

## Electronic Supplementary Information

# Unraveling Mechanisms of the Uncoordinated Nucleophiles: Theoretical Elucidations of the Cleavage of Bis(*p*- nitrophenyl) Phosphate Mediated by Zinc-Complexes with Apical Nucleophiles

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**1. The pKa values of the mono-deprotonations of [Zn<sup>II</sup>(L<sup>n</sup>H)(H<sub>2</sub>O)<sub>2</sub>]<sup>+</sup> (n=1, 2 and 3) complexes using B3LYP, TPSS and PBE functions**

**Table S1.** The pKa values of the mono-deprotonations of [Zn<sup>II</sup>(L<sup>n</sup>H)(H<sub>2</sub>O)<sub>2</sub>]<sup>+</sup> (n=1, 2 and 3) complexes using B3LYP, TPSS and PBE functions.

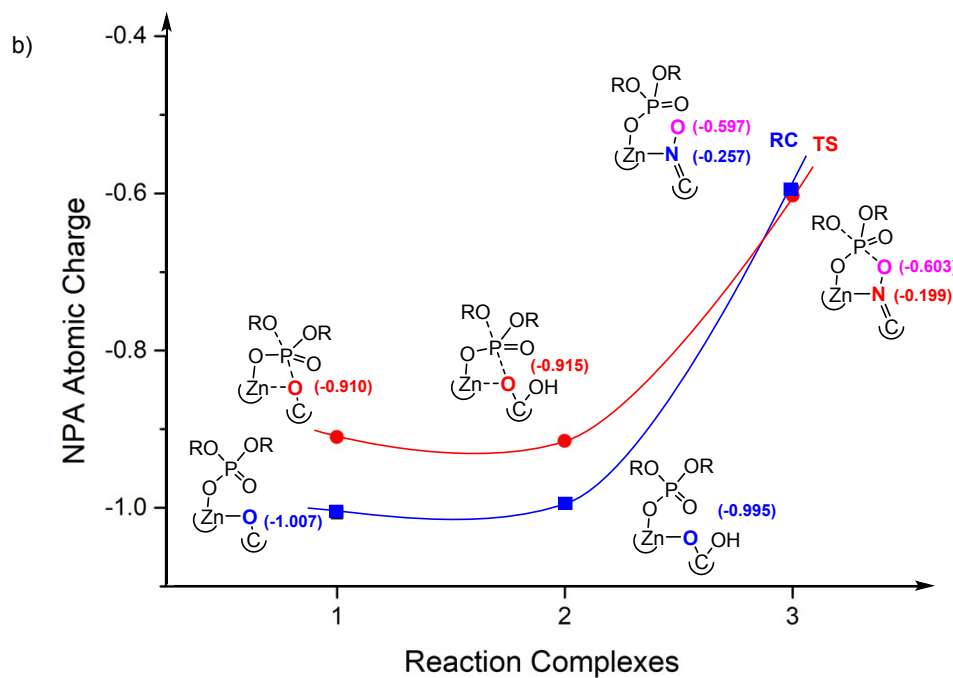
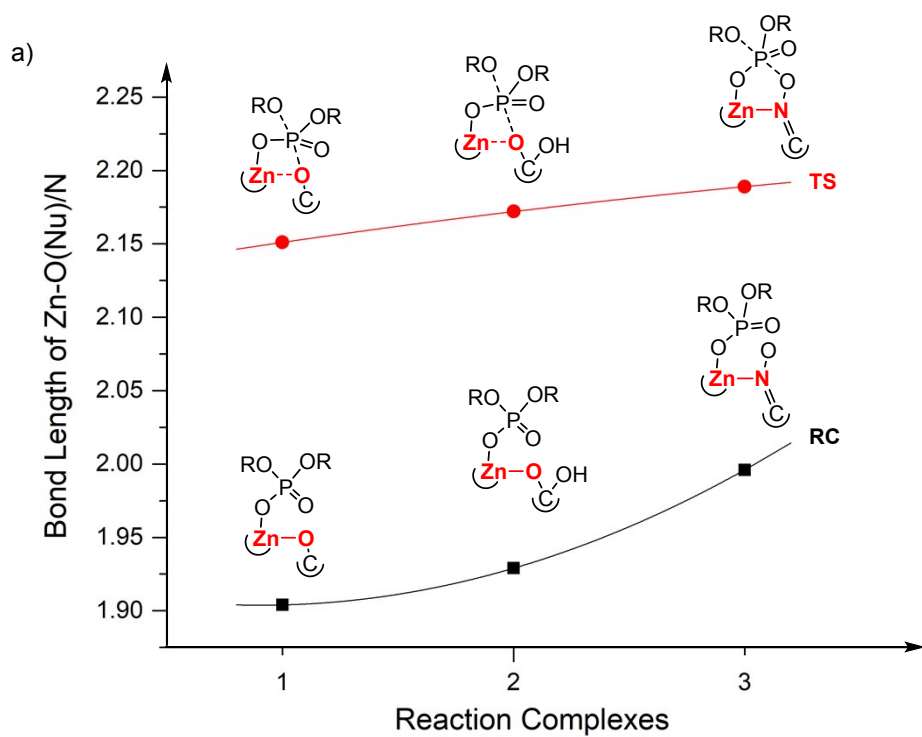
	structures	Zn-L <sup>1</sup>	Zn-L <sup>2</sup>	Zn-L <sup>3</sup>
B3LYP	[Zn <sup>II</sup> L <sup>n</sup> (H <sub>2</sub> O) <sub>2</sub> ] <sup>+</sup>	14.5	10.0	8.8
	[Zn <sup>II</sup> L <sup>n</sup> H(H <sub>2</sub> O)(OH)] <sup>+</sup>	12.6	10.3	11.4
TPSS	[Zn <sup>II</sup> L <sup>n</sup> (H <sub>2</sub> O) <sub>2</sub> ] <sup>+</sup>	13.6	9.0	8.1
	[Zn <sup>II</sup> L <sup>n</sup> H(H <sub>2</sub> O)(OH)] <sup>+</sup>	12.0	10.2	10.8
PBE	[Zn <sup>II</sup> L <sup>n</sup> (H <sub>2</sub> O) <sub>2</sub> ] <sup>+</sup>	11.7	8.4	5.7
	[Zn <sup>II</sup> L <sup>n</sup> H(H <sub>2</sub> O)(OH)] <sup>+</sup>	10.2	8.4	9.4

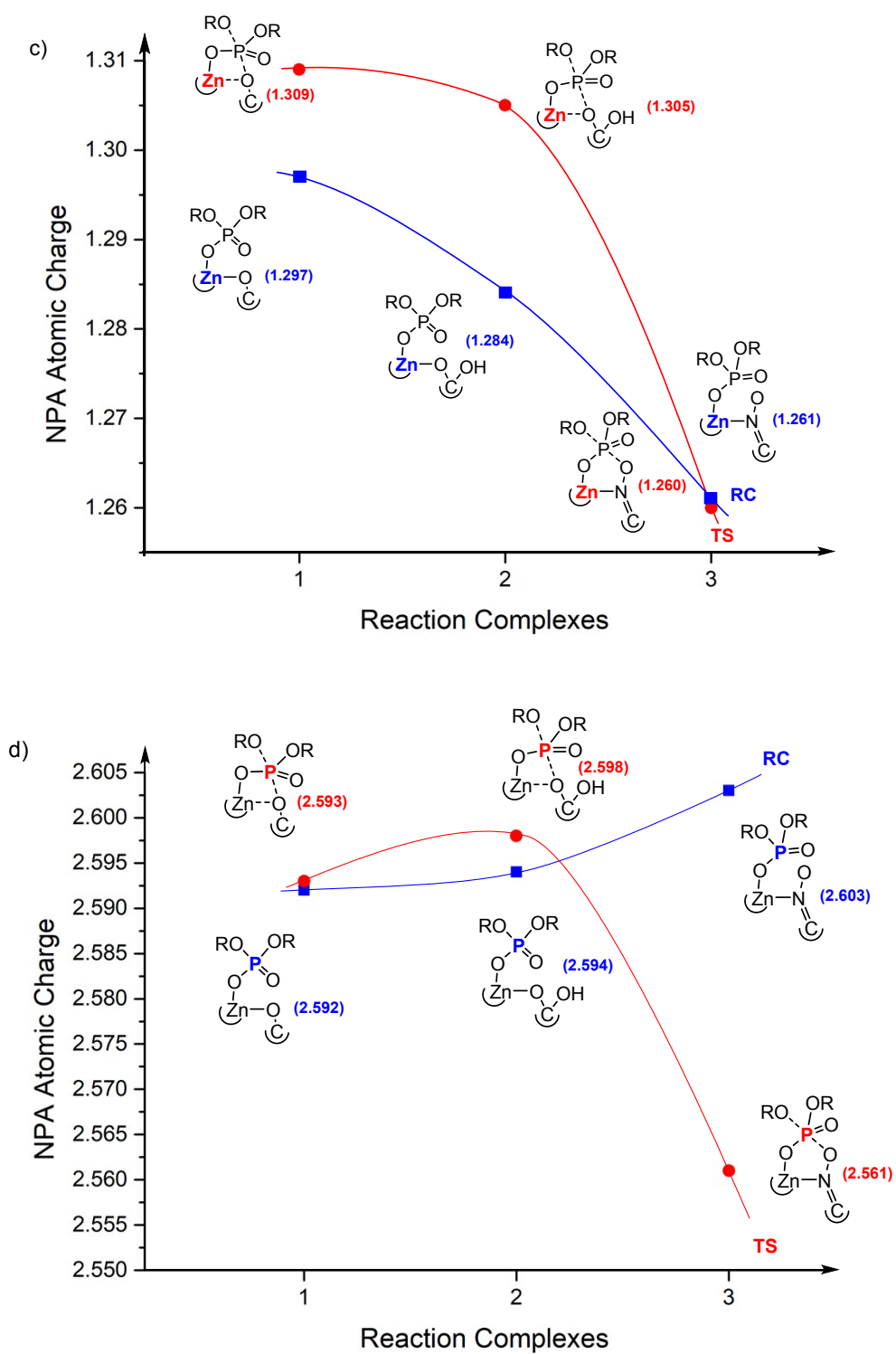
**2. The analysis of Fukui function for the [Zn(L<sup>n</sup>)(η-H<sub>2</sub>O)]<sup>+</sup> complexes and [Zn(L<sup>n</sup>)(η-H<sub>2</sub>O)]<sup>+</sup> complexes.**

**Table S2.** The analysis of Fukui function for the [Zn(L<sup>n</sup>)(η-H<sub>2</sub>O)]<sup>+</sup> complexes and [Zn(L<sup>n</sup>)(η-H<sub>2</sub>O)]<sup>+</sup> complexes.

	<i>N</i>	<i>N-1</i>	<i>N+1</i>	<i>f</i> <sup>-</sup>	<i>f</i> <sup>+</sup>	Δ <i>f</i>
[Zn(L <sup>1</sup> )(η-H <sub>2</sub> O)] <sup>+</sup>	-0.305	-0.101	-0.311	0.204	0.006	-0.199
[Zn(L <sup>1</sup> H)(η-OH)] <sup>+</sup>	-0.388	-0.336	-0.391	0.051	0.003	-0.048
[Zn(L <sup>2</sup> )(η-H <sub>2</sub> O)] <sup>+</sup>	-0.303	-0.124	-0.308	0.179	0.005	-0.174
[Zn(L <sup>2</sup> H)(η-OH)] <sup>+</sup>	-0.385	-0.334	-0.389	0.051	0.003	-0.048
[Zn(L <sup>3</sup> )(η-H <sub>2</sub> O)] <sup>+</sup>	-0.374	-0.033	-0.381	0.340	0.007	-0.333
[Zn(L <sup>3</sup> H)(η-OH)] <sup>+</sup>	-0.358	-0.251	-0.364	0.106	0.006	-0.100

### 3. The length of Zn-O/N(Nu) and NPA atomic charge distribution analysis.





**Figure S1.** (a) The length of Zn-O/N(Nu), in Å. (b) NPA atomic charge distribution analysis of O/N(Nu) atom, (c) NPA atomic charge distribution analysis of Zn atom and (d) NPA atomic charge distribution analysis of P atom.

## 4. The optimized structures.

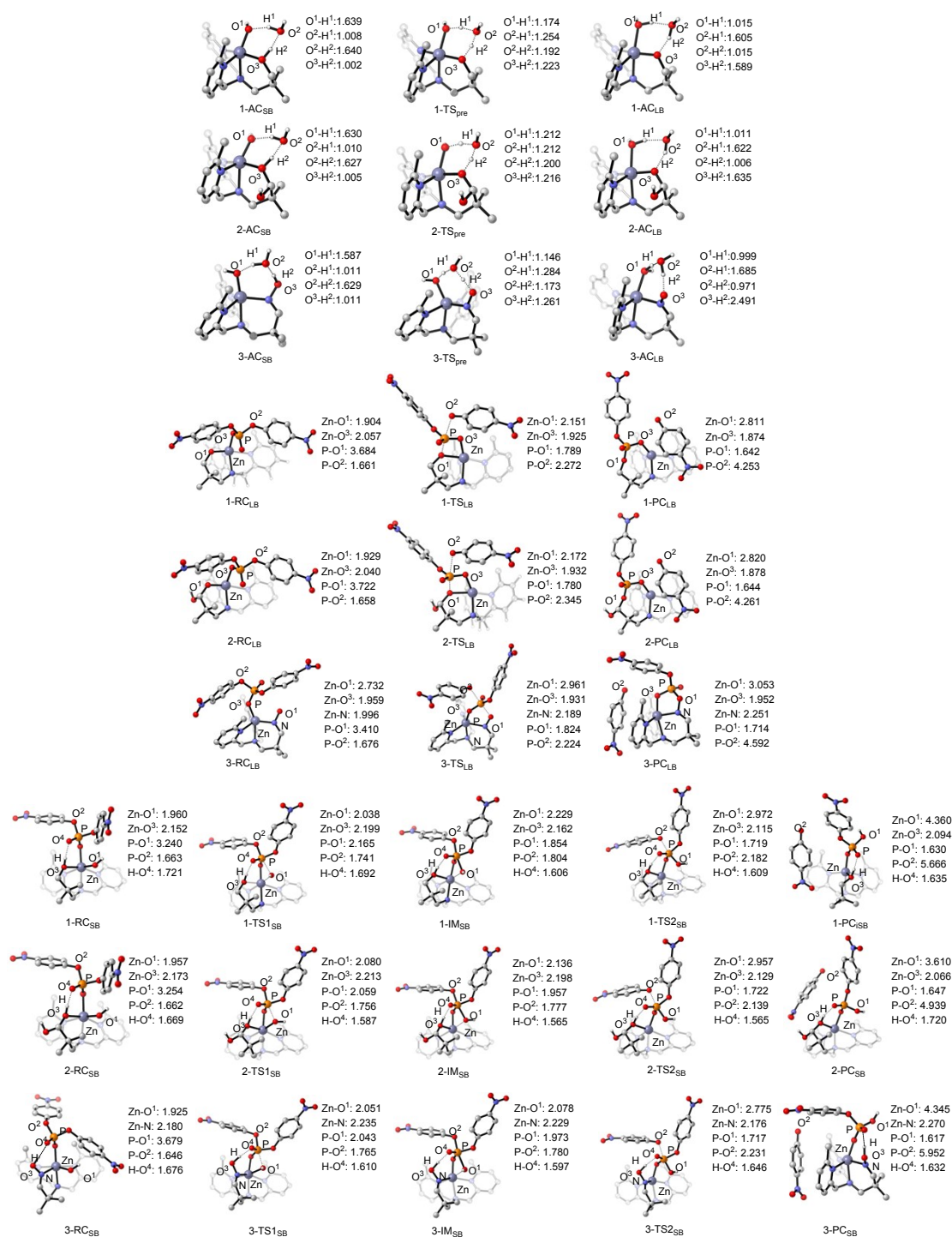
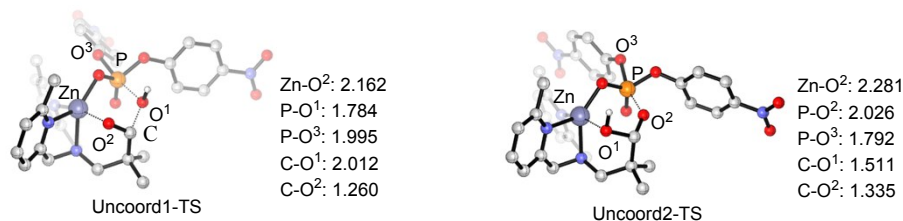
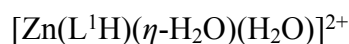


Figure S2. The optimized structures



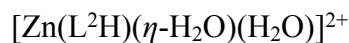
**Figure S3.** The optimized structures of Uncoord1-TS and Uncoord2-TS.

