000	C 1.03530000	-2.89150000	-0.08230000

H	5.65600000	0.89500000	1.48100000
H	-0.08970000	-5.66580000	-1.64320000
P	0.43350000	-0.36210000	-0.00550000
O	1.88690000	-0.25270000	-0.78220000
O	0.58850000	-1.83990000	0.70650000
O	0.34440000	0.62430000	1.13360000
O	-0.62080000	-0.36740000	-1.08230000
C	-3.51540000	1.68910000	-0.86620000
N	-2.26490000	1.79310000	-1.39080000
C	-1.58390000	2.87680000	-1.98180000
C	-0.39280000	2.55740000	-2.66340000
C	-1.99970000	4.21660000	-1.91260000
C	0.33800000	3.55500000	-3.29670000
H	-0.05700000	1.52510000	-2.68480000
C	-1.25360000	5.20520000	-2.55760000
H	-2.89630000	4.48940000	-1.37180000
C	-0.08850000	4.88570000	-3.25410000
H	1.24130000	3.28460000	-3.83440000
H	-1.58790000	6.23790000	-2.50140000
H	0.48630000	5.66330000	-3.74890000
C	-1.00410000	3.84350000	1.22620000
C	-1.89060000	4.81590000	1.53130000
C	-2.81770000	2.44490000	1.69370000
N	-1.45480000	2.56440000	1.41420000
H	-0.80740000	1.74750000	1.26960000
H	-0.00120000	3.97230000	0.84890000
H	-1.75450000	5.88450000	1.45700000
H	-3.36250000	2.17990000	0.54590000
S	-3.39210000	4.12430000	2.13470000
C	-3.27330000	1.32200000	2.59300000
C	-4.59380000	1.29490000	3.06760000
C	-2.40020000	0.28410000	2.95060000
C	-5.03160000	0.26150000	3.89340000
H	-5.28350000	2.09560000	2.81010000
C	-2.84860000	-0.75410000	3.76870000
H	-1.37260000	0.27400000	2.60070000
C	-4.15900000	-0.77130000	4.24470000
H	-6.05490000	0.26190000	4.25830000
H	-2.15670000	-1.54710000	4.03610000
H	-4.50030000	-1.58230000	4.88210000
H	-1.66600000	0.94230000	-1.28830000
C	-4.64670000	2.53230000	-1.38040000
C	-5.70110000	2.90470000	-0.53450000
C	-4.73830000	2.84130000	-2.74800000
C	-6.80860000	3.59020000	-1.03380000
H	-5.65870000	2.65290000	0.52020000
C	-5.84910000	3.51840000	-3.24670000
H	-3.94260000	2.54000000	-3.42120000
C	-6.88490000	3.90180000	-2.39140000
H	-7.61160000	3.87690000	-0.36060000
H	-5.90690000	3.74280000	-4.30830000
H	-7.74790000	4.43340000	-2.78250000
C	-3.91640000	0.25350000	-0.55530000
H	-3.09060000	-0.31520000	-0.12240000

H	-4.77310000	0.23390000	0.11930000
H	-4.21380000	-0.23060000	-1.49270000
H	-9.36290000	-3.04300000	1.58360000
H	1.97490000	9.89890000	-1.16850000
C	6.48390000	-1.51380000	2.27240000
C	3.53290000	1.88040000	0.15540000
C	-1.31840000	-3.73730000	-0.20550000
C	2.37800000	-6.09850000	-2.55910000
C	0.12660000	-3.84990000	-0.52560000
C	3.85690000	0.45400000	0.40410000

(Z)-anti-TS-R

C	-7.74160000	1.32000000	-2.23350000
C	-8.76650000	1.98390000	-1.55370000
C	-8.45660000	2.93470000	-0.57690000
C	-7.12140000	3.21810000	-0.27340000
C	-6.08690000	2.54590000	-0.94440000
C	-6.40580000	1.60240000	-1.93450000
C	-1.65100000	4.49640000	-2.20050000
C	-2.18240000	4.88680000	-3.42650000
C	-3.51350000	4.63270000	-3.74320000
C	-4.35080000	3.97380000	-2.84660000
C	-4.96600000	1.68490000	1.63750000
C	-4.44470000	1.34770000	2.88380000
C	-3.13180000	1.66200000	3.22090000
C	-2.30220000	2.32750000	2.32310000
C	3.67000000	-7.20690000	2.52050000
C	4.49680000	-8.06100000	1.78560000
C	5.21920000	-7.56790000	0.69540000
C	5.11170000	-6.22120000	0.33490000
C	4.27450000	-5.35930000	1.06260000
C	3.56060000	-5.86000000	2.16330000
C	5.07460000	-0.51130000	2.03510000
C	5.67180000	-0.86220000	3.24240000
C	5.80580000	-2.19670000	3.61330000
C	5.33470000	-3.21960000	2.79410000
C	2.92220000	-4.61470000	-1.44530000
C	2.38080000	-4.26030000	-2.67860000
C	2.41160000	-2.94130000	-3.12180000
C	2.95230000	-1.93210000	-2.32980000
C	-2.80680000	2.73750000	0.98420000
C	-4.14440000	2.43430000	0.64730000
C	-4.67020000	2.82960000	-0.60620000
C	-3.83800000	3.50670000	-1.52860000
C	-2.49240000	3.78320000	-1.20040000
C	4.55290000	-1.55790000	1.11320000
C	4.65630000	-2.91130000	1.50440000
C	4.14880000	-3.93370000	0.66750000
C	3.54820000	-3.58820000	-0.56690000
C	3.51060000	-2.24030000	-0.98620000
H	-7.98200000	0.58850000	-2.99420000
H	-9.25110000	3.45100000	-0.05390000
H	-6.89200000	3.95410000	0.48740000
H	-5.62150000	1.09570000	-2.48090000

H -0.61450000	4.73060000	-1.99730000	C 1.82150000	3.25690000	0.21930000
H -5.38310000	3.82670000	-3.13260000	C 2.11310000	4.32820000	1.09900000
H -5.97810000	1.37880000	1.41140000	C 1.04990000	5.13190000	1.57170000
H -5.06390000	0.81650000	3.59490000	C -0.26800000	4.83250000	1.20860000
H -2.74660000	1.37190000	4.19000000	C -0.57180000	3.72870000	0.41260000
H -1.28340000	2.53130000	2.62470000	C 0.47970000	2.94530000	-0.05740000
H 4.13130000	3.61630000	1.44890000	H 5.78390000	0.12800000	-1.62640000
H 3.56240000	4.77800000	2.64900000	H -1.08270000	5.46110000	1.56550000
H 4.06270000	5.33140000	1.05110000	P 0.37050000	0.34040000	-0.17900000
H 3.11670000	-7.58730000	3.36930000	O 1.83010000	0.49060000	0.58250000
H 5.86200000	-8.22940000	0.12920000	O 0.21050000	1.84070000	-0.85000000
H 5.67520000	-5.84990000	-0.51230000	O 0.46070000	-0.58820000	-1.36390000
H 2.93350000	-5.20450000	2.75180000	O -0.63910000	0.07700000	0.90210000
H 5.70180000	1.22760000	-4.13830000	H -9.80050000	1.76470000	-1.78660000
H 6.69600000	4.12210000	-1.09600000	H 4.58100000	-9.10360000	2.06350000
H 8.53950000	4.95910000	-2.50860000	C -3.43230000	-1.83380000	-0.46390000
H 8.97830000	3.93570000	-4.72340000	N -2.93530000	-1.46290000	0.76080000
H 7.56200000	2.06750000	-5.52950000	C -3.20690000	-0.75940000	-1.52110000
H 5.00500000	0.53980000	1.78800000	H -3.79870000	0.12690000	-1.27200000
H 5.49250000	-4.23890000	3.11750000	H -2.15850000	-0.45240000	-1.54430000
H 2.85060000	-5.64870000	-1.13640000	H -3.48610000	-1.11510000	-2.51510000
H 1.92840000	-5.02110000	-3.30160000	C -3.30990000	-1.78500000	2.08450000
H 1.99440000	-2.69410000	-4.08940000	C -2.29000000	-1.75000000	3.05270000
H 2.94310000	-0.92000000	-2.71250000	C -4.63550000	-2.00880000	2.49340000
H 0.01810000	5.57140000	4.05100000	C -2.58970000	-1.96780000	4.39410000
H 0.39910000	7.52610000	5.51190000	H -1.27780000	-1.51850000	2.73870000
H 1.87610000	9.37220000	4.76630000	C -4.91790000	-2.23700000	3.83890000
H 2.96650000	9.26770000	2.54240000	H -5.44520000	-1.96980000	1.77680000
H 2.58540000	7.32980000	1.06100000	C -3.90190000	-2.22530000	4.79600000
H -1.55390000	5.40410000	-4.14010000	H -1.79010000	-1.93080000	5.12900000
H -3.90550000	4.95940000	-4.69790000	H -5.94880000	-2.40350000	4.14040000
H 6.04680000	-0.08640000	3.89770000	H -4.13320000	-2.39680000	5.84350000
H 6.28990000	-2.44320000	4.54960000	C -1.14190000	-2.65590000	-3.72170000
H 2.74600000	4.75660000	-1.59140000	C -2.00830000	-3.61390000	-4.11490000
H 4.41880000	5.08200000	-1.14470000	C -1.57550000	-3.55670000	-1.60810000
H 4.04020000	4.48820000	-2.76160000	N -0.81230000	-2.68820000	-2.38900000
C 2.11590000	7.35510000	2.03650000	H -0.25730000	-1.90970000	-1.95690000
C 2.32790000	8.45760000	2.86990000	H -0.68520000	-1.89630000	-4.34390000
C 1.71150000	8.51770000	4.12280000	H -2.39540000	-3.79910000	-5.10560000
C 0.87860000	7.47700000	4.54280000	H -2.53300000	-2.80100000	-1.02880000
C 0.66370000	6.37270000	3.71260000	S -2.45680000	-4.64540000	-2.76000000
C 3.54220000	4.52520000	1.58290000	C -0.95820000	-4.16180000	-0.37980000
C 3.76990000	4.39620000	-1.70350000	C 0.05250000	-3.47230000	0.30640000
C 6.86550000	3.67770000	-2.06880000	C -1.43070000	-5.37630000	0.14000000
C 7.91550000	4.14880000	-2.86290000	C 0.55990000	-3.98250000	1.50000000
C 8.16440000	3.57050000	-4.11060000	H 0.45100000	-2.54450000	-0.08790000
C 7.36600000	2.51720000	-4.56470000	C -0.91350000	-5.88500000	1.32940000
C 6.31470000	2.04310000	-3.77400000	H -2.19520000	-5.93760000	-0.38980000
C 4.95760000	0.76410000	-1.31180000	C 0.07530000	-5.18290000	2.02050000
C 4.94250000	2.11390000	-1.68030000	H 1.33490000	-3.42760000	2.02080000
C 3.89620000	2.95380000	-1.23530000	H -1.28270000	-6.83140000	1.71450000
C 2.89190000	2.41120000	-0.39670000	H 0.46610000	-5.57510000	2.95500000
C 2.88620000	1.02840000	-0.13980000	H -2.08410000	-0.86460000	0.72370000
C 3.92760000	0.20090000	-0.55930000	C -4.68100000	-2.66220000	-0.56910000

C -4.76180000 -3.92710000 0.04010000
 C -5.77670000 -2.21390000 -1.32160000
 C -5.90890000 -4.70610000 -0.08520000
 H -3.92460000 -4.29290000 0.62540000
 C -6.93110000 -2.98950000 -1.43650000
 H -5.73890000 -1.24810000 -1.81050000
 C -7.00160000 -4.23820000 -0.81990000
 H -5.95140000 -5.68000000 0.39480000
 H -7.77300000 -2.61400000 -2.01170000
 H -7.89810000 -4.84500000 -0.91320000
 C 3.99180000 -1.22060000 -0.13810000
 C 6.05060000 2.62720000 -2.52380000
 C 1.28890000 6.29950000 2.45650000
 C -1.97700000 3.40830000 0.05980000

(E)-syn-TS-S

C -7.47170000 -4.00520000 -0.80760000
 C -8.82480000 -3.65510000 -0.83960000
 C -9.20850000 -2.32470000 -0.64450000
 C -8.23960000 -1.34170000 -0.42030000
 C -6.87950000 -1.68720000 -0.39520000
 C -6.50080000 -3.02540000 -0.58330000
 C -4.23080000 2.21790000 -2.05450000
 C -4.92860000 2.16510000 -3.25820000
 C -5.90470000 1.19760000 -3.47870000
 C -6.21500000 0.25640000 -2.50030000
 C -5.52810000 -1.49670000 2.20300000
 C -4.81440000 -1.45730000 3.39830000
 C -3.76770000 -0.55740000 3.57840000
 C -3.41610000 0.34240000 2.57590000
 C 6.91350000 -4.20320000 1.54030000
 C 8.28330000 -3.98990000 1.72350000
 C 8.82270000 -2.71130000 1.54850000
 C 7.99360000 -1.64410000 1.18870000
 C 6.61990000 -1.85610000 1.00070000
 C 6.08260000 -3.13880000 1.18090000
 C 3.47260000 1.76640000 2.36650000
 C 3.71490000 1.45300000 3.70140000
 C 4.58400000 0.42360000 4.04960000
 C 5.24370000 -0.31690000 3.07280000
 C 6.39660000 -0.99810000 -1.79580000
 C 6.23480000 -0.62170000 -3.12670000
 C 5.25450000 0.29510000 -3.49610000
 C 4.42840000 0.88450000 -2.54210000
 C -4.14500000 0.35600000 1.27810000
 C -5.17440000 -0.58800000 1.07730000
 C -5.84780000 -0.65070000 -0.16330000
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 C 4.11970000 0.99040000 1.27090000
 C 5.02550000 -0.03230000 1.62800000
 C 5.73160000 -0.73490000 0.62900000
 C 5.56670000 -0.37940000 -0.72640000
 C 4.61590000 0.59800000 -1.09230000

H -7.17530000 -5.03560000 -0.95500000
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 H -5.45640000 -3.30720000 -0.55230000
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 H -6.33940000 -2.20690000 2.11670000
 H -5.07610000 -2.13740000 4.19860000
 H -3.22250000 -0.55390000 4.51350000
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 H 1.08260000 4.93980000 1.54730000
 H -0.04200000 5.55760000 2.75680000
 H 0.06970000 6.33130000 1.17660000
 H 6.49540000 -5.19200000 1.67790000
 H 9.88280000 -2.54740000 1.69260000
 H 8.41790000 -0.65640000 1.05670000
 H 5.02250000 -3.31010000 1.04450000
 H 3.91430000 4.53770000 -3.81230000
 H 2.43570000 7.18290000 -0.73960000
 H 3.38480000 9.10990000 -1.95540000
 H 4.60490000 8.76390000 -4.08540000
 H 4.87300000 6.47700000 -5.00440000
 H 2.82220000 2.60390000 2.15680000
 H 5.91670000 -1.10070000 3.39420000
 H 7.15140000 -1.73690000 -1.56230000
 H 6.85680000 -1.07360000 -3.88850000
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 H -4.17780000 6.01370000 5.66070000
 H -4.00230000 8.37890000 4.93930000
 H -3.05290000 8.93090000 2.71690000
 H -2.28260000 7.13170000 1.21270000
 H -4.70610000 2.88450000 -4.03580000
 H -6.42460000 1.17160000 -4.42770000
 H 3.22840000 2.02590000 4.48050000
 H 4.75570000 0.20120000 5.09490000
 H -0.86840000 5.08280000 -1.62640000
 H 0.11070000 6.40820000 -1.00510000
 H 0.36970000 5.81910000 -2.64690000
 C -2.67980000 6.87720000 2.18750000
 C -3.12220000 7.89840000 3.03380000
 C -3.65940000 7.58720000 4.28580000
 C -3.75850000 6.25370000 4.69220000
 C -3.31690000 5.22920000 3.84920000
 C 0.08570000 5.36010000 1.68650000
 C 0.13920000 5.50250000 -1.62330000
 C 2.95000000 7.01910000 -1.67840000
 C 3.49380000 8.11200000 -2.35990000
 C 4.18370000 7.91680000 -3.55960000
 C 4.33490000 6.62750000 -4.07740000
 C 3.79230000 5.53160000 -3.39930000
 C 3.38530000 3.52340000 -1.09260000
 C 2.52140000 4.55470000 -1.47550000

C	1.15410000	4.47660000	-1.13850000	H	0.82090000	-1.97240000	1.93150000
C	0.70060000	3.36850000	-0.38200000	C	3.21970000	-3.95660000	3.29790000
C	1.55980000	2.27600000	-0.16750000	H	3.20120000	-6.11540000	3.29080000
C	2.92310000	2.35860000	-0.47510000	H	2.92750000	-1.82380000	3.15540000
C	-0.64330000	3.38010000	0.26790000	H	4.15990000	-3.88050000	3.83740000
C	-0.98930000	4.40400000	1.18640000	H	-0.10930000	-2.21970000	-1.76320000
C	-2.30640000	4.44550000	1.69400000	H	-0.20480000	-4.24180000	-0.12670000
C	-3.21320000	3.44060000	1.34560000	C	1.63110000	-4.08810000	-1.59820000
C	-2.84720000	2.36640000	0.53350000	C	2.45700000	-5.03790000	-0.97110000
C	-1.55430000	2.34290000	0.00980000	C	2.23750000	-3.07260000	-2.35390000
H	4.45050000	3.61500000	-1.30300000	C	3.84150000	-4.97800000	-1.09470000
H	-4.23060000	3.47680000	1.73330000	H	2.01580000	-5.82810000	-0.37340000
P	-0.08830000	0.18230000	-0.21750000	C	3.62180000	-3.03440000	-2.49900000
O	1.06570000	1.14870000	0.46600000	H	1.63810000	-2.32000000	-2.84950000
O	-1.14760000	1.30430000	-0.81500000	C	4.43170000	-3.97910000	-1.87190000
O	0.43120000	-0.57290000	-1.41320000	H	4.45870000	-5.71470000	-0.58830000
O	-0.69510000	-0.56510000	0.94560000	H	4.05440000	-2.26740000	-3.12950000
H	-9.57600000	-4.41470000	-1.01330000	H	5.51140000	-3.94170000	-1.98740000
H	8.92630000	-4.81460000	2.00240000				
C	3.08590000	5.72100000	-2.19960000				
C	3.87830000	1.28200000	-0.09500000	(E)-anti-TS-S			
C	-2.76500000	5.53440000	2.59350000	C	6.82280000	-4.49070000	1.60810000
C	-3.82400000	1.28350000	0.26240000	C	8.18690000	-4.28740000	1.83780000
C	0.13750000	-4.24550000	-1.56460000	C	8.73550000	-3.00740000	1.70880000
N	-0.56750000	-3.13450000	-1.95810000	C	7.92140000	-1.92920000	1.34770000
C	-0.35800000	-5.63040000	-1.95900000	C	6.55340000	-2.13100000	1.11180000
H	-1.15540000	-6.00340000	-1.31010000	C	6.00650000	-3.41500000	1.24810000
H	-0.73070000	-5.60970000	-2.98930000	C	3.38110000	1.53980000	2.42080000
H	0.46410000	-6.34500000	-1.91310000	C	3.52710000	1.14440000	3.69290000
C	-1.87010000	-2.97700000	-2.46730000	C	4.31000000	0.03860000	4.04740000
C	-2.15670000	-1.70900000	-3.01950000	C	4.98310000	-0.68080000	3.13960000
C	-2.87930000	-3.95700000	-2.46560000	C	6.50460000	-1.13920000	-1.66790000
C	-3.39210000	-1.45690000	-3.59830000	C	6.40990000	-0.73660000	-2.94250000
H	-1.39730000	-0.93480000	-2.97960000	C	5.45540000	0.19570000	-3.36020000
C	-4.11590000	-3.68510000	-3.05610000	C	4.56400000	0.78330000	-2.46460000
H	-2.72590000	-4.92050000	-2.00520000	C	-7.80080000	-3.55780000	-1.25180000
C	-4.38110000	-2.44570000	-3.63160000	C	-9.12940000	-3.13000000	-1.17250000
H	-3.57850000	-0.47890000	-4.03130000	C	-9.41860000	-1.80020000	-0.85150000
H	-4.88000000	-4.45830000	-3.05150000	C	-8.37980000	-0.89610000	-0.60940000
H	-5.34530000	-2.24740000	-4.09040000	C	-7.04460000	-1.32050000	-0.68950000
C	-2.70990000	-3.46090000	1.04320000	C	-6.75980000	-2.65670000	-1.01090000
C	-3.00120000	-4.77750000	1.12440000	C	-4.19500000	2.54670000	-2.20440000
C	-0.50790000	-4.23730000	1.15130000	C	-4.89140000	2.55060000	-3.34940000
N	-1.38910000	-3.14160000	1.19760000	C	-5.92130000	1.63450000	-3.60220000
H	-1.06650000	-2.14670000	1.08410000	C	-6.28340000	0.70060000	-2.71170000
H	-3.40650000	-2.65820000	0.85970000	C	-5.58160000	-1.34530000	1.87960000
H	-3.96880000	-5.25120000	1.05490000	C	-4.86860000	-1.36380000	3.01450000
S	-1.54050000	-5.71840000	1.42360000	C	-3.78650000	-0.50110000	3.23240000
C	0.78650000	-4.14380000	1.90820000	C	-3.40600000	0.41100000	2.32760000
C	1.47610000	-5.30050000	2.30070000	C	4.65110000	0.47400000	-1.01780000
C	1.33070000	-2.88810000	2.21610000	C	5.61820000	-0.57820000	-0.61480000
C	2.68480000	-5.20840000	2.98850000	C	5.68560000	-0.99920000	0.72640000
H	1.06480000	-6.28340000	2.08260000	C	4.91400000	-0.33640000	1.69790000
C	2.53590000	-2.80440000	2.91110000	C	4.03420000	0.79470000	1.31310000
				C	-4.48720000	1.55020000	-1.14490000

C -5.59440000	0.59620000	-1.40130000	C -3.59790000	6.26990000	4.70970000
C -5.94410000	-0.36600000	-0.43320000	C -3.18370000	5.26890000	3.82550000
C -5.23510000	-0.40820000	0.78280000	C -3.10620000	3.58950000	1.24810000
C -4.11880000	0.53540000	1.03190000	C -2.17070000	4.54690000	1.64960000
H 6.39800000	-5.48100000	1.70900000	C -0.84870000	4.47970000	1.15750000
H 9.79130000	-2.85110000	1.88810000	C -0.52730000	3.48270000	0.20220000
H 8.35370000	-0.94110000	1.24880000	C -1.47570000	2.50210000	-0.12840000
H 4.95090000	-3.57950000	1.07480000	C -2.77060000	2.54350000	0.38730000
H 2.78480000	2.42050000	2.22580000	C 0.83710000	3.41670000	-0.39910000
H 5.58350000	-1.51360000	3.48210000	C 1.37830000	4.51190000	-1.11360000
H 7.24930000	-1.88430000	-1.42110000	C 2.75760000	4.51360000	-1.40780000
H 7.07500000	-1.16710000	-3.68060000	C 3.54620000	3.42740000	-1.01690000
H 5.39670000	0.45600000	-4.40930000	C 2.99870000	2.28050000	-0.43530000
H 3.81970000	1.46600000	-2.85120000	C 1.62310000	2.27120000	-0.17660000
H -0.58960000	5.25400000	-1.63500000	H -4.12500000	3.64080000	1.63040000
H 0.71650000	5.93220000	-2.60980000	H 4.62120000	3.46150000	-1.19120000
H 0.45630000	6.50090000	-0.96090000	P -0.13750000	0.28710000	-0.39970000
H -7.57760000	-4.58730000	-1.49980000	O -0.89840000	-0.45350000	0.67870000
H 10.44760000	-1.47040000	-0.78990000	O -1.08760000	1.49330000	-1.00290000
H -8.61300000	0.13200000	-0.36070000	O 1.03020000	1.15780000	0.40340000
H -5.73540000	-2.99850000	-1.07460000	O 0.43330000	-0.48480000	-1.55580000
H -3.30610000	4.22960000	4.10540000	C 0.41630000	-4.24020000	-1.12350000
H -2.03880000	7.24920000	1.29400000	N -0.34510000	-3.21850000	-1.64370000
H -2.76190000	9.00580000	2.87020000	C -0.17430000	-5.64250000	-1.09880000
H -3.76360000	8.38930000	5.05230000	H 0.25270000	-6.21430000	-0.27070000
H -4.03930000	6.00210000	5.66090000	H -1.25640000	-5.61640000	-0.96640000
H -3.41340000	3.28350000	-2.07240000	H 0.06170000	-6.18800000	-2.01890000
H -7.08190000	0.01890000	-2.97380000	C 1.66410000	-2.10620000	2.27470000
H -6.40950000	-2.03470000	1.77820000	C 2.42830000	-3.14550000	2.67440000
H -5.13550000	-2.07030000	3.79050000	C 0.20780000	-3.81240000	1.61470000
H -3.24440000	-0.57150000	4.16710000	N 0.41940000	-2.44830000	1.81290000
H -2.56090000	1.04710000	2.55780000	H -0.19820000	-1.69880000	1.39780000
H 4.21270000	4.44020000	-3.70540000	H 1.92090000	-1.05530000	2.29370000
H 5.32490000	6.33110000	-4.84030000	H 3.42490000	-3.12970000	3.08710000
H 5.17390000	8.61770000	-3.89460000	H 0.40040000	-4.03180000	0.32750000
H 3.91590000	9.01140000	-1.79520000	S 1.57180000	-4.66620000	2.45780000
H 2.81310000	7.13190000	-0.63600000	C -1.18790000	-4.35640000	1.77630000
H 3.02870000	1.70160000	4.47640000	C -2.27230000	-3.62400000	1.26710000
H 4.38340000	-0.23390000	5.09280000	C -1.41990000	-5.61950000	2.33780000
H -4.65120000	3.28560000	-4.10740000	C -3.55460000	-4.16900000	1.30070000
H -6.44170000	1.68550000	-4.55040000	H -2.12210000	-2.63360000	0.84810000
H 0.29090000	6.35700000	1.21840000	C -2.70880000	-6.14920000	2.38490000
H 0.10700000	5.55740000	2.77890000	H -0.59610000	-6.18850000	2.75900000
H 1.23390000	4.91610000	1.58440000	C -3.78020000	-5.42900000	1.85650000
C 3.34300000	6.94870000	-1.56240000	H -4.38030000	-3.60850000	0.87820000
C 3.97380000	8.01420000	-2.21170000	H -2.87150000	-7.12500000	2.83420000
C 4.68500000	7.79190000	-3.39410000	H -4.78420000	-5.84330000	1.88040000
C 4.77030000	6.50280000	-3.92690000	H 0.01870000	-2.25040000	-1.55370000
C 4.14050000	5.43440000	-3.28110000	C 1.89450000	-4.15550000	-1.35700000
C 0.44190000	5.60900000	-1.59930000	C 2.75570000	-5.16530000	-0.88360000
C 0.25240000	5.37600000	1.70810000	C 2.44280000	-3.12010000	-2.13570000
C -2.46050000	6.96560000	2.25040000	C 4.11450000	-5.14770000	-1.19090000
C -2.87560000	7.96320000	3.13760000	H 2.36750000	-5.98090000	-0.28520000
C -3.44210000	7.61580000	4.36700000	C 3.79600000	-3.12340000	-2.45660000

H 1.81720000 -2.31900000 -2.51040000
 C 4.64080000 -4.12990000 -1.98660000
 H 4.75910000 -5.93770000 -0.81540000
 H 4.17760000 -2.34150000 -3.10260000
 H 5.69650000 -4.12530000 -2.24360000
 C -1.58330000 -3.28780000 -2.32530000
 C -2.49490000 -2.22910000 -2.17090000
 C -1.87700000 -4.31070000 -3.24350000
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 H -2.27450000 -1.42730000 -1.47490000
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 H -4.90520000 -3.22780000 -4.36600000
 H -9.93460000 -3.82860000 -1.35940000
 H 8.81840000 -5.12090000 2.11650000
 C 3.88180000 1.14860000 -0.04520000
 C 3.41270000 5.65190000 -2.09900000
 C -2.60280000 5.60990000 2.59220000
 C -3.77900000 1.50590000 0.07020000

On MOF-fcu
 (Z)-syn-TS-R

H 2.02660000 -5.78820000 10.30450000
 H -1.12040000 -9.93710000 5.76500000
 H -8.92780000 -0.34310000 7.58780000
 H -6.24690000 -9.84280000 -0.42450000
 H -10.62070000 -5.03870000 2.49170000
 H -3.35010000 1.29180000 11.30010000
 H 7.63400000 0.48070000 9.18260000
 H 8.93900000 0.35570000 7.11580000
 H 4.98070000 -10.64500000 0.26660000
 H 9.60030000 -6.24820000 -2.77900000
 H 1.35780000 -0.88490000 -7.86290000
 H -1.17160000 -0.63190000 8.10670000
 H 1.24370000 -7.84670000 2.82700000
 H -1.68370000 -7.50970000 -2.56450000
 H 7.45060000 -3.29780000 -0.47470000
 H -7.63250000 -2.29600000 0.99910000
 O -3.14020000 -0.69130000 6.41060000
 O 2.02360000 -5.92360000 4.39290000
 O -2.03600000 -5.60070000 -4.16840000
 H 5.66480000 -4.91690000 -0.06940000
 H -6.12570000 -4.17060000 0.58680000
 H -3.37530000 -7.65470000 1.93190000
 H 2.13090000 -7.73480000 -1.16810000
 H 8.07590000 0.18180000 1.43660000
 H -8.04010000 -0.41710000 -1.19830000
 H 0.78990000 -2.62730000 7.63040000
 H -0.70810000 -2.86660000 -7.51390000
 H -5.00260000 -5.84630000 2.23310000
 H 3.95070000 -6.15340000 -1.56800000

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 O 0.19650000 -4.16440000 5.62670000
 O -0.27970000 -4.53890000 -5.65310000
 C 2.51240000 -13.29340000 2.93890000
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 O 0.43770000 -14.46880000 1.36880000
 H -2.81930000 -5.64080000 -10.10320000
 H -0.82150000 -10.49390000 -5.59950000
 H -7.46500000 -0.64860000 -8.96340000
 C -4.22750000 -13.09920000 -2.44540000
 C -1.36070000 -16.30980000 -2.69900000
 C -4.04450000 -16.07570000 0.67720000
 O -1.24400000 -16.73900000 -1.43330000
 O -0.83740000 -16.65970000 2.12620000
 O 0.73610000 -16.79870000 0.14580000
 O -2.81750000 -16.60210000 0.54740000
 O -2.28240000 -14.38830000 -0.80470000
 Zr -0.97910000 -15.51600000 0.31310000
 H 11.28890000 -1.62810000 3.68460000
 H 9.90920000 -1.57530000 5.69650000
 H 3.25210000 5.61390000 10.23760000
 H 3.09100000 7.33130000 8.51230000
 H 0.83330000 10.29970000 5.73200000
 H 1.09010000 8.51890000 7.39540000
 C 6.17130000 -0.40820000 15.59340000
 C 2.87100000 -3.12890000 16.16450000
 C 5.31030000 -3.40690000 12.60660000
 O 3.93820000 -1.42460000 14.13990000
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 H 4.34370000 -1.50840000 7.22430000
 H -0.63370000 7.54190000 -2.34210000
 H 2.68330000 7.78970000 2.75550000
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 H 7.60110000 2.42270000 -2.22710000
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 H 7.04970000 0.54270000 -4.14430000
 H -6.80280000 1.50310000 4.31770000
 H 1.35830000 2.77830000 7.58480000
 H -3.41220000 3.63930000 -7.65590000
 O -4.48860000 1.61060000 5.49590000
 H -4.39670000 10.64840000 2.32660000
 O -6.44830000 9.13850000 2.85120000
 H -9.84920000 6.28890000 1.24300000
 O -8.13560000 8.19020000 0.81030000
 C 1.65290000 -5.44330000 9.34870000
 C 1.37880000 -6.38770000 8.35570000
 C -3.54290000 -12.94960000 3.61510000
 C -9.26910000 0.62770000 5.05680000
 C -0.89760000 0.25900000 10.66730000
 C 1.76150000 -3.06170000 10.14520000
 C -0.26220000 -10.07530000 3.18060000

C	-12.51730000	-2.20050000	5.66720000	O	1.51460000	0.08600000	16.91070000
C	-0.66170000	-2.78110000	13.70430000	O	5.01930000	-0.28230000	16.26910000
C	-10.17170000	-2.38480000	2.03310000	O	3.08240000	-1.87920000	16.60410000
C	-3.71930000	-9.97760000	0.56920000	O	3.45120000	1.68390000	16.57530000
C	-8.02060000	0.57190000	5.84700000	O	1.78190000	1.27830000	14.56180000
C	-2.10180000	0.33310000	9.80990000	Zr	3.05470000	-0.08520000	15.42260000
C	1.45620000	-4.07360000	9.10430000	C	-8.01750000	0.04360000	7.14650000
C	0.00940000	-9.01180000	4.16770000	C	-6.83430000	-0.00470000	7.88670000
C	-9.25150000	-3.51790000	1.77350000	C	-15.23900000	1.08940000	6.31820000
C	-4.68990000	-8.88020000	0.72760000	C	-11.99640000	3.87950000	5.70290000
C	-5.63010000	0.47790000	7.34630000	C	-15.60860000	4.20130000	3.35420000
C	-4.39770000	0.45550000	8.17000000	C	-3.29440000	0.89300000	10.29480000
C	0.91090000	-5.98510000	7.09380000	C	-4.42940000	0.95250000	9.48350000
C	0.58830000	-7.00360000	6.06460000	O	-13.91570000	0.97480000	6.50640000
C	-7.51270000	-5.68550000	1.27080000	O	-10.41750000	0.67770000	5.75510000
C	-6.55720000	-6.79990000	1.08090000	O	-0.97920000	-1.47960000	13.77860000
C	-0.49820000	-9.10040000	5.47170000	O	-0.61010000	2.08210000	13.75110000
C	-0.21650000	-8.10340000	6.40820000	O	-1.10400000	0.32290000	11.99470000
O	-2.24080000	-13.01930000	3.93070000	O	-0.47510000	0.28330000	15.52890000
O	1.31320000	-13.21050000	3.53470000	O	-12.31980000	-0.95510000	6.12480000
O	1.96370000	-3.52150000	11.39320000	O	-12.01410000	2.61300000	6.14550000
O	2.59860000	-3.57150000	14.92790000	O	1.52810000	-1.17170000	14.58110000
O	4.03080000	-3.73380000	12.84370000	O	-13.73590000	2.20930000	4.16960000
O	0.52500000	-3.36650000	13.48270000	Zr	0.36740000	0.17940000	13.55620000
O	-0.55760000	-14.90570000	3.78550000	Zr	-12.41410000	0.85680000	4.97510000
O	-0.38590000	-11.32120000	3.67090000	O	-16.46500000	-0.58450000	3.41390000
O	-1.87680000	-11.87600000	1.57570000	O	-16.16200000	2.98220000	3.43700000
O	1.08540000	-1.14780000	12.16490000	O	-16.67610000	1.23940000	1.66890000
O	-11.54130000	-0.44720000	3.65040000	O	-15.94380000	1.15700000	5.17860000
Zr	2.40070000	-2.37070000	13.15840000	O	-13.94510000	-0.24160000	4.15560000
Zr	-0.59670000	-13.14660000	2.55380000	Zr	-15.15530000	1.10200000	3.18080000
H	-11.11530000	1.68770000	-3.37730000	H	9.09920000	-1.48910000	-7.35250000
C	-5.97140000	-8.97490000	0.16280000	O	7.10050000	-1.50440000	-9.01030000
C	-6.90800000	-7.95030000	0.34310000	H	6.11100000	10.06000000	-1.98300000
C	-16.48700000	1.23040000	0.34060000	O	7.96400000	8.30430000	-2.48260000
C	-13.76670000	-2.05340000	-0.30330000	H	10.86640000	4.90680000	-0.88720000
C	-16.12480000	-1.87820000	3.31440000	O	9.44450000	7.03790000	-0.44600000
C	-9.64950000	-4.83680000	2.05710000	C	16.59930000	-1.25380000	-0.00430000
C	-8.80210000	-5.91690000	1.79320000	C	13.34990000	-4.05340000	0.50980000
O	-13.55950000	-2.53710000	0.93080000	C	15.75730000	-4.18140000	-3.06560000
O	-12.81480000	-2.62520000	4.43000000	O	14.36990000	-2.26900000	-1.46960000
O	-4.43220000	-14.79170000	0.69270000	H	3.59290000	0.83890000	-11.13010000
O	-4.23700000	-11.21690000	0.54530000	O	5.89200000	0.86790000	-9.91910000
O	-11.44710000	-2.71510000	2.29570000	H	0.29290000	4.76660000	-9.53330000
O	-14.93350000	-2.43640000	3.05370000	H	0.68010000	6.44010000	-7.78480000
O	-4.53920000	-13.05490000	-1.14150000	H	-0.02480000	10.35590000	-5.56440000
O	-4.13790000	-12.94800000	2.41270000	H	-0.55770000	8.61400000	-7.18330000
O	-2.00510000	-14.33330000	1.64310000	C	4.74520000	-9.67190000	-0.14700000
O	-14.44810000	-0.18260000	1.74280000	C	5.79170000	-8.77690000	-0.38940000
Zr	-13.09010000	-1.39630000	2.68980000	C	1.82740000	-13.42500000	-3.12190000
Zr	-3.15920000	-13.07210000	0.50480000	C	1.09500000	0.01220000	-10.43580000
C	0.19890000	0.22160000	16.68700000	C	9.45650000	-0.56630000	-4.82110000
C	3.49750000	2.94330000	16.11540000	C	12.20210000	-3.81960000	-5.47560000
C	-0.03260000	3.28910000	13.65360000	C	2.32450000	-10.30500000	-0.23680000

C	9.77740000	-3.69000000	-1.86360000	C	1.51940000	10.21030000	3.09390000
C	0.41290000	-2.95760000	-13.52990000	C	2.40960000	3.00910000	10.09610000
C	2.32140000	-0.03310000	-9.60980000	C	5.93880000	2.66290000	12.57100000
C	8.23520000	-0.47080000	-5.64940000	C	3.77310000	10.00430000	-0.58160000
C	-1.79780000	-4.08920000	-8.96540000	C	10.29790000	2.39700000	-1.78210000
C	-1.22250000	-9.16500000	-3.91930000	C	9.78700000	-0.73610000	2.39830000
C	3.41550000	-9.32270000	-0.43620000	C	5.88340000	-0.48740000	8.35310000
C	8.67350000	-4.65290000	-1.64600000	C	1.71910000	9.16640000	4.11480000
C	4.68370000	-0.18390000	-8.06960000	C	2.32590000	4.05450000	9.04650000
C	5.91730000	-0.27460000	-7.25080000	C	4.74060000	8.89970000	-0.77280000
C	-1.53590000	-6.11650000	-6.98080000	C	9.35750000	3.52430000	-1.59260000
C	-1.42150000	-7.15330000	-5.93050000	C	8.18930000	-0.68970000	4.72700000
C	5.51760000	-7.49390000	-0.90970000	C	7.38700000	-0.62890000	5.97130000
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C	8.75250000	-5.95240000	-2.17300000	C	2.15510000	6.04520000	7.04550000
C	7.74270000	-6.88900000	-1.93010000	C	6.61440000	6.80940000	-1.09350000
O	12.39450000	-4.32260000	-4.24700000	C	7.57290000	5.69170000	-1.27580000
O	13.06400000	-4.45970000	-0.73620000	C	7.19360000	0.01260000	8.31080000
O	2.70040000	-11.59450000	-0.17610000	C	7.93720000	-0.05590000	7.13020000
O	2.53120000	-15.17790000	-0.09420000	O	11.94240000	-0.92190000	1.36200000
O	14.48430000	-4.53570000	-2.83430000	O	15.45240000	-1.16920000	0.68630000
O	10.97430000	-4.22770000	-2.15720000	O	6.25750000	1.36170000	12.50110000
O	2.82340000	-13.35300000	1.63520000	O	5.88680000	-2.19920000	12.51180000
O	2.42360000	-13.42330000	-1.92020000	O	6.39370000	-0.44180000	14.27100000
O	0.29040000	-12.06660000	-1.14990000	O	5.74280000	-0.37410000	10.74350000
O	11.49350000	-1.97870000	-3.41330000	O	13.55510000	-2.81600000	0.98530000
O	-1.07950000	-1.14300000	-11.93290000	O	13.83960000	0.75120000	1.07270000
Zr	12.83780000	-3.20680000	-2.46590000	O	3.75290000	1.05290000	11.69830000
Zr	1.44360000	-13.32800000	-0.01140000	O	12.17320000	0.38390000	-0.93870000
C	-2.29630000	-5.38460000	-9.18490000	O	2.38180000	11.95270000	0.99380000
C	-2.17050000	-6.36920000	-8.20720000	Zr	4.91110000	-0.29710000	12.72390000
C	-6.06730000	0.35890000	-15.25700000	Zr	13.47730000	-0.98620000	-0.13740000
C	-3.16940000	-2.76690000	-15.95070000	C	-5.16280000	0.66400000	-6.81960000
C	-5.57730000	-2.80360000	-12.36570000	C	5.34260000	-1.08840000	7.20500000
C	-1.05040000	-9.48100000	-5.27720000	C	2.28560000	-0.53200000	-8.29650000
C	-1.14120000	-8.49020000	-6.25180000	C	-2.07030000	-0.16980000	8.49710000
O	0.52430000	-13.36910000	-3.43610000	C	-0.61710000	7.78810000	-3.39670000
O	-3.02770000	-13.17110000	-3.04100000	C	0.81180000	-7.91370000	3.81870000
O	-2.94070000	-3.27160000	-14.72910000	C	2.32170000	7.94960000	3.76410000
O	-2.26730000	-3.40450000	-11.21700000	C	-1.50610000	-7.83440000	-3.58600000
O	-0.84060000	-3.38300000	-13.31150000	C	-7.21320000	4.29920000	2.08380000
O	-4.35620000	-3.29250000	-12.62960000	C	7.54080000	-4.29120000	-0.89690000
O	-1.15140000	-11.47910000	-3.27680000	C	-7.97190000	-3.29700000	1.23500000
O	-1.34490000	-15.06120000	-3.18920000	C	7.98960000	3.36900000	-1.87150000
O	0.15990000	-14.52360000	-1.07900000	C	-5.95810000	0.74680000	-5.67380000
O	-3.97030000	-0.98710000	-13.86960000	C	6.07950000	-1.15540000	6.01870000
Zr	-2.56100000	-2.15260000	-12.93550000	C	3.45490000	-0.60640000	-7.53530000
Zr	-1.11970000	-13.24920000	-2.05830000	C	-3.19940000	-0.10090000	7.67410000
C	10.28780000	-1.22070000	3.61820000	C	-0.96230000	6.79500000	-4.32240000
C	9.49830000	-1.19480000	4.76920000	C	1.10210000	-6.91090000	4.75090000
C	10.62050000	-0.76690000	1.17440000	C	2.47300000	6.92920000	4.70730000
C	5.07090000	-0.36850000	9.57920000	C	-1.61270000	-6.85260000	-4.56880000
C	4.63360000	13.07340000	2.31220000	C	-6.18280000	5.22920000	1.92210000
C	13.86820000	2.02440000	0.65110000	C	6.52090000	-5.21730000	-0.66140000

C	-7.11080000	-4.36890000	0.99230000	O	-0.98220000	-9.74150000	-1.60680000
C	7.10810000	4.44090000	-1.71450000	O	-9.32530000	2.40720000	1.99500000
C	-4.88030000	0.14370000	-9.25560000	O	9.46390000	-2.39020000	-1.73170000
C	-10.51000000	0.71870000	-0.90620000	O	-9.63340000	-1.15490000	1.97220000
C	-2.71210000	13.37280000	-2.19880000	O	9.75740000	1.16750000	-1.75060000
C	0.05850000	10.14400000	-2.83930000	O	-2.42920000	-9.61170000	0.48780000
C	-1.80770000	3.09080000	-9.75780000	O	1.08140000	-9.80190000	-0.15550000
C	-13.26150000	4.02490000	-0.26410000	O	2.51780000	9.64040000	-0.27140000
C	-9.65090000	3.70830000	2.07410000	O	-0.95260000	9.83390000	0.51850000
C	-2.16110000	10.34130000	0.81090000	O	9.27020000	-0.55300000	-3.49090000
C	-5.37170000	3.28960000	-12.14840000	O	9.95980000	-0.63970000	0.01170000
C	-5.69980000	0.18120000	-8.02560000	O	-9.10900000	0.62980000	3.72430000
C	-9.69140000	0.63330000	-2.13550000	O	-9.83210000	0.63740000	0.24890000
C	-0.28180000	9.08730000	-3.82290000	O	2.19250000	1.74810000	9.68660000
C	-1.57840000	4.08010000	-8.70400000	O	1.80600000	-1.78970000	9.71900000
C	-8.54930000	4.67250000	1.86360000	O	-1.84140000	-1.75680000	-9.50210000
C	-3.24170000	9.35740000	1.02960000	O	-1.82360000	1.81220000	-9.35460000
C	-7.30630000	0.35170000	-5.71060000	O	11.96210000	-2.07100000	-0.99740000
C	-8.14030000	0.44810000	-4.48810000	O	3.49910000	-1.40070000	11.72160000
C	-0.91980000	7.07770000	-5.70320000	O	0.56960000	-12.01450000	1.29930000
C	-1.15180000	6.01510000	-6.70870000	O	-11.83890000	2.07060000	1.25050000
C	-6.46610000	6.55040000	1.53750000	O	-3.41630000	1.38130000	-11.37990000
C	-5.36040000	7.52370000	1.36820000	O	-0.58380000	12.06850000	-0.82790000
C	-4.34890000	-7.73810000	1.46590000	Zr	0.84410000	10.92860000	0.10410000
C	3.14480000	-8.03680000	-0.93550000	Zr	-0.73490000	-10.89280000	0.18380000
C	4.50310000	7.63480000	-0.20890000	Zr	-10.63810000	0.72490000	2.22920000
C	-3.19090000	8.09080000	0.42400000	Zr	10.77550000	-0.70820000	-1.97000000
C	7.07090000	0.13240000	-5.14640000	Zr	-2.04210000	0.07760000	-10.59440000
C	8.47950000	-0.22200000	2.35720000	Zr	2.22480000	-0.03760000	10.87340000
C	-6.81880000	1.06120000	5.30660000	C	-10.16080000	1.17660000	-3.34130000
C	-8.43010000	0.01290000	-2.11280000	C	-9.40350000	1.08120000	-4.51350000
C	1.75710000	3.76360000	7.79360000	C	-7.03690000	-0.24430000	-8.05410000
C	0.97070000	-3.67320000	7.84600000	C	-7.84130000	-0.15500000	-6.91450000
C	-1.14380000	-3.83210000	-7.75500000	O	-11.83620000	0.86380000	-1.08170000
C	-2.51070000	4.24070000	-7.67080000	O	-15.35070000	1.13870000	-0.36660000
C	-5.27510000	-6.70960000	1.64130000	O	-5.98460000	-1.53240000	-12.23320000
C	4.18500000	-7.13240000	-1.16780000	O	-5.86470000	2.04210000	-12.11520000
C	5.43010000	6.60210000	-0.36750000	O	-6.27260000	0.32270000	-13.93190000
C	-4.24010000	7.18360000	0.59200000	O	-5.55860000	0.18440000	-10.41610000
C	5.92450000	0.22940000	-5.93940000	O	-13.45490000	2.77900000	-0.72200000
C	7.67580000	-0.20920000	3.50190000	O	-13.74500000	-0.78720000	-0.74620000
C	-5.62730000	1.00950000	6.03810000	O	-3.49890000	-1.08380000	-11.45270000
C	-7.66350000	-0.07770000	-3.27650000	O	-12.04980000	-0.38470000	1.23790000
C	1.68370000	4.73780000	6.79210000	O	-2.15510000	-11.92980000	-0.87310000
C	0.71530000	-4.61180000	6.84170000	Zr	-4.76030000	0.22330000	-12.41030000
C	-1.00880000	-4.82890000	-6.79400000	Zr	-13.36350000	0.96880000	0.43030000
C	-2.30970000	5.20450000	-6.67420000	C	2.80510000	5.35390000	9.28630000
O	-3.55160000	0.08790000	-9.07430000	C	2.71650000	6.33760000	8.29860000
O	3.74690000	-0.26290000	9.38440000	C	-1.29100000	13.43930000	3.73150000
O	-0.06740000	0.00790000	-9.76400000	C	1.83940000	16.30900000	2.95480000
O	0.26950000	0.12770000	10.01740000	C	-1.84280000	16.45040000	0.69820000
O	0.34780000	9.72170000	-1.59750000	C	1.29970000	9.36740000	5.43810000
O	-0.33080000	-9.67540000	1.90070000	C	1.44490000	8.35050000	6.38590000
O	1.23560000	9.76280000	1.85980000	O	0.04050000	13.38060000	3.88350000