### 5. Cartesian coordinates of optimized structures.



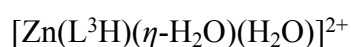
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N	1.48628900	-0.82537200	0.27717100
O	0.85556300	1.85370000	1.63717100
C	-2.56974900	-1.83985800	0.67987000
C	-3.76229800	-2.30187100	0.11456900
H	-4.25066300	-3.17285700	0.53960000
C	-4.29657900	-1.65678700	-0.99692900
H	-5.22043300	-2.00805600	-1.44619800
C	-3.60853500	-0.57455500	-1.54896600
H	-3.97205300	-0.07541100	-2.44159400
C	-2.43248300	-0.15045500	-0.94295700
C	-1.63302000	1.00585600	-1.51791500
H	-1.75135300	1.02760000	-2.61020000
H	-2.02703700	1.95104000	-1.13794600
C	0.44286000	-0.23639500	-1.84434400
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H	-0.29969700	-1.03661500	-1.92520900
C	1.62891700	-0.77645800	-1.06916500
C	2.77338300	-1.25336200	-1.69489200
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H	4.69099200	-2.18957700	-1.36659600
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H	4.40465300	-2.26662500	1.11211500
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H	-0.85539200	0.99312400	3.46110800
H	-1.87360500	-0.13630500	3.03434200
H	0.49844600	2.32869800	2.41515000
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H	-0.91599300	3.30873300	4.25986800
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H	2.03455900	-0.30246900	2.88171900
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H	-1.94919600	-3.64147000	1.66948700
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H	2.43002300	4.14454200	-1.42041800
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H	-1.29753700	4.17871600	-0.68472300
H	-1.23965200	2.99424900	0.63950500



Zn	0.58836300	0.40210300	0.53145100
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H	5.83780200	-1.47021700	-1.59261200
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H	3.66189800	-2.61441100	-2.08327700
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H	-0.87036200	-0.37653700	2.64553900
H	0.70938800	0.94786200	3.25914300
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H	-1.18763900	4.30820400	1.55977900
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H	-0.50694400	-0.17396900	5.06410500
H	-1.30833100	1.08125900	4.62802900



Zn	-0.18405000	-0.16935800	0.71650400
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N	0.27701800	0.84194700	-1.14446000



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C	-4.49472500	-0.24286200	-0.37868400
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C	-4.54158300	0.79983800	-1.29937000
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C	-0.86580900	1.74597500	-1.36162200
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H	-0.75439800	2.60145400	-0.69255000
C	0.27617700	-0.28814600	-2.10346400
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H	-0.76187000	-0.58942400	-2.27676700
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C	1.72411600	-2.33664500	-2.40183700
H	1.71978100	-2.15959800	-3.47251000
C	2.41282300	-3.41754700	-1.85200100
H	2.95033800	-4.11238700	-2.48996000
C	2.42667600	-3.57169800	-0.46886900
H	2.98252600	-4.38126300	-0.00797900
C	1.73479700	-2.66756400	0.34208900
C	1.62089900	1.47936000	-1.12835900
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C	1.87564300	2.64758100	-0.13960700
C	3.39087000	2.61524300	0.22465500
H	3.98604800	2.69078700	-0.69189000
H	3.65928400	1.68612100	0.73868100
H	3.66089700	3.45972800	0.86582900
C	1.58444400	4.02859900	-0.78976800
H	0.54282900	4.15221400	-1.09685900
H	2.21330000	4.14999500	-1.67686600
H	1.82759500	4.84300600	-0.10028600
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H	1.16887500	3.49539200	1.77825400
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O	-0.65442700	-1.03819300	2.60124800
H	-0.14611300	-0.86733200	3.42869300
H	-0.99706700	-1.94297500	2.66045000
H	0.12460400	1.26782000	3.55384100
C	1.77770200	-2.80643100	1.83995900

H	1.81755300	-1.82731200	2.32402800
H	0.89533400	-3.34057500	2.21275300
H	2.65433700	-3.38131900	2.14792700
C	-3.20774100	-1.75957200	1.16542900
H	-2.32913400	-2.38144400	0.95445000
H	-3.15824800	-1.39722900	2.19805000
H	-4.09182500	-2.39465600	1.07651000
O	0.57276200	-0.03869400	4.81998800
H	1.49203800	-0.09410800	5.13445100
H	0.02370500	0.04206000	5.62074200

[Zn(L<sup>1</sup>)( $\eta$ -H<sub>2</sub>O)(H<sub>2</sub>O)]<sup>+</sup>

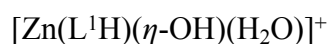
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N	0.05908400	-0.90626100	-1.14199900
N	-0.26570000	1.83299400	-0.58475800
O	-1.05908500	-0.11973500	1.68511400
C	3.58747000	0.71871300	-0.05867400
C	4.82404600	0.23803300	-0.49829900
H	5.71777200	0.83048600	-0.33360400
C	4.89120000	-0.98440400	-1.16559400
H	5.84600600	-1.36916200	-1.51120400
C	3.71427700	-1.68599500	-1.41958300
H	3.72132800	-2.61449700	-1.98184700
C	2.51271100	-1.16458500	-0.94532000
C	1.18776200	-1.85157300	-1.23001900
H	1.23183500	-2.33241700	-2.21978700
H	1.02024400	-2.64627700	-0.49967300
C	0.11627000	0.09289500	-2.24199400
H	-0.35076200	-0.30069800	-3.15445500
H	1.16676400	0.28777200	-2.47888300
C	-0.52098000	1.41030500	-1.84019000
C	-1.29333200	2.16511000	-2.71681800
H	-1.49351400	1.80274300	-3.71997800
C	-1.80351600	3.38746600	-2.27361700
H	-2.40873800	3.99963600	-2.93555100
C	-1.54501100	3.80626800	-0.97062200
H	-1.94480200	4.74248200	-0.59620000
C	-0.77510100	2.99680600	-0.12938400
C	-1.26856100	-1.60053200	-1.13748900
H	-1.19425500	-2.49326100	-1.77778400
H	-1.97132600	-0.91971600	-1.62835000
C	-1.88421800	-1.97514000	0.23025000
C	-2.18124100	-0.70029600	1.06760100

H	-2.90231900	-0.97595500	1.85211000
C	-3.23079400	-2.65561500	-0.09193800
H	-3.09151300	-3.54265200	-0.72099300
H	-3.91163800	-1.97323700	-0.61633100
H	-3.72614600	-2.97773100	0.82981700
C	-1.00747600	-2.93666200	1.04590200
H	-0.07711200	-2.46010000	1.37281600
H	-0.76897200	-3.84427000	0.47758300
H	-1.53338100	-3.24261200	1.95670100
O	1.57586100	0.52638300	2.52095700
H	2.40318700	0.02411100	2.58852700
H	-0.74989600	-0.46594700	3.20465300
C	3.44138400	2.08912700	0.54826200
H	2.95783000	2.75607900	-0.17741100
H	2.81791500	2.07183400	1.44482800
H	4.41484700	2.51623400	0.80099000
C	-0.49784700	3.33169400	1.30928200
H	0.58146000	3.35765400	1.49960100
H	-0.92450400	4.29694300	1.59079000
H	-0.92264700	2.54930500	1.95103200
O	-0.20434100	-0.55977400	4.05496400
H	0.98141000	0.18379300	3.26939500
H	-0.67328700	-0.10507600	4.77047600
H	-2.69091300	0.03332300	0.41585100
[Zn(L <sup>2</sup> )( $\eta$ -H <sub>2</sub> O)(H <sub>2</sub> O)] <sup>+</sup>			
Zn	0.42500500	0.36090000	0.61988300
N	2.45288700	-0.00576100	-0.21676300
N	0.05249100	-0.87666600	-1.17068500
N	-0.30253100	1.87060000	-0.61316800
O	-1.09233900	-0.23448300	1.66626800
O	-2.87941300	0.16084500	0.22888900
C	3.58596700	0.70220700	-0.00250700
C	4.82442000	0.21769000	-0.43793900
H	5.72024900	0.80145400	-0.25206300
C	4.88887800	-0.99157000	-1.12360500
H	5.84336300	-1.38042700	-1.46620300
C	3.70577400	-1.67420200	-1.40318600
H	3.70865800	-2.59213100	-1.98284100
C	2.50481800	-1.14690100	-0.93837000
C	1.18257100	-1.81950900	-1.25854200
H	1.23992300	-2.27856300	-2.25792000
H	1.00336600	-2.63015600	-0.54997600
C	0.12332000	0.13107200	-2.26239500
H	-0.32103100	-0.26297100	-3.18566200

H	1.17732700	0.33586700	-2.47447100
C	-0.53425400	1.44067600	-1.87064700
C	-1.30737400	2.17732800	-2.76056200
H	-1.48844000	1.80526900	-3.76362400
C	-1.84953000	3.38856600	-2.32964800
H	-2.46079500	3.98472900	-3.00068400
C	-1.61505300	3.81727600	-1.02519600
H	-2.03759600	4.74726300	-0.65973800
C	-0.83954500	3.02770800	-0.17170500
C	-1.27162400	-1.58011600	-1.20252900
H	-1.18329700	-2.45048800	-1.87013500
H	-1.97762600	-0.88743100	-1.66236200
C	-1.88759600	-2.02308700	0.14327900
C	-2.19794900	-0.79765100	1.05095800
H	-2.88760700	-1.13675700	1.84215500
C	-3.21756800	-2.72219100	-0.21141600
H	-3.04118200	-3.61178600	-0.82747000
H	-3.88948700	-2.04958000	-0.75252900
H	-3.72974600	-3.04910200	0.69988700
C	-1.00551100	-2.99898300	0.93757200
H	-0.07724200	-2.53101600	1.27998600
H	-0.76724200	-3.88848500	0.34205400
H	-1.53350800	-3.33664800	1.83635200
H	-3.15235000	0.89305100	0.80265500
O	1.40726900	0.82752600	2.46970200
H	0.86936600	0.43073500	3.22870800
C	3.48679100	2.04766500	0.67096500
H	2.45300900	2.39065100	0.71924600
H	3.88514100	2.02311100	1.69237100
H	4.07720000	2.78552400	0.11806100
C	-0.59114800	3.38578800	1.26765000
H	-0.97830100	2.59380500	1.92044900
H	0.48158100	3.46948100	1.47311200
H	-1.06960700	4.33079800	1.53496700
O	-0.17937400	-0.47592300	4.07154200
H	-0.70678600	-0.09553400	4.78950600
H	-0.74788700	-0.50323700	3.24163700
H	2.30201900	0.46878300	2.57103100
[Zn(L <sup>3</sup> )( $\eta$ -H <sub>2</sub> O)(H <sub>2</sub> O)] <sup>+</sup>			
Zn	-1.45743300	-0.40424000	-0.00885000
N	-1.65924600	-0.32423800	-2.17253900
N	-3.61672900	-0.84598900	-0.34091000
N	-2.15950800	1.48318000	0.54962800
C	-0.78989900	0.27015700	-3.02601900

C	-0.96036200	0.14717800	-4.40816000
H	-0.25388100	0.62701500	-5.07694500
C	-2.04294100	-0.57107300	-4.91098900
H	-2.18589700	-0.67190800	-5.98267400
C	-2.95949700	-1.12777500	-4.02092800
H	-3.83896900	-1.65716300	-4.37409400
C	-2.73384800	-0.97985100	-2.65487000
C	-3.71190900	-1.54308700	-1.63958600
H	-4.73438100	-1.48587100	-2.04315500
H	-3.49873400	-2.60101400	-1.47766500
C	-4.16779000	0.53336600	-0.46422100
H	-5.25629000	0.52848600	-0.32468100
H	-3.97713700	0.87715300	-1.48606300
C	-3.51322400	1.52648500	0.47577300
C	-4.25156000	2.48068800	1.15862900
H	-5.33438500	2.48778600	1.08827100
C	-3.56964500	3.43048600	1.92828000
H	-4.12048600	4.18875900	2.47660700
C	-2.18405500	3.39104700	1.98126600
H	-1.62631100	4.11422800	2.56702800
C	-1.48732600	2.39070300	1.28599300
C	-4.30156900	-1.60397700	0.74902900
H	-5.16709800	-2.12991000	0.31931100
H	-4.69226000	-0.86625700	1.45509600
C	-3.43228800	-2.60236900	1.56540300
C	-4.40182900	-3.35873500	2.49877000
H	-5.12069500	-3.95133200	1.92265100
H	-4.96155200	-2.66709400	3.13908200
H	-3.84787400	-4.04278800	3.14992900
C	-2.69451300	-3.63179300	0.68188000
H	-1.96234700	-3.15505100	0.01905100
H	-3.39650300	-4.21326600	0.07147200
H	-2.14215400	-4.33311000	1.31498800
C	-2.44033800	-1.84836900	2.43437000
H	-2.48716500	-1.93460400	3.52123500
N	-1.52804700	-1.08285900	1.93841400
O	-0.73022000	-0.40881200	2.76702800
C	0.00923600	2.30676100	1.35907900
H	0.31326800	1.95832500	2.34985800
H	0.41589200	1.60000900	0.63287600
H	0.46086900	3.28902400	1.18254300
C	0.32342000	1.09034200	-2.43791400
H	-0.08112000	1.79685000	-1.70443700
H	1.04046600	0.44975200	-1.91703600

H	0.84646200	1.65702900	-3.21160800
H	1.08668000	-0.99452600	0.49329300
O	0.49507800	-1.16058500	-0.33171900
H	0.52639900	-2.11474100	-0.50633000
O	1.64890400	-0.49098100	1.83504200
H	0.74075500	-0.45899900	2.31953000
H	2.25234600	-1.03973100	2.35765600



Zn	0.57656800	0.40648900	0.65834100
N	2.53311100	0.03951500	-0.35512000
N	0.07157300	-0.86411500	-1.09357400
N	-0.27817500	1.86942600	-0.53137400
O	-1.41333300	0.09266500	1.52114900
C	3.67760000	0.72794200	-0.14652700
C	4.89891900	0.22419000	-0.60323600
H	5.81131900	0.78367100	-0.42560600
C	4.92678700	-0.98715300	-1.29401100
H	5.86816900	-1.38975100	-1.65585400
C	3.73268200	-1.66615400	-1.53326300
H	3.71560700	-2.59839700	-2.08937100
C	2.55094300	-1.11627100	-1.04081500
C	1.21080900	-1.79874000	-1.25288500
H	1.18942900	-2.27194000	-2.24656200
H	1.09115300	-2.59792900	-0.51750200
C	0.08038300	0.14037100	-2.19702300
H	-0.40459900	-0.26351000	-3.09468300
H	1.12077700	0.34973100	-2.46117900
C	-0.55903500	1.45007000	-1.78171200
C	-1.33955800	2.21058800	-2.64495400
H	-1.55906800	1.85117700	-3.64513100
C	-1.82505100	3.44059700	-2.19379500
H	-2.43375900	4.06024500	-2.84550800
C	-1.53195000	3.86025800	-0.89888100
H	-1.90698400	4.80532900	-0.52111100
C	-0.75856500	3.04233500	-0.06799600
C	-1.23522200	-1.60422100	-1.09727900
H	-1.11638700	-2.49315800	-1.73346000
H	-1.96091700	-0.95766400	-1.60046900
C	-1.85672200	-2.01568600	0.25882200
C	-2.41929000	-0.77961800	0.99142800
H	-3.06182100	-1.10665400	1.81706200
C	-3.06138600	-2.91962200	-0.08239900
H	-2.73703900	-3.82318100	-0.60996900

H	-3.79191800	-2.40187800	-0.71633100
H	-3.57487200	-3.23616500	0.83119900
C	-0.88612100	-2.78079200	1.17216800
H	-0.01977700	-2.17746800	1.46353900
H	-0.53193700	-3.69900000	0.68909000
H	-1.38795100	-3.06690600	2.10225800
O	1.31556300	0.41116000	2.41349100
H	2.19016800	-0.00071300	2.47327100
H	-1.25667200	-0.13380600	2.48426000
C	3.55835900	2.05718300	0.54895400
H	3.08057900	2.78393800	-0.12099800
H	2.93039200	1.97015700	1.44163100
H	4.53730900	2.45088200	0.83293300
C	-0.45942800	3.37846600	1.36489100
H	-1.04201600	2.71819400	2.01889200
H	0.59621100	3.20295500	1.59779100
H	-0.70971300	4.41595500	1.59765400
O	-0.57394200	-0.55164500	3.91527400
H	0.28839500	-0.18637200	3.54180600
H	-0.76517300	-0.07774800	4.73817900
H	-3.03379500	-0.18411500	0.30544000
[Zn(L <sup>2</sup> H)( $\eta$ -OH)(H <sub>2</sub> O)] <sup>+</sup>			
Zn	0.59407800	0.40167700	0.63890300
N	2.54707500	0.02570900	-0.34937500
N	0.07960100	-0.86634000	-1.10386300
N	-0.25550500	1.87322200	-0.53361500
O	-1.43417600	0.09448000	1.49796200
O	-3.20366400	-0.02651600	0.03944500
C	3.69257000	0.71045200	-0.13413200
C	4.91138500	0.21487600	-0.60584500
H	5.82471900	0.77101200	-0.42274200
C	4.93545000	-0.98375500	-1.31854400
H	5.87485400	-1.37958900	-1.69273100
C	3.74015500	-1.65863300	-1.56336100
H	3.72017600	-2.58079200	-2.13588200
C	2.56077900	-1.11832600	-1.05505100
C	1.22007800	-1.79839700	-1.26883400
H	1.19789500	-2.26811400	-2.26396600
H	1.10076400	-2.60065000	-0.53607200
C	0.08371200	0.14591600	-2.20101300
H	-0.39934600	-0.25445200	-3.10072300
H	1.12333000	0.36334500	-2.46287300
C	-0.56380900	1.44733000	-1.77444600
C	-1.38293600	2.19087600	-2.61577200

H	-1.62636800	1.82385100	-3.60737500
C	-1.88304000	3.40882400	-2.15061700
H	-2.52592200	4.01329700	-2.78352200
C	-1.55939800	3.83741100	-0.86522500
H	-1.94109300	4.77615400	-0.47818700
C	-0.74341100	3.03802200	-0.05882400
C	-1.22655700	-1.61072800	-1.11655400
H	-1.09316900	-2.51528200	-1.72549500
H	-1.94864900	-0.97967500	-1.63587100
C	-1.86177400	-2.00481000	0.23545500
C	-2.43881400	-0.76379500	0.95972900
H	-3.05911500	-1.10561000	1.80089400
C	-3.04657400	-2.93877200	-0.09824700
H	-2.68959500	-3.86281300	-0.56567800
H	-3.75844300	-2.45697600	-0.77481400
H	-3.58302900	-3.21719700	0.81519000
C	-0.89656800	-2.73554200	1.18285800
H	-0.02426000	-2.13194400	1.45327400
H	-0.55147700	-3.67210200	0.73060400
H	-1.40006600	-2.98912900	2.12187000
H	-3.62878500	0.70981000	0.50590400
O	1.28816200	0.38473900	2.41279300
H	2.15170800	-0.04665800	2.49286000
H	-1.30297800	-0.10148800	2.47503200
C	3.57669800	2.02673300	0.58605400
H	3.09170900	2.76441000	-0.06717200
H	2.95561400	1.92266200	1.48207800
H	4.55748700	2.41736800	0.86893800
C	-0.39701100	3.38710600	1.36092300
H	-0.89814800	2.68833200	2.04145800
H	0.67881100	3.28316500	1.53736300
H	-0.70194900	4.40519700	1.61315000
O	-0.64476800	-0.46751700	3.91697800
H	0.23391700	-0.14571200	3.53731700
H	-0.82106900	0.03426500	4.72654800
[Zn(L <sup>3</sup> H)( $\eta$ -OH)(H <sub>2</sub> O)] <sup>+</sup>			
Zn	-0.29631500	-0.20562100	0.84978600
N	-2.29591300	0.17258800	-0.12862200
N	0.21979600	0.76831600	-1.09739700
N	1.12710500	-1.61463000	-0.13499500
C	-3.49650200	-0.37053700	0.19268200
C	-4.65781400	0.00861700	-0.49470800
H	-5.60680400	-0.43449900	-0.21256300
C	-4.58592300	0.93183000	-1.53121700



H	-5.47968800	1.22396900	-2.07437300
C	-3.34384700	1.46832400	-1.86691400
H	-3.23753400	2.18565600	-2.67456400
C	-2.23075900	1.07019000	-1.13490200
C	-0.87791200	1.69529400	-1.40088500
H	-0.82254700	2.07212800	-2.43304300
H	-0.78195000	2.55269400	-0.73229200
C	0.23572100	-0.38046900	-2.02873000
H	0.59663000	-0.08019800	-3.02366600
H	-0.79485500	-0.73123400	-2.14746600
C	1.08655500	-1.50917900	-1.48014300
C	1.78632300	-2.36821600	-2.31831100
H	1.73439000	-2.24582700	-3.39556000
C	2.56315300	-3.37290700	-1.73818800
H	3.12308200	-4.06426900	-2.36082700
C	2.63660300	-3.45392500	-0.35211900
H	3.26242500	-4.19892200	0.12845300
C	1.91147400	-2.55317300	0.44100500
C	1.56683100	1.39390700	-1.05927100
H	1.86188200	1.68700700	-2.07898400
H	2.24597300	0.59761600	-0.74926300
C	1.80462200	2.61652900	-0.13453500
C	3.31874900	2.60259200	0.22811400
H	3.91999400	2.62317300	-0.68823300
H	3.58145700	1.70641500	0.79963000
H	3.58658800	3.48096800	0.82359000
C	1.51997200	3.96197600	-0.85291900
H	0.47882700	4.07725000	-1.16343500
H	2.14855200	4.04196700	-1.74575400
H	1.76502000	4.80566100	-0.19960000
C	1.07331800	2.60472900	1.18381700
H	1.13920800	3.51760000	1.77994100
N	0.44129800	1.62083200	1.70633300
O	-0.12074000	1.95380900	2.93574300
O	-0.77337700	-1.23666800	2.38481100
H	-0.81331200	-2.19151300	2.23342400
H	0.05967800	1.16005100	3.53491100
C	2.01126500	-2.60294700	1.94192400
H	1.77474200	-1.64106300	2.39788000
H	1.31099400	-3.33994400	2.35430600
H	3.01676200	-2.91032000	2.24483700
C	-3.56082400	-1.40370800	1.27992200
H	-3.10832000	-2.34186600	0.93302100
H	-2.98928000	-1.08703900	2.15467000

H	-4.59742300	-1.61178300	1.55587000
O	0.48728300	-0.18888300	4.34144800
H	-0.04803300	-0.78058000	3.72036800
H	0.12380600	-0.27517300	5.23533600
[Zn <sub>2</sub> (L <sup>1</sup> H) <sub>2</sub> (μ-OH)] <sup>3+</sup>			
Zn	-0.01956600	-0.54888700	0.83143400
N	-2.13728900	-0.67204800	0.36286700
N	-0.29500300	1.20353400	-0.41277900
N	1.03872900	-1.23462800	-0.80042300
O	1.75778500	0.21283300	1.79562900
C	-2.94870400	-1.75242200	0.47078000
C	-4.32950800	-1.62261500	0.29808900
H	-4.96613800	-2.49708400	0.38437800
C	-4.86952300	-0.37641900	-0.01798200
H	-5.93889300	-0.26340300	-0.16953700
C	-4.01715000	0.71843200	-0.16990800
H	-4.40251900	1.69374300	-0.45077000
C	-2.65243200	0.53290300	0.03062000
C	-1.67163400	1.68350400	-0.12913500
H	-2.02004900	2.35464100	-0.92678200
H	-1.64288500	2.27369000	0.78979200
C	-0.25418000	0.58379000	-1.77531000
H	-0.14912500	1.35519200	-2.54698900
H	-1.20989800	0.08170400	-1.95345000
C	0.84451100	-0.45105400	-1.88886000
C	1.56907700	-0.63715100	-3.05960300
H	1.39796700	0.00665000	-3.91634400
C	2.50769200	-1.67106800	-3.11093900
H	3.08359900	-1.84465200	-4.01489000
C	2.69960500	-2.47366900	-1.98803200
H	3.42412600	-3.28105500	-2.00000800
C	1.95513900	-2.22790200	-0.83210200
C	0.71144100	2.32254800	-0.35216500
H	0.21055000	3.24655700	-0.66930500
H	1.46756900	2.10352900	-1.11165000
C	1.45879500	2.57381300	0.97856100
C	2.42238000	1.41686400	1.30834200
H	2.97852500	1.09647100	0.42375400
H	3.14544100	1.72711000	2.06914500
O	-0.45687700	-1.12402800	2.71273800
H	-1.41697000	-1.23413300	2.64208700
H	1.56568000	0.30614600	2.74294600
C	2.15595100	-3.01805400	0.43112000
H	2.86623100	-2.49365400	1.08540600

H	1.20696700	-3.14189900	0.96445900
H	2.56544600	-4.00991600	0.22442500
C	-2.30779700	-3.09608800	0.70828100
H	-2.01713200	-3.54353400	-0.25090600
H	-1.40505400	-3.01382800	1.32157300
H	-3.00214200	-3.78733200	1.19381300
Zn	-0.19169300	-1.62114000	4.64719600
N	-2.33481800	-1.95664200	4.79115300
N	-0.27164500	-3.40862900	5.86541200
N	0.43084000	-0.74651500	6.40866900
O	1.83958100	-1.95628400	3.98507400
C	-3.33232600	-1.06983800	4.55539500
C	-4.66573300	-1.48902200	4.54152100
H	-5.45388100	-0.76689100	4.35488500
C	-4.97031800	-2.82443600	4.80223500
H	-6.00264500	-3.16138600	4.80922900
C	-3.93579100	-3.71762900	5.08662500
H	-4.14264100	-4.75539500	5.32919600
C	-2.62631800	-3.24687400	5.07050500
C	-1.45640400	-4.16564200	5.38463900
H	-1.76632200	-4.91345000	6.12786400
H	-1.16544100	-4.71422200	4.48563500
C	-0.56711900	-2.81770600	7.20928700
H	-0.41404000	-3.56117600	8.00001200
H	-1.62393800	-2.53576100	7.23679700
C	0.25342300	-1.57252900	7.46812600
C	0.73913300	-1.25369600	8.73019500
H	0.58842300	-1.93438400	9.56189500
C	1.41032400	-0.04036900	8.90418000
H	1.79485800	0.23854800	9.88053900
C	1.58359100	0.80570200	7.81061500
H	2.10269400	1.75227800	7.91791200
C	1.09051700	0.42344400	6.56093800
C	0.94688100	-4.28843900	5.97387600
H	0.60995100	-5.30449700	6.21750500
H	1.51235800	-3.93322200	6.84016200
C	1.92779300	-4.34396300	4.77957400
C	2.65910600	-3.00005200	4.59081700
H	2.98236200	-2.58624000	5.54926900
H	3.54513500	-3.13245900	3.96219100
H	1.82806100	-2.06833700	3.02061600
C	1.29591300	1.26220300	5.33023100
H	1.42990300	2.31752400	5.58061400
H	2.19932000	0.92805900	4.80132200

H	0.43652600	1.17538900	4.65608200
C	-2.96297900	0.38161400	4.38341700
H	-2.92913700	0.87506600	5.36326600
H	-1.97888200	0.49891700	3.91942200
H	-3.70358300	0.91093000	3.77745000
C	0.50834000	2.83124900	2.15841400
H	1.07903800	3.06419800	3.06418700
H	-0.14002800	3.69062300	1.95839300
H	-0.12811600	1.96364000	2.37559700
C	2.33929500	3.82368500	0.74391000
H	1.72472500	4.69055400	0.48125700
H	2.89998600	4.07946200	1.64881600
H	3.06165600	3.66658400	-0.06549400
C	1.25020100	-4.77695000	3.46979000
H	1.99128700	-4.86324200	2.66746700
H	0.78021500	-5.75989400	3.57924300
H	0.48239700	-4.06407900	3.14236700
C	3.00978300	-5.37988700	5.16541500
H	2.56288100	-6.36281900	5.34479100
H	3.74341500	-5.49337100	4.36074700
H	3.54953300	-5.08591600	6.07305100
$[\text{Zn}_2(\text{L}^2\text{H})_2(\mu\text{-OH})]^{3+}$			
Zn	2.65624600	-1.86049000	-0.64072900
N	0.69037800	-1.19028200	-0.10856700
N	2.17058000	-3.25822900	0.93912500
N	3.92597000	-1.03354500	0.75923400
O	5.39054100	-5.18236700	-1.71332900
O	4.32493600	-3.26095800	-1.21774600
C	0.15223900	0.03217800	-0.31105800
C	-1.14004800	0.32607200	0.13790300
H	-1.54787300	1.31853600	-0.02326800
C	-1.87906400	-0.65071200	0.79646300
H	-2.88101100	-0.43592500	1.15575400
C	-1.30104100	-1.90344000	1.02372600
H	-1.83400300	-2.67499700	1.57048100
C	-0.01181300	-2.13314800	0.56286500
C	0.69783700	-3.44847700	0.81969000
H	0.29369600	-3.91700100	1.72710600
H	0.51785400	-4.13827100	-0.00875400
C	2.47635500	-2.42177500	2.14642500
H	2.53484800	-3.04789900	3.04356800
H	1.64479600	-1.72781900	2.30039300
C	3.73523700	-1.59448000	1.97865600
C	4.60000700	-1.34796100	3.03708200

H	4.42965500	-1.81169100	4.00340300
C	5.68094600	-0.48481700	2.83264300
H	6.37200000	-0.27063000	3.64231600
C	5.86242100	0.09547000	1.58010300
H	6.69126700	0.77130800	1.39650200
C	4.96708100	-0.19736200	0.54607500
C	2.87440400	-4.58028300	1.06440000
H	2.19457900	-5.27352200	1.57534200
H	3.71861000	-4.42563800	1.74318000
C	3.42746400	-5.26594800	-0.20878000
C	4.70123400	-4.52679900	-0.67301600
H	5.37493700	-4.36845100	0.18265300
C	3.85501400	-6.68650700	0.22538400
H	2.99755500	-7.24451000	0.61333900
H	4.61787800	-6.66174000	1.01346000
H	4.25226200	-7.24885500	-0.62412700
C	2.41890900	-5.36658800	-1.36233300
H	2.06973500	-4.38451100	-1.69375400
H	1.55244700	-5.96730800	-1.06638100
H	2.89272500	-5.85299400	-2.21996700
H	5.12066100	-2.83842900	-1.58034000
C	0.97148800	1.06261100	-1.03807200
H	0.77982400	2.06527400	-0.64566100
H	2.04301400	0.85976400	-0.95131000
H	0.69630900	1.07060900	-2.09971000
C	5.10361100	0.42851100	-0.81716700
H	4.60249000	1.40511500	-0.83551300
H	6.15350100	0.60052600	-1.07097000
H	4.64214600	-0.18921300	-1.59514300
Zn	2.69725900	-2.25382500	-4.34553500
N	3.83287800	-3.95334400	-4.59313300
N	1.27687900	-3.39116700	-5.49920000
N	2.88256900	-1.10575900	-6.03439800
O	-1.40593100	-0.51432400	-3.04334600
O	0.49644400	-0.66533000	-4.29231300
C	5.17768300	-4.04315300	-4.52849400
C	5.82454800	-5.24171500	-4.84463600
H	6.90713200	-5.29425100	-4.79335400
C	5.07338000	-6.34724100	-5.22669700
H	5.56156400	-7.28385500	-5.47867600
C	3.68125300	-6.23306500	-5.31128200
H	3.07059900	-7.06841800	-5.63878900
C	3.09321400	-5.01700400	-4.99455800
C	1.59614900	-4.79610100	-5.10766100