O	3.51580000	13.14590000	3.05070000	O	-1.47500000	1.41120000	-14.26870000
O	3.31830000	3.41210000	14.87150000	Zr	-0.21030000	0.10850000	-13.30910000
O	2.69150000	3.43560000	11.33970000	Zr	12.59880000	-0.81000000	-4.68910000
O	1.24820000	3.61420000	13.42230000	O	-1.40360000	0.25210000	-16.64530000
O	4.75160000	3.24720000	12.79140000	O	-4.91910000	0.34370000	-15.95070000
O	1.64210000	11.48090000	3.51260000	O	-3.10590000	2.08750000	-16.24140000
O	1.88140000	15.05410000	3.42690000	O	-3.21870000	-1.48990000	-16.35840000
O	4.19150000	1.02540000	14.12100000	O	-1.55490000	-1.04870000	-14.34540000
O	0.11810000	14.54730000	1.51370000	Zr	-2.93300000	0.25330000	-15.13640000
Zr	2.87870000	2.24840000	13.12070000	C	5.91640000	9.10300000	-1.51400000
Zr	1.50110000	13.25720000	2.31330000	C	6.85390000	8.07580000	-1.66880000
C	-4.34810000	9.68830000	1.82720000	C	3.21110000	13.03260000	-3.62170000
C	-5.40540000	8.78890000	1.99290000	C	0.41020000	16.25250000	-2.97930000
C	-8.83040000	5.98510000	1.45140000	C	4.08520000	16.11040000	-0.71900000
C	-7.80670000	6.92410000	1.29800000	C	9.82150000	4.76960000	-1.13770000
O	-12.21660000	4.36400000	4.47130000	C	8.94660000	5.85160000	-0.98850000
O	-12.97160000	4.45080000	0.97440000	O	13.68000000	2.52810000	-0.57790000
O	-2.51650000	11.63360000	0.91600000	O	12.99050000	2.66590000	-4.08870000
O	-2.35240000	15.21690000	0.83290000	O	4.46340000	14.82590000	-0.79790000
O	-14.34010000	4.55440000	3.09860000	O	4.26160000	11.24780000	-0.73060000
O	-10.85550000	4.24750000	2.32710000	O	11.58570000	2.73090000	-1.97390000
O	-2.86160000	13.40650000	-0.86600000	O	15.08840000	2.45570000	-2.67990000
O	-2.02900000	13.44560000	2.61160000	O	4.78440000	13.04680000	0.97940000
O	-0.01170000	12.08510000	1.56820000	O	3.95020000	13.02580000	-2.50220000
O	-11.33830000	2.01250000	3.66340000	O	14.58200000	0.18390000	-1.41360000
O	1.33810000	1.30730000	12.14150000	O	1.93450000	14.38650000	-1.45560000
Zr	-12.69890000	3.22320000	2.71600000	Zr	13.23740000	1.41420000	-2.36050000
Zr	-1.28920000	13.36590000	0.59700000	Zr	3.21450000	13.10670000	-0.48570000
O	-14.24190000	2.26810000	1.75750000	C	-0.43500000	4.88330000	-8.73920000
C	15.44290000	-1.01780000	-5.99310000	C	-0.21750000	5.83520000	-7.74360000
C	12.70310000	2.25850000	-5.33430000	C	-0.28160000	9.36940000	-5.19920000
C	16.28250000	1.89940000	-2.93230000	C	-0.58590000	8.37330000	-6.12750000
O	16.62240000	0.60680000	-3.04740000	O	1.87960000	13.09430000	-3.77300000
O	16.31380000	-2.96220000	-3.12560000	O	-1.59460000	13.30460000	-2.93800000
O	16.80820000	-1.24530000	-1.32940000	O	-1.96550000	3.58540000	-10.99630000
O	16.12920000	-1.10790000	-4.84400000	O	-2.72720000	3.74000000	-14.49980000
O	14.11460000	0.27790000	-3.82980000	O	-4.11890000	3.71450000	-12.37250000
Zr	15.30860000	-1.08230000	-2.85880000	O	-0.61720000	3.62530000	-13.11370000
C	8.22410000	-0.99030000	-6.95360000	O	0.23920000	14.98930000	-3.39710000
C	7.08430000	-0.88910000	-7.75710000	O	0.03790000	11.40800000	-3.29800000
C	-0.07890000	0.19680000	-16.44060000	O	1.80890000	11.92610000	-1.40670000
C	-2.98330000	3.33020000	-15.75110000	O	-0.99970000	1.31960000	-11.85230000
C	0.60510000	3.13550000	-13.36990000	O	11.70830000	0.47680000	-3.36020000
C	3.54370000	0.41880000	-10.13290000	Zr	-2.40750000	2.48420000	-12.78720000
C	4.71900000	0.33900000	-9.38010000	Zr	0.42100000	13.21500000	-2.20080000
O	14.12290000	-0.89740000	-6.19960000	O	-3.88950000	1.47330000	-13.78890000
O	10.61540000	-0.65980000	-5.49590000	O	1.56470000	16.75480000	1.71980000
O	1.01360000	1.86380000	-13.49200000	O	0.72650000	16.72100000	-1.76270000
O	0.90250000	-1.70940000	-13.57470000	O	-0.59450000	16.83720000	0.39520000
O	1.28320000	0.04790000	-11.76680000	O	2.88450000	16.63800000	-0.43700000
O	0.61250000	0.13480000	-15.29270000	O	2.50850000	14.40700000	0.94000000
O	12.50660000	1.01980000	-5.81070000	Zr	1.08360000	15.55370000	0.00510000
O	12.23070000	-2.54680000	-5.89790000	O	-0.45580000	14.52290000	-0.88150000
O	13.90460000	-2.17530000	-3.88530000	H	-0.62650000	-16.92080000	4.14710000

H	2.72980000	-17.21660000	-0.07220000	O	7.83750000	-8.14030000	-2.54210000
H	-1.48640000	-17.08970000	-3.43700000	H	-2.60160000	-7.35130000	-8.38090000
H	-4.84290000	-16.79650000	0.78560000	H	-0.97380000	-8.75060000	-7.29330000
H	2.92920000	-3.89700000	16.92310000	O	-9.87800000	1.71700000	-5.66230000
H	5.97920000	-4.24530000	12.47090000	O	-9.14100000	-0.65830000	-6.97640000
H	-12.42200000	-2.98130000	6.40880000	O	5.52490000	-1.81800000	4.92350000
H	-17.38880000	1.30930000	-0.25050000	H	3.40330000	-1.01120000	-6.53180000
H	-16.93470000	-2.57770000	3.46770000	O	-1.26730000	5.51520000	-3.85410000
H	-0.41170000	0.29210000	17.57630000	O	3.15740000	5.77350000	4.33350000
H	3.71220000	3.69550000	16.86160000	H	-5.16210000	4.92080000	2.11300000
H	-0.70210000	4.12840000	13.78060000	H	6.05990000	4.29630000	-1.94650000
H	-15.82790000	1.13380000	7.22380000	H	5.22640000	5.63980000	0.08630000
H	-16.28910000	5.02520000	3.51830000	H	-4.18570000	6.21990000	0.10010000
H	17.49170000	-1.34260000	0.59930000	H	5.04250000	0.70800000	-5.53140000
H	16.43910000	-5.00440000	-3.22880000	O	6.41890000	0.39450000	3.42230000
H	-6.96460000	0.40760000	-15.85800000	O	1.03740000	4.41320000	5.59740000
H	-3.34020000	-3.50170000	-16.72500000	O	-3.34650000	5.45030000	-5.77050000
H	-6.35150000	-3.54780000	-12.24130000	P	-2.91310000	5.10960000	-4.14240000
H	6.76530000	3.34500000	12.42850000	O	-3.16020000	3.46630000	-3.82950000
H	-13.35400000	4.80510000	-1.00670000	O	-3.79230000	5.92080000	-3.21820000
H	-6.09460000	4.07230000	-11.96560000	P	7.02930000	-0.36290000	-10.29110000
H	2.06050000	17.07890000	3.68080000	O	6.56200000	-1.15190000	-11.71290000
H	-2.54560000	17.25610000	0.85860000	O	8.39340000	0.25790000	-10.48750000
H	16.04580000	-1.04680000	-6.89000000	H	6.22190000	-0.43160000	-12.30150000
H	12.61560000	3.04960000	-6.06590000	P	-1.09950000	-4.24500000	-4.25930000
H	17.09550000	2.59990000	-3.06290000	O	-2.07110000	-3.10340000	-4.44120000
H	0.52370000	0.20340000	-17.33810000	O	-0.07230000	-4.19010000	-3.15900000
H	-3.11010000	4.12260000	-16.47550000	P	-10.31020000	0.59550000	-6.88850000
H	0.27200000	17.00870000	-3.73940000	O	-11.66200000	-0.00140000	-6.57000000
H	4.86770000	16.83080000	-0.91260000	O	-10.38820000	1.39980000	-8.37480000
H	13.42740000	-4.84430000	1.24280000	H	-10.30950000	0.68350000	-9.05420000
H	14.07420000	2.75660000	1.41930000	P	-7.90910000	9.41460000	1.99260000
H	-11.76960000	4.62350000	6.45360000	O	-9.07000000	9.39960000	2.96060000
H	-1.48910000	-3.46260000	13.84430000	O	-7.83720000	10.92100000	1.22600000
H	7.05570000	-0.49590000	16.20880000	H	-7.39070000	11.51620000	1.87960000
H	5.55370000	13.02900000	2.87790000	P	-9.43170000	-8.24070000	0.82690000
H	-1.85520000	13.49050000	4.65220000	P	8.08330000	-9.39950000	-1.40060000
H	3.77460000	12.98020000	-4.54280000	P	9.42360000	8.32930000	-1.57830000
H	2.50000000	-13.47960000	-3.96650000	O	-10.74010000	-7.91390000	0.14420000
H	-4.21560000	-12.88440000	4.45880000	O	-9.47080000	-9.84190000	1.37180000
H	-13.98450000	-2.79800000	-1.05610000	O	9.53280000	-9.41320000	-0.97200000
H	1.13980000	-3.74060000	-13.69420000	O	7.69640000	-10.88230000	-2.11760000
H	11.99290000	-4.55210000	-6.24270000	O	9.54520000	9.79740000	-0.74640000
H	-3.63330000	13.40560000	-2.76360000	O	10.59760000	8.18930000	-2.52000000
H	3.35760000	-13.31570000	3.61260000	H	7.53590000	-11.49640000	-1.35740000
H	-5.07250000	-13.07390000	-3.11930000	H	9.20450000	10.47680000	-1.38150000
H	1.37860000	3.87950000	-13.49950000	H	-9.26880000	-10.38680000	0.56980000
H	1.54170000	-7.43690000	8.56990000	P	-3.24590000	0.47400000	5.15370000
H	-0.62690000	-8.19160000	7.40680000	O	-1.76630000	1.28440000	5.02250000
O	-8.14430000	-8.05260000	-0.29530000	O	-3.55100000	-0.22430000	3.84830000
O	-9.21620000	-7.19520000	2.17390000	H	-1.91780000	1.97780000	4.33170000
H	-6.85790000	-0.42370000	8.88530000	P	2.11330000	4.41450000	4.25790000
H	-5.33640000	1.39060000	9.88200000	O	3.04060000	3.00150000	4.27570000
O	7.08570000	-9.15090000	-0.02560000	O	1.31520000	4.47330000	2.97640000

H	3.59880000	3.07710000	5.09030000	H	1.05030000	-2.19110000	1.16370000
P	1.33160000	-4.35170000	4.35250000	C	0.70740000	0.85660000	2.63140000
O	2.55970000	-3.20030000	4.52030000	H	-0.06760000	2.61340000	1.64700000
O	0.63570000	-4.14640000	3.02810000	H	1.43540000	-1.05460000	3.31640000
H	3.04290000	-3.46330000	5.34370000	H	0.86690000	1.35240000	3.58460000
P	5.13930000	-0.72860000	3.65390000	C	-1.10980000	-10.20060000	-2.86290000
O	4.91440000	-1.50670000	2.37770000	C	-1.97910000	-3.01040000	-9.96550000
O	3.72800000	0.11380000	4.04860000				
H	3.85220000	0.39290000	4.99030000				
H	-3.19610000	3.03640000	-4.72100000	(E)-syn-TS-S			
C	0.01110000	-1.16940000	-1.11980000	H	1.58290000	-6.49070000	10.02550000
N	-0.49050000	-2.43550000	-1.09250000	H	-0.18990000	-10.53970000	4.71960000
C	-1.20620000	-3.10830000	-0.07540000	H	-9.72400000	-2.47340000	6.24200000
C	-1.05680000	-4.50720000	-0.03290000	H	-4.48840000	-10.62710000	-1.91460000
C	-2.01260000	-2.46750000	0.87790000	H	-9.77250000	-6.76050000	0.82020000
C	-1.63910000	-5.23780000	0.99720000	H	-4.99040000	-0.49470000	10.88280000
H	-0.46450000	-4.99550000	-0.80050000	H	6.13770000	0.69950000	10.12440000
C	-2.59240000	-3.21630000	1.90300000	H	7.68400000	0.98790000	8.25270000
H	-2.16770000	-1.39650000	0.83740000	H	6.63110000	-9.73990000	0.11100000
C	-2.39060000	-4.59390000	1.98420000	H	10.79460000	-4.39130000	-1.91210000
H	-1.48420000	-6.31240000	1.03830000	H	2.43720000	0.44710000	-7.54140000
H	-3.19850000	-2.71230000	2.65050000	H	-2.15830000	-1.71990000	7.86220000
H	-2.80640000	-5.15850000	2.81310000	H	2.19490000	-7.82880000	2.36370000
C	-3.87010000	-1.39790000	-1.90150000	H	-0.24130000	-7.44010000	-3.38840000
C	-4.22640000	-0.30280000	-1.19460000	H	7.89220000	-2.06040000	0.27440000
C	-2.06930000	-0.04130000	-2.53910000	H	-7.24330000	-3.47940000	-0.40300000
N	-2.76530000	-1.23780000	-2.70050000	O	-3.86340000	-1.86520000	5.90900000
H	-2.43650000	-2.00060000	-3.35330000	O	2.45400000	-5.99730000	4.18710000
H	-4.36870000	-2.35870000	-1.89970000	O	-0.72930000	-5.45170000	-4.86760000
H	-5.05570000	-0.19400000	-0.51120000	H	6.37410000	-3.97480000	0.29840000
S	-3.16020000	1.04900000	-1.55660000	H	-5.39560000	-5.03810000	-0.75140000
C	-1.42740000	0.58920000	-3.75350000	H	-2.14570000	-8.05820000	0.63670000
C	-0.62090000	1.72970000	-3.61220000	H	3.54290000	-7.18150000	-1.49150000
C	-1.63400000	0.05950000	-5.03510000	H	7.63200000	1.26270000	2.51900000
C	-0.04360000	2.33670000	-4.72600000	H	-7.59710000	-1.39520000	-2.27800000
H	-0.45010000	2.15750000	-2.62720000	H	0.22930000	-3.28450000	7.46210000
C	-1.04090000	0.66340000	-6.14560000	H	0.48500000	-2.04870000	-7.58310000
H	-2.23670000	-0.83090000	-5.16960000	H	-4.05680000	-6.54720000	0.87200000
C	-0.24940000	1.80170000	-5.99980000	H	5.10870000	-5.30830000	-1.51710000
H	0.56830000	3.22540000	-4.59830000	H	-5.99890000	-1.12530000	-4.10580000
H	-1.20650000	0.23460000	-7.12950000	O	0.21490000	-4.66520000	5.26570000
H	0.20670000	2.26790000	-6.86880000	O	0.94600000	-3.80000000	-5.80950000
H	-0.27480000	-3.04560000	-1.91360000	C	4.27660000	-13.01960000	2.18400000
H	-1.05680000	-0.35120000	-1.76300000	C	1.55310000	-16.35720000	1.88530000
C	1.09670000	-0.98330000	-2.17400000	C	4.65980000	-15.84020000	-1.06650000
H	2.01890000	-1.46000000	-1.81710000	O	2.63540000	-14.30300000	0.22960000
H	0.81820000	-1.45290000	-3.12110000	H	-0.24500000	-4.88050000	-10.79750000
H	1.30380000	0.07460000	-2.34350000	H	1.95620000	-9.69270000	-6.37840000
C	0.24290000	-0.44750000	0.18210000	H	-6.01070000	-0.85440000	-9.88650000
C	-0.03950000	0.91560000	0.33230000	C	-1.64660000	-13.19550000	-4.08870000
C	0.80160000	-1.14080000	1.26930000	C	1.69190000	-15.92660000	-4.20420000
C	0.18460000	1.56200000	1.54890000	C	-1.41090000	-16.44680000	-1.25010000
H	-0.46410000	1.47540000	-0.49290000	O	1.71040000	-16.46980000	-2.97760000
C	1.02460000	-0.49530000	2.48200000	O	1.62990000	-16.72230000	0.59660000
				O	3.45180000	-16.41920000	-1.13760000

O	-0.11050000	-16.77570000	-1.24340000	C	0.32680000	-9.59570000	4.59660000
O	0.24490000	-14.37360000	-2.30240000	C	0.31540000	-8.67500000	5.64530000
Zr	1.55030000	-15.41970000	-1.11010000	O	-0.54880000	-13.53930000	2.49130000
H	10.74260000	-0.28910000	5.08180000	O	3.01180000	-13.17640000	2.60320000
H	9.10480000	-0.63790000	6.85590000	O	1.04380000	-4.37340000	11.27210000
H	1.33460000	4.80230000	10.78830000	O	1.29200000	-4.66570000	14.84290000
H	1.07020000	6.61560000	9.16900000	O	2.94750000	-4.38300000	12.94560000
H	-1.21610000	9.79620000	6.74800000	O	-0.61730000	-4.66370000	13.17420000
H	-0.96350000	7.90690000	8.27390000	O	1.41320000	-15.13820000	2.42770000
C	4.16310000	-1.03950000	16.18890000	O	1.03460000	-11.57190000	2.65250000
C	1.34780000	-4.30830000	16.13450000	O	-0.06400000	-12.10580000	0.32520000
C	4.16770000	-3.82750000	12.89200000	O	-0.31600000	-2.26470000	12.11420000
O	2.31190000	-2.25970000	14.39670000	O	-11.69050000	-2.55520000	1.95810000
H	-3.35110000	1.17450000	-7.15950000	Zr	1.07900000	-3.34540000	13.16240000
H	3.45280000	-1.50690000	7.56690000	Zr	1.26100000	-13.27900000	1.36330000
H	-1.50670000	7.60730000	-1.82270000	H	-10.70500000	0.31130000	-4.74090000
H	0.32620000	7.38640000	3.51430000	C	-4.38950000	-9.74320000	-1.29600000
H	-7.70190000	1.97660000	1.69210000	C	-5.49100000	-8.89270000	-1.14980000
H	7.28570000	3.72070000	-0.87590000	C	-16.34700000	-1.36180000	-1.92990000
H	-4.97730000	0.88710000	-5.35680000	C	-13.02720000	-4.07760000	-2.40590000
H	2.23220000	7.81670000	1.52060000	C	-15.86020000	-4.66530000	0.80470000
H	-3.63370000	7.37440000	0.07860000	C	-8.82710000	-6.37520000	0.45850000
H	7.44180000	2.34220000	-3.13490000	C	-7.78100000	-7.27540000	0.23660000
H	-7.49410000	0.01940000	3.51570000	O	-12.90890000	-4.64790000	-1.19730000
H	-0.83780000	2.14800000	8.17090000	O	-12.66160000	-4.98100000	2.35680000
H	-2.92710000	3.85850000	-7.72400000	O	-1.99360000	-15.24070000	-1.17920000
O	-5.40910000	0.32370000	5.03770000	O	-2.34130000	-11.67940000	-0.96350000
H	-6.38840000	9.60260000	2.54420000	O	-11.00980000	-4.62350000	0.47080000
O	-8.21740000	7.75800000	2.66810000	O	-14.56500000	-4.99330000	0.68680000
H	-10.89090000	4.58440000	0.40190000	O	-2.12940000	-13.34220000	-2.84570000
O	-9.48250000	6.76480000	0.35880000	O	-2.21800000	-13.57970000	0.72460000
C	1.29410000	-6.10610000	9.05540000	O	0.18720000	-14.54760000	0.15510000
C	1.32280000	-6.96860000	7.95600000	O	-14.30570000	-2.56630000	-0.34700000
C	-1.79270000	-13.62580000	1.99620000	Zr	-12.89990000	-3.63700000	0.69830000
C	-9.86110000	-1.29320000	3.78180000	Zr	-0.99150000	-13.34760000	-1.02340000
C	-2.33940000	-1.06340000	10.49810000	C	-1.91060000	-1.51320000	16.58630000
C	0.90860000	-3.82930000	10.04930000	C	0.90110000	1.75850000	16.64210000
C	1.02400000	-10.27530000	2.29530000	C	-2.34660000	1.76060000	13.79690000
C	-12.61850000	-4.64550000	3.65480000	O	-0.62330000	-1.45080000	16.95870000
C	-1.90530000	-4.30680000	13.29200000	O	2.94060000	-1.17120000	16.72560000
C	-9.78890000	-4.06400000	0.42700000	O	1.28850000	-3.09030000	16.69370000
C	-2.03110000	-10.38680000	-0.76640000	O	1.02760000	0.46950000	16.99150000
C	-8.74420000	-1.24650000	4.74950000	O	-0.31730000	-0.00460000	14.76170000
C	-3.43200000	-1.09150000	9.50000000	Zr	1.07420000	-1.21790000	15.66260000
C	0.91040000	-4.76350000	8.89790000	C	-8.83600000	-1.91030000	5.98240000
C	0.98820000	-9.29560000	3.39820000	C	-7.77350000	-1.87000000	6.88780000
C	-8.65850000	-4.99950000	0.22590000	C	-15.93450000	-1.92290000	4.13740000
C	-3.17400000	-9.45890000	-0.65360000	C	-13.17360000	1.40190000	4.25420000
C	-6.59840000	-1.16310000	6.58230000	C	-16.42760000	1.38040000	1.41030000
C	-5.49520000	-1.11390000	7.57150000	C	-4.74910000	-0.76890000	9.86330000
C	0.97990000	-6.50600000	6.67460000	C	-5.76950000	-0.78140000	8.90890000
C	0.97620000	-7.44050000	5.52390000	O	-14.65070000	-1.84050000	4.51770000
C	-6.52490000	-6.80030000	-0.19720000	O	-11.08660000	-1.49860000	4.29530000
C	-5.37890000	-7.72340000	-0.36740000	O	-2.45260000	-3.08930000	13.42760000