H	1.17146000	-5.50729900	-5.82846000
H	1.11939100	-4.98596200	-4.14283500
C	1.80579700	-3.12074600	-6.87873400
H	1.07891100	-3.42725600	-7.63865100
H	2.69666500	-3.73891200	-7.02796800
C	2.21939700	-1.67493800	-7.06959300
C	2.01453900	-0.99597400	-8.26346300
H	1.47850600	-1.47020100	-9.07924300
C	2.52307100	0.30036300	-8.39189800
H	2.38108900	0.85557900	-9.31423600
C	3.21310100	0.87253200	-7.32546200
H	3.62122100	1.87484000	-7.40250500
C	3.38205800	0.14644300	-6.14191300
C	-0.21346700	-3.16027700	-5.49715600
H	-0.68309400	-4.10469600	-5.79855900
H	-0.41751400	-2.44756500	-6.30103800
C	-0.92202100	-2.63058600	-4.21963600
C	-0.86330200	-1.08252800	-4.21702200
H	-1.39850400	-0.70539100	-5.09974800
C	-2.41451500	-3.01154400	-4.35961400
H	-2.53915400	-4.09863100	-4.33453000
H	-2.84308300	-2.64825500	-5.30129900
H	-2.99912100	-2.59508500	-3.53365800
C	-0.38856000	-3.21169800	-2.90281200
H	0.67371800	-3.00798900	-2.75177100
H	-0.54827400	-4.29434000	-2.86771500
H	-0.92836600	-2.76482000	-2.06414000
H	0.51971000	0.27708100	-4.52754900
C	5.95757300	-2.81087100	-4.15943900
H	6.78520400	-3.05869700	-3.48731800
H	6.39621700	-2.35265900	-5.05455300
H	5.32093400	-2.05582600	-3.68452300
C	4.14225300	0.69832600	-4.96543600
H	5.17880900	0.33729300	-4.98400100
H	4.17675600	1.79041800	-4.99006900
H	3.69570900	0.37724300	-4.01775600
H	-2.30656300	-0.19095600	-3.20358400
H	6.05239500	-5.79126400	-1.34685300
O	2.56382000	-1.46269400	-2.57752300
H	1.77909200	-0.89838800	-2.70931700
[Zn <sub>2</sub> (L <sup>1</sup> )(L <sup>1</sup> H)(μ-OH)] <sup>2+</sup>			
Zn	-1.63685400	0.48067800	0.10315300
N	-2.99802600	2.13959100	0.18740200
N	-2.99107500	0.16157800	-1.73005300

N	-3.08437300	-1.17752500	0.79304100
O	-0.40288800	-1.21290300	-0.67610200
C	-3.25096200	2.92186700	1.25767600
C	-3.94715200	4.12656300	1.11006300
H	-4.13959800	4.74451200	1.98072700
C	-4.40071800	4.50725700	-0.15060100
H	-4.95137500	5.43420800	-0.27970600
C	-4.15557400	3.67377700	-1.24323300
H	-4.51227000	3.92903800	-2.23609400
C	-3.43999300	2.49891200	-1.03604100
C	-3.10385000	1.56604700	-2.18449300
H	-3.86473300	1.67054500	-2.97237500
H	-2.13793500	1.85174100	-2.61292000
C	-4.27434700	-0.28631100	-1.12663400
H	-4.98735500	-0.59449700	-1.90184600
H	-4.72909800	0.55268700	-0.59577600
C	-4.05561400	-1.39161900	-0.12281700
C	-4.86688700	-2.52225900	-0.11057000
H	-5.62878200	-2.65303800	-0.87238000
C	-4.68952700	-3.46381500	0.90316700
H	-5.30507400	-4.35732900	0.94396500
C	-3.71853700	-3.22659600	1.86959600
H	-3.56725600	-3.92414900	2.68674400
C	-2.92749900	-2.07293200	1.79210900
C	-2.65919200	-0.76162500	-2.86926900
H	-2.98819900	-0.28756100	-3.80449100
H	-3.28247300	-1.65145500	-2.74179800
C	-1.21093400	-1.26306400	-3.04416900
C	-0.74769300	-2.04561300	-1.80341900
H	-1.53837500	-2.70825300	-1.43948200
H	0.12397000	-2.66394200	-2.05100200
Zn	1.33245400	1.38083800	0.58651400
N	2.53268700	-0.21330600	-0.30502800
N	2.68425400	2.50706700	-0.77013300
N	2.57336000	2.42209500	2.01763400
O	-0.13882400	1.85945200	-0.73115500
C	2.76880600	-1.45309100	0.19186100
C	3.58479200	-2.35479100	-0.49650200
H	3.76107900	-3.34196600	-0.08258700
C	4.17622700	-1.96756300	-1.69752400
H	4.81765400	-2.65524600	-2.24058500
C	3.95872400	-0.67589900	-2.17822500
H	4.43304900	-0.32904300	-3.09066600
C	3.13405500	0.17919000	-1.45288900

C	2.85981900	1.59637100	-1.91320700
H	3.66104000	1.93518400	-2.58617000
H	1.92784900	1.59928200	-2.47531700
C	3.93536200	2.65209700	0.00023700
H	4.60124300	3.39956800	-0.45284100
H	4.46973000	1.69585600	-0.01972900
C	3.65655700	3.00050500	1.44764100
C	4.51816300	3.82984000	2.15724500
H	5.36832600	4.28287600	1.65762200
C	4.26557500	4.06181300	3.50850400
H	4.91712300	4.70714900	4.08982000
C	3.16166200	3.45406200	4.09843500
H	2.93811000	3.61032200	5.14825300
C	2.32487600	2.63387200	3.33452700
C	2.18228600	3.86077300	-1.14803700
H	2.86685100	4.29884900	-1.89289000
H	2.28488800	4.45846100	-0.23644800
C	0.72210500	4.02048200	-1.63832700
C	-0.27903300	3.27165400	-0.73249100
H	-0.19644700	3.67560900	0.29502000
H	-1.27914700	3.55515800	-1.08146700
H	0.46198900	-0.80078600	-0.83892500
O	-0.21599300	0.57559900	1.53622100
H	-0.11021500	-0.12499400	2.19017100
C	-1.88091300	-1.80295300	2.83913200
H	-2.04679700	-2.41714000	3.72751100
H	-0.88462100	-2.04624000	2.45097200
H	-1.89645400	-0.75060100	3.13625200
C	1.14370100	1.94784600	3.96136900
H	0.24945400	2.06498400	3.34748000
H	1.33398500	0.87035800	4.04844100
H	0.95331900	2.33552600	4.96470300
C	2.10468400	-1.81744900	1.48999700
H	2.20073300	-1.00045300	2.21313900
H	1.03794400	-1.99578400	1.31621200
H	2.54342800	-2.72019400	1.92118300
C	-2.78923700	2.42134300	2.59738500
H	-3.44753300	1.61180700	2.93912600
H	-1.77924600	2.00905300	2.52095100
H	-2.81045700	3.21307200	3.35039100
C	0.51218500	3.61649900	-3.11065200
H	-0.45775700	3.98883900	-3.46124900
H	1.28180600	4.05166100	-3.75813500
H	0.50680300	2.53602900	-3.25771100



C	0.41570200	5.53237200	-1.51925200
H	1.10395600	6.12576800	-2.13158500
H	-0.60082600	5.74657100	-1.86670100
H	0.49754000	5.88361100	-0.48349400
C	-0.23372600	-0.12157900	-3.35293500
H	-0.51707300	0.38687200	-4.28150300
H	-0.21337000	0.61475000	-2.54482300
H	0.78272100	-0.51434300	-3.49435800
C	-1.23911800	-2.26023500	-4.22342600
H	-0.23012700	-2.62519200	-4.44328200
H	-1.87206600	-3.13010000	-4.00957900
H	-1.62207700	-1.78229000	-5.13142000
$[\text{Zn}_2(\text{L}^2)(\text{L}^2\text{H})(\mu\text{-OH})]^{2+}$			
Zn	-1.68337300	0.44052000	0.05731600
N	-3.04537000	2.12452000	0.12292300
N	-2.98819600	0.12476400	-1.76106700
N	-3.11961800	-1.14417500	0.79148300
O	-0.37414200	-1.16923200	-0.73679800
C	-3.33588900	2.91457800	1.17908700
C	-4.00206100	4.13145800	0.99692300
H	-4.21723600	4.75964100	1.85492700
C	-4.40023600	4.50967800	-0.28372400
H	-4.92655300	5.44636500	-0.44070600
C	-4.13499400	3.66004400	-1.35894900
H	-4.45675100	3.91031000	-2.36498700
C	-3.44541800	2.47553100	-1.11803700
C	-3.09786800	1.52002800	-2.24523300
H	-3.85334600	1.60688700	-3.04033800
H	-2.12955100	1.80059800	-2.66874100
C	-4.28344200	-0.31552000	-1.17412000
H	-4.96972000	-0.66029800	-1.95736000
H	-4.76268300	0.53824200	-0.69009500
C	-4.08522100	-1.38056200	-0.12290000
C	-4.91017000	-2.49960000	-0.07423900
H	-5.66574200	-2.65151900	-0.83809400
C	-4.74672700	-3.40782000	0.96995000
H	-5.37069900	-4.29386600	1.03697800
C	-3.77643000	-3.14900100	1.93314000
H	-3.63687200	-3.82010800	2.77428200
C	-2.97545100	-2.00674400	1.82144700
C	-2.64300700	-0.82835700	-2.87358300
H	-3.02820300	-0.40919700	-3.81333500
H	-3.20476900	-1.74309600	-2.68248100
C	-1.17830100	-1.25578500	-3.10021000

C	-0.62146500	-2.02047200	-1.88340800
H	0.34634300	-2.47229900	-2.15079700
Zn	1.29897300	1.49854600	0.61994300
N	2.47340700	-0.18886000	-0.28794100
N	2.65922500	2.51756900	-0.78338000
N	2.67913500	2.34821200	2.02550800
O	-0.19588600	1.85104200	-0.85920400
C	2.72302600	-1.41287700	0.23747100
C	3.54571800	-2.32511400	-0.42876200
H	3.73450300	-3.29936900	0.00982400
C	4.12968000	-1.96245200	-1.64178800
H	4.77524400	-2.65780200	-2.17005200
C	3.90070400	-0.68429500	-2.15248400
H	4.37099400	-0.35495500	-3.07351800
C	3.07163400	0.18128200	-1.44341200
C	2.79390600	1.59124000	-1.92087900
H	3.57790100	1.91560800	-2.62021300
H	1.84412100	1.59472700	-2.45208300
C	3.93666900	2.64973600	-0.04609800
H	4.58578500	3.40417000	-0.51028700
H	4.46906200	1.69413600	-0.10209600
C	3.71339900	2.97059200	1.41791800
C	4.57505400	3.81926000	2.10535100
H	5.38835800	4.30978700	1.58038800
C	4.36900000	4.02251700	3.46934100
H	5.02218000	4.68094900	4.03386400
C	3.30901800	3.37208300	4.09476300
H	3.12173400	3.50914700	5.15433900
C	2.47027700	2.53817000	3.34939400
C	2.16796700	3.87316800	-1.16795700
H	2.81747300	4.28104700	-1.95845600
H	2.32104100	4.48615100	-0.27675100
C	0.68551000	4.04244100	-1.59217300
C	-0.26999600	3.21927000	-0.69688700
H	-1.28655900	3.59343400	-0.86987100
H	0.49319000	-0.73468800	-0.82803800
O	-0.28448200	0.66112100	1.49930300
H	-0.17630200	-0.01299000	2.18070400
C	-1.93219300	-1.70912300	2.86538900
H	-2.09173800	-2.31130000	3.76307000
H	-0.93071700	-1.94396100	2.48499800
H	-1.96059200	-0.65299500	3.14861400
C	1.31657200	1.81852800	3.99278400
H	0.38695300	2.00909700	3.44982300

H	1.48490300	0.73427200	3.97678000
H	1.19356100	2.12275600	5.03462400
C	2.06404000	-1.74389400	1.54727500
H	2.19217000	-0.91951800	2.25678700
H	0.98996400	-1.89021300	1.38995500
H	2.48094800	-2.65294600	1.98697200
C	-2.95764200	2.40962800	2.54664800
H	-3.70124600	1.67697500	2.88643300
H	-1.98992400	1.89798000	2.52483100
H	-2.93035700	3.22049800	3.27941100
C	0.41050100	3.69339600	-3.06712800
H	-0.61969600	3.96535500	-3.32755300
H	1.07296600	4.26291700	-3.72785500
H	0.52581900	2.63310900	-3.29175200
C	0.36620500	5.54450000	-1.40478000
H	1.03601500	6.16280500	-2.01299900
H	-0.65932000	5.76052100	-1.72494400
H	0.46683100	5.84781200	-0.35914900
C	-0.25266100	-0.07697600	-3.42531900
H	-0.58288400	0.41888000	-4.34472800
H	-0.23488700	0.65743500	-2.61800800
H	0.77209800	-0.43219400	-3.60112400
C	-1.19338800	-2.23885200	-4.29370900
H	-0.18008300	-2.59701600	-4.50767700
H	-1.82587000	-3.10883300	-4.09504400
H	-1.56162100	-1.74020000	-5.19640400
O	-1.54310900	-2.98331600	-1.48446000
H	-1.14847200	-3.56552100	-0.81708900
O	0.08662000	3.54832600	0.68528500
H	-0.64892300	3.25991300	1.24892500
$[\text{Zn}_2(\text{L}^1\text{H})_2(\mu\text{-OH})_2]^{2+}$			
Zn	-0.26598500	1.96747100	-1.90093700
N	-1.98658600	1.57817000	-3.14612800
N	0.31026600	2.86976300	-3.89858800
N	1.17142000	0.35802900	-2.84039500
O	1.74622600	2.77899800	-1.09269600
C	-2.94227900	0.64534200	-2.96640700
C	-4.15992900	0.73729500	-3.64857200
H	-4.91881600	-0.02466000	-3.50344000
C	-4.37287600	1.80079700	-4.52434800
H	-5.31094900	1.88698400	-5.06451100
C	-3.35362100	2.73290400	-4.73233000
H	-3.47229200	3.54356200	-5.44456600
C	-2.16240700	2.58379400	-4.02677200

C	-0.97859000	3.51682500	-4.24649000
H	-0.98115600	3.85489300	-5.29355700
H	-1.07328400	4.40392100	-3.61358500
C	0.54237000	1.68386500	-4.76936700
H	0.91993900	1.98908300	-5.75335700
H	-0.40930300	1.17584400	-4.93671100
C	1.47683000	0.69643500	-4.11188500
C	2.54511800	0.13498100	-4.80545700
H	2.75621200	0.44223000	-5.82483500
C	3.32462700	-0.82891600	-4.16467800
H	4.16899300	-1.28495900	-4.67274600
C	2.99431400	-1.20094600	-2.86581300
H	3.56829000	-1.95977900	-2.34430000
C	1.90452800	-0.59635300	-2.22355900
C	1.46491600	3.82146000	-4.08138800
H	1.13827100	4.62935000	-4.74891900
H	2.23852500	3.27168700	-4.62478900
C	2.15362300	4.45638500	-2.85195900
C	2.76609300	3.39102700	-1.93098300
H	3.25415100	2.60466800	-2.51911300
H	3.50935700	3.85172200	-1.27098700
O	-0.41312300	1.33099700	-0.02911600
H	-0.92617700	0.51503100	0.04401300
H	2.10729100	1.98727700	-0.65997100
Zn	-1.39516100	3.10849300	0.82892700
N	-3.13130800	1.77543500	1.07852500
N	-1.28462700	2.39839800	2.99935900
N	-2.14787100	4.88096900	1.97542500
O	0.54748900	4.00942700	1.05507300
C	-4.25810900	1.74554200	0.33909400
C	-5.14584600	0.66817500	0.43551900
H	-6.05492200	0.66371300	-0.15715300
C	-4.85695600	-0.37906400	1.30832100
H	-5.53485900	-1.22270900	1.39776800
C	-3.70736100	-0.31299600	2.09772100
H	-3.48025300	-1.08790900	2.82335100
C	-2.86940100	0.79206000	1.96398900
C	-1.64422900	0.97214400	2.85076100
H	-1.84127100	0.50636300	3.82875600
H	-0.78345500	0.46056700	2.41212300
C	-2.39130400	3.14503000	3.65577200
H	-2.35842800	3.01829300	4.74570700
H	-3.34596700	2.73540800	3.31858500
C	-2.35470000	4.60881700	3.28190900

C	-2.56046800	5.60485900	4.23127000
H	-2.71520200	5.34188400	5.27281200
C	-2.56322500	6.93595300	3.81306200
H	-2.71966300	7.73910000	4.52689600
C	-2.35490300	7.21623600	2.46663200
H	-2.34737700	8.24010400	2.10812200
C	-2.14515300	6.16795600	1.56167300
C	-0.03829400	2.58174700	3.81981500
H	0.04973700	1.72712100	4.50594400
H	-0.21068200	3.46114200	4.44708100
C	1.32237200	2.80719100	3.12097100
C	1.30787500	4.09330000	2.27215600
H	0.86797300	4.91857400	2.84181900
H	2.33632000	4.37679300	2.01743000
O	-1.27063200	3.61246800	-1.10550000
H	-2.06381100	3.96454100	-1.52750900
H	1.08754300	3.65321400	0.31685000
C	-4.51409300	2.91052300	-0.57936800
H	-4.16749800	3.84010500	-0.11763800
H	-3.97537100	2.77751700	-1.52391900
H	-5.57812600	3.00551600	-0.81115500
C	-2.62956800	-0.48007900	-2.01701100
H	-1.57374900	-0.75640900	-2.09840000
H	-2.82464300	-0.17660500	-0.98257800
H	-3.24403100	-1.35960500	-2.22575700
C	-1.91408200	6.43784100	0.10145100
H	-2.76679700	6.08195700	-0.49066400
H	-1.79741900	7.50763300	-0.08789100
H	-1.02923600	5.90306200	-0.24833600
C	1.49895100	-1.02397100	-0.83812400
H	0.55028300	-1.57468700	-0.88049700
H	2.24793100	-1.68340000	-0.39305900
H	1.32875200	-0.16565200	-0.18444100
C	1.76271100	1.60240100	2.27853600
H	2.75955900	1.78409300	1.85237900
H	1.84098000	0.70255500	2.90030500
H	1.05744200	1.41010200	1.46669100
C	2.34344100	3.04056300	4.25852100
H	3.35097900	3.17400400	3.85031900
H	2.10128900	3.93107900	4.85136300
H	2.37503200	2.18298800	4.93915700
C	1.21731100	5.39501100	-2.07705200
H	0.88380200	6.21014100	-2.73060500
H	0.34004500	4.87033900	-1.69394800

H	1.74211800	5.85046000	-1.22867300
C	3.34456400	5.26759300	-3.41664900
H	3.85215900	5.81290900	-2.61443900
H	4.08426700	4.62581200	-3.91107400
H	2.99931700	6.00560400	-4.14818100
$[\text{Zn}_2(\text{L}^2\text{H})_2(\mu\text{-OH})_2]^{2+}$			
Zn	2.89590000	-1.81696500	-1.01297400
N	0.93923300	-1.17209200	-0.23319900
N	2.55476800	-3.21671900	0.69570000
N	4.03865900	-0.76980900	0.52996200
O	6.16980600	-5.16907200	-1.45759100
O	5.29904300	-3.22966300	-0.62588400
C	0.27759300	-0.02242900	-0.46837700
C	-1.09647700	0.07198200	-0.24233400
H	-1.61818100	0.99976600	-0.44956500
C	-1.78211300	-1.03982700	0.24627100
H	-2.85130600	-0.98703400	0.42664600
C	-1.07986500	-2.21489100	0.51239000
H	-1.58153800	-3.08986700	0.91402900
C	0.28863000	-2.24582000	0.25242800
C	1.10817800	-3.50215200	0.49007400
H	0.69244100	-4.04779200	1.34978700
H	1.02972100	-4.14052500	-0.39351600
C	2.74304000	-2.32234400	1.87729100
H	2.81982100	-2.90635500	2.80164100
H	1.86037300	-1.68810500	1.98189800
C	3.93437500	-1.40525400	1.71748900
C	4.81690400	-1.16969600	2.76591100
H	4.70516800	-1.70349000	3.70433400
C	5.83408900	-0.23015500	2.58513800
H	6.54331600	-0.02525500	3.38158800
C	5.91712200	0.44825900	1.37350500
H	6.68209900	1.19995900	1.20889000
C	4.99849700	0.16552600	0.35342600
C	3.30958000	-4.49585700	0.95800300
H	2.60490700	-5.19269400	1.43075800
H	4.06114700	-4.26429400	1.71826000
C	4.04649500	-5.24441700	-0.18330400
C	5.44679700	-4.60992600	-0.37037200
H	6.02279300	-4.74809900	0.55777200
C	4.28560600	-6.68357800	0.32849900
H	3.33440900	-7.21005700	0.45573200
H	4.80718100	-6.69701100	1.29375800
H	4.88139200	-7.25449500	-0.39081700

C	3.26314900	-5.31199100	-1.49777200
H	3.02579700	-4.33396800	-1.90984500
H	2.31703400	-5.84356700	-1.34451000
H	3.83988200	-5.86508800	-2.24225600
H	6.16496000	-2.79829300	-0.53894200
C	1.10555900	1.12728900	-0.97728200
H	0.49085100	1.99770100	-1.22299800
H	1.84228900	1.42769300	-0.22252400
H	1.67439200	0.82786200	-1.86732600
C	5.01928500	0.91454800	-0.95005200
H	4.21253800	1.65917000	-0.96262300
H	5.96360700	1.44812900	-1.08646400
H	4.85214200	0.23034700	-1.78603800
Zn	2.74438200	-2.32927500	-4.05237100
N	3.56777400	-4.21099000	-4.66313200
N	1.06876000	-3.27343500	-5.54760600
N	2.75280600	-1.03102900	-5.72197100
O	-2.14193900	-0.59470200	-3.36255900
O	0.06881800	-0.81336100	-3.78758100
C	4.87025700	-4.57048200	-4.61684600
C	5.24954400	-5.90726200	-4.78352100
H	6.30127300	-6.16922300	-4.73801100
C	4.27995200	-6.87419100	-5.02067300
H	4.55897800	-7.91506800	-5.15471000
C	2.94521700	-6.48084800	-5.12604200
H	2.16660200	-7.19907200	-5.36245400
C	2.62348600	-5.13976000	-4.94759900
C	1.18783500	-4.67541700	-5.10152700
H	0.67272800	-5.36307400	-5.79193800
H	0.69238100	-4.75062000	-4.13209000
C	1.82371900	-3.01555000	-6.79817800
H	1.24084200	-3.28063700	-7.69114100
H	2.72156400	-3.63614000	-6.81787600
C	2.25507200	-1.56636300	-6.86115800
C	2.16582400	-0.83586800	-8.04196300
H	1.75738600	-1.29969200	-8.93396000
C	2.60443200	0.48750100	-8.05155400
H	2.54863600	1.08166300	-8.95868300
C	3.10067900	1.03883600	-6.87464500
H	3.43751500	2.06887900	-6.84194200
C	3.16321800	0.25892500	-5.71383100
C	-0.35593300	-2.90758400	-5.82845200
H	-0.78912600	-3.73800100	-6.40899900
H	-0.31686800	-2.05251000	-6.51165600

C	-1.38291700	-2.52740800	-4.72241400
C	-1.21152500	-1.03583100	-4.34119400
H	-1.32496100	-0.42273700	-5.25060100
C	-2.76784800	-2.62976400	-5.41099000
H	-2.96596500	-3.65977600	-5.72312900
H	-2.83487300	-1.99254000	-6.30182500
H	-3.56758100	-2.34422800	-4.72048600
C	-1.39717000	-3.43963200	-3.48669900
H	-0.43765300	-3.47039500	-2.97109400
H	-1.66395700	-4.46135400	-3.77947900
H	-2.15281400	-3.08604300	-2.77921700
H	0.07134200	0.09385100	-3.43964200
C	5.91426300	-3.51138500	-4.39709600
H	6.26817200	-3.55327800	-3.36051900
H	6.78075000	-3.69341200	-5.04062100
H	5.52569200	-2.51338700	-4.61108900
C	3.68726200	0.82702200	-4.42678800
H	4.63263100	0.35206600	-4.15123400
H	3.83495900	1.90673000	-4.50340900
H	2.99849100	0.61562100	-3.60371800
H	-2.94929200	-0.27239900	-3.79234800
H	6.79650600	-5.83561900	-1.13803400
O	4.05877600	-1.59822700	-2.63913400
H	4.82655900	-2.16562300	-2.47294500
O	1.65208100	-2.66338600	-2.45271300
H	0.85276000	-2.12450100	-2.57381300
[Zn <sub>2</sub> (L <sup>1</sup> H)(L <sup>n</sup> )] <sup>3+</sup>			
Zn	-2.45693700	-0.49194000	0.20045900
N	-2.08064300	1.27405100	1.39619400
N	-2.87795000	1.09729900	-1.19614500
N	-4.50622200	-0.76518000	0.11947500
O	-1.62243500	-1.81990100	-1.06133200
C	-2.11227400	1.40979500	2.74657600
C	-1.72230000	2.60535700	3.35656800
H	-1.75674900	2.68894000	4.43825700
C	-1.33131300	3.68672800	2.57077600
H	-1.02981500	4.62275600	3.03110700
C	-1.38873100	3.56613600	1.18137700
H	-1.15946600	4.40882100	0.53650500
C	-1.77484600	2.35027000	0.62908000
C	-1.93200400	2.19129400	-0.87130600
H	-2.27126800	3.14158200	-1.30688300
H	-0.96867200	1.96119400	-1.32779900
C	-4.26488100	1.48595700	-0.80155200



H	-4.72961500	2.10159100	-1.58084100
H	-4.20805900	2.10312000	0.10037100
C	-5.12347800	0.27706100	-0.48841100
C	-6.48757300	0.26004700	-0.75639000
H	-6.95675700	1.10442600	-1.25101800
C	-7.23401900	-0.85683600	-0.37551900
H	-8.30180200	-0.89521900	-0.56883600
C	-6.59060000	-1.92675300	0.24531200
H	-7.14511400	-2.80972500	0.54473700
C	-5.21613400	-1.86091400	0.47897700
C	-2.85442100	0.73697400	-2.64880000
H	-2.71047500	1.65493600	-3.23534200
H	-3.85478400	0.36418800	-2.88883300
C	-1.84389800	-0.34027400	-3.09824400
C	-2.13280900	-1.69581400	-2.40757200
H	-3.21706700	-1.87209600	-2.38532100
H	-1.69644600	-2.48874900	-3.02138500
Zn	-0.25451200	-3.17091900	-0.77366700
N	1.54955200	-2.76476000	-1.76741100
N	1.19127600	-3.73684100	0.75826900
N	-0.58579200	-5.20390900	-0.83766000
O	-0.98107400	-1.50188800	1.55690900
C	1.81150700	-2.76143800	-3.09538100
C	3.03953100	-2.28923600	-3.57236100
H	3.23180000	-2.28804400	-4.64059900
C	4.01118400	-1.86048600	-2.67321800
H	4.96887500	-1.49490700	-3.03125700
C	3.76297900	-1.96527800	-1.30061200
H	4.52879400	-1.71477000	-0.57329800
C	2.52427000	-2.43077500	-0.88354800
C	2.21570500	-2.67030200	0.58547300
H	3.14261000	-2.92035600	1.11888500
H	1.81127400	-1.76088200	1.03465400
C	1.64138800	-5.03769900	0.14962900
H	2.26971400	-5.59357100	0.85393000
H	2.25580100	-4.83043000	-0.72805800
C	0.45607300	-5.87589400	-0.28479900
C	0.45758000	-7.25999700	-0.17645200
H	1.30100200	-7.77155500	0.27597200
C	-0.64261800	-7.97255500	-0.66125900
H	-0.66944600	-9.05574100	-0.59041100
C	-1.70765300	-7.27656600	-1.22795600
H	-2.57522600	-7.80488600	-1.60886200
C	-1.66191300	-5.88194400	-1.30782600

C	0.90795600	-4.06261000	2.19991200
H	1.86740300	-4.29446500	2.68407300
H	0.34177300	-4.99767700	2.15830900
C	0.11355000	-3.11135400	3.12270200
C	-1.17849800	-2.63356700	2.45116300
H	-1.60815200	-3.41737900	1.82287900
H	-1.91953500	-2.35757700	3.20570800
H	-0.55459100	-0.78889700	2.06142300
C	0.79025500	-3.33876400	-4.03763800
H	-0.02878900	-3.81779300	-3.49427300
H	0.37605000	-2.57808800	-4.70682600
H	1.25720500	-4.09923300	-4.67301800
C	-2.77116300	-5.08835000	-1.93957800
H	-2.93072500	-4.14472700	-1.41034800
H	-2.52505900	-4.85046600	-2.98246100
H	-3.70705100	-5.65214000	-1.94721000
C	-4.45841400	-2.97672800	1.14291000
H	-3.52119700	-3.16535400	0.60763800
H	-4.21192300	-2.71304900	2.17899600
H	-5.04057500	-3.90083100	1.16695300
C	-2.63695700	0.26729400	3.57638800
H	-3.14447800	-0.47169800	2.95169900
H	-1.83909300	-0.22767300	4.14302300
H	-3.35691700	0.63736300	4.31323300
C	-0.31596900	-3.98682300	4.32869400
H	0.55198200	-4.46966300	4.78899500
H	-0.79836000	-3.37613500	5.09829000
H	-1.01855200	-4.77380600	4.02977100
C	0.94371800	-1.93130200	3.66860900
H	0.36122700	-1.35181100	4.39480900
H	1.82652300	-2.30358900	4.19755200
H	1.30654500	-1.24179200	2.89860700
C	-2.10737300	-0.53522100	-4.60954800
H	-1.97676300	0.40386600	-5.15693900
H	-1.41204400	-1.26268000	-5.03952900
H	-3.12526200	-0.89479000	-4.80177500
C	-0.38151600	0.07749900	-2.88001100
H	0.29545500	-0.63368500	-3.35847200
H	-0.18236500	1.05937900	-3.32270800
H	-0.11516900	0.10189100	-1.81812200
[Zn <sub>2</sub> (L <sup>2</sup> H)(L <sup>n</sup> )] <sup>3+</sup>			
Zn	0.14026800	-0.45031100	0.52441800
N	-1.80237400	-1.08130900	0.22560200
N	-0.44231700	1.01139700	-0.88648700

N	1.22511800	-1.26119300	-1.00945900
O	0.91917200	0.72062800	1.90864600
O	2.64445100	1.01542100	0.49125500
C	-2.31835400	-2.31486500	0.44186000
C	-3.67591500	-2.56123000	0.22180400
H	-4.07835100	-3.55217600	0.40521700
C	-4.48986700	-1.54136600	-0.27026900
H	-5.54465900	-1.72169200	-0.45504800
C	-3.92440000	-0.29856700	-0.56488300
H	-4.51999700	0.49863000	-0.99838900
C	-2.57290700	-0.10049000	-0.30688400
C	-1.88577200	1.22010700	-0.61822800
H	-2.38242400	1.70835300	-1.46758000
H	-1.98006400	1.89130800	0.23677800
C	-0.24925400	0.29956400	-2.18588500
H	-0.19016000	1.01546300	-3.01382100
H	-1.13238800	-0.32205600	-2.36782500
C	0.96453300	-0.61159200	-2.17140500
C	1.72313400	-0.83343200	-3.31262100
H	1.50175500	-0.29633100	-4.22933500
C	2.76687000	-1.76204300	-3.25641300
H	3.37647700	-1.95527700	-4.13390300
C	3.01680900	-2.43375500	-2.06300900
H	3.81795400	-3.16206300	-1.99220000
C	2.22849900	-2.16210300	-0.94113000
C	0.37412400	2.26422400	-0.86535200
H	-0.18147800	3.06266200	-1.37629300
H	1.25337800	2.04489100	-1.47440300
C	0.88352100	2.78614500	0.49808500
C	1.70539800	1.72733900	1.28980600
H	2.23422700	2.27276900	2.07276900
C	1.83865600	3.95806800	0.16076000
H	1.29912800	4.76569000	-0.34406500
H	2.65799300	3.65729400	-0.50335500
H	2.27447400	4.37902300	1.07389300
C	-0.22141600	3.33343600	1.42096000
H	-0.87615600	2.54571100	1.79822700
H	-0.82968000	4.08024100	0.90014000
H	0.22434500	3.82643900	2.29280100
H	3.33326300	1.61161200	0.15416600
C	-1.36617100	-3.41376000	0.82784500
H	-0.54273300	-3.03213800	1.43772300
H	-1.87118300	-4.21773800	1.36996300
H	-0.93105800	-3.85528100	-0.07785400