O	-2.71090000	0.47100000	13.73100000	O	13.40280000	-1.90420000	-2.77630000
O	-2.69980000	-1.15750000	11.79070000	O	13.58990000	-2.31770000	0.77090000
O	-2.45640000	-1.44970000	15.36260000	O	4.60350000	-10.98220000	-0.72010000
O	-12.70720000	-3.43920000	4.23470000	O	4.98770000	-14.54340000	-0.96530000
O	-13.03050000	0.10990000	4.58610000	O	15.28070000	-1.94590000	-1.07890000
O	-0.13880000	-2.45270000	14.55660000	O	11.71160000	-2.25710000	-0.92810000
O	-14.36710000	-0.35730000	2.34290000	O	4.76120000	-12.89000000	0.93960000
Zr	-1.40170000	-1.21720000	13.50630000	O	4.84830000	-12.63770000	-2.62930000
Zr	-12.95390000	-1.55580000	3.23180000	O	2.44540000	-11.68750000	-2.06140000
O	-16.43230000	-3.46130000	0.95470000	O	12.01320000	0.16870000	-1.89970000
O	-16.76520000	0.08620000	1.30880000	O	0.66040000	-0.01370000	-11.98520000
O	-16.71690000	-1.52220000	-0.65020000	Zr	13.39930000	-0.93340000	-0.86030000
O	-16.47520000	-1.85240000	2.91160000	Zr	3.62340000	-12.88700000	-0.88280000
O	-14.13960000	-2.79530000	2.10140000	C	-0.01120000	-4.62670000	-9.76630000
Zr	-15.41950000	-1.57000000	1.06200000	C	0.16410000	-5.67290000	-8.86450000
H	10.06070000	0.52860000	-6.04170000	C	-4.06230000	0.96030000	-15.85080000
O	8.30670000	0.37370000	-7.95640000	C	-0.61530000	-1.59340000	-16.34760000
H	4.50420000	10.97140000	-0.35550000	C	-3.40210000	-2.32580000	-13.13330000
O	6.66680000	9.57800000	-0.73660000	C	1.41590000	-8.81260000	-6.03820000
H	9.90510000	6.58960000	1.00750000	C	1.28680000	-7.73810000	-6.91540000
O	8.09880000	8.41700000	1.39320000	O	3.18000000	-12.69320000	-4.39630000
C	16.39330000	1.29080000	2.31750000	O	-0.38280000	-13.02940000	-4.50690000
C	13.62200000	-2.01140000	2.07650000	O	-0.45650000	-2.15980000	-15.14200000
C	16.49580000	-1.37760000	-1.07640000	O	-0.19880000	-2.48350000	-11.58550000
O	14.59550000	0.11360000	0.44010000	O	1.44230000	-2.05820000	-13.46650000
H	4.89010000	2.40540000	-10.51020000	O	-2.09250000	-2.58910000	-13.25700000
O	7.00760000	2.63340000	-9.02360000	O	1.24330000	-11.07570000	-4.31400000
H	0.61810000	5.89040000	-9.07640000	O	1.57530000	-14.64260000	-4.57520000
H	0.47720000	7.42400000	-7.16930000	O	2.69300000	-14.12940000	-2.22780000
H	-1.18420000	10.84660000	-4.66560000	O	-1.95440000	-0.15160000	-14.28280000
H	-1.21640000	9.23710000	-6.49660000	Zr	-0.49370000	-1.15430000	-13.24440000
C	6.29230000	-8.77980000	-0.25880000	Zr	1.37000000	-12.95080000	-3.26810000
C	7.19740000	-7.71430000	-0.28700000	C	9.70930000	-0.02430000	4.89530000
C	4.42310000	-12.59660000	-3.90100000	C	8.77250000	-0.22810000	5.90980000
C	2.41100000	1.33320000	-10.13670000	C	10.30850000	0.72880000	2.57980000
C	9.98640000	1.42160000	-3.47990000	C	3.72130000	-0.56530000	10.10450000
C	13.30340000	-1.30620000	-3.97290000	C	2.09840000	13.22510000	4.02980000
C	4.03770000	-9.76240000	-0.72810000	C	13.08660000	4.02200000	2.81230000
C	10.41260000	-1.94360000	-0.78320000	C	-0.65240000	9.86910000	4.07260000
C	2.62280000	-1.42120000	-13.48670000	C	0.45380000	2.22940000	10.56050000
C	3.52290000	1.40320000	-9.15970000	C	3.72480000	2.23520000	13.41830000
C	8.89160000	1.44390000	-4.46990000	C	2.08070000	10.43990000	0.76480000
C	0.07920000	-3.28970000	-9.34160000	C	9.88160000	4.10120000	-0.10330000
C	0.88680000	-8.73780000	-4.74010000	C	9.31500000	0.50740000	3.65640000
C	4.97030000	-8.61320000	-0.70280000	C	4.67030000	-0.41130000	8.98310000
C	9.46910000	-3.08310000	-0.80780000	C	-0.47580000	8.73540000	5.00830000
C	5.67960000	1.46460000	-7.33540000	C	0.28220000	3.33330000	9.59470000
C	6.80370000	1.48250000	-6.36830000	C	3.22530000	9.51570000	0.61050000
C	0.44570000	-5.44290000	-7.50940000	C	8.74600000	5.04030000	0.03600000
C	0.61320000	-6.56050000	-6.55430000	C	7.41960000	0.09020000	5.70960000
C	6.78010000	-6.44580000	-0.74420000	C	6.45520000	-0.07720000	6.82290000
C	7.71660000	-5.29680000	-0.76770000	C	-0.19620000	6.54820000	6.77360000
C	9.83740000	-4.29520000	-1.41400000	C	-0.02150000	5.42600000	7.72630000
C	8.98090000	-5.40000000	-1.38820000	C	5.44240000	7.78170000	0.38620000

C	6.59130000	6.85280000	0.25970000	C	-4.89750000	8.63820000	1.30640000
C	5.88060000	0.27500000	9.16170000	C	-6.44740000	-0.12160000	-6.58740000
C	6.76200000	0.44250000	8.09180000	C	-7.43210000	-0.27620000	-5.48860000
O	11.59790000	0.75910000	2.95930000	C	-1.39610000	7.49740000	-5.22240000
O	15.16290000	1.12260000	2.82470000	C	-1.31700000	6.53270000	-6.34370000
O	4.27180000	1.01780000	13.28290000	C	-7.65900000	5.34000000	1.16440000
O	4.53030000	-2.53770000	12.96200000	C	-6.71740000	6.48360000	1.21390000
O	4.52950000	-0.90580000	14.90540000	C	-3.06590000	-8.29130000	0.11740000
O	4.25540000	-0.59130000	11.33830000	C	4.55500000	-7.34400000	-1.14170000
O	13.54400000	-0.81700000	2.68210000	C	3.14030000	8.18830000	1.06200000
O	13.21400000	2.72130000	3.11490000	C	-4.57450000	7.46280000	0.60820000
O	1.96000000	0.38260000	12.15440000	C	7.62880000	1.95190000	-4.12770000
O	11.93260000	2.32430000	0.84330000	C	7.96110000	0.82950000	3.45570000
O	0.22450000	11.96900000	2.30460000	C	-7.57510000	-0.52810000	4.44690000
Zr	3.21940000	-0.85310000	13.20440000	C	-7.93930000	-0.96220000	-3.21000000
Zr	13.32110000	1.09090000	1.72040000	C	-0.40300000	3.11650000	8.38790000
C	-4.28120000	0.66240000	-7.37180000	C	0.54410000	-4.30910000	7.61770000
C	4.36740000	-0.94590000	7.71950000	C	0.37510000	-3.04860000	-7.99380000
C	3.37270000	0.89120000	-7.85900000	C	-2.17560000	4.62800000	-7.59060000
C	-3.16000000	-1.43920000	8.16500000	C	-4.15680000	-7.43210000	0.25690000
C	-1.44680000	7.97650000	-2.83910000	C	5.45040000	-6.27240000	-1.16040000
C	1.64630000	-8.06150000	3.26880000	C	4.23750000	7.33090000	0.95030000
C	0.02610000	7.50530000	4.54840000	C	-5.47570000	6.39650000	0.56300000
C	0.21860000	-7.56580000	-4.36470000	C	6.59790000	1.97690000	-5.07000000
C	-8.07700000	2.95720000	1.42690000	C	7.01330000	0.61190000	4.46210000
C	8.20460000	-2.98050000	-0.20420000	C	-6.50270000	-0.48940000	5.34450000
C	-7.40680000	-4.53260000	-0.21050000	C	-7.02470000	-0.81060000	-4.25520000
C	7.46470000	4.68610000	-0.41920000	C	-0.55130000	4.14620000	7.45290000
C	-5.21280000	0.50350000	-6.34240000	C	0.59370000	-5.16160000	6.51190000
C	5.24350000	-0.77770000	6.64140000	C	0.56100000	-4.10290000	-7.10340000
C	4.43920000	0.92480000	-6.95710000	C	-2.27860000	5.50930000	-6.50730000
C	-4.17310000	-1.43930000	7.20160000	O	-2.31990000	0.55440000	-9.41560000
C	-1.50250000	7.05200000	-3.88880000	O	2.42770000	-0.65750000	9.75840000
C	1.64440000	-7.13120000	4.31510000	O	1.19020000	1.09650000	-9.62880000
C	0.15400000	6.41260000	5.41270000	O	-1.10230000	-0.94790000	9.99180000
C	0.07320000	-6.50700000	-5.25670000	O	-1.09210000	9.81150000	-0.75670000
C	-7.20590000	4.04810000	1.47880000	O	1.06260000	-9.75380000	1.05940000
C	7.33780000	-4.07570000	-0.18590000	O	-0.72620000	9.54200000	2.77260000
C	-6.35100000	-5.42370000	-0.41590000	O	0.89110000	-9.53280000	-2.48800000
C	6.40000000	5.58260000	-0.30780000	O	-9.80100000	0.77570000	0.89680000
C	-3.60530000	0.40660000	-9.77270000	O	9.86870000	-0.72870000	-0.60170000
C	-10.26040000	-0.76190000	-2.27920000	O	-9.47130000	-2.76290000	0.53520000
C	-4.59520000	13.04640000	-1.40900000	O	9.55760000	2.80690000	-0.25410000
C	-1.29470000	10.33130000	-1.97800000	O	-0.81300000	-9.83550000	-0.63770000
C	-1.04440000	3.84460000	-9.65750000	O	2.73100000	-9.45740000	-0.77700000
C	-13.60900000	1.96440000	-1.80530000	O	0.86940000	9.86870000	0.87100000
C	-10.35650000	1.99190000	1.02640000	O	-2.66730000	9.48860000	1.14060000
C	-3.96410000	9.78340000	1.32660000	O	9.61550000	1.26480000	-2.19870000
C	-4.26010000	3.68040000	-12.48930000	O	9.80780000	0.87450000	1.34190000
C	-4.56380000	0.19520000	-8.66690000	O	-9.51980000	-1.12070000	2.49490000
C	-9.28220000	-0.57990000	-3.37530000	O	-9.74340000	-0.85300000	-1.04390000
C	-1.33770000	9.35660000	-3.09560000	O	0.48560000	0.99670000	10.03000000
C	-1.13460000	4.75940000	-8.51860000	O	0.77950000	-2.53120000	9.73550000
C	-9.42040000	3.13650000	1.05760000	O	-0.29180000	-0.95110000	-9.72100000

O	-0.89360000	2.54930000	-9.34520000	O	-13.57180000	2.29980000	-0.50690000
O	12.14690000	-0.11290000	0.54430000	O	-4.52190000	10.99110000	1.51980000
O	2.13970000	-2.07060000	11.95260000	O	-4.89760000	14.54660000	1.81310000
O	2.39050000	-11.86240000	0.39730000	O	-15.21750000	1.95830000	1.38280000
O	-12.08920000	0.11780000	-0.25020000	O	-11.66000000	2.30070000	1.13370000
O	-2.11990000	2.04800000	-11.59080000	O	-4.91110000	12.89830000	-0.11350000
O	-2.47870000	11.89370000	0.10660000	O	-4.52760000	12.63890000	3.43410000
Zr	-1.01930000	10.85950000	1.11000000	O	-2.21490000	11.70290000	2.54830000
Zr	1.08250000	-10.82650000	-0.79400000	O	-11.92430000	-0.11090000	2.19870000
Zr	-10.81760000	-1.11090000	0.79090000	O	-0.49520000	0.18920000	12.31750000
Zr	10.89810000	1.15000000	-0.48310000	Zr	-13.33160000	0.95700000	1.15250000
Zr	-0.65240000	0.91670000	-10.71220000	Zr	-3.54350000	12.90180000	1.54300000
Zr	0.74430000	-0.85930000	11.06680000	O	-14.53620000	-0.12900000	-0.10530000
C	-9.68400000	-0.02170000	-4.59890000	C	16.06950000	1.99890000	-3.73730000
C	-8.77740000	0.12320000	-5.65380000	C	12.75450000	4.72580000	-3.24040000
C	-5.78260000	-0.45870000	-8.90410000	C	15.96770000	4.66000000	-0.34570000
C	-6.72380000	-0.61200000	-7.88220000	O	16.53250000	3.45510000	-0.51540000
O	-11.55450000	-0.82060000	-2.64270000	O	16.84230000	-0.08840000	-0.94400000
O	-15.12530000	-1.19480000	-2.45830000	O	16.78230000	1.47660000	1.04710000
O	-4.03250000	-1.15190000	-12.97780000	O	16.59220000	1.89170000	-2.50650000
O	-4.53510000	2.37220000	-12.60380000	O	14.25090000	2.83250000	-1.70700000
O	-4.41990000	0.77660000	-14.57110000	Zr	15.50770000	1.57420000	-0.67940000
O	-4.13200000	0.43880000	-11.00960000	C	9.10140000	0.95050000	-5.76650000
O	-13.51650000	0.75830000	-2.38500000	C	8.07460000	0.97190000	-6.71630000
O	-13.17010000	-2.78550000	-2.73750000	C	1.96610000	1.85780000	-16.21840000
O	-1.77410000	-0.38220000	-11.83620000	C	-1.48770000	4.41520000	-15.72520000
O	-11.86250000	-2.32440000	-0.49100000	C	1.76110000	4.58620000	-12.89360000
O	-0.00680000	-11.93120000	-2.13520000	C	4.75370000	1.97470000	-9.52580000
Zr	-3.11140000	0.78520000	-12.86810000	C	5.82920000	1.99710000	-8.63270000
Zr	-13.26910000	-1.12380000	-1.38020000	O	14.79070000	1.93630000	-4.13740000
C	0.79990000	4.60850000	9.86660000	O	11.22820000	1.55820000	-3.97600000
C	0.65160000	5.64300000	8.94040000	O	2.39070000	3.41110000	-13.04120000
C	-3.94030000	12.59540000	4.63930000	O	2.89570000	-0.11190000	-13.38300000
C	-1.21490000	15.93920000	4.60140000	O	2.75080000	1.50650000	-11.42600000
C	-4.56930000	15.84560000	1.87690000	O	2.51120000	1.80750000	-14.99370000
C	-0.82220000	8.86390000	6.36300000	O	12.83740000	3.53110000	-3.84530000
C	-0.68240000	7.78250000	7.23520000	O	13.17740000	-0.00580000	-4.27650000
O	-2.64400000	12.69840000	4.96860000	O	14.46620000	0.39770000	-2.00270000
O	0.90070000	13.05180000	4.60900000	O	0.12880000	2.63880000	-14.18100000
O	0.77780000	2.31240000	15.42660000	Zr	1.46740000	1.47490000	-13.14650000
O	0.55750000	2.58060000	11.85410000	Zr	13.07540000	1.62530000	-2.88280000
O	-1.12520000	2.31370000	13.74840000	O	0.68680000	1.71770000	-16.59720000
O	2.43690000	2.59130000	13.53740000	O	-2.85150000	1.18800000	-16.38180000
O	-0.73230000	11.09290000	4.62450000	O	-1.33760000	3.21650000	-16.30830000
O	-1.03920000	14.65450000	4.94530000	O	-0.82890000	-0.30990000	-16.67370000
O	2.13290000	0.18780000	14.60290000	O	0.47620000	0.21390000	-14.42970000
O	-2.45570000	14.14510000	2.76210000	Zr	-0.99440000	1.34390000	-15.31290000
Zr	0.74240000	1.27120000	13.54850000	C	4.42220000	9.96080000	0.02580000
Zr	-1.00070000	12.97070000	3.61250000	C	5.52790000	9.11110000	-0.07960000
C	-6.12870000	8.71750000	1.97600000	C	1.44020000	13.70180000	-2.01790000
C	-7.03950000	7.65830000	1.92700000	C	-1.87640000	16.40270000	-1.45120000
C	-9.86800000	4.42430000	0.72080000	C	1.46890000	16.49960000	1.27470000
C	-9.00590000	5.52270000	0.78230000	C	8.93440000	6.30320000	0.62110000
O	-13.30330000	1.97090000	3.04620000	C	7.87560000	7.21150000	0.72530000

O	12.99040000	4.62170000	1.61610000	H	-0.56340000 -2.27590000 -17.18440000
O	12.79100000	5.03410000	-1.93520000	H	-4.04830000 -3.19190000 -13.16410000
O	2.04560000	15.29860000	1.11960000	H	4.42970000 3.05460000 13.43480000
O	2.38540000	11.74830000	0.79380000	H	-13.73330000 2.79270000 -2.48880000
O	11.10860000	4.64970000	-0.07210000	H	-5.12190000 4.31910000 -12.35480000
O	14.67360000	4.99590000	-0.23730000	H	-1.20510000 16.63900000 5.42530000
O	2.41380000	13.38080000	2.73510000	H	-5.40100000 16.52160000 2.01810000
O	2.02730000	13.66420000	-0.81220000	H	16.78910000 2.16020000 -4.52780000
O	14.38250000	2.54850000	0.73640000	H	12.64000000 5.56920000 -3.90690000
O	-0.28590000	14.59570000	0.07410000	H	16.66180000 5.48670000 -0.28720000
Zr	12.99780000	3.65420000	-0.30180000	H	2.66470000 2.03900000 -17.02330000
Zr	1.04490000	13.39870000	1.07970000	H	-1.65630000 5.23770000 -16.40620000
C	-0.19080000	5.77920000	-8.36420000	H	-2.03340000 17.21860000 -2.14280000
C	-0.27420000	6.65150000	-7.27910000	H	2.14990000 17.33910000 1.26600000
C	-1.27190000	9.79360000	-4.42940000	H	13.72750000 -2.85640000 2.74260000
C	-1.29020000	8.87360000	-5.47890000	H	13.05660000 4.68900000 3.66250000
O	0.14420000	13.59510000	-2.34720000	H	-13.18560000 2.09000000 5.08790000
O	-3.39810000	13.22300000	-1.98820000	H	-2.61050000 -5.12600000 13.27440000
O	-1.12320000	4.41460000	-10.87090000	H	4.97770000 -1.04120000 16.89960000
O	-1.46020000	4.74970000	-14.42640000	H	2.93800000 13.24090000 4.71050000
O	-3.07950000	4.31750000	-12.51490000	H	-4.61480000 12.45720000 5.47270000
O	0.45140000	4.85130000	-12.77650000	H	2.11470000 13.83900000 -2.85150000
O	-1.80000000	15.18760000	-2.01430000	H	5.20130000 -12.46580000 -4.63990000
O	-1.46410000	11.62460000	-2.30690000	H	-2.57180000 -13.75160000 2.73510000
O	-0.03850000	12.15390000	-0.14300000	H	-13.00360000 -4.76440000 -3.24040000
O	0.31200000	2.41340000	-11.73310000	H	3.48630000 -2.06090000 -13.60410000
O	11.80480000	2.60800000	-1.60430000	H	13.32960000 -1.97440000 -4.82240000
Zr	-1.14670000	3.41600000	-12.77250000	H	-5.43390000 13.01910000 -2.09060000
Zr	-1.49850000	13.32390000	-0.99020000	H	5.01910000 -12.99330000 2.96930000
O	-2.30190000	2.27370000	-14.03040000	H	-2.38980000 -13.21390000 -4.87360000
O	-1.40090000	16.48850000	3.39160000	H	2.40790000 5.45200000 -12.86650000
O	-1.78780000	16.76070000	-0.16120000	H	1.62520000 -7.99810000 8.10380000
O	-3.36680000	16.43410000	1.79260000	H	-0.21030000 -8.92800000 6.55800000
O	0.17620000	16.81830000	1.43850000	O	-6.65680000 -9.18070000 -1.86000000
O	-0.02090000	14.40690000	2.51690000	O	-7.97980000 -8.61780000 0.56540000
Zr	-1.47790000	15.44980000	1.51260000	H	-7.86580000 -2.39960000 7.82820000
O	-2.72030000	14.33110000	0.31940000	H	-6.77640000 -0.52360000 9.21370000
H	1.61280000	-17.17000000	2.59560000	O	8.47900000 -7.91500000 0.22650000
H	5.49730000	-16.52330000	-1.09490000	O	9.36550000 -6.55430000 -2.07310000
H	1.78570000	-16.63150000	-5.01850000	H	0.05260000 -6.69750000 -9.20820000
H	-2.09390000	-17.28160000	-1.32420000	H	1.73050000 -7.80120000 -7.90520000
H	1.45750000	-5.12720000	16.83170000	O	-9.21170000 0.76050000 -6.81760000
H	4.98380000	-4.52650000	12.77370000	O	-7.88880000 -1.33030000 -8.15310000
H	-12.49330000	-5.47390000	4.33800000	O	4.94460000 -1.41140000 5.43420000
H	-17.15790000	-1.36810000	-2.64490000	H	4.30150000 0.51200000 -5.96610000
H	-16.54820000	-5.49860000	0.77440000	O	-1.58250000 5.69180000 -3.58240000
H	-2.61620000	-1.63270000	17.39660000	O	0.73320000 5.24050000 4.92180000
H	0.89840000	2.45810000	17.46630000	H	-6.17760000 3.88540000 1.77800000
H	-3.16240000	2.46160000	13.90550000	H	5.42480000 5.28760000 -0.67600000
H	-16.64170000	-2.06850000	4.94200000	H	4.15020000 6.31560000 1.31760000
H	-17.25780000	2.06190000	1.53280000	H	-5.20950000 5.50630000 0.00600000
H	17.19400000	1.27400000	3.04370000	H	5.63500000 2.38350000 -4.78520000
H	17.32220000	-2.06340000	-1.20030000	O	5.69970000 1.03040000 4.23960000
H	-4.87410000	0.91830000	-16.56350000	O	-1.32360000 3.90540000 6.31520000

O	-3.42430000	5.44940000	-5.71010000	H	0.63380000	-4.71590000	-0.99990000
P	-3.08290000	5.01800000	-4.08220000	C	-2.13760000	-3.82220000	1.54190000
O	-3.02630000	3.33330000	-3.94770000	H	-2.09440000	-1.85340000	0.70920000
O	-4.18470000	5.54360000	-3.19050000	C	-1.62690000	-5.11770000	1.51550000
P	8.29160000	1.51430000	-9.24040000	H	-0.22830000	-6.44410000	0.53820000
O	8.08400000	0.69570000	-10.70640000	H	-2.93220000	-3.56550000	2.23740000
O	9.60640000	2.25970000	-9.26510000	H	-1.99900000	-5.87010000	2.20480000
H	7.75430000	1.38510000	-11.33640000	C	-3.32490000	-1.62350000	-2.29540000
P	-0.13800000	-3.94410000	-4.57440000	C	-3.86210000	-0.62460000	-1.56130000
O	-1.30750000	-3.00760000	-4.77210000	C	-1.64930000	-0.03750000	-2.69720000
O	0.66970000	-3.88270000	-3.30650000	N	-2.17330000	-1.29330000	-2.96710000
P	-9.27180000	-0.31370000	-8.15560000	H	-1.73660000	-1.97080000	-3.65750000
O	-10.51870000	-1.16310000	-8.06290000	H	-3.71120000	-2.62880000	-2.40500000
O	-9.30990000	0.58480000	-9.58870000	H	-4.75730000	-0.65130000	-0.95720000
H	-9.01300000	-0.04720000	-10.29110000	S	-2.91310000	0.84870000	-1.72070000
P	-9.59590000	7.88780000	1.65300000	C	-0.99000000	0.73970000	-3.80510000
O	-10.84120000	7.60010000	2.46010000	C	-0.30460000	1.92790000	-3.51010000
O	-9.68630000	9.45500000	1.02200000	C	-1.08030000	0.31330000	-5.13800000
H	-9.41890000	10.04490000	1.77130000	C	0.25560000	2.69350000	-4.53050000
P	-7.94210000	-9.63770000	-0.81660000	H	-0.21710000	2.26170000	-2.47920000
P	9.67170000	-7.86600000	-1.00770000	C	-0.49910000	1.07530000	-6.15280000
P	7.98950000	9.77030000	0.34140000	H	-1.58990000	-0.61150000	-5.38470000
O	-9.25360000	-9.52400000	-1.55960000	C	0.16030000	2.26820000	-5.85750000
O	-7.71880000	-11.23860000	-0.31720000	H	0.76920000	3.61970000	-4.28890000
O	11.03570000	-7.69460000	-0.37920000	H	-0.57370000	0.73240000	-7.18060000
O	9.63610000	-9.31270000	-1.88400000	H	0.60070000	2.86160000	-6.65420000
O	7.76650000	11.17190000	1.26230000	H	0.43550000	-2.73150000	-1.90140000
O	9.26920000	9.89230000	-0.45380000	H	-0.63480000	-0.26370000	-1.84980000
H	9.48440000	-10.01650000	-1.20390000	C	-0.08810000	-0.18230000	0.30220000
H	7.39180000	11.83400000	0.62820000	C	1.02050000	-9.86050000	-3.78320000
H	-7.38560000	-11.71020000	-1.12190000	C	-0.15040000	-2.16420000	-10.28120000
P	-3.97400000	-0.58340000	4.77200000	H	0.20750000	0.86620000	0.26840000
O	-2.62910000	0.42940000	4.94370000	H	-1.16650000	-0.18840000	0.45310000
O	-3.99380000	-1.15570000	3.37300000	H	0.38530000	-0.65480000	1.17140000
H	-2.85160000	1.23780000	4.41650000	C	1.61720000	-0.46200000	-1.61860000
P	-0.38270000	3.93460000	4.87890000	C	2.41980000	0.53200000	-1.02850000
O	0.46460000	2.47780000	4.73460000	C	2.09260000	-1.08050000	-2.79020000
O	-1.29820000	4.09650000	3.68720000	C	3.65750000	0.87580000	-1.57300000
H	1.05750000	2.45280000	5.52740000	H	2.11260000	1.02660000	-0.11490000
P	1.57330000	-4.52090000	4.22750000	C	3.32760000	-0.73260000	-3.33060000
O	2.58010000	-3.28610000	4.79640000	H	1.52820000	-1.86720000	-3.27760000
O	1.11020000	-4.17180000	2.83350000	C	4.12020000	0.24270000	-2.72470000
H	3.00630000	-3.66040000	5.60830000	H	4.26390000	1.63250000	-1.08190000
P	4.59990000	-0.28850000	4.18110000	H	3.67060000	-1.24310000	-4.22580000
O	4.72030000	-0.98250000	2.84370000	H	5.09160000	0.49540000	-3.13720000
O	3.02110000	0.28970000	4.36600000				
H	3.01590000	0.72470000	5.25560000	On MOF-bct			
H	-2.94780000	3.00250000	-4.87780000	(Z)-syn-TS-R			
C	0.30850000	-0.88550000	-0.98380000	O	-13.66970000	10.14630000	-3.80170000
N	0.02390000	-2.23160000	-1.09760000	O	-12.86400000	8.76690000	-1.97480000
C	-0.60830000	-3.13950000	-0.21420000	C	-12.99510000	9.09530000	-3.27720000
C	-0.13150000	-4.46640000	-0.27290000	C	-12.38220000	8.14830000	-4.24020000
C	-1.64690000	-2.83620000	0.68190000	C	-11.46890000	7.17850000	-3.79050000
C	-0.63320000	-5.43680000	0.58530000	C	-10.94930000	6.22010000	-4.66420000

C	-12.18450000	7.23750000	-6.48920000	O	16.11860000	-10.06700000	3.94090000
O	-10.02180000	5.30130000	-4.17020000	O	16.88940000	-8.60390000	2.14380000
C	-11.30960000	6.24080000	-6.02780000	C	16.74490000	-8.98490000	3.42890000
C	-12.72030000	8.17880000	-5.60440000	O	-6.14890000	3.71790000	10.70620000
O	-12.88940000	-13.96100000	-2.83280000	O	-5.31930000	1.93310000	9.28510000
O	-12.07510000	-15.35740000	-1.00190000	C	-5.48450000	3.22650000	9.63210000
C	-12.21500000	-15.00070000	-2.29440000	C	-4.93710000	4.21230000	8.66980000
O	0.92790000	10.67330000	-3.82890000	C	-3.98700000	3.80620000	7.71620000
O	1.72710000	9.24850000	-2.03420000	C	-3.54310000	4.68380000	6.72450000
C	2.16880000	8.66200000	-4.32150000	C	-4.93020000	6.43420000	7.67560000
C	2.79600000	7.48130000	-3.89950000	O	-2.58840000	4.23240000	5.81180000
C	3.26860000	6.55420000	-4.82170000	C	-4.01880000	6.01070000	6.69370000
C	2.54050000	7.95650000	-6.62000000	C	-5.39030000	5.54250000	8.65130000
O	3.92480000	5.42680000	-4.35020000	O	-6.20580000	2.74170000	-13.57470000
C	3.13690000	6.75820000	-6.20400000	O	-5.36970000	0.99300000	-15.06130000
C	2.06120000	8.89130000	-5.70400000	C	-5.55930000	2.26660000	-14.66200000
O	1.64930000	-13.44410000	-2.83970000	O	8.33580000	4.14810000	10.64250000
O	2.50500000	-14.84200000	-1.02940000	O	9.10100000	2.35710000	9.19550000
C	2.34330000	-14.47900000	-2.31740000	C	8.93030000	3.65480000	9.53060000
O	15.46430000	11.02750000	-3.81960000	C	9.38080000	4.64910000	8.52420000
O	16.27080000	9.60170000	-2.00830000	C	9.85130000	4.22190000	7.26970000
C	16.12650000	9.97260000	-3.29630000	C	10.22110000	5.14390000	6.28760000
O	16.24490000	-13.01570000	-2.78070000	C	9.72280000	6.95680000	7.82220000
O	17.05280000	-14.44490000	-0.97300000	O	10.70570000	4.66070000	5.07090000
C	16.91340000	-14.06770000	-2.25960000	C	10.17350000	6.52630000	6.56440000
O	-13.74040000	13.21790000	2.85700000	C	9.31860000	6.02950000	8.78800000
O	-12.99230000	14.65410000	1.02860000	O	8.47550000	3.13160000	-13.50710000
C	-13.12040000	14.29200000	2.32080000	O	9.35760000	1.36840000	-14.94860000
O	-13.02490000	-10.89790000	3.83010000	C	9.16700000	2.64550000	-14.56110000
O	-12.28570000	-9.47530000	2.00850000	O	-6.05050000	-3.02650000	13.61490000
C	-12.40670000	-9.81050000	3.31010000	O	-5.32430000	-1.22550000	15.09690000
C	-11.85560000	-8.82900000	4.27710000	C	-5.43160000	-2.50910000	14.69900000
C	-11.01210000	-7.79660000	3.82990000	O	-5.84280000	-3.99020000	-10.66980000
C	-10.55860000	-6.80770000	4.70660000	O	-5.14710000	-2.15670000	-9.24150000
C	-11.71570000	-7.91500000	6.52980000	C	-5.22260000	-3.45840000	-9.58850000
O	-9.70490000	-5.81980000	4.21380000	C	-4.62640000	-4.41040000	-8.61850000
C	-10.91410000	-6.85750000	6.07030000	C	-3.84490000	-3.93040000	-7.55120000
C	-12.18710000	-8.88800000	5.64220000	C	-3.37120000	-4.79420000	-6.56130000
O	0.81300000	13.57890000	2.89990000	C	-4.37020000	-6.66670000	-7.73920000
O	1.54740000	15.06660000	1.10720000	O	-2.60500000	-4.26440000	-5.52130000
C	1.42190000	14.67220000	2.39020000	C	-3.63310000	-6.17640000	-6.64920000
O	1.56000000	-10.43170000	3.84940000	C	-4.87050000	-5.79220000	-8.70990000
O	2.24810000	-8.97400000	2.03500000	O	8.59370000	-2.55050000	13.63860000
C	2.12760000	-9.31420000	3.33730000	O	9.35380000	-0.71880000	15.06440000
C	2.60500000	-8.31040000	4.32230000	C	9.24420000	-2.00990000	14.69220000
C	2.99220000	-7.02560000	3.90010000	O	8.60370000	-3.60150000	-10.60020000
C	3.37440000	-6.04900000	4.82540000	O	9.26960000	-1.78960000	-9.12960000
C	3.06500000	-7.65200000	6.62220000	C	9.18600000	-3.08820000	-9.49060000
O	3.77760000	-4.80000000	4.34710000	C	9.74630000	-4.06640000	-8.52510000
C	3.42470000	-6.36280000	6.20120000	C	9.50710000	-5.44530000	-8.67130000
C	2.64840000	-8.61180000	5.69560000	C	10.02080000	-6.36650000	-7.74920000
O	15.39770000	14.00150000	2.89400000	C	11.00010000	-4.53490000	-6.49370000
O	16.16570000	15.45500000	1.08790000	O	9.68180000	-7.71330000	-7.89140000
C	16.02850000	15.07750000	2.37480000	C	10.75750000	-5.90920000	-6.63650000

C 10.50570000 -3.62510000 -7.42750000
 O -16.30020000 12.74620000 -3.96580000
 O -17.12680000 14.34740000 -2.31740000
 C -16.97570000 13.84310000 -3.55840000
 O -15.51940000 -11.37510000 -3.00840000
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 C -16.20210000 -10.28140000 -2.60460000
 O -1.74210000 13.23480000 -3.93880000
 O -2.58310000 14.79270000 -2.25620000
 C -2.42860000 14.31580000 -3.50770000
 O -0.99260000 -10.85610000 -2.95370000
 O -1.80170000 -9.29680000 -1.27970000
 C -1.65060000 -9.74520000 -2.54430000
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C	4.8486000	5.1026000	-9.1658000	C	12.2641000	9.8973000	-3.3024000
O	-16.2992000	13.1511000	2.8632000	C	11.6761000	8.9471000	-4.2717000
O	-17.1263000	14.5461000	1.0373000	C	10.6287000	8.0989000	-3.8747000
C	-16.9748000	14.1921000	2.3292000	C	10.1285000	7.1229000	-4.7409000
O	-15.5808000	-10.9805000	3.8233000	C	11.6712000	7.8793000	-6.4563000
O	-16.3979000	-9.5878000	1.9911000	O	9.0561000	6.3378000	-4.3154000
C	-16.2541000	-9.9406000	3.2843000	C	10.6602000	6.9963000	-6.0413000
O	-1.7525000	13.4876000	2.8960000	C	12.1755000	8.8456000	-5.5801000
O	-2.5893000	14.9160000	1.1001000	O	13.6873000	-13.0783000	-2.7980000
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C	-2.2207000	-8.5047000	4.3334000	C	-9.2918000	-2.5831000	14.6303000
C	-2.9018000	-7.3599000	3.8820000	O	-8.3723000	-4.1183000	-10.6349000
C	-3.3774000	-6.4034000	4.7819000	O	-9.1969000	-2.3694000	-9.1664000
C	-2.5753000	-7.7600000	6.6267000	C	-9.0027000	-3.6563000	-9.5294000
O	-4.0536000	-5.2918000	4.2768000	C	-9.4889000	-4.6803000	-8.5725000
C	-3.2210000	-6.6004000	6.1695000	C	-9.0585000	-6.0171000	-8.6634000
C	-2.0704000	-8.6976000	5.7190000	C	-9.5099000	-6.9816000	-7.7522000
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C	3.53590000	6.23230000	6.68460000	O	2.21030000	-9.13390000	-1.31590000
C	5.05740000	5.80440000	8.53620000	C	2.07950000	-9.60310000	-2.57700000
O	5.91250000	3.04730000	-13.58060000	C	2.50880000	-8.68980000	-3.66190000
O	5.22040000	1.23280000	-15.06190000	C	2.61160000	-7.30830000	-3.42620000
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C	-12.99940000	9.43830000	2.61040000	C	3.26390000	-6.93050000	-5.74000000
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C	-12.26630000	-14.65980000	3.59030000	C	-5.53920000	3.38330000	14.51260000
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O	1.69890000	9.35250000	1.29670000	O	-5.25130000	1.16450000	-9.37610000
C	1.54660000	9.78610000	2.56600000	C	-5.46160000	2.42400000	-9.81120000
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O	3.50290000	5.48570000	3.89070000	O	-2.07220000	3.90020000	-6.60450000
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O	1.67540000	-13.09970000	3.98940000	O	8.39750000	4.27910000	13.31720000
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O	15.43870000	11.33920000	3.01680000	O	8.37680000	3.21810000	-10.83250000
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O	17.02450000	-14.30400000	2.38430000	C	9.81440000	3.57740000	-7.44690000
C	16.86370000	-13.82050000	3.63220000	C	10.18100000	4.57950000	-6.54500000
O	-13.74050000	12.81220000	-3.96810000	C	9.79020000	6.24780000	-8.26420000
O	-12.99310000	14.45530000	-2.32300000	O	10.61730000	4.20100000	-5.27380000
C	-13.12090000	13.94250000	-3.56310000	C	10.18900000	5.92940000	-6.95630000
O	-12.95990000	-11.29260000	-2.97570000	C	9.38800000	5.24300000	-9.14970000
O	-12.26410000	-9.66170000	-1.32080000	O	-6.01560000	-3.10580000	10.93380000
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C	-3.73120000	-5.59940000	7.13650000	O	-3.52990000	-0.55680000	-13.39790000
C	-5.11730000	-5.04730000	9.06130000	C	-0.71770000	-0.50780000	-13.42340000
O	-5.87400000	-4.08580000	-13.35810000	Zr	8.84740000	0.73850000	10.57240000
O	-5.21250000	-2.36260000	-14.95780000	O	10.96690000	0.82820000	10.88230000
C	-5.27660000	-3.62060000	-14.47730000	Zr	8.99080000	-0.27970000	-13.63020000
O	8.53760000	-2.67120000	10.96630000	O	11.09220000	-0.20070000	-13.19530000
O	9.22880000	-0.98540000	9.36240000	Zr	-5.71810000	0.40670000	13.76680000
C	9.13170000	-2.25100000	9.82460000	O	-3.59930000	0.44340000	13.42430000
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C	9.39160000	-4.66460000	9.17030000	Zr	-5.59260000	-0.56090000	-10.58610000
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C	10.99220000	-3.95300000	6.99520000	C	-0.71810000	-0.40980000	-11.00540000
O	9.50890000	-6.98400000	8.54720000	Zr	8.90260000	0.88770000	13.72090000
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C	10.49990000	-2.96630000	7.84920000	Zr	8.89720000	-0.17280000	-10.47960000
O	8.68840000	-3.69910000	-13.27230000	O	11.02020000	-0.10190000	-10.77060000
O	9.46190000	-1.98790000	-14.83360000	Zr	-16.71240000	13.18600000	-0.56550000
C	9.35040000	-3.24460000	-14.35890000	O	-18.81660000	12.76670000	-0.54040000
Zr	-13.26980000	10.13180000	-0.38390000	Zr	-15.96910000	-10.94650000	0.39060000
O	-11.16660000	10.53810000	-0.40520000	O	-18.07180000	-11.37330000	0.39710000
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Zr	-12.51150000	-14.00160000	0.59780000	O	-4.24760000	13.14060000	-0.51590000
O	-10.41210000	-13.55980000	0.59090000	C	-7.03610000	13.05680000	-0.53730000
C	-7.61360000	-13.47290000	0.59580000	Zr	-1.40730000	-10.49210000	0.44780000
Zr	1.32050000	10.57880000	-0.41190000	O	-3.50440000	-10.92110000	0.47030000
O	3.41760000	11.01010000	-0.41230000	C	-6.29730000	-11.01190000	0.47010000
C	6.20850000	11.09670000	-0.41300000	Zr	12.44400000	14.04660000	-0.54310000
Zr	2.07190000	-13.50270000	0.58500000	O	10.33780000	13.62770000	-0.52940000
O	4.16480000	-13.04070000	0.56200000	C	7.53150000	13.55570000	-0.52430000
C	6.95150000	-12.95900000	0.55640000	Zr	13.19180000	-10.04240000	0.49170000
Zr	15.86530000	10.94530000	-0.38910000	O	11.08730000	-10.44500000	0.49080000
O	17.97310000	11.34620000	-0.39950000	C	8.28480000	-10.50670000	0.45880000
Zr	16.62740000	-13.11190000	0.64920000	Zr	-16.63140000	10.03440000	-0.37850000
O	18.73260000	-12.69630000	0.64960000	O	-18.75430000	10.34460000	-0.39700000
Zr	-13.34590000	13.27460000	-0.57120000	Zr	-15.87740000	-14.09790000	0.57360000
O	-11.22600000	12.94450000	-0.55270000	O	-18.00130000	-13.79530000	0.53750000
C	-8.43190000	13.01880000	-0.53680000	Zr	-2.03720000	10.45320000	-0.41850000
Zr	-12.60770000	-10.85900000	0.41440000	O	-4.16320000	10.73090000	-0.44580000
O	-10.48650000	-11.15370000	0.44580000	C	-6.96850000	10.64080000	-0.42970000
C	-7.69330000	-11.05820000	0.46700000	Zr	-1.29390000	-13.63360000	0.60330000
Zr	1.21140000	13.72250000	-0.52650000	O	-3.41840000	-13.32830000	0.59480000
O	3.33510000	13.41840000	-0.51630000	C	-6.21710000	-13.42660000	0.59880000
C	6.13460000	13.51280000	-0.52140000	Zr	12.50410000	10.90290000	-0.39940000
Zr	1.95090000	-10.35710000	0.42650000	O	10.38900000	11.21970000	-0.41760000
O	4.07830000	-10.63360000	0.42580000	C	7.60390000	11.13960000	-0.41590000
C	6.88680000	-10.54310000	0.44760000	Zr	13.25970000	-13.19100000	0.62420000
Zr	15.81170000	14.10000000	-0.53330000	O	11.14080000	-12.85410000	0.58930000
O	17.93190000	13.77050000	-0.51040000	C	8.34720000	-12.92260000	0.56740000

Zr	-9.02580000	0.24510000	10.55720000	O	7.13000000	1.85520000	10.37240000
O	-11.14650000	0.20620000	10.86990000	O	7.27460000	0.83380000	-13.89430000
Zr	-9.01260000	-0.82140000	-13.65610000	O	-7.38350000	-0.79650000	13.94900000
O	-11.11640000	-0.91140000	-13.23650000	O	-7.20910000	-1.80690000	-10.32920000
Zr	5.49030000	0.64410000	10.63930000	O	7.25530000	-0.32600000	13.98210000
O	3.38900000	0.59860000	11.02670000	O	7.24950000	-1.39740000	-10.30540000
C	0.61090000	0.49950000	11.03410000	O	-15.03390000	13.33660000	-1.75380000
Zr	5.62160000	-0.38890000	-13.72150000	O	-14.28100000	-10.79040000	-0.78310000
O	3.49810000	-0.44170000	-13.39330000	O	-0.47500000	13.79510000	-1.71150000
C	0.68080000	-0.48260000	-13.42340000	O	0.25890000	-10.31010000	-0.74330000
Zr	-9.08580000	0.34280000	13.70640000	O	14.12960000	14.19490000	-1.72230000
O	-11.19250000	0.29330000	13.29530000	O	14.87700000	-9.86960000	-0.68020000
Zr	-8.94660000	-0.71880000	-10.50690000	O	-14.94370000	9.97280000	0.80450000
O	-11.06650000	-0.82000000	-10.81130000	O	-14.19970000	-14.15760000	1.77120000
Zr	5.53370000	0.79270000	13.78160000	O	-0.35540000	10.38120000	0.76530000
O	3.41500000	0.70760000	13.43550000	O	0.40060000	-13.68750000	1.77790000
C	0.60460000	0.59980000	13.45170000	O	14.18050000	10.79530000	0.79060000
Zr	5.54160000	-0.27990000	-10.57460000	O	14.93770000	-13.27950000	1.81940000
O	3.44670000	-0.32310000	-10.98540000	O	-7.32040000	-0.90330000	10.44700000
C	0.67550000	-0.38490000	-11.00540000	O	-7.27740000	-1.92250000	-13.83140000
Zr	-14.98710000	11.51780000	-2.75920000	O	7.19870000	-0.49160000	10.48100000
Zr	-14.21780000	-12.60450000	-1.79070000	O	7.34840000	-1.51480000	-13.81150000
Zr	-0.40880000	12.00160000	-2.75970000	O	-7.42650000	1.55660000	13.87480000
Zr	0.32180000	-12.10960000	-1.76940000	O	-7.31970000	0.54060000	-10.40190000
Zr	14.16190000	12.38930000	-2.75280000	O	7.18710000	2.02340000	13.87240000
Zr	14.92550000	-11.67020000	-1.71430000	O	7.17710000	0.95230000	-10.39090000
Zr	-14.98620000	11.78900000	1.80970000	O	-13.18740000	11.62940000	-1.73910000
Zr	-14.25820000	-12.34020000	2.77890000	O	-12.42740000	-12.49790000	-0.75460000
Zr	-0.41940000	12.16620000	1.81600000	O	1.38870000	12.10730000	-1.73340000
Zr	0.33790000	-11.88010000	2.80100000	O	2.12690000	-11.98830000	-0.75780000
Zr	14.14530000	12.59830000	1.82080000	O	15.95920000	12.46700000	-1.72160000
Zr	14.88710000	-11.47830000	2.85450000	O	16.71800000	-11.58440000	-0.67690000
Zr	-7.41330000	2.61400000	12.08450000	O	-13.18670000	11.77960000	0.78370000
Zr	-7.40820000	1.59600000	-12.18470000	O	-12.44980000	-12.35150000	1.76840000
Zr	7.12660000	3.05080000	12.06620000	O	1.38400000	12.19850000	0.79580000
Zr	7.19100000	2.00330000	-12.17860000	O	2.13450000	-11.86100000	1.76780000
Zr	-7.33040000	-1.96330000	12.22860000	O	15.95000000	12.58210000	0.79980000
Zr	-7.18700000	-2.97600000	-12.04110000	O	16.69680000	-11.47850000	1.84360000
Zr	7.25850000	-1.52010000	12.28040000	O	-5.59460000	1.62440000	12.15400000
Zr	7.33510000	-2.56550000	-12.01820000	O	-5.56000000	0.65800000	-12.19760000
O	-14.94340000	9.83310000	-1.54590000	O	8.95730000	2.07900000	12.08380000
O	-14.17890000	-14.29360000	-0.57930000	O	9.02350000	1.03990000	-12.09420000
O	-0.34700000	10.29720000	-1.58260000	O	-5.54820000	-0.90550000	12.23410000
O	0.39230000	-13.80600000	-0.57190000	O	-5.43820000	-1.86870000	-12.11820000
O	14.18890000	10.68770000	-1.56250000	O	9.02970000	-0.44620000	12.20230000
O	14.95750000	-13.37820000	-0.53100000	O	9.10260000	-1.48450000	-12.00630000
O	-15.03350000	13.47610000	0.59620000	O	-16.78800000	11.53230000	-1.73170000
O	-14.30120000	-10.65430000	1.56750000	O	-16.02780000	-12.59840000	-0.77880000
O	-0.48080000	13.87970000	0.64120000	O	-2.21270000	11.97390000	-1.73970000
O	0.26840000	-10.19010000	1.60260000	O	-1.47560000	-12.12820000	-0.73810000
O	14.12110000	14.30230000	0.62980000	O	12.35790000	12.41270000	-1.73430000
O	14.85750000	-9.77100000	1.67230000	O	13.11690000	-11.67140000	-0.70430000
O	-7.36390000	1.44570000	10.37270000	O	-16.78750000	11.68190000	0.78810000
O	-7.39050000	0.42810000	-13.90520000	O	-16.05010000	-12.45260000	1.74140000