C	2.43736000	-2.88239500	0.36157800
H	2.04633700	-2.29419600	1.19791000
H	1.92264100	-3.85133600	0.35199200
H	3.49820600	-3.07430200	0.54450000
Zn	1.03070400	0.54730500	3.88325100
N	1.66709300	2.48247300	4.51482500
N	-0.35278900	0.90201500	5.47596100
N	1.98781100	-0.68634600	5.22214600
O	-0.24006700	-1.39118400	3.30662600
O	-1.14913800	-2.61157700	4.98767500
C	2.87414900	3.07662900	4.36470400
C	3.05494200	4.41525600	4.72873500
H	4.02677500	4.87991300	4.59564200
C	1.99494000	5.12731300	5.28497500
H	2.12315000	6.16547600	5.57627800
C	0.77638700	4.47799700	5.50339600
H	-0.05157100	4.98881700	5.98490400
C	0.65073700	3.15220300	5.10820300
C	-0.62312300	2.36495800	5.36029200
H	-1.11204700	2.74168900	6.26872700
H	-1.32341100	2.50693400	4.53251700
C	0.51878300	0.62654500	6.66657400
H	-0.09060300	0.49645000	7.56663800
H	1.15344100	1.49984500	6.84058100
C	1.43431600	-0.56328200	6.45501500
C	1.77275800	-1.42183700	7.49133800
H	1.31138000	-1.31010000	8.46714700
C	2.72285000	-2.42029500	7.25418100
H	3.00566200	-3.10660600	8.04660800
C	3.30769100	-2.51946800	5.99480000
H	4.06039400	-3.27359800	5.78877100
C	2.92263600	-1.63363900	4.98315400
C	-1.63356000	0.12470900	5.62876600
H	-2.36812300	0.78218600	6.10922400
H	-1.43118400	-0.68800000	6.32732700
C	-2.28028000	-0.51058500	4.38153100
C	-1.49774800	-1.76049800	3.92266900
H	-2.08823300	-2.29978700	3.17258000
C	-3.67460800	-1.01117000	4.82876900
H	-4.31470400	-0.16856500	5.10706500
H	-3.60913600	-1.67969500	5.69346000
H	-4.17602600	-1.54831100	4.01559600
C	-2.45414900	0.46362300	3.20774000
H	-1.49655200	0.80635800	2.80523000

H	-3.03889900	1.33580900	3.51814400
H	-3.00152400	-0.01848500	2.39262900
H	-1.72275900	-3.39302000	5.02458100
C	4.02669600	2.24703100	3.86169900
H	3.69466600	1.30144200	3.42480800
H	4.61709700	2.79013400	3.11680600
H	4.70102800	2.00904200	4.69396600
C	3.55922600	-1.67377500	3.61947700
H	2.99496700	-1.08757700	2.88647900
H	4.57281000	-1.25616600	3.66263500
H	3.65315700	-2.70125600	3.25453800
H	0.36880000	-2.11656700	3.53553200
[Zn <sub>2</sub> (L <sup>1</sup> ) <sub>2</sub> ] <sup>2+</sup>			
Zn	-1.50473000	-0.39651500	0.37385900
N	-2.59100000	0.56173100	2.02073500
N	-2.99747700	0.92114500	-0.63151100
N	-2.93892900	-1.86854800	-0.06581600
O	-0.27868800	-0.47367000	-1.24955700
C	-2.66986100	0.13311300	3.29919600
C	-3.09595800	0.99753500	4.31261500
H	-3.14009800	0.64443200	5.33779300
C	-3.48929400	2.29439400	3.98630100
H	-3.82621800	2.97658100	4.76102100
C	-3.48559900	2.69319100	2.64870900
H	-3.83740300	3.67700900	2.35403500
C	-3.02807200	1.79324500	1.69099500
C	-3.02448900	2.13835300	0.21117800
H	-3.90229600	2.76061800	-0.02062800
H	-2.14040600	2.73404500	-0.02749100
C	-4.25869700	0.14610300	-0.46712300
H	-5.03081300	0.50992300	-1.15612100
H	-4.63903700	0.30713400	0.54535700
C	-4.05100400	-1.34618500	-0.63466800
C	-5.00157300	-2.15002900	-1.25198000
H	-5.87836600	-1.70453600	-1.71076400
C	-4.80732600	-3.53391200	-1.26055300
H	-5.53075500	-4.18653200	-1.73984200
C	-3.68156100	-4.06475700	-0.63995200
H	-3.51353200	-5.13646400	-0.61301500
C	-2.75362000	-3.20479800	-0.04028400
C	-2.81260600	1.24495900	-2.08302200
H	-3.32278800	2.19724500	-2.29304600
H	-3.35238000	0.47243000	-2.63896300
C	-1.37954200	1.27678500	-2.65133100

C	-0.71674300	-0.11818700	-2.54380100
H	-1.42737200	-0.87832700	-2.90717700
H	0.13220700	-0.12641400	-3.23411100
Zn	1.51530000	-0.36184300	-0.39550400
N	2.59343100	0.66370000	-2.00864900
N	2.99208500	0.94011000	0.65468400
N	2.97036300	-1.82915500	-0.00570200
O	0.29185600	-0.51202300	1.22246500
C	2.67942900	0.27888700	-3.30051700
C	3.09448300	1.18236800	-4.28387500
H	3.14438900	0.86442600	-5.32022300
C	3.46921700	2.47308500	-3.91384700
H	3.79733600	3.18530400	-4.66496000
C	3.45852800	2.82717000	-2.56383800
H	3.79623300	3.80548400	-2.23618900
C	3.01248500	1.88953200	-1.63728900
C	3.00199800	2.18479800	-0.14692000
H	3.87016400	2.81205400	0.10684600
H	2.10890700	2.75916600	0.10991700
C	4.26365100	0.18799100	0.46539400
H	5.02989500	0.53747100	1.16823400
H	4.64342000	0.38976000	-0.53995200
C	4.07585800	-1.31201600	0.58028500
C	5.03773200	-2.12411700	1.16866600
H	5.90883700	-1.68319300	1.64245500
C	4.86235700	-3.50997400	1.12864500
H	5.59506800	-4.16913400	1.58430600
C	3.74317100	-4.03396300	0.49048300
H	3.58957100	-5.10624300	0.42605900
C	2.80304900	-3.16604900	-0.07798000
C	2.80208500	1.21264800	2.11600500
H	3.29907500	2.16416000	2.35840500
H	3.35196100	0.42938700	2.64650300
C	1.36837700	1.20485300	2.68388900
C	0.72617800	-0.19525800	2.52775600
H	1.44857600	-0.95704700	2.86350000
H	-0.12183600	-0.24038300	3.21766500
C	-2.37830300	-1.31967200	3.56883800
H	-1.67812700	-1.72971600	2.83788900
H	-1.97405200	-1.47104600	4.57348000
H	-3.30979300	-1.89612400	3.49610500
C	-1.56058400	-3.74005100	0.70394600
H	-0.77303800	-2.98842000	0.80590900
H	-1.86185700	-4.04780600	1.71351700

H	-1.14967800	-4.62236200	0.20604100
C	2.40669700	-1.16793400	-3.61727600
H	1.70187500	-1.60634200	-2.90752100
H	2.01628800	-1.29325700	-4.63088000
H	3.34312500	-1.73690300	-3.54945300
C	1.61631900	-3.69070900	-0.83952700
H	0.81973400	-2.94563700	-0.91592600
H	1.92078700	-3.96052300	-1.85892600
H	1.21654900	-4.59429800	-0.37158900
C	1.51053800	1.48172600	4.19605200
H	1.99581300	2.44609000	4.38268900
H	0.52474600	1.50989200	4.67330800
H	2.10240700	0.70522800	4.69579200
C	0.46523700	2.27619500	2.06002900
H	-0.48824800	2.32459500	2.59547500
H	0.92495200	3.26992700	2.11184900
H	0.23989500	2.04391300	1.01521900
C	-1.52620800	1.60424800	-4.15298300
H	-2.02580600	2.56727100	-4.30589400
H	-0.54099700	1.66345100	-4.62865200
H	-2.10679500	0.83706300	-4.67962000
C	-0.49097100	2.33779600	-1.99015400
H	0.46335800	2.41510900	-2.52088000
H	-0.96255400	3.32709600	-2.01029300
H	-0.26594800	2.07325100	-0.95302900
[Zn <sub>2</sub> (L <sup>2</sup> ) <sub>2</sub> ] <sup>2+</sup>			
Zn	-0.13598400	-0.34796600	0.90679100
N	-2.04024800	-1.03570700	0.00955400
N	-0.31875400	0.85615800	-0.92014200
N	1.14051100	-1.51908500	-0.24178200
O	1.10658700	1.06911100	1.80449700
O	2.87939700	1.66557900	0.54943700
C	-2.69343600	-2.20173600	0.22436800
C	-4.00739800	-2.37557400	-0.22065300
H	-4.51896300	-3.31289300	-0.02745300
C	-4.63321500	-1.35603700	-0.93510100
H	-5.65270500	-1.47735000	-1.28859100
C	-3.91601000	-0.19728900	-1.23069600
H	-4.34779400	0.59248900	-1.83769300
C	-2.61725500	-0.07727700	-0.74334900
C	-1.76526100	1.13166400	-1.08478900
H	-1.98491400	1.45036600	-2.11501800
H	-2.02958600	1.96731100	-0.43537100
C	0.14413500	-0.10740800	-1.96134300

H	0.42952500	0.42308800	-2.87756100
H	-0.69483100	-0.76037200	-2.22063900
C	1.26936500	-1.00765100	-1.48717300
C	2.30798500	-1.38800900	-2.32749800
H	2.39838300	-0.95349900	-3.31768000
C	3.21914700	-2.34438300	-1.87218800
H	4.04678800	-2.65588400	-2.50231200
C	3.04202900	-2.90900900	-0.61262300
H	3.71312800	-3.68086700	-0.25029500
C	1.98019700	-2.48323300	0.19312900
C	0.49142000	2.11063300	-1.02835200
H	0.02805500	2.75261400	-1.79197500
H	1.47045400	1.81051300	-1.40698600
C	0.75220100	2.92629000	0.25114700
C	1.70437300	2.15898600	1.21191100
H	2.01022900	2.88349700	1.98156800
C	1.45288300	4.22609800	-0.20104300
H	0.77327700	4.85554400	-0.78497000
H	2.32966900	4.02944600	-0.82980600
H	1.77904000	4.81261700	0.66586300
C	-0.50914000	3.29729400	1.04765700
H	-1.02805700	2.40925000	1.42027000
H	-1.20194500	3.89688500	0.44678200
H	-0.23438800	3.89908000	1.92319200
H	3.46489000	2.40314300	0.31446200
C	-1.92949100	-3.33428800	0.85555300
H	-1.15197500	-2.98293000	1.53361200
H	-2.59465000	-4.00933600	1.40200200
H	-1.44263600	-3.92273600	0.06666100
C	1.67984700	-3.13103900	1.51749200
H	1.21613700	-2.43964200	2.22625000
H	0.97474100	-3.95709500	1.36491100
H	2.57834200	-3.55812500	1.96766500
Zn	0.95953500	0.64671000	3.72412000
N	1.64498000	2.51818300	4.68521900
N	-0.15131100	0.69847000	5.61536900
N	2.22287100	-0.65703700	4.74482200
O	-0.47906100	-0.57720100	2.83415300
O	-0.96093400	-2.43525700	4.01388900
C	2.78331800	3.21168800	4.44941900
C	2.95159000	4.50181300	4.96154300
H	3.86581700	5.04697300	4.75034500
C	1.95886900	5.05911700	5.76458400
H	2.07684600	6.05885800	6.17153900



C	0.83361600	4.29702700	6.07719100
H	0.06847000	4.67275400	6.74946000
C	0.71558600	3.02667100	5.51995500
C	-0.45460500	2.12613700	5.87115400
H	-0.72914500	2.28244100	6.92536300
H	-1.32634900	2.40114500	5.27596900
C	0.87504000	0.20879100	6.58170200
H	0.39862200	-0.13690400	7.50688800
H	1.52049400	1.04994400	6.85244400
C	1.77616300	-0.86652100	6.00423500
C	2.21889300	-1.93997900	6.76632800
H	1.83453000	-2.09489700	7.76913500
C	3.17146500	-2.80162500	6.21621100
H	3.53086800	-3.65483700	6.78361000
C	3.67033600	-2.54181200	4.94335600
H	4.43838100	-3.17239800	4.50769400
C	3.18260100	-1.44833700	4.21893200
C	-1.37675100	-0.15183200	5.74465300
H	-1.98624300	0.24921700	6.56791100
H	-1.03006900	-1.14139500	6.04903800
C	-2.25716100	-0.36613400	4.50014000
C	-1.51935100	-1.23957500	3.44643900
H	-2.27517100	-1.52237800	2.69835300
C	-3.50768000	-1.13154700	4.98612000
H	-4.11927700	-0.50521500	5.64390300
H	-3.24877100	-2.03539600	5.55062500
H	-4.13636000	-1.42662200	4.13779100
C	-2.71262700	0.92392500	3.79948700
H	-1.86658100	1.49100500	3.40060000
H	-3.29159100	1.56427300	4.47446700
H	-3.36203200	0.67796900	2.94974800
H	-1.66991500	-3.05360400	4.25280400
C	3.89881100	2.51521600	3.71769000
H	3.53161000	1.75412400	3.02983100
H	4.51626600	3.22569500	3.16022200
H	4.55139900	2.01789700	4.44741800
C	3.75793800	-1.06173100	2.88358900
H	3.02099100	-0.58201200	2.23388500
H	4.57180400	-0.34220300	3.03440000
H	4.18657200	-1.92322300	2.36726800
[Zn <sub>2</sub> (L <sup>3</sup> ) <sub>2</sub> ] <sup>2+</sup>			
Zn	-1.67036500	-0.21915800	0.35498400
N	-1.86917100	2.00711400	0.54338000
N	-3.54626200	0.22316600	-0.72013000

N	-3.11439400	-1.49875200	1.33621100
C	-1.24057700	2.84217400	1.40755400
C	-1.46513000	4.22315200	1.36131100
H	-0.95038900	4.86788900	2.06557400
C	-2.35459200	4.75364100	0.43220100
H	-2.54490600	5.82211900	0.39584100
C	-3.01348300	3.88557200	-0.43618900
H	-3.73175400	4.25245000	-1.16256800
C	-2.74170000	2.52355000	-0.35093100
C	-3.39333600	1.55405800	-1.31615000
H	-4.35138200	1.95778600	-1.67546600
H	-2.73701700	1.45597100	-2.18297200
C	-4.54272000	0.22330900	0.37407800
H	-5.56803800	0.25449400	-0.02213600
H	-4.39519500	1.13314100	0.96579900
C	-4.36374700	-0.98975200	1.26821800
C	-5.43375400	-1.54586700	1.95819200
H	-6.42523500	-1.11255500	1.87300600
C	-5.20121000	-2.67663900	2.74222200
H	-6.01197000	-3.13651000	3.29912100
C	-3.92493900	-3.23063900	2.76714600
H	-3.72617600	-4.13690400	3.32954400
C	-2.88735000	-2.63094400	2.04289700
C	-3.85661200	-0.86306000	-1.68552700
H	-4.85670200	-0.69614500	-2.11399000
H	-3.92001300	-1.77018700	-1.08186300
C	-2.87860000	-1.13562300	-2.86123700
C	-3.04693600	-2.64190700	-3.21523000
H	-4.09611900	-2.86110100	-3.44447600
H	-2.73202000	-3.28094100	-2.38317900
H	-2.45287300	-2.90509200	-4.09618000
C	-3.25809600	-0.32599900	-4.13079600
H	-3.17440500	0.75580400	-3.99635400
H	-4.28979100	-0.55035200	-4.42081100
H	-2.61244900	-0.60329200	-4.97043400
C	-1.40608100	-0.92742000	-2.59233900
H	-0.74840100	-1.05724000	-3.45540800
N	-0.81965300	-0.67478400	-1.47223200
O	0.53228400	-0.61398700	-1.54986400
Zn	1.86466900	-0.21049400	-0.17525100
N	2.05216300	2.01679200	-0.36256200
N	3.73829000	0.24100500	0.90002600
N	3.31547700	-1.48184900	-1.15748800
C	1.41932700	2.84893400	-1.22642100

C	1.63664600	4.23104100	-1.17952100
H	1.11863900	4.87340400	-1.88356100
C	2.52318700	4.76570800	-0.25001100
H	2.70790200	5.83515100	-0.21310000
C	3.18648700	3.90069300	0.61808800
H	3.90269600	4.27100400	1.34475900
C	2.92185000	2.53731200	0.53213900
C	3.57833500	1.57065700	1.49691100
H	4.53416800	1.97915900	1.85670700
H	2.92230200	1.46853000	2.36348200
C	4.73478700	0.24700900	-0.19410800
H	5.75989800	0.28309200	0.20222500
H	4.58267200	1.15653700	-0.78513100
C	4.56211200	-0.96625600	-1.08918800
C	5.63502200	-1.51605800	-1.77970900
H	6.62416900	-1.07749600	-1.69424700
C	5.40847700	-2.64741400	-2.56464600
H	6.22163600	-3.10246700	-3.12200500
C	4.13519300	-3.20822100	-2.58989200
H	3.94124300	-4.11509200	-3.15299100
C	3.09446300	-2.61469300	-1.86505800
C	4.05396200	-0.84437300	1.86464000
H	5.05331700	-0.67304500	2.29306500
H	4.12150100	-1.75082500	1.26042100
C	3.07743900	-1.12216300	3.04037800
C	3.25252300	-2.62790000	3.39338100
H	4.30272100	-2.84269900	3.62215500
H	2.94013200	-3.26778200	2.56102700
H	2.65989900	-2.89423800	4.27435500
C	3.45369700	-0.31157400	4.31029900
H	3.36563700	0.76994000	4.17630300
H	4.48632100	-0.53184700	4.60012800
H	2.80927000	-0.59186000	5.14987700
C	1.60391700	-0.92035400	2.77196600
H	0.94706000	-1.05290100	3.63524800
N	1.01611700	-0.67049800	1.65195100
O	-0.33600100	-0.61536400	1.72978500
C	1.72746900	-3.24230900	-1.82947600
H	1.24834500	-3.07679400	-0.86103000
H	1.07761800	-2.79082400	-2.58487100
H	1.79757100	-4.31679200	-2.02043800
C	0.47466400	2.26296300	-2.23695500
H	0.93738200	1.43483500	-2.77901600
H	-0.40183400	1.84766000	-1.73467900

H	0.14645900	3.02850600	-2.94432100
C	-1.51694900	-3.25108400	2.00692900
H	-1.03914200	-3.08320300	1.03822600
H	-0.86927400	-2.79586900	2.76195000
H	-1.58107800	-4.32589300	2.19811400
C	-0.29287400	2.26080100	2.41790900
H	-0.75159800	1.43061100	2.96020700
H	0.58548200	1.84954000	1.91556300
H	0.03180200	3.02799800	3.12510900
1-AC <sub>SB</sub>			
Zn	-0.43515700	-1.35113400	-0.27147900
N	-0.66517900	-2.79426300	-1.99820600
N	-1.01100100	-3.36434800	0.66969400
N	-2.75797900	-1.20445100	0.21673900
O	-0.36280100	-0.50374100	1.70496200
C	-0.75137700	-2.50226900	-3.31073700
C	-0.32759700	-3.42241200	-4.27611500
H	-0.39693500	-3.16868300	-5.32900400
C	0.17286400	-4.65707200	-3.86743400
H	0.50476300	-5.38509100	-4.60248600
C	0.23018400	-4.95420200	-2.50670900
H	0.59944500	-5.91241500	-2.15389300
C	-0.19113000	-3.98701300	-1.59570900
C	-0.10771200	-4.24031500	-0.09988700
H	-0.31810500	-5.30392800	0.10479200
H	0.91339300	-4.01164200	0.21208000
C	-2.42090900	-3.60624000	0.29552600
H	-2.82318800	-4.49332000	0.80797700
H	-2.46812000	-3.80474100	-0.77696900
C	-3.27538700	-2.39274100	0.58208700
C	-4.53022500	-2.51940500	1.17488300
H	-4.89945000	-3.49954700	1.46095300
C	-5.28420600	-1.36706700	1.39195100
H	-6.26744500	-1.42641600	1.85034400
C	-4.74683100	-0.13869900	1.02578500
H	-5.29616100	0.78196900	1.19407900
C	-3.47046100	-0.08057500	0.44621800
C	-0.86238900	-3.54402500	2.14694000
H	-0.58424900	-4.59320200	2.33695900
H	-1.86212700	-3.40874900	2.57348200
C	0.08457100	-2.62746100	2.96360600
C	-0.40802000	-1.16393100	2.96896700
H	0.19066700	-0.59120600	3.68762700
P	0.90180300	1.42388500	-0.65768700

O	-0.20021500	0.52566200	-1.20616700
O	2.27939800	1.12055000	-1.48262600
O	0.63511100	2.94196200	-1.28334700
O	1.12232100	1.50179900	0.83019300
C	3.52381400	1.19486800	-0.87850600
C	3.90273700	0.23219700	0.06264500
C	4.38915200	2.21394100	-1.28239000
C	5.17736100	0.29969800	0.61282000
H	3.19236000	-0.54959200	0.32177900
C	5.66584100	2.28126900	-0.73398700
H	4.05019600	2.93688200	-2.01657700
C	6.04244700	1.32258400	0.21039600
H	5.50966200	-0.42791100	1.34293900
H	6.36293500	3.05859900	-1.02090800
C	-0.48398800	3.64387800	-0.90711300
C	-1.41110600	3.97538800	-1.90225000
C	-0.67898000	4.04272200	0.42301400
C	-2.55523000	4.69004100	-1.56990300
H	-1.22236500	3.65346100	-2.92050700
C	-1.82498100	4.75311700	0.76071300
H	0.05848000	3.77076700	1.16908600
C	-2.75467700	5.06137500	-0.23690600
H	-3.29435100	4.95051900	-2.31737100
H	-2.00888000	5.06609200	1.78114000
N	7.38729100	1.39007400	0.79260400
O	8.14063700	2.29257800	0.41386300
O	7.69992000	0.54128100	1.63327000
N	-3.97897400	5.78053500	0.12620100
O	-4.15213800	6.06932500	1.31434900
O	-4.78143900	6.05221300	-0.77259300
C	-1.31596900	-1.15490800	-3.66733600
H	-2.31187100	-1.03595200	-3.22389400
H	-0.69154200	-0.35991300	-3.24641900
H	-1.39378600	-1.02703800	-4.75055800
C	-2.84144000	1.23633200	0.10446200
H	-3.54111200	2.06324900	0.25250900
H	-1.96674400	1.39405000	0.74247100
H	-2.47526100	1.24739700	-0.92344400
H	0.33502800	0.20009700	1.63394400
O	1.47963100	-1.75172100	-0.37553300
H	1.79951400	-1.55674400	-1.26963900
C	1.55239600	-2.71428500	2.52338100
H	1.70675500	-2.33129100	1.51133200
H	2.18015300	-2.13179700	3.21001300

H	1.90232400	-3.75429500	2.56439200
C	-0.03387300	-3.12189200	4.42465600
H	0.29971200	-4.16221900	4.51176400
H	0.59767800	-2.51811800	5.08559600
H	-1.06437500	-3.06498000	4.79896500
H	-1.45287400	-1.13351400	3.30803000
1-TS1 <sub>SB</sub>			
Zn	-1.42650700	-0.86038400	-0.12555000
N	-1.63736500	-2.54584500	-1.55438000
N	-3.13210100	-2.11505100	0.70495400
N	-3.22884400	0.35291200	-0.62047500
C	-1.05171800	-2.63541900	-2.76557900
C	-0.78962300	-3.88586600	-3.33586700
H	-0.31362300	-3.94168800	-4.30931100
C	-1.14489700	-5.04238300	-2.64587100
H	-0.94765800	-6.02049200	-3.07554500
C	-1.76642700	-4.93152700	-1.40318500
H	-2.06824100	-5.81068600	-0.84177100
C	-1.98555500	-3.65705800	-0.88596100
C	-2.60969600	-3.47717800	0.48891100
H	-3.39958300	-4.23254800	0.63771400
H	-1.83517400	-3.65798400	1.23735300
C	-4.23895300	-1.81742400	-0.23569200
H	-5.18560100	-2.25326000	0.11612900
H	-4.00773400	-2.27552100	-1.19974700
C	-4.37998500	-0.32507000	-0.44426100
C	-5.62501800	0.29545100	-0.46872200
H	-6.52767600	-0.28711800	-0.31268000
C	-5.67630600	1.67244300	-0.69076600
H	-6.62995700	2.19222800	-0.71521700
C	-4.48768500	2.37081900	-0.86618200
H	-4.49061000	3.44367200	-1.02807100
C	-3.26158600	1.68927500	-0.82038700
C	-3.62095100	-1.90087900	2.10276900
H	-4.04444500	-2.85171500	2.46501300
H	-4.45758700	-1.19836200	2.03019300
C	-2.66922700	-1.33409200	3.18532300
C	-2.26103600	0.12604900	2.88010800
H	-1.75635400	0.54465400	3.76052000
P	1.28206600	0.04226400	0.06892100
O	0.08821900	0.25286800	-0.89117100
O	2.45722200	-0.96118000	-0.52396300
O	2.21026500	1.42135500	-0.44721700
O	1.20717700	0.27492200	1.57671000

C	3.77600600	-0.94212800	-0.18801900
C	4.27844300	-0.35809600	0.98688100
C	4.63627600	-1.60224700	-1.07969800
C	5.63846800	-0.43448400	1.25719500
H	3.60232400	0.14353900	1.66820100
C	5.99336100	-1.68139100	-0.80853900
H	4.21439400	-2.04356900	-1.97624600
C	6.48651000	-1.09413100	0.36192000
H	6.05055800	0.00842100	2.15563900
H	6.67324100	-2.18481200	-1.48466900
C	1.64832900	2.64969100	-0.38712200
C	1.50319800	3.37029200	-1.58600000
C	1.22532500	3.22328000	0.82859800
C	0.91179500	4.62496400	-1.58573900
H	1.84405500	2.90925700	-2.50669500
C	0.62991700	4.47706900	0.83446100
H	1.35400900	2.65708600	1.74237500
C	0.46473200	5.16475800	-0.37356400
H	0.77585700	5.18387700	-2.50356100
H	0.28717000	4.92902300	1.75739000
N	7.91388300	-1.17702800	0.65536100
O	8.64215300	-1.76876700	-0.15079900
O	8.32806700	-0.65368900	1.69616500
N	-0.20761800	6.45812500	-0.37329800
O	-0.60627800	6.91190200	0.70696700
O	-0.36290400	7.03807600	-1.45584800
C	-0.70132700	-1.34635100	-3.45201000
H	-1.58908600	-0.70729900	-3.53270800
H	0.02794200	-0.79289100	-2.85116500
H	-0.30133000	-1.52318600	-4.45395000
C	-1.95999200	2.41786200	-0.96262600
H	-2.12003600	3.47511900	-1.18760400
H	-1.38331400	2.33251500	-0.03691500
H	-1.33478600	1.96824600	-1.73694500
O	0.27427500	-1.84133900	0.42003900
H	0.54962900	-2.03506200	1.32608700
H	-0.44531000	0.29829000	1.94146900
O	-1.42878300	0.30203600	1.74081100
H	-3.16458600	0.72382400	2.70218900
C	-1.42850200	-2.20637200	3.40627700
H	-1.70885900	-3.23147600	3.67815600
H	-0.81514200	-2.23797900	2.50703100
H	-0.81201700	-1.80056200	4.21662200
C	-3.49881900	-1.29465000	4.48842700

H	-2.89783000	-0.89894300	5.31433100
H	-4.38835100	-0.66012700	4.38668600
H	-3.83140300	-2.29941500	4.77319000
1-IM <sub>SB</sub>			
Zn	1.65207600	-0.68523300	0.09191300
N	2.09887800	-2.18518100	1.63952500
N	3.36365500	-1.90952800	-0.77021600
N	3.30357800	0.69866800	0.26508400
C	1.60821100	-2.16697400	2.89680100
C	1.50372900	-3.35275100	3.63181900
H	1.10087000	-3.32360100	4.63878100
C	1.92131200	-4.55355500	3.06302500
H	1.84483100	-5.48194500	3.62186600
C	2.45118200	-4.54946300	1.77381700
H	2.80211900	-5.46338900	1.30383200
C	2.51335300	-3.33783200	1.09010400
C	3.03720500	-3.28026800	-0.33556700
H	3.91255900	-3.94411100	-0.43338300
H	2.26460100	-3.66681600	-1.00291000
C	4.51809300	-1.38023100	0.00002700
H	5.46801600	-1.75299600	-0.40911800
H	4.44095700	-1.74276000	1.02808200
C	4.50477000	0.13356300	0.03564400
C	5.66002100	0.89041800	-0.12662700
H	6.61058300	0.40252600	-0.31845100
C	5.55877900	2.28096000	-0.04006400
H	6.43957200	2.90473000	-0.16336800
C	4.31557200	2.85818800	0.19258800
H	4.20315700	3.93558100	0.25273100
C	3.18337400	2.04247000	0.33742900
C	3.68489200	-1.84102600	-2.23081800
H	4.19229800	-2.77813400	-2.51173200
H	4.42553800	-1.04272800	-2.34506600
C	2.55965300	-1.54760800	-3.25211600
C	2.01402200	-0.11275300	-3.08409600
H	1.37077800	0.12731600	-3.94057900
P	-1.17076400	-0.45050300	-0.05520700
O	0.01041700	0.15878600	0.78366000
O	-2.30699500	-1.44833800	0.67201400
O	-2.25043200	0.91409300	0.42153300
O	-1.25659800	-0.28040100	-1.58388100
C	-3.66017700	-1.30458400	0.58085000
C	-4.30369800	-0.92447000	-0.60887200
C	-4.40612100	-1.64852000	1.71629600



C	-5.68956900	-0.88613900	-0.65339200
H	-3.70433000	-0.65092700	-1.46965700
C	-5.79297300	-1.61634000	1.67342100
H	-3.87753800	-1.93622200	2.61881500
C	-6.42517000	-1.23441700	0.48596100
H	-6.21044900	-0.59263000	-1.55654600
H	-6.38907400	-1.87577000	2.53955800
C	-1.85422200	2.17585800	0.22304000
C	-1.74828600	3.02862900	1.34225400
C	-1.55546400	2.68703600	-1.06115600
C	-1.31127900	4.33547000	1.20005400
H	-1.99395300	2.62173200	2.31748200
C	-1.11772900	3.99420800	-1.20904500
H	-1.65518300	2.02580400	-1.91251200
C	-0.98027200	4.80952500	-0.07721400
H	-1.20353300	4.98983100	2.05672700
H	-0.87283700	4.39442100	-2.18568200
N	-7.88360400	-1.20215400	0.43399700
O	-8.51202300	-1.51713300	1.45220900
O	-8.42368300	-0.86228000	-0.62513900
N	-0.45506900	6.15505100	-0.22502400
O	-0.14892300	6.54795100	-1.36031600
O	-0.31649300	6.84922500	0.79305400
C	1.19306000	-0.83590900	3.45396800
H	2.02823400	-0.12679900	3.39743100
H	0.38271100	-0.41749200	2.84709300
H	0.87547800	-0.92183200	4.49633900
C	1.81365100	2.61203500	0.54504900
H	1.84758700	3.69530100	0.68108800
H	1.17775700	2.38130400	-0.31585100
H	1.31642800	2.15049800	1.40168700
O	-0.13977800	-1.98822500	-0.15347900
H	-0.52807700	-2.54768300	-0.84314700
H	0.28103800	-0.04424000	-1.98259100
O	1.28463600	0.10639100	-1.88616600
H	2.84924600	0.60060600	-3.08813800
C	1.40854000	-2.55841000	-3.18405500
H	1.76786300	-3.58136200	-3.35229100
H	0.91211600	-2.50506200	-2.21517300
H	0.65724400	-2.33548400	-3.94990400
C	3.22474800	-1.61722700	-4.64392500
H	2.49096000	-1.40680100	-5.42952800
H	4.04008500	-0.88928000	-4.74354000
H	3.63768500	-2.61449100	-4.83502500