O	-2.21760000	12.06490000	0.78960000	P	-10.66550000	3.70940000	-4.11940000
O	-1.46660000	-12.00230000	1.78970000	P	-2.34410000	3.69050000	-4.92190000
O	12.34890000	12.52800000	0.79120000	P	3.09400000	4.00150000	-4.33800000
O	13.09520000	-11.56550000	1.81850000	P	9.52770000	4.70880000	-4.04610000
O	-9.15090000	-0.97270000	12.16760000	H	-11.16420000	7.14640000	-2.75160000
O	-9.03620000	-2.03820000	-12.03750000	H	-12.47610000	7.26910000	-7.53200000
O	5.42840000	-0.54870000	12.26920000	H	-13.41700000	8.91410000	-5.98660000
O	5.50240000	-1.60100000	-12.10490000	H	-11.75990000	-15.67180000	-3.00950000
O	-9.19630000	1.55570000	12.08840000	H	2.93030000	7.22600000	-2.85250000
O	-9.15860000	0.48700000	-12.11700000	H	2.41850000	8.13850000	-7.68440000
O	5.35460000	1.97880000	12.15070000	H	1.58670000	9.78770000	-6.09560000
O	5.42280000	0.92390000	-12.19430000	H	2.79650000	-15.14000000	-3.04290000
C	-10.60150000	11.75530000	-0.48010000	H	16.56630000	9.30180000	-4.02120000
C	-9.11670000	11.79190000	-0.48200000	H	17.36350000	-14.73050000	-2.98550000
C	-9.85480000	-12.33770000	0.52190000	H	-12.70660000	14.98780000	3.03740000
C	-8.37080000	-12.28940000	0.52890000	H	-10.71410000	-7.73760000	2.79030000
C	3.97060000	12.23420000	-0.46460000	H	-12.00200000	-7.97040000	7.57300000
C	5.45440000	12.28260000	-0.46580000	H	-12.83020000	-9.67130000	6.02300000
C	4.71610000	-11.81610000	0.49380000	H	1.82800000	15.35460000	3.12380000
C	6.20120000	-11.77030000	0.49730000	H	2.97590000	-6.76020000	2.85030000
C	18.52460000	12.56810000	-0.45330000	H	3.09100000	-7.91080000	7.67370000
C	19.27670000	-11.47070000	0.60240000	H	2.36280000	-9.59100000	6.05850000
C	-2.98830000	0.42260000	12.22630000	H	16.44380000	15.76100000	3.10230000
C	-1.50480000	0.47020000	12.23780000	H	17.14890000	-8.29970000	4.16100000
C	-2.91780000	-0.51280000	-12.20120000	H	-3.59900000	2.79490000	7.71970000
C	-1.43480000	-0.47320000	-12.21330000	H	-5.31010000	7.44860000	7.66750000
C	11.56020000	0.89470000	12.08390000	H	-6.12230000	5.88750000	9.37070000
C	11.62800000	-0.13190000	-11.96650000	H	-5.17780000	3.02190000	-15.33480000
C	-19.35750000	11.54100000	-0.46780000	H	9.91540000	3.16760000	7.03150000
C	-18.60850000	-12.60120000	0.46330000	H	9.67460000	8.01400000	8.05310000
C	-4.80000000	11.91500000	-0.48160000	H	8.96270000	6.39680000	9.74220000
C	-6.28460000	11.86880000	-0.48340000	H	9.59170000	3.39390000	-15.21550000
C	-4.05580000	-12.14520000	0.53400000	H	-4.99840000	-3.23730000	15.37050000
C	-5.53990000	-12.19550000	0.53520000	H	-3.62000000	-2.87490000	-7.45980000
C	9.76890000	12.40990000	-0.47340000	H	-4.58590000	-7.72500000	-7.82120000
C	8.28490000	12.36950000	-0.47170000	H	-5.46790000	-6.19760000	-9.51680000
C	10.51910000	-11.66240000	0.53410000	H	9.70590000	-2.72300000	15.36100000
C	9.03390000	-11.69660000	0.51980000	H	8.91300000	-5.81650000	-9.49690000
C	-11.74170000	0.23840000	12.07190000	H	11.57500000	-4.16420000	-5.65370000
C	-11.66310000	-0.89230000	-12.01090000	H	10.71600000	-2.57310000	-7.28180000
C	2.80780000	0.63210000	12.23710000	H	-17.42100000	14.42810000	-4.35100000
C	1.32460000	0.57760000	12.24370000	H	-16.63960000	-9.69440000	-3.40010000
C	2.87850000	-0.39490000	-12.19970000	H	-2.88290000	14.91140000	-4.28720000
C	1.39510000	-0.42200000	-12.21340000	H	-3.26550000	-7.56860000	-2.23280000
P	11.05020000	-8.70360000	-8.21300000	H	-2.13570000	-8.41640000	-6.98620000
P	1.87600000	-4.12820000	-4.96560000	H	-1.29370000	-9.93510000	-5.26470000
P	-3.46060000	-4.29530000	-4.03170000	H	11.75600000	15.34100000	-4.31360000
P	-10.19260000	-9.44720000	-8.20080000	H	13.24200000	-9.57580000	-5.20920000
P	-10.47360000	-4.28480000	4.16270000	H	10.35850000	-5.73800000	-3.96680000
P	-3.14200000	-3.85020000	4.48270000	H	11.27900000	-7.15560000	-2.21400000
P	2.67470000	-3.55710000	4.78840000	H	-17.25270000	8.75160000	3.41030000
P	10.82740000	-7.99580000	8.98760000	H	-16.53670000	-15.38270000	4.35390000
P	-3.25390000	4.05350000	4.23840000	H	-3.39320000	7.21870000	2.24950000
P	-10.89180000	8.85080000	8.28020000	H	-2.94210000	8.48190000	7.02350000

H	-2.18170000	10.03480000	5.29700000	H	3.12470000	3.07300000	7.88530000
H	-1.90010000	-14.95090000	4.38020000	H	4.94800000	7.66750000	7.47800000
H	10.23230000	8.36330000	2.28940000	H	5.85850000	6.15500000	9.17530000
H	12.01260000	8.49060000	6.91610000	H	4.87380000	3.23960000	-15.34630000
H	12.89880000	10.04050000	5.24100000	H	-13.15480000	9.80110000	5.32720000
H	12.58600000	-14.52910000	4.38210000	H	-10.55870000	5.76560000	4.07570000
H	-10.52480000	-2.42580000	7.41090000	H	-11.46660000	7.18820000	2.32560000
H	-9.61570000	-7.19180000	8.43410000	H	-11.82420000	-15.24320000	4.38590000
H	-8.87020000	-5.46770000	9.99800000	H	2.59500000	7.28150000	2.25870000
H	-9.53430000	-4.60140000	-15.00340000	H	2.56850000	8.75230000	6.99480000
H	3.24170000	-2.15590000	8.17420000	H	1.73060000	10.26460000	5.26610000
H	5.37290000	-6.63340000	8.08000000	H	2.82110000	-14.76960000	4.35320000
H	6.17920000	-4.94580000	9.66280000	H	16.53850000	9.63930000	3.38270000
H	5.10230000	-4.16250000	-15.08340000	H	17.30090000	-14.41980000	4.41860000
H	-9.85070000	4.07970000	15.05760000	H	-12.70720000	14.54840000	-4.35710000
H	-10.60830000	1.84540000	-7.35640000	H	-12.44560000	-10.52890000	-5.29520000
H	-10.04690000	6.66090000	-8.39750000	H	-10.15040000	-6.32070000	-4.02380000
H	-9.18790000	4.98980000	-9.96040000	H	-10.98610000	-7.79540000	-2.28070000
H	4.77000000	4.54300000	15.09140000	H	1.83770000	15.09580000	-4.28060000
H	3.61050000	2.36260000	-7.54830000	H	2.39750000	-6.89960000	-2.44620000
H	4.58150000	7.12120000	-8.48170000	H	3.40120000	-8.71720000	-6.95130000
H	5.43900000	5.43690000	10.01550000	H	2.71540000	-10.24040000	-5.16320000
H	-17.42000000	14.86670000	3.04710000	H	16.47060000	15.42300000	-4.30040000
H	-16.70490000	-9.26630000	3.99890000	H	17.20990000	-8.60990000	-3.24480000
H	-2.89450000	15.18500000	3.11580000	H	-5.13330000	4.16750000	15.13630000
H	-3.04850000	-7.18290000	2.82380000	H	-3.23560000	2.27930000	-8.27070000
H	-2.44120000	-7.92770000	7.68840000	H	-5.52970000	6.65960000	-7.89090000
H	-1.55550000	-9.56800000	6.10550000	H	-6.40290000	4.96770000	-9.43360000
H	11.73030000	15.68030000	3.08810000	H	9.49370000	4.67620000	15.01250000
H	13.09130000	-9.14470000	6.13750000	H	9.83760000	2.54950000	-7.10720000
H	10.39700000	-5.30510000	4.52980000	H	9.78400000	7.27820000	-8.59810000
H	11.32450000	-6.87170000	2.91300000	H	9.07680000	5.52520000	-10.14750000
H	-17.25360000	8.31220000	-3.98840000	H	-3.55590000	-2.27500000	7.83480000
H	-16.47170000	-15.80990000	-3.04470000	H	-4.89410000	-7.02990000	8.26880000
H	-2.77060000	6.80500000	-2.87450000	H	-5.81110000	-5.37650000	9.82470000
H	-3.29940000	8.04700000	-7.64570000	H	-4.82240000	-4.37640000	-15.10270000
H	-2.58160000	9.74390000	-6.03490000	H	8.75380000	-4.95890000	9.99430000
H	-1.93130000	-15.31760000	-3.01870000	H	11.60940000	-3.65930000	6.15480000
H	10.20170000	8.18070000	-2.88230000	H	10.75390000	-1.93390000	7.64490000
H	12.09480000	7.79790000	-7.44990000	H	9.82140000	-4.00850000	-14.96170000
H	12.98090000	9.48740000	-5.91520000	H	-8.85520000	9.63790000	-0.38650000
H	12.64990000	-14.84150000	-3.01840000	H	-8.09670000	-14.44050000	0.64480000
H	-9.72000000	-3.32750000	15.28710000	H	5.72400000	10.12930000	-0.36940000
H	-8.36010000	-6.31860000	-9.43440000	H	6.46360000	-13.92460000	0.59560000
H	-11.47480000	-4.96440000	-5.82150000	H	-8.97160000	13.95650000	-0.57860000
H	-10.72820000	-3.30500000	-7.43970000	H	-8.23870000	-10.12430000	0.41520000
H	4.98780000	-2.85550000	15.44110000	H	5.59050000	14.44790000	-0.56330000
H	2.97270000	-3.07740000	-8.34270000	H	6.34620000	-9.60620000	0.40200000
H	5.52360000	-7.18340000	-7.22480000	H	-1.29200000	0.38840000	10.07720000
H	6.41350000	-5.61720000	-8.88670000	H	-1.23410000	-0.55750000	-14.37370000
H	-8.84090000	5.87570000	9.50590000	H	-1.31230000	0.56760000	14.39840000
H	-11.80390000	4.31010000	5.85090000	H	-1.23050000	-0.38070000	-10.05190000
H	-10.95450000	2.70290000	7.47120000	H	-6.54910000	14.02280000	-0.58010000
H	-9.89390000	2.79840000	-15.23470000	H	-5.81480000	-10.04390000	0.42020000

H	8.01810000	14.52190000	-0.56790000	H	-12.20020000	-4.87510000	2.99510000
H	8.77550000	-9.54230000	0.42040000	H	-1.34960000	-4.59310000	3.51910000
H	-6.42680000	9.70430000	-0.38700000	H	1.66710000	-3.88920000	2.89770000
H	-5.67110000	-14.36000000	0.65020000	H	10.11680000	-9.64650000	7.77830000
H	8.14600000	10.20320000	-0.37420000	H	10.35160000	-10.29560000	-6.92070000
H	8.88520000	-13.86090000	0.61450000	H	0.10360000	-5.26220000	-4.45080000
H	1.12600000	0.47930000	10.08190000	H	-1.90150000	-4.92900000	-2.66350000
H	1.19930000	-0.51170000	-14.37340000	H	-9.36820000	-10.90070000	-6.82250000
H	1.11770000	0.65860000	14.40320000	H	-3.74190000	2.04970000	-5.13870000
H	1.18560000	-0.33750000	-10.05140000	H	-8.79290000	2.83320000	-4.76760000
H	19.60560000	12.58660000	-0.45010000	C	5.20700000	2.68960000	-9.79440000
H	20.35750000	-11.44540000	0.61050000	C	1.58930000	9.60260000	-3.32950000
H	12.64060000	0.92780000	12.06350000	C	3.72510000	0.45320000	-1.65510000
H	12.70800000	-0.09400000	-11.93580000	N	3.02060000	0.68890000	-2.79850000
H	-20.43830000	11.51330000	-0.46610000	C	1.78980000	0.17140000	-3.25350000
H	-19.68920000	-12.63310000	0.45580000	C	1.37810000	0.57530000	-4.53950000
H	-12.82240000	0.21610000	12.05200000	C	0.95210000	-0.66960000	-2.50170000
H	-12.74280000	-0.94160000	-11.98670000	C	0.16980000	0.13020000	-5.06360000
O	11.42680000	-8.58620000	-9.73900000	H	2.00850000	1.24600000	-5.11440000
O	10.66690000	-10.31280000	-7.85940000	C	-0.25270000	-1.11670000	-3.04800000
O	0.37970000	-4.34240000	-4.20810000	H	1.22990000	-0.97860000	-1.50320000
O	2.27980000	-2.60740000	-4.90440000	C	-0.65230000	-0.72750000	-4.32530000
O	-4.52790000	-3.13560000	-4.02060000	H	-0.13110000	0.45990000	-6.05400000
O	-2.38000000	-4.06670000	-2.75030000	H	-0.88480000	-1.77130000	-2.45460000
O	-9.61910000	-10.98110000	-7.77720000	H	-1.59320000	-1.07980000	-4.73860000
O	-10.48880000	-9.41740000	-9.74850000	C	0.21460000	2.20310000	-1.10120000
O	-11.49000000	-4.20940000	2.81260000	C	-0.07260000	1.57710000	0.06210000
O	-9.37790000	-3.15710000	4.05260000	C	2.35190000	2.33390000	-0.15830000
O	-4.08760000	-2.60390000	4.29060000	N	1.48640000	2.71240000	-1.18510000
O	-1.90520000	-3.79550000	3.33000000	H	1.78050000	3.24710000	-2.04390000
O	1.31530000	-3.62100000	3.78380000	H	-0.44750000	2.33500000	-1.94640000
O	3.37580000	-2.15410000	4.63120000	H	-0.99990000	1.10380000	0.34870000
O	11.15150000	-7.78800000	10.51590000	S	1.29590000	1.64250000	1.16260000
O	10.39960000	-9.61140000	8.72680000	C	3.40120000	3.31420000	0.29930000
O	8.37830000	4.04860000	3.87130000	C	4.34200000	2.92460000	1.26350000
O	10.41730000	4.74810000	2.30340000	C	3.44910000	4.61780000	-0.21170000
O	-2.08660000	3.96920000	3.18280000	C	5.30620000	3.82060000	1.71800000
O	-4.16800000	2.63160000	4.17310000	H	4.31950000	1.91510000	1.66740000
O	-11.24110000	8.74120000	9.93180000	C	4.42340000	5.51040000	0.24010000
O	-10.46180000	10.32830000	7.93870000	H	2.73570000	4.93370000	-0.96550000
O	-9.39760000	2.59380000	-4.02060000	C	5.35070000	5.11920000	1.20540000
O	-11.59030000	3.55970000	-2.85190000	H	6.02060000	3.50350000	2.47190000
O	-0.99080000	3.91790000	-4.14810000	H	4.45260000	6.51720000	-0.16670000
O	-2.89470000	2.11790000	-4.63050000	H	6.10400000	5.81860000	1.55720000
O	4.08920000	2.89030000	-4.12520000	H	3.39400000	1.47550000	-3.37330000
O	1.88750000	4.10030000	-3.43640000	H	3.03980000	1.32880000	-0.64340000
O	10.28790000	4.58470000	-2.54000000	C	5.10220000	1.10880000	-1.65130000
O	8.24950000	3.78600000	-4.06400000	H	11.21310000	5.33650000	2.33880000
O	1.08070000	4.20950000	3.39830000	H	0.60940000	5.05520000	3.60680000
O	3.19490000	2.84040000	4.27270000	H	9.71800000	5.11280000	-1.92580000
P	9.62810000	5.00420000	3.77740000	C	3.70410000	-0.91150000	-1.01820000
P	2.44990000	4.22410000	4.39110000	C	3.84020000	-2.05030000	-1.83080000
H	-4.93910000	2.80060000	4.77120000	C	3.69130000	-1.07770000	0.37260000
H	-10.35610000	8.71270000	10.37530000	C	3.94340000	-3.31830000	-1.26300000

H	3.88220000	-1.93250000	-2.90840000	C	11.27010000	6.73080000	5.79180000
C	3.78540000	-2.35000000	0.93830000	C	12.56300000	8.73800000	5.31710000
H	3.59420000	-0.21400000	1.02090000	O	-1.10060000	-13.44620000	3.24610000
C	3.90730000	-3.47480000	0.12430000	O	-1.88020000	-14.95790000	1.49290000
H	4.06270000	-4.18730000	-1.90240000	C	-1.74110000	-14.53450000	2.76520000
H	3.76950000	-2.45860000	2.01730000	O	-1.10140000	10.63670000	3.69580000
H	3.98230000	-4.46470000	0.56610000	O	-1.89290000	9.16820000	1.93440000
H	5.77910000	0.50900000	-2.27380000	C	-1.73050000	9.53410000	3.22420000
H	5.06740000	2.11810000	-2.06730000	C	-2.23900000	8.57410000	4.23740000
H	5.51240000	1.13450000	-0.64000000	C	-2.86290000	7.38120000	3.83030000
(E)-syn-TS-S				C	-3.27680000	6.42990000	4.76570000
O	13.40790000	-10.57870000	-3.69280000	C	-2.52600000	7.88430000	6.55700000
O	12.67760000	-9.14030000	-1.87980000	O	-3.90080000	5.26970000	4.30390000
C	12.77540000	-9.49740000	-3.17740000	C	-3.11560000	6.67920000	6.14450000
C	12.17660000	-8.54870000	-4.14730000	C	-2.08200000	8.81770000	5.61420000
C	11.30110000	-7.54320000	-3.70040000	O	-15.61210000	-13.42730000	3.46310000
C	10.79870000	-6.58310000	-4.58210000	O	-16.44950000	-14.92860000	1.72830000
C	11.97370000	-7.66860000	-6.40780000	C	-16.27680000	-14.50730000	2.99720000
O	9.90740000	-5.62810000	-4.09020000	O	-15.70380000	10.60520000	3.94550000
C	11.13740000	-6.63750000	-5.95020000	O	-16.51040000	9.09710000	2.20220000
C	12.49310000	-8.61190000	-5.51550000	C	-16.35040000	9.51700000	3.47320000
O	13.33030000	13.62510000	-3.26070000	O	6.29310000	-3.61600000	10.73550000
O	12.55050000	15.07380000	-1.45560000	O	5.47770000	-1.85020000	9.28070000
C	12.67870000	14.68870000	-2.74100000	C	5.61650000	-3.13640000	9.66410000
O	-1.15250000	-10.72690000	-3.55440000	C	5.01390000	-4.13300000	8.75060000
O	-1.91080000	-9.22840000	-1.80270000	C	3.96690000	-3.75180000	7.89480000
C	-2.37750000	-8.72410000	-4.10640000	C	3.45940000	-4.63800000	6.94190000
C	-3.07040000	-7.56780000	-3.72080000	C	4.98930000	-6.34610000	7.74020000
C	-3.55770000	-6.67660000	-4.67130000	O	2.39890000	-4.21750000	6.13770000
C	-2.70800000	-8.06820000	-6.42590000	C	3.97770000	-5.94670000	6.85000000
O	-4.29420000	-5.58610000	-4.23670000	C	5.50550000	-5.44700000	8.68040000
C	-3.36860000	-6.89230000	-6.04700000	O	6.03810000	-3.14910000	-13.49300000
C	-2.21990000	-8.96930000	-5.48120000	O	5.24340000	-1.41460000	-15.01820000
O	-1.29220000	13.47820000	-3.06600000	C	5.39560000	-2.68260000	-14.58630000
O	-2.03490000	14.95760000	-1.27020000	O	-8.24020000	-3.61280000	10.86130000
C	-1.92920000	14.55320000	-2.55180000	O	-8.98830000	-1.81670000	9.41110000
O	-15.75500000	-10.69910000	-3.35370000	C	-8.85130000	-3.11440000	9.76040000
O	-16.49570000	-9.19220000	-1.58010000	C	-9.36480000	-4.10410000	8.78010000
C	-16.38490000	-9.61230000	-2.85640000	C	-10.07680000	-3.67260000	7.64660000
O	-15.83400000	13.33540000	-2.86930000	C	-10.50170000	-4.58140000	6.67450000
O	-16.60730000	14.83490000	-1.10370000	C	-9.57170000	-6.39830000	7.98770000
C	-16.48280000	14.41390000	-2.37820000	O	-11.23200000	-4.09970000	5.58650000
O	13.51790000	-13.51380000	3.02770000	C	-10.25870000	-5.96030000	6.84450000
O	12.69470000	-14.96630000	1.24500000	C	-9.12040000	-5.48010000	8.94110000
C	12.85780000	-14.58090000	2.52650000	O	-8.65290000	-3.15230000	-13.39530000
O	13.43050000	10.69150000	3.46120000	O	-9.46770000	-1.35770000	-14.83770000
O	12.65810000	9.24760000	1.67060000	C	-9.32710000	-2.64070000	-14.44850000
C	12.79190000	9.60480000	2.96510000	O	6.39140000	3.20250000	13.46350000
C	12.23180000	8.65020000	3.95350000	O	5.63750000	1.45940000	14.99960000
C	11.38010000	7.61450000	3.52970000	C	5.77200000	2.72910000	14.56710000
C	10.91680000	6.65090000	4.42900000	O	5.93680000	3.67170000	-10.77110000
C	12.08160000	7.79100000	6.22690000	O	5.13490000	1.90400000	-9.30760000
O	10.05380000	5.65980000	3.95900000	C	5.26700000	3.18920000	-9.69730000
				C	4.66230000	4.18680000	-8.79170000

C	3.50340000	3.86450000	-8.06800000	O	15.96530000	13.38920000	3.54570000
C	2.97370000	4.75370000	-7.12740000	O	16.72040000	14.98290000	1.85620000
C	4.73280000	6.34050000	-7.66900000	C	16.59810000	14.50020000	3.10890000
O	1.77170000	4.41760000	-6.49990000	O	1.43400000	-10.75570000	3.26470000
C	3.60040000	6.00120000	-6.90810000	O	2.17300000	-9.21980000	1.53740000
C	5.25740000	5.44340000	-8.60430000	C	2.04250000	-9.63180000	2.81730000
O	-8.20700000	3.13850000	13.75690000	C	2.56370000	-8.70370000	3.85300000
O	-8.99730000	1.35740000	15.23000000	C	3.03230000	-7.42890000	3.48870000
C	-8.85200000	2.63780000	14.83350000	C	3.46360000	-6.51710000	4.45520000
O	-8.49340000	3.58690000	-10.49220000	C	3.04120000	-8.16900000	6.18200000
O	-9.24030000	1.80510000	-9.02130000	O	3.93720000	-5.27400000	4.03170000
C	-9.09230000	3.09940000	-9.38020000	C	3.48160000	-6.88720000	5.81670000
C	-9.59360000	4.10550000	-8.41260000	C	2.57530000	-9.06390000	5.21290000
C	-9.19670000	5.45220000	-8.50480000	O	1.44800000	13.31670000	3.70540000
C	-9.66820000	6.40500000	-7.59300000	O	2.18280000	14.88790000	1.98610000
C	-10.90870000	4.66350000	-6.44400000	C	2.07880000	14.41970000	3.24590000
O	-9.18470000	7.71160000	-7.68250000	O	-13.03560000	-10.76510000	3.41310000
C	-10.51900000	6.00830000	-6.54010000	O	-12.30450000	-9.24830000	1.66620000
C	-10.45620000	3.72390000	-7.37110000	C	-12.39670000	-9.66540000	2.94600000
O	15.95650000	-13.26020000	-3.85100000	C	-11.78730000	-8.76650000	3.95730000
O	16.76900000	-14.84960000	-2.18440000	C	-10.94560000	-7.71440000	3.55230000
C	16.60820000	-14.36730000	-3.43290000	C	-10.44480000	-6.79640000	4.47940000
O	15.90840000	10.98480000	-3.39300000	C	-11.54580000	-8.02130000	6.26240000
O	16.73150000	9.40830000	-1.71910000	O	-9.59960000	-5.78180000	4.02610000
C	16.57040000	9.88590000	-2.96950000	C	-10.74890000	-6.94190000	5.84890000
O	1.46030000	-13.34550000	-3.59960000	C	-12.06520000	-8.92120000	5.32670000
O	2.25300000	-14.88660000	-1.87870000	O	-13.17370000	13.29300000	3.93000000
C	2.11380000	-14.43580000	-3.14160000	O	-12.42280000	14.83680000	2.19310000
O	1.27360000	10.82030000	-3.19640000	C	-12.54030000	14.38970000	3.45940000
O	2.05070000	9.25580000	-1.51100000	O	8.86160000	3.19850000	10.71150000
C	1.87680000	9.68170000	-2.78160000	O	9.56070000	1.45980000	9.16960000
C	2.32580000	8.74990000	-3.84390000	C	9.44090000	2.74280000	9.57560000
C	2.57410000	7.40130000	-3.53750000	C	9.93850000	3.77130000	8.62710000
C	2.93630000	6.49320000	-4.53520000	C	10.61510000	3.38600000	7.45610000
C	2.87980000	8.28500000	-6.16970000	C	11.02590000	4.33520000	6.51680000
O	3.17130000	5.16670000	-4.17410000	C	10.15480000	6.09820000	7.93910000
C	3.11200000	6.93430000	-5.86310000	O	11.72070000	3.89670000	5.38830000
C	2.47490000	9.18090000	-5.17390000	C	10.80490000	5.70750000	6.75790000
O	-13.21540000	-13.37780000	-3.43560000	C	9.71720000	5.14100000	8.85980000
O	-12.39620000	-14.92100000	-1.72880000	O	8.49900000	3.72680000	-13.43800000
C	-12.56260000	-14.47360000	-2.98950000	O	9.32950000	2.00640000	-14.95990000
O	-13.24560000	10.68850000	-2.91800000	C	9.16520000	3.27060000	-14.52140000
O	-12.45140000	9.16050000	-1.20990000	O	-5.67350000	3.19840000	11.05500000
C	-12.59370000	9.58340000	-2.48400000	O	-4.92360000	1.48670000	9.50570000
C	-12.01700000	8.70090000	-3.53140000	C	-5.04650000	2.75930000	9.93680000
C	-12.16640000	9.00780000	-4.89670000	C	-4.49330000	3.78970000	9.02610000
C	-11.63550000	8.16950000	-5.88540000	C	-3.58380000	3.41820000	8.02050000
C	-10.82300000	6.67330000	-4.15690000	C	-3.13640000	4.34530000	7.07710000
O	-11.87190000	8.48350000	-7.22490000	C	-4.43520000	6.07260000	8.18330000
C	-10.98110000	6.97560000	-5.51750000	O	-2.21740000	3.92530000	6.11370000
C	-11.32630000	7.52820000	-3.17560000	C	-3.56500000	5.68690000	7.14970000
O	16.08290000	-10.85790000	3.08720000	C	-4.90040000	5.13230000	9.10970000
O	16.84810000	-9.27600000	1.39110000	O	-6.03320000	3.66460000	-13.24540000
C	16.72590000	-9.75480000	2.64540000	O	-5.30410000	1.97270000	-14.84890000

C	-5.42100000	3.22640000	14.36740000	C	-10.66170000	6.60130000	4.96640000
O	8.91040000	-3.65300000	13.35440000	O	-11.71150000	8.27700000	8.10950000
O	9.75300000	-1.92640000	14.86280000	C	-10.81570000	6.84850000	6.33830000
C	9.59230000	-3.19170000	14.42590000	C	-11.18650000	7.48330000	4.02240000
O	8.56420000	-3.12080000	-10.79370000	O	15.96330000	-10.59650000	-3.75000000
O	9.27360000	-1.37710000	-9.26260000	O	16.78820000	-9.14690000	-1.96600000
C	9.16140000	-2.66050000	-9.66930000	C	16.62190000	-9.52890000	-3.24820000
C	9.69390000	-3.68500000	-8.73620000	O	15.89000000	13.64860000	-3.29020000
C	10.37060000	-3.29430000	-7.56720000	O	16.68320000	15.11020000	-1.50170000
C	10.81740000	-4.24270000	-6.64390000	C	16.53300000	14.72380000	-2.78440000
C	9.98190000	-6.01280000	-8.07820000	O	1.39070000	-10.65260000	-3.56800000
O	11.50580000	-3.79870000	-5.51390000	O	2.13670000	-9.16300000	-1.80290000
C	10.63230000	-5.61740000	-6.89890000	C	1.98540000	-9.53110000	-3.09370000
C	9.50910000	-5.05770000	-8.98320000	C	2.45320000	-8.54590000	-4.10200000
O	-5.68540000	-3.71490000	13.53390000	C	2.79630000	-7.24080000	-3.70530000
O	-4.88180000	-2.02820000	15.10750000	C	3.18080000	-6.27910000	-4.64320000
C	-5.03020000	-3.28150000	14.63340000	C	2.95900000	-7.93330000	-6.40510000
O	-6.00870000	-3.25260000	-10.80910000	O	3.53550000	-5.00890000	-4.18480000
O	-5.19600000	-1.56860000	-9.26230000	C	3.28260000	-6.62550000	-6.00710000
C	-4.77400000	-3.89340000	-8.83180000	C	2.53490000	-8.88000000	-5.46530000
C	-4.04880000	-3.54790000	-7.68240000	O	1.27890000	13.49510000	-3.12850000
C	-3.58990000	-4.52300000	-6.80400000	O	2.10720000	14.97210000	-1.36860000
C	-4.51960000	-6.23050000	-8.20140000	C	1.93720000	14.57100000	-2.64430000
O	-2.84430000	-4.12440000	-5.70450000	O	-13.19460000	-10.70410000	-3.39790000
C	-3.82930000	-5.88810000	-7.03030000	O	-12.38810000	-9.21400000	-1.66230000
C	-4.98870000	-5.25910000	-9.08600000	C	-12.53940000	-9.60850000	-2.94370000
O	16.07750000	-13.52160000	2.98410000	C	-11.97220000	-8.69650000	-3.96980000
O	16.82860000	-14.97790000	1.17310000	C	-12.19650000	-8.91870000	-5.34100000
C	16.71260000	-14.59260000	2.45980000	C	-11.68320000	-8.04040000	-6.30480000
O	15.98610000	10.72560000	3.44490000	C	-10.73240000	-6.67940000	-4.53530000
O	16.76870000	9.28040000	1.63850000	O	-11.99840000	-8.26100000	-7.64640000
C	16.63670000	9.66200000	2.92470000	C	-10.97080000	-6.89240000	-5.90060000
O	1.46490000	-13.42790000	3.23900000	C	-11.21920000	-7.57310000	-3.58210000
O	2.26200000	-14.92340000	1.48000000	O	-13.27560000	13.35620000	-2.90610000
C	2.12200000	-14.50420000	2.75360000	O	-12.47060000	14.86670000	-1.16400000
O	1.43840000	10.63700000	3.63240000	C	-12.62700000	14.44350000	-2.43420000
O	2.15880000	9.17830000	1.83210000	O	8.95890000	3.18750000	13.38880000
C	2.05130000	9.53860000	3.12950000	O	9.77570000	1.43440000	14.88060000
C	2.60550000	8.57450000	4.11580000	C	9.63320000	2.70610000	14.45610000
C	3.19890000	7.37680000	3.67740000	O	8.47250000	3.70720000	-10.77000000
C	3.65400000	6.42190000	4.59030000	O	9.24430000	1.97530000	-9.25520000
C	3.00730000	7.88100000	6.41760000	C	9.09850000	3.25660000	-9.65750000
O	4.24570000	5.25800000	4.09720000	C	9.64000000	4.29100000	-8.74120000
C	3.56710000	6.67180000	5.97560000	C	9.33560000	5.65270000	-8.92630000
C	2.52110000	8.81800000	5.49900000	C	9.83430000	6.62710000	-8.05140000
O	-13.05230000	-13.44000000	3.40010000	C	10.92810000	4.88360000	-6.76540000
O	-12.31880000	-14.95290000	1.62860000	O	9.43170000	7.95230000	-8.22750000
C	-12.42350000	-14.52810000	2.90360000	C	10.61830000	6.24010000	-6.94510000
O	-13.14250000	10.62700000	3.89220000	C	10.45020000	3.92140000	-7.65390000
O	-12.40140000	9.13190000	2.13170000	O	-5.63790000	3.12020000	13.74260000
C	-12.50330000	9.53160000	3.41710000	O	-4.86590000	1.32960000	15.21380000
C	-11.89440000	8.62900000	4.42760000	C	-4.99340000	2.61140000	14.81590000
C	-12.03310000	8.88550000	5.80460000	O	-5.95850000	3.56290000	-10.57180000
C	-11.48020000	8.01930000	6.75710000	O	-5.18170000	1.76530000	-9.14050000

C	-5.30950000	3.06200000	-9.49330000	O	-3.99670000	-5.45150000	3.98850000
C	-4.73810000	4.04890000	-8.54150000	C	-3.19600000	-6.89860000	5.79450000
C	-4.06020000	3.61090000	-7.38860000	C	-2.12610000	-9.00500000	5.21450000
C	-3.60540000	4.52320000	-6.43320000	O	-1.11790000	13.31090000	3.76780000
C	-4.41270000	6.35030000	-7.81010000	O	-1.95570000	14.87160000	2.08590000
O	-2.95630000	4.03690000	-5.29810000	C	-1.78270000	14.40650000	3.33940000
C	-3.77830000	5.90670000	-6.63950000	O	-15.59310000	-10.76160000	3.48800000
C	-4.89790000	5.43170000	-8.74650000	O	-16.41540000	-9.22240000	1.77930000
O	8.82680000	-3.63290000	10.68460000	C	-16.24480000	-9.66580000	3.04100000
O	9.56000000	-1.89170000	9.16060000	O	-15.73200000	13.27090000	3.96970000
C	9.42700000	-3.17510000	9.56090000	O	-16.55700000	14.80340000	2.25660000
C	9.94920000	-4.20390000	8.62800000	C	-16.39480000	14.35840000	3.51870000
C	9.61930000	-5.56240000	8.79190000	O	13.39590000	-13.25070000	-3.80340000
C	10.09820000	-6.53090000	7.89990000	O	12.63460000	-14.83710000	-2.10960000
C	11.22120000	-4.78800000	6.63920000	C	12.75250000	-14.35400000	-3.36260000
O	9.67760000	-7.85240000	8.05630000	O	13.34880000	10.95360000	-3.35110000
C	10.88700000	-6.14120000	6.79860000	O	12.62360000	9.37170000	-1.66100000
C	10.76320000	-3.83150000	7.54460000	C	12.72330000	9.82940000	-2.92650000
O	8.60530000	-3.11220000	-13.46820000	C	12.12870000	8.96020000	-3.97320000
O	9.38080000	-1.35380000	-14.97540000	C	12.35160000	9.21190000	-5.33960000
C	9.25620000	-2.62620000	-14.54790000	C	11.81490000	8.36910000	-6.32280000
O	-5.71770000	-3.62690000	10.85030000	C	10.83970000	6.98830000	-4.58200000
O	-4.94400000	-1.83720000	9.40470000	O	12.13280000	8.61400000	-7.65990000
C	-5.08850000	-3.13170000	9.75750000	C	11.07900000	7.22750000	-5.94270000
C	-4.55840000	-4.11840000	8.78640000	C	11.35100000	7.84630000	-3.60970000
C	-3.66390000	-3.70650000	7.78250000	O	-1.10470000	-13.38780000	-3.59410000
C	-3.22870000	-4.59730000	6.79840000	O	-1.88560000	-14.92710000	-1.86550000
C	-4.51670000	-6.36520000	7.85080000	C	-1.74710000	-14.48260000	-3.13070000
O	-2.32330000	-4.14350000	5.83770000	O	-1.24580000	10.78980000	-3.13210000
C	-3.65520000	-5.94050000	6.82640000	O	-1.97060000	9.24570000	-1.40410000
C	-4.97030000	-5.46210000	8.81780000	C	-1.85420000	9.66650000	-2.68210000
O	-6.08840000	-3.16870000	-13.47900000	C	-2.38930000	8.74320000	-3.71140000
O	-5.32950000	-1.38340000	-14.96280000	C	-3.27080000	7.71210000	-3.34350000
C	-5.46750000	-2.66490000	-14.56820000	C	-3.71550000	6.77760000	-4.28220000
O	13.52330000	-10.84150000	3.11870000	C	-2.45700000	7.93330000	-6.00670000
O	12.74230000	-9.26330000	1.45040000	O	-4.62360000	5.80030000	-3.87030000
C	12.88150000	-9.71950000	2.71280000	C	-3.31020000	6.88430000	-5.62930000
C	12.31630000	-8.85100000	3.77680000	C	-1.99500000	8.85010000	-5.05680000
C	12.54460000	-9.12690000	5.13780000	O	-15.77440000	-13.36460000	-3.37650000
C	12.03420000	-8.28710000	6.13770000	O	-16.52930000	-14.89770000	-1.63170000
C	11.07910000	-6.85830000	4.42410000	C	-16.41680000	-14.45320000	-2.89940000
O	12.36190000	-8.55740000	7.46800000	O	-15.80720000	10.67010000	-2.89590000
C	11.32290000	-7.12260000	5.77940000	O	-16.56140000	9.12910000	-1.15780000
C	11.56200000	-7.71410000	3.43570000	C	-16.43980000	9.57310000	-2.42490000
O	13.40450000	13.36360000	3.57120000	O	6.34390000	-3.63510000	13.42260000
O	12.58500000	14.94450000	1.89960000	O	5.62340000	-1.90030000	14.98380000
C	12.74170000	14.46270000	3.14870000	C	5.73620000	-3.16650000	14.53490000
O	-1.11030000	-10.76240000	3.26040000	O	6.03240000	-3.16040000	-10.81240000
O	-1.87470000	-9.24050000	1.53300000	O	5.19560000	-1.43470000	-9.32080000
C	-1.73910000	-9.64900000	2.81230000	C	5.35900000	-2.71190000	-9.72630000
C	-2.27680000	-8.72610000	3.84420000	C	4.78470000	-3.74090000	-8.83180000
C	-2.91930000	-7.53290000	3.46390000	C	3.68320000	-3.42880000	-8.01800000
C	-3.35380000	-6.61300000	4.42190000	C	3.18020000	-4.35900000	-7.10310000
C	-2.59050000	-8.10510000	6.17810000	C	4.84230000	-5.96490000	-7.84810000

O	2.04830000	-4.01950000	-6.36020000	Zr	-16.08510000	-10.48440000	0.07930000
C	3.76710000	-5.63890000	-7.00390000	O	-18.20070000	-10.83900000	0.12660000
C	5.34730000	-5.02520000	-8.75300000	Zr	-16.19100000	13.54930000	0.55870000
O	-8.25600000	-3.69920000	13.54420000	O	-18.30220000	13.16710000	0.58680000
O	-9.02060000	-2.00240000	15.12610000	Zr	13.05550000	-13.63110000	-0.39040000
C	-8.89360000	-3.25760000	14.65060000	O	10.94650000	-13.23980000	-0.33710000
O	-8.54330000	-3.23860000	-10.71840000	C	8.15230000	-13.23410000	-0.26100000
O	-9.25620000	-1.54660000	-9.13000000	Zr	12.99830000	10.59450000	0.04900000
C	-9.12830000	-2.81680000	-9.57260000	O	10.88240000	10.92830000	0.08140000
C	-9.63110000	-3.87560000	-8.66340000	C	8.08230000	10.89480000	0.10930000
C	-9.28840000	-5.22490000	-8.86900000	Zr	-1.50800000	-13.66660000	-0.17510000
C	-9.75120000	-6.22450000	-8.00360000	O	-3.62310000	-13.29660000	-0.17020000
C	-10.87380000	-4.52910000	-6.67780000	C	-6.42620000	-13.30330000	-0.14890000
O	-9.31550000	-7.53580000	-8.20430000	Zr	-1.59060000	10.49790000	0.28720000
C	-10.53420000	-5.87490000	-6.88370000	O	-3.70380000	10.84060000	0.34170000
C	-10.43320000	-3.54190000	-7.55870000	C	-6.50050000	10.81960000	0.38900000
O	6.33260000	3.21490000	10.78190000	Zr	-16.10150000	-13.64220000	0.05080000
O	5.50550000	1.48060000	9.29840000	O	-18.21330000	-13.26600000	0.10440000
C	5.65980000	2.76090000	9.69730000	Zr	-16.16760000	10.39080000	0.52870000
C	5.07980000	3.78360000	8.79350000	O	-18.28430000	10.74010000	0.56420000
C	4.12250000	3.41100000	7.83390000	Zr	5.89370000	-0.19630000	10.56370000
C	3.63170000	4.33700000	6.90990000	O	3.79520000	-0.18870000	10.97750000
C	4.99190000	6.06290000	7.94130000	C	1.00980000	-0.20480000	11.02850000
O	2.66010000	3.91850000	5.99920000	Zr	5.59080000	0.26460000	13.73470000
C	4.06710000	5.67810000	6.95640000	O	3.47390000	0.23560000	-13.37580000
C	5.49890000	5.12440000	8.84720000	C	0.66230000	0.22220000	-13.36850000
O	5.93290000	3.68710000	-13.45580000	Zr	-8.64260000	-0.18890000	10.75530000
O	5.19590000	1.94580000	-15.00190000	O	-10.75660000	-0.19680000	11.11260000
C	5.30720000	3.21300000	-14.55570000	Zr	-9.03440000	0.27630000	-13.52180000
O	-8.20230000	3.21590000	11.08010000	O	-11.13650000	0.27860000	-13.08540000
O	-8.98930000	1.52640000	9.52430000	Zr	5.97800000	-0.21590000	13.70910000
C	-8.83730000	2.79560000	9.96060000	O	3.85540000	-0.21290000	13.38820000
C	-9.37710000	3.85290000	9.07220000	C	1.04980000	-0.24480000	13.44760000
C	-8.99610000	5.19760000	9.23450000	Zr	5.56470000	0.24770000	-10.58650000
C	-9.48980000	6.19260000	8.38030000	O	3.46240000	0.21380000	-10.96470000
C	-10.73010000	4.50100000	7.15870000	C	0.68700000	0.17130000	-10.94900000
O	-9.01610000	7.49730000	8.52990000	Zr	-8.63270000	-0.28570000	13.90450000
C	-10.34660000	5.84110000	7.31640000	O	-10.74840000	-0.25880000	13.53930000
C	-10.25610000	3.51950000	8.02780000	Zr	-8.93950000	0.16910000	-10.37140000
O	-8.59770000	3.68270000	-13.16540000	O	-11.06400000	0.19040000	-10.66050000
O	-9.44100000	2.00210000	-14.72420000	Zr	16.42250000	-13.64020000	-0.45030000
C	-9.27990000	3.25380000	-14.24990000	O	18.53800000	-13.28190000	-0.47430000
Zr	13.07290000	-10.48480000	-0.26950000	Zr	16.36100000	10.61510000	0.01250000
O	10.95850000	-10.83010000	-0.24290000	O	18.47180000	11.00020000	0.00370000
C	8.15570000	-10.81530000	-0.21810000	Zr	1.86010000	-13.63620000	-0.18440000
Zr	12.96490000	13.74100000	0.16910000	O	3.96650000	-13.23710000	-0.18660000
O	10.85760000	13.33800000	0.17290000	C	6.75610000	-13.23250000	-0.23810000
C	8.06150000	13.31290000	0.18140000	Zr	1.76870000	10.50800000	0.20310000
Zr	-1.52700000	-10.51910000	-0.14250000	O	3.88090000	10.86840000	0.15430000
O	-3.63450000	-10.88540000	-0.12420000	C	6.68460000	10.88250000	0.12030000
C	-6.42470000	-10.88400000	-0.10460000	Zr	-12.73540000	-13.66220000	-0.02920000
Zr	-1.60540000	13.64380000	0.36600000	O	-10.62260000	-13.29360000	-0.07220000
O	-3.71510000	13.25160000	0.40250000	C	-7.82340000	-13.30210000	-0.13260000
C	-6.51410000	13.23830000	0.44260000	Zr	-12.80460000	10.42470000	0.47810000

O	-10.69520000	10.79900000	0.45100000	Zr	7.63000000	2.07230000	12.09270000
C	-7.89760000	10.81130000	0.40590000	Zr	7.22450000	2.56940000	-12.12440000
Zr	16.43560000	-10.48450000	-0.32960000	Zr	-6.93790000	2.04100000	12.38780000
O	18.54800000	-10.85660000	-0.38160000	Zr	-7.28370000	2.49700000	-11.91790000
Zr	16.33210000	13.77070000	0.13300000	O	14.73160000	-10.25900000	-1.46870000
O	18.44950000	13.42540000	0.09650000	O	14.63390000	13.97670000	-1.01840000
Zr	1.83190000	-10.48800000	-0.15190000	O	0.14580000	-10.31360000	-1.32060000
O	3.94970000	-10.82500000	-0.17860000	O	0.04970000	13.85810000	-0.84600000
C	6.75760000	-10.81370000	-0.19580000	O	-14.42900000	-10.30730000	-1.13620000
Zr	1.76200000	13.65570000	0.28530000	O	-14.52590000	13.75090000	-0.64120000
O	3.87270000	13.27930000	0.23420000	O	14.75910000	-13.85690000	0.74890000
C	6.66500000	13.30060000	0.19230000	O	14.69190000	10.37950000	1.20010000
Zr	-12.72360000	-10.51310000	-0.00140000	O	0.18110000	-13.84080000	0.99510000
O	-10.61470000	-10.88210000	-0.05470000	O	0.11840000	10.29510000	1.41550000
C	-7.82100000	-10.88290000	-0.08840000	O	-14.39140000	-13.83900000	1.18610000
Zr	-12.82330000	13.57610000	0.50860000	O	-14.46500000	10.21730000	1.67890000
O	-10.70960000	13.21070000	0.47780000	O	7.55820000	-1.38290000	10.32430000
C	-7.91110000	13.23000000	0.45920000	O	7.29470000	-0.88640000	-13.89860000
Zr	9.25130000	-0.21890000	10.46010000	O	-6.96990000	-1.36790000	10.53620000
O	11.37590000	-0.22440000	10.74860000	O	-7.36420000	-0.90440000	-13.78960000
Zr	8.95980000	0.31430000	-13.69900000	O	7.67440000	0.95000000	13.84230000
O	11.06950000	0.34560000	-13.30120000	O	7.22320000	1.44930000	-10.37780000
Zr	-5.28350000	-0.21120000	10.74670000	O	-6.93960000	0.87450000	14.10900000
O	-3.17190000	-0.22950000	11.08910000	O	-7.24510000	1.32680000	-10.20650000
C	-0.38540000	-0.22180000	11.05060000	O	14.71750000	-13.76670000	-1.60320000
Zr	-5.66550000	0.25370000	-13.62330000	O	14.66590000	10.46900000	-1.15240000
O	-3.54340000	0.22730000	-13.30030000	O	0.17510000	-13.81680000	-1.35810000
C	-0.73550000	0.21560000	-13.35290000	O	0.06000000	10.35760000	-0.93150000
Zr	9.34570000	-0.23640000	13.61070000	O	-14.44730000	-13.81770000	-1.16770000
O	11.44800000	-0.24930000	13.17490000	O	-14.50060000	10.23920000	-0.67540000
Zr	8.92310000	0.29860000	-10.54600000	O	14.77360000	-10.34920000	0.88330000
O	11.04190000	0.32230000	-10.87380000	O	14.65980000	13.88730000	1.33410000
Zr	-5.26360000	-0.30730000	13.89070000	O	0.15420000	-10.33730000	1.03010000
O	-3.15290000	-0.29860000	13.49970000	O	0.10640000	13.79720000	1.50620000
C	-0.34760000	-0.26220000	13.46970000	O	-14.37270000	-10.32870000	1.21750000
Zr	-5.58240000	0.14670000	-10.47660000	O	-14.49080000	13.72890000	1.71170000
O	-3.48550000	0.15310000	-10.89010000	O	7.57350000	0.96830000	10.33850000
C	-0.70700000	0.16440000	-10.93340000	O	7.25960000	1.46690000	-13.88670000
Zr	14.70320000	-11.96870000	-2.64650000	O	-6.95480000	0.98030000	10.60710000
Zr	14.63550000	12.26360000	-2.19600000	O	-7.34590000	1.44640000	-13.70990000
Zr	0.15900000	-12.05000000	-2.45230000	O	7.65940000	-1.40400000	13.82880000
Zr	0.02900000	12.13150000	-2.00250000	O	7.25820000	-0.90330000	-10.39070000
Zr	-14.46190000	-12.05070000	-2.26290000	O	-6.95510000	-1.47850000	14.03730000
Zr	-14.52800000	12.00460000	-1.76830000	O	-7.26260000	-1.02330000	-10.28620000
Zr	14.78390000	-12.14410000	1.92670000	O	12.92110000	-12.00700000	-1.59070000
Zr	14.68630000	12.08950000	2.37770000	O	12.84690000	12.21280000	-1.15250000
Zr	0.16960000	-12.09680000	2.12560000	O	-1.63980000	-12.07920000	-1.42310000
Zr	0.13980000	12.01400000	2.57350000	O	-1.74840000	12.10010000	-0.93620000
Zr	-14.35330000	-12.09230000	2.31300000	O	-16.23890000	-12.05100000	-1.19400000
Zr	-14.45950000	11.96180000	2.80530000	O	-16.31420000	11.98090000	-0.71610000
Zr	7.60010000	-2.50620000	12.06700000	O	12.96560000	-12.10420000	0.93500000
Zr	7.29290000	-2.00660000	-12.14730000	O	12.87440000	12.11650000	1.37330000
Zr	-6.96890000	-2.53670000	12.24760000	O	-1.63500000	-12.10470000	1.10680000
Zr	-7.31940000	-2.07470000	-12.07270000	O	-1.68710000	12.03670000	1.59430000

O	-16.17900000	-12.07400000	1.32970000	C	-10.10750000	12.00810000	0.45750000
O	-16.27640000	11.95730000	1.80700000	C	-8.62230000	12.01650000	0.44040000
O	5.80700000	-1.47050000	12.12980000	C	11.98410000	-0.23980000	11.94440000
O	5.47640000	-1.00980000	-12.16630000	C	11.62790000	0.34190000	-12.08070000
O	-8.76470000	-1.50130000	12.28960000	C	-2.56790000	-0.26160000	12.28900000
O	-9.11380000	-1.04010000	-11.98470000	C	-1.08380000	-0.25060000	12.27110000
O	5.82230000	1.06010000	12.14480000	C	-2.92070000	0.18850000	-12.10850000
O	5.43890000	1.51860000	-12.15310000	C	-1.43790000	0.18800000	-12.13440000
O	-8.74710000	1.02820000	12.36740000	P	-10.42050000	8.84080000	-8.07450000
O	-9.09400000	1.48690000	-11.89930000	P	-3.93050000	4.22850000	-3.89650000
O	16.52270000	-12.01430000	-1.65310000	P	1.96780000	4.12520000	-4.81830000
O	16.44850000	12.24190000	-1.18970000	P	10.74630000	8.99590000	-8.60290000
O	1.96360000	-12.04610000	-1.43400000	P	10.80490000	4.11520000	3.95110000
O	1.85580000	12.11350000	-1.02340000	P	3.26830000	3.87650000	4.39310000
O	-12.63790000	-12.07480000	-1.28150000	P	-2.91580000	3.88290000	4.54470000
O	-12.71230000	12.01190000	-0.77110000	P	-10.25870000	8.60160000	8.97050000
O	16.56720000	-12.11090000	0.86900000	P	2.88730000	-3.99930000	4.50580000
O	16.47640000	12.14580000	1.33270000	P	10.98040000	-8.91060000	8.42990000
O	1.96890000	-12.07260000	1.09670000	P	10.59880000	-4.05550000	-4.07800000
O	1.91570000	12.04790000	1.50570000	P	2.41570000	-3.81000000	-4.69580000
O	-12.57840000	-12.09750000	1.24520000	P	-3.59560000	-4.08810000	-4.23370000
O	-12.67500000	11.98790000	1.75400000	P	-10.60460000	-8.60550000	-8.59270000
O	9.42490000	1.03620000	12.03720000	H	11.01340000	-7.48480000	-2.65790000
O	9.04070000	1.57140000	-12.11370000	H	12.24800000	-7.72640000	-7.45410000
O	-5.14390000	1.00530000	12.35390000	H	13.16080000	-9.37480000	-5.89530000
O	-5.49220000	1.46230000	-12.00860000	H	12.23450000	15.35430000	-3.46800000
O	9.40800000	-1.49260000	12.02360000	H	-3.25000000	-7.30800000	-2.68160000
O	9.07900000	-0.95530000	-12.12580000	H	-2.54040000	-8.25740000	-7.48280000
O	-5.16000000	-1.52560000	12.27670000	H	-1.69410000	-9.84870000	-5.84480000
O	-5.51190000	-1.06370000	-12.09410000	H	-2.38220000	15.21020000	-3.28120000
C	10.35740000	-12.03180000	-0.27900000	H	-16.82500000	-8.95870000	-3.59660000
C	8.87210000	-12.02610000	-0.25200000	H	-16.92780000	15.05960000	-3.12240000
C	10.27500000	12.12630000	0.13110000	H	12.43850000	-15.24920000	3.26560000
C	8.78980000	12.11060000	0.14070000	H	11.08280000	7.53330000	2.49140000
C	-4.22340000	-12.09290000	-0.14430000	H	12.36650000	7.86930000	7.26900000
C	-5.70800000	-12.09430000	-0.13350000	H	13.21260000	9.52430000	5.68040000
C	-4.30430000	12.04250000	0.38290000	H	-2.16530000	-15.18600000	3.51650000
C	-5.78940000	12.03340000	0.40660000	H	-3.01190000	7.16360000	2.78010000
C	-18.77900000	-12.04960000	0.12910000	H	-2.38880000	8.09270000	7.61100000
C	-18.86540000	11.94930000	0.58410000	H	-1.60960000	9.72560000	5.96710000
C	3.23090000	-0.20390000	12.19680000	H	-16.69080000	-15.15430000	3.75800000
C	1.74710000	-0.21570000	12.22630000	H	-16.75920000	8.86200000	4.23000000
C	2.87430000	0.21730000	-12.17190000	H	3.54880000	-2.75370000	7.94810000
C	1.39130000	0.20180000	-12.16600000	H	5.40320000	-7.34550000	7.68460000
C	-11.32490000	-0.22480000	12.32770000	H	6.31210000	-5.77000000	9.32650000
C	-11.67230000	0.23800000	-11.85540000	H	4.98210000	-3.44280000	-15.23430000
C	19.11520000	-12.07120000	-0.43820000	H	-10.29550000	-2.62270000	7.49660000
C	19.03280000	12.21830000	0.04400000	H	-9.37080000	-7.45260000	8.13420000
C	4.55320000	-12.02710000	-0.18810000	H	-8.57300000	-5.85050000	9.79850000
C	6.03870000	-12.02280000	-0.20610000	H	-9.78280000	-3.37270000	-15.10080000
C	4.47160000	12.07610000	0.18410000	H	5.36370000	3.48500000	15.22350000
C	5.95680000	12.08550000	0.16300000	H	3.00750000	2.91410000	-8.22640000
C	-10.02410000	-12.08930000	-0.07510000	H	5.23240000	7.28910000	-7.51410000
C	-8.53970000	-12.09190000	-0.10070000	H	6.15170000	5.71610000	-9.15050000

H	-9.27380000	3.37710000	15.50000000	H	2.28140000	-9.87570000	-5.80700000
H	-8.51100000	5.77200000	-9.27990000	H	2.34830000	15.23270000	-3.39400000
H	-11.56990000	4.34020000	-5.64910000	H	-12.77910000	-9.76880000	-5.67320000
H	-10.78430000	2.69710000	-7.26910000	H	-10.17530000	-5.81070000	-4.20510000
H	17.02090000	-14.98160000	-4.22100000	H	-11.01690000	-7.36920000	-2.53830000
H	16.99340000	9.27450000	-3.75440000	H	-12.21290000	15.09490000	-3.19120000
H	2.55130000	-15.06290000	-3.90580000	H	10.08680000	3.45650000	15.08850000
H	2.45670000	7.03400000	-2.52550000	H	8.70100000	5.96860000	-9.74470000
H	3.00570000	8.64470000	-7.18350000	H	11.54030000	4.56740000	-5.92930000
H	2.29310000	10.21360000	-5.44390000	H	10.71200000	2.88530000	-7.48040000
H	-12.15370000	-15.10990000	-3.76200000	H	-4.55450000	3.34510000	15.47760000
H	-12.69890000	9.89820000	-5.20660000	H	-3.90730000	2.55510000	-7.20150000
H	-10.31310000	5.76700000	-3.85310000	H	-4.55960000	7.40920000	-7.98420000
H	-11.18570000	7.25680000	-2.13710000	H	-5.41130000	5.80770000	-9.62240000
H	17.16750000	-9.14110000	3.41810000	H	8.97960000	-5.87950000	9.60590000
H	17.02930000	15.11740000	3.88480000	H	11.83670000	-4.46990000	5.80630000
H	3.04340000	-7.11830000	2.45140000	H	11.04340000	-2.79750000	7.38780000
H	3.04260000	-8.47140000	7.22210000	H	9.70380000	-3.37340000	-15.18830000
H	2.22710000	-10.03820000	5.53150000	H	-3.30990000	-2.68360000	7.74410000
H	2.52640000	15.04280000	4.00760000	H	-4.85820000	-7.39260000	7.88700000
H	-10.68860000	-7.58250000	2.50850000	H	-5.66120000	-5.81220000	9.57450000
H	-11.79320000	-8.14880000	7.30920000	H	-5.06230000	-3.40230000	-15.24710000
H	-12.70460000	-9.72210000	5.67590000	H	13.13010000	-9.98830000	5.43380000
H	-12.10420000	15.02740000	4.21560000	H	10.52070000	-5.97800000	4.12920000
H	10.81620000	2.34190000	7.25110000	H	11.35550000	-7.47010000	2.40130000
H	9.97030000	7.14650000	8.14040000	H	12.31340000	15.06990000	3.93390000
H	9.19820000	5.47690000	9.74850000	H	-3.06640000	-7.29050000	2.41860000
H	9.58890000	4.03690000	-15.15540000	H	-2.45480000	-8.33920000	7.22690000
H	-3.22970000	2.39720000	7.94610000	H	-1.64040000	-9.91370000	5.54660000
H	-4.77910000	7.09730000	8.25420000	H	-2.19700000	15.02660000	4.12200000
H	-5.60010000	5.45170000	9.87170000	H	-16.64880000	-9.02580000	3.81310000
H	-5.00370000	4.00170000	-14.99470000	H	-16.81720000	14.98980000	4.28790000
H	10.03480000	-3.95470000	15.05100000	H	12.30590000	-14.96390000	-4.13550000
H	10.54290000	-2.24750000	-7.35040000	H	12.95390000	10.05560000	-5.65260000
H	9.82530000	-7.06340000	-8.29040000	H	10.26370000	6.12530000	-4.27020000
H	8.99280000	-5.39800000	-9.87180000	H	11.14720000	7.62280000	-2.57010000
H	-4.60060000	-4.06040000	15.24780000	H	-2.17090000	-15.12200000	-3.89260000
H	-3.81970000	-2.52000000	-7.41760000	H	-3.61080000	7.61650000	-2.31960000
H	-4.72640000	-7.27910000	-8.39870000	H	-2.12980000	8.02850000	-7.03490000
H	-5.54420000	-5.59380000	-9.95870000	H	-1.31200000	9.62830000	-5.37390000
H	17.15230000	-15.26480000	3.18340000	H	-16.86680000	-15.08640000	-3.65140000
H	17.07690000	8.99340000	3.65140000	H	-16.87160000	8.93260000	-3.18120000
H	2.56020000	-15.14980000	3.50190000	H	5.31870000	-3.92430000	15.18320000
H	3.29140000	7.15820000	2.62100000	H	3.21210000	-2.45530000	-8.08340000
H	2.92710000	8.09040000	7.47730000	H	5.31130000	-6.93920000	-7.78500000
H	2.07410000	9.72910000	5.87580000	H	6.19870000	-5.29310000	-9.36650000
H	-11.97900000	-15.17840000	3.64400000	H	-9.32650000	-4.03090000	15.26980000
H	-12.57790000	9.75460000	6.15120000	H	-8.65020000	-5.51110000	-9.69580000
H	-10.14230000	5.71410000	4.62450000	H	-11.48350000	-4.24120000	-5.82970000
H	-11.05090000	7.25240000	2.97350000	H	-10.71870000	-2.51520000	-7.36760000
H	17.03690000	-8.85740000	-3.98680000	H	3.75980000	2.39160000	7.78390000
H	16.94760000	15.39840000	-3.52050000	H	5.34310000	7.08630000	7.99080000
H	2.74390000	-6.94710000	-2.66430000	H	6.23690000	5.44480000	9.57200000
H	3.02550000	-8.21880000	-7.44780000	H	4.87070000	3.96700000	-15.19580000

H	-8.30320000	5.48240000	10.01650000	O	1.61380000	-3.99610000	3.57690000
H	-11.39840000	4.21270000	6.35620000	O	3.69370000	-2.52030000	4.35270000
H	-10.57600000	2.49650000	7.87440000	O	11.38840000	-8.73730000	10.06240000
H	-9.72310000	4.03510000	-14.85140000	O	10.53070000	-10.39770000	8.16360000
H	8.67240000	-9.86380000	-0.21060000	O	9.36630000	-2.90120000	-3.97680000
H	8.56740000	14.26980000	0.20560000	O	11.54940000	-3.91230000	-2.82890000
H	-5.91010000	-9.93130000	-0.09250000	O	1.09110000	-3.93380000	-3.84960000
H	-6.00500000	14.19360000	0.45700000	O	3.09170000	-2.27770000	-4.45780000
H	8.66480000	-14.18750000	-0.28600000	O	-4.71230000	-3.07770000	-4.22560000
H	8.60550000	9.94740000	0.07740000	O	-2.51280000	-4.01720000	-3.18330000
H	-5.91180000	-14.25570000	-0.17190000	O	-10.10810000	-10.19550000	-8.29720000
H	-5.98060000	9.87030000	0.36110000	O	-10.96440000	-8.45000000	-10.11940000
H	1.50750000	-0.18340000	10.06720000	O	-1.84100000	-3.92770000	3.10360000
H	1.16880000	0.24590000	-14.32510000	O	-3.96830000	-2.77180000	4.22040000
H	1.58100000	-0.25510000	14.39090000	P	-10.35250000	-4.24020000	4.11720000
H	1.20940000	0.15430000	-10.00070000	P	-3.04760000	-4.04920000	4.28290000
H	6.24180000	-14.18520000	-0.24750000	H	4.52020000	-2.62790000	4.88780000
H	6.17730000	9.92620000	0.09740000	H	10.51970000	-8.68760000	10.53540000
H	-8.33920000	-14.25390000	-0.14360000	H	12.54540000	4.65570000	2.77990000
H	-8.40680000	9.85590000	0.39070000	H	1.44710000	4.66550000	3.52580000
H	6.24300000	-9.86150000	-0.17110000	H	-1.14770000	4.66490000	3.56800000
H	6.14340000	14.24870000	0.22550000	H	-9.50190000	10.15750000	7.66720000
H	-8.33420000	-9.92970000	-0.06380000	H	-9.65150000	10.33410000	-6.70660000
H	-8.43100000	14.17920000	0.48660000	H	-2.18460000	4.57710000	-2.66320000
H	-0.91380000	-0.21190000	10.10560000	H	0.12780000	5.21760000	-4.46240000
H	-1.26290000	0.23390000	-14.29830000	H	9.99590000	10.59610000	-7.35060000
H	-0.84820000	-0.28340000	14.42940000	H	2.49670000	-1.66030000	-4.95360000
H	-1.20850000	0.14280000	-9.97390000	H	8.74310000	-3.13350000	-4.71070000
H	-19.85990000	-12.04430000	0.15490000	C	-5.34420000	-2.83510000	-9.70530000
H	-19.94640000	11.94110000	0.60040000	C	-1.79280000	-9.63020000	-3.08600000
H	-12.40600000	-0.22000000	12.33130000	C	-4.99750000	-0.42500000	-1.71570000
H	-12.75290000	0.24430000	-11.82270000	N	-4.25030000	-0.70130000	-2.83820000
H	20.19610000	-12.07490000	-0.45770000	C	-4.81220000	0.93680000	-1.04850000
H	20.11380000	12.22870000	0.03240000	H	-3.98930000	0.94410000	-0.32610000
H	13.06470000	-0.24470000	11.91200000	H	-4.60270000	1.69970000	-1.80200000
H	12.70890000	0.35620000	-12.06800000	H	-5.71970000	1.22750000	-0.52020000
O	-10.70190000	8.78350000	-9.62420000	C	-3.17330000	-0.01620000	-3.43850000
O	-9.90240000	10.39750000	-7.66260000	C	-2.98510000	-0.25300000	-4.81640000
O	-2.98460000	4.01360000	-2.51110000	C	-2.27610000	0.83720000	-2.77420000
O	-5.08450000	3.15530000	-3.91820000	C	-1.95430000	0.36990000	-5.50840000
O	2.40010000	2.62620000	-4.59430000	H	-3.65660000	-0.93770000	-5.32390000
O	0.49920000	4.40920000	-4.02690000	C	-1.24350000	1.45590000	-3.48380000
O	10.28930000	10.59550000	-8.29650000	H	-2.35520000	1.00810000	-1.71060000
O	11.10490000	8.84620000	-10.13030000	C	-1.07790000	1.23740000	-4.84920000
O	11.82810000	3.99450000	2.60940000	H	-1.83380000	0.17540000	-6.57060000
O	9.69670000	2.99800000	3.86210000	H	-0.56130000	2.11060000	-2.94850000
O	4.13380000	2.57410000	4.19580000	H	-0.27520000	1.72600000	-5.39340000
O	1.97440000	3.85730000	3.30350000	C	-1.41980000	-1.79250000	-0.90120000
O	-1.68660000	3.85490000	3.38300000	C	-1.30630000	-1.04960000	0.22150000
O	-3.79820000	2.58490000	4.39930000	C	-3.59470000	-2.13660000	-0.10290000
O	-10.53700000	8.47640000	10.51680000	N	-2.62120000	-2.44020000	-1.04620000
O	-9.74840000	10.17720000	8.62620000	H	-2.74760000	-3.08570000	-1.87180000
O	-9.25060000	-3.11500000	4.06070000	H	-0.67470000	-1.92770000	-1.67420000
O	-11.40850000	-4.05230000	2.80920000	H	-0.46600000	-0.45300000	0.54430000

S	-2.76490000	-1.16220000	1.19580000	C	-6.42060000	-0.93750000	-1.74540000
C	-4.54250000	-3.20880000	0.35540000	C	-7.22330000	-0.81910000	-0.59530000
C	-5.43270000	-2.94930000	1.40790000	C	-6.99900000	-1.49190000	-2.89940000
C	-4.55390000	-4.47260000	-0.25100000	C	-8.55460000	-1.22470000	-0.59910000
C	-6.30000000	-3.93770000	1.86400000	H	-6.80490000	-0.40690000	0.31820000
H	-5.43970000	-1.97250000	1.88570000	C	-8.33300000	-1.90050000	-2.89940000
C	-5.43580000	-5.45570000	0.20130000	H	-6.42100000	-1.62300000	-3.80370000
H	-3.87850000	-4.69730000	-1.07000000	C	-9.11860000	-1.76630000	-1.75610000
C	-6.30540000	-5.19670000	1.26030000	H	-9.15120000	-1.11790000	0.30290000
H	-6.96910000	-3.72470000	2.69210000	H	-8.75440000	-2.32360000	-3.80710000
H	-5.43570000	-6.42980000	-0.27930000	H	-10.15870000	-2.08060000	-1.76410000
H	-6.98470000	-5.96770000	1.61350000	H	-12.11300000	-4.73300000	2.95510000
H	-4.49450000	-1.57450000	-3.34580000	H	-1.28540000	-4.73800000	3.22740000
H	-4.42200000	-1.26480000	-0.73060000	H	-10.94650000	-10.72240000	-8.28030000