1-TS2<sub>SB</sub>

Zn	1.76842900	-0.66133500	0.04115300
N	2.16280100	-2.25356900	1.50868800
N	3.39119700	-1.90202300	-0.89396800
N	3.34554400	0.65113100	0.26842000
O	1.23155700	0.07110400	-1.86860300
C	1.66882000	-2.26299600	2.76664700
C	1.51862800	-3.47107900	3.45367100
H	1.11608700	-3.46841800	4.46119500
C	1.89233200	-4.66450600	2.83517000
H	1.77622500	-5.61064800	3.35594700
C	2.42804100	-4.63098600	1.54905900
H	2.74266700	-5.53863500	1.04309300
C	2.54258300	-3.39481000	0.91462500
C	3.07073000	-3.28985100	-0.50480500
H	3.94944500	-3.94448500	-0.62429000
H	2.29566900	-3.65420300	-1.18119200
C	4.57242200	-1.39804100	-0.14086000
H	5.50868300	-1.73892200	-0.60386000
H	4.53802300	-1.81317100	0.87009200
C	4.54704200	0.11401700	-0.02649400
C	5.67708000	0.90774900	-0.17716500
H	6.63336800	0.45697200	-0.42257300
C	5.54453100	2.29088100	-0.01437400
H	6.40763800	2.93938400	-0.13380600
C	4.29949400	2.83205500	0.28948800
H	4.16533600	3.90183200	0.40889700
C	3.19286800	1.98335200	0.42626900
C	3.66922100	-1.78757000	-2.36231300
H	4.18735400	-2.70600700	-2.68093300
H	4.38951800	-0.97012000	-2.47283100
C	2.50473400	-1.49228800	-3.33626400
C	1.94046500	-0.07761400	-3.09650000
H	1.26496700	0.18977200	-3.91800500
P	-1.11762600	-1.18038900	-0.23171900
O	-0.05237300	-0.47170500	0.66945300
O	-2.39069000	-1.84417900	0.58815300
O	-2.29726100	0.59544300	0.23228400
O	-1.18096900	-0.87518300	-1.71821400
C	-3.72342200	-1.57474800	0.42267100
C	-4.28373000	-1.30967000	-0.83448900
C	-4.52394600	-1.67180200	1.56514300
C	-5.65651700	-1.13942600	-0.94103800
H	-3.63559900	-1.21689800	-1.69774900

C	-5.89831100	-1.50653900	1.46059400
H	-4.05146500	-1.86781100	2.52148800
C	-6.45342000	-1.24246200	0.20515500
H	-6.11924800	-0.92784700	-1.89701900
H	-6.54101000	-1.57310100	2.32950800
C	-1.84049400	1.77471900	-0.03886500
C	-1.71736600	2.75261600	0.99966000
C	-1.43025600	2.17080000	-1.35421900
C	-1.14683600	3.98641900	0.76910900
H	-2.06570800	2.47374400	1.98964300
C	-0.86268900	3.40742300	-1.58695600
H	-1.56607400	1.45946800	-2.15920100
C	-0.68809400	4.31361800	-0.52279500
H	-1.02054300	4.70542500	1.57046300
H	-0.52878100	3.69145800	-2.57849900
N	-7.90004700	-1.07442300	0.08827000
O	-8.58340800	-1.16560900	1.11534800
O	-8.37360800	-0.85148600	-1.03149500
N	0.04449400	5.52519400	-0.73224000
O	0.42362300	5.81074400	-1.88492100
O	0.31358300	6.24083300	0.25500300
C	1.28947700	-0.93818000	3.36456700
H	2.10550800	-0.21747100	3.23397300
H	0.41626300	-0.53942900	2.83604700
H	1.06683500	-1.02896600	4.43072100
C	1.80974300	2.47288500	0.72018900
H	1.78356400	3.55056400	0.88953600
H	1.14093200	2.23732700	-0.11557600
H	1.39275600	1.96361000	1.59561000
H	0.25912000	-0.20237400	-1.96956000
O	-0.34887400	-2.71572900	-0.31954200
H	-0.48205600	-3.20981500	0.50472700
C	1.37763200	-2.53446500	-3.28195600
H	0.85031200	-2.54241500	-2.32616400
H	0.62562400	-2.31239200	-4.04713600
H	1.76929100	-3.53983400	-3.48429400
C	3.13335400	-1.49087900	-4.74739200
H	3.56094700	-2.47094100	-4.98817000
H	2.37259700	-1.26763300	-5.50283000
H	3.92977900	-0.74131100	-4.84111000
H	2.75520500	0.65743500	-3.08326900
1-PC <sub>SB</sub>			
Zn	1.53218700	-1.18883100	0.24776200
N	2.60371000	-2.78110400	1.21668800

N	3.43090500	-1.26630100	-0.96152500
N	2.35436300	0.63562000	0.83267800
O	0.79008200	-1.90243400	-1.57560500
C	2.35775700	-3.29047200	2.44697400
C	3.10644400	-4.36831500	2.93143800
H	2.89106200	-4.76357900	3.91844700
C	4.12149200	-4.91216200	2.15004200
H	4.71206000	-5.74633000	2.51756700
C	4.38345900	-4.35729300	0.89943300
H	5.18230400	-4.73578700	0.26975400
C	3.59995200	-3.29216200	0.46252600
C	3.81827100	-2.68234000	-0.90743500
H	4.86564300	-2.82638000	-1.21714100
H	3.19173500	-3.22256100	-1.61533300
C	4.32842700	-0.43646800	-0.12995400
H	5.23276700	-0.15214700	-0.68558400
H	4.65292800	-1.03799800	0.72688300
C	3.63237400	0.79546600	0.40715500
C	4.30487100	2.00039400	0.51941200
H	5.30899300	2.10135500	0.12229500
C	3.64923900	3.07997600	1.11320500
H	4.13381200	4.04765900	1.18291800
C	2.36085000	2.90003200	1.59595400
H	1.81634200	3.71979900	2.04827700
C	1.71038700	1.67216600	1.42758000
C	3.41041500	-0.71364900	-2.35233200
H	4.39576800	-0.90107600	-2.81235800
H	3.30228400	0.36696400	-2.22969400
C	2.30569000	-1.17126300	-3.34216400
C	0.92131200	-1.00816100	-2.70957100
H	0.14092600	-1.25894200	-3.43619800
P	-1.60994100	-1.83854700	0.56267300
O	-0.26700600	-1.31820900	1.08446200
O	-2.59347200	-0.53759800	0.68073800
O	-3.19783500	3.59654900	0.77933300
O	-1.63195000	-2.49461100	-0.79057800
C	-3.93136400	-0.49559000	0.31458800
C	-4.61306500	-1.59625400	-0.22176400
C	-4.56812700	0.73312400	0.51696600
C	-5.95885600	-1.46357500	-0.54806800
H	-4.10133300	-2.53428800	-0.39725600
C	-5.91159300	0.86237400	0.18460200
H	-4.01439400	1.59206200	0.88928000
C	-6.59562700	-0.23884900	-0.33833800

H	-6.51338700	-2.29535500	-0.96437700
H	-6.42154600	1.80798400	0.32153500
C	-2.11360700	3.57577700	0.14381500
C	-1.05572900	4.54946300	0.37960800
C	-1.82374700	2.57136100	-0.87420500
C	0.16031600	4.46679100	-0.24141400
H	-1.27238400	5.34592600	1.08557800
C	-0.59678300	2.48126900	-1.47258700
H	-2.61917100	1.88183900	-1.13751000
C	0.43670900	3.40032900	-1.14295000
H	0.94392500	5.19002500	-0.04401900
H	-0.39971700	1.72097200	-2.21873100
N	-8.01497100	-0.10785000	-0.68243800
O	-8.56461400	0.97741000	-0.47668500
O	-8.59001000	-1.09216000	-1.15995300
N	1.72460200	3.22671700	-1.65291500
O	1.98815200	2.17459000	-2.31472900
O	2.61784300	4.07882600	-1.42189000
C	1.26520000	-2.67171100	3.27211600
H	1.28791000	-1.58135900	3.19682000
H	0.28501000	-2.98720500	2.90164700
H	1.36108500	-2.96365700	4.32126500
C	0.29668300	1.48570800	1.89159200
H	-0.06745300	2.38867100	2.38422300
H	-0.36605500	1.27650600	1.04786700
H	0.21445800	0.63579500	2.57426900
H	-0.16661500	-2.18045900	-1.44363700
O	-2.23466700	-2.87821400	1.65146500
H	-2.45045500	-2.43776300	2.49064100
C	2.47339100	-2.60808800	-3.88022000
H	2.12156100	-3.36537900	-3.17434400
H	1.87959300	-2.73159800	-4.79286000
H	3.51905500	-2.81774200	-4.13533100
C	2.39881300	-0.19381600	-4.53795700
H	3.37599500	-0.28219600	-5.02767000
H	1.63413900	-0.43638200	-5.28465600
H	2.26197700	0.84433500	-4.22354600
H	0.78262300	0.02451400	-2.37727200
2-AC <sub>SB</sub>			
Zn	-0.42053300	-1.39223200	-0.34488500
N	-0.66163100	-2.83414900	-2.03197100
N	-1.00055900	-3.36850200	0.65209400
N	-2.77551800	-1.20921400	0.11384600
O	-0.36048900	-0.53499800	1.65076100

C	-0.76541600	-2.56006600	-3.34684900
C	-0.39588100	-3.51080600	-4.30449500
H	-0.47931300	-3.27273600	-5.35999400
C	0.06948100	-4.75546700	-3.88449300
H	0.35881100	-5.50733700	-4.61345700
C	0.14704400	-5.03135500	-2.52022700
H	0.49003200	-5.99602000	-2.15874500
C	-0.22038200	-4.03534900	-1.61706600
C	-0.11468600	-4.26276600	-0.11880000
H	-0.32647500	-5.32152400	0.10663800
H	0.91244700	-4.03372700	0.17503400
C	-2.41911700	-3.59881400	0.29849300
H	-2.82143300	-4.47868000	0.82184900
H	-2.48386300	-3.80108100	-0.77244400
C	-3.25390700	-2.37405900	0.59112000
C	-4.44825400	-2.46676700	1.30138300
H	-4.78360600	-3.42825600	1.67726200
C	-5.18150200	-1.30359700	1.52761900
H	-6.11263800	-1.33482900	2.08634600
C	-4.69453900	-0.10065900	1.02880000
H	-5.23814700	0.82650900	1.18126300
C	-3.48251900	-0.07904400	0.32198900
C	-0.83916200	-3.54566300	2.13193900
H	-0.52242800	-4.58323800	2.31824100
H	-1.83361500	-3.43497800	2.56787000
C	0.08996500	-2.60941500	2.94222400
C	-0.41203400	-1.14670800	2.92618000
H	0.21613800	-0.55242400	3.60689300
P	0.89493700	1.41747200	-0.66322200
O	-0.19045800	0.51373400	-1.23252200
O	2.28871500	1.12955100	-1.46108800
O	0.63108200	2.94042700	-1.27459100
O	1.08369000	1.48670700	0.83187600
C	3.52168600	1.20858400	-0.83240700
C	3.89859200	0.22525600	0.08741000
C	4.37634600	2.25279600	-1.19136000
C	5.16182400	0.29727100	0.66315700
H	3.19621000	-0.57470500	0.31055600
C	5.64169800	2.32452900	-0.61755100
H	4.03904400	2.99053500	-1.91145500
C	6.01663600	1.34510800	0.30585500
H	5.49293100	-0.44553500	1.37836100
H	6.33127100	3.12044900	-0.86953200
C	-0.47804000	3.64730600	-0.87553500

C	-1.43869700	3.95978400	-1.84407200
C	-0.62853200	4.06757900	0.45371800
C	-2.57511900	4.67368100	-1.48362200
H	-1.28357500	3.62203800	-2.86284200
C	-1.76555200	4.77907600	0.81916000
H	0.13564100	3.81092300	1.17789000
C	-2.73067300	5.06539800	-0.15081900
H	-3.34086400	4.91827100	-2.20937500
H	-1.91511800	5.11028100	1.83947200
N	7.35000000	1.41753200	0.91460000
O	8.09449900	2.34255200	0.57526200
O	7.66113700	0.55021800	1.73636800
N	-3.94660500	5.78394200	0.24288800
O	-4.07073100	6.10943000	1.42731700
O	-4.79022600	6.01737700	-0.62834100
C	-1.28977400	-1.19892000	-3.71280900
H	-2.28130600	-1.04774700	-3.26928300
H	-0.64212100	-0.41881600	-3.29909700
H	-1.36521500	-1.07652200	-4.79676400
C	-2.92728600	1.21524200	-0.19616500
H	-3.69040400	1.99852800	-0.20446100
H	-2.09921100	1.54873000	0.43757700
H	-2.51119700	1.09508100	-1.19668300
H	0.29536400	0.21690200	1.57469900
O	1.49690000	-1.77241200	-0.43714900
H	1.82341000	-1.55506500	-1.32370300
O	-1.75912400	-1.13329800	3.36707900
H	-2.14115200	-0.28028400	3.10755600
C	1.55637600	-2.65177000	2.48926500
H	1.69411700	-2.28949900	1.46794000
H	2.17289400	-2.03744500	3.15843600
H	1.93549600	-3.67967200	2.55267100
C	0.00510400	-3.10426700	4.40589900
H	0.41106600	-4.11893200	4.48970400
H	0.60032900	-2.45686800	5.05983100
H	-1.02341900	-3.10569700	4.77900800
2-TS1 <sub>SB</sub>			
Zn	-1.43255900	-0.78367200	-0.23007800
N	-1.63325500	-2.39868000	-1.75554600
N	-3.08118500	-2.09760400	0.55924200
N	-3.18374500	0.43631900	-0.65684700
O	-1.37906400	0.23665700	1.73294200
C	-1.10286000	-2.40847900	-2.99646200
C	-0.90472000	-3.61810700	-3.67137000

H	-0.47101400	-3.61295400	-4.66599000
C	-1.27448900	-4.81374900	-3.05793200
H	-1.12818700	-5.76063500	-3.56992300
C	-1.84640200	-4.78238800	-1.78662900
H	-2.16104700	-5.69313300	-1.28613700
C	-2.00346800	-3.54630100	-1.16166400
C	-2.57340000	-3.44505700	0.24365900
H	-3.35773400	-4.20851700	0.37733300
H	-1.77342700	-3.66303300	0.95507800
C	-4.21858900	-1.72968400	-0.31932400
H	-5.15861800	-2.16717900	0.04554600
H	-4.03540800	-2.13710900	-1.31667000
C	-4.33746000	-0.22431200	-0.43900100
C	-5.56085200	0.42885200	-0.34061600
H	-6.46751500	-0.13684600	-0.15121000
C	-5.58421700	1.81772800	-0.47206700
H	-6.52034900	2.36286400	-0.39128800
C	-4.39102600	2.49617300	-0.69567200
H	-4.37447900	3.57650400	-0.79597700
C	-3.18759000	1.78163500	-0.78216600
C	-3.52306900	-1.98315100	1.98783600
H	-3.93807000	-2.95736200	2.29010700
H	-4.34722200	-1.26794800	1.99761000
C	-2.53100600	-1.51456100	3.07758600
C	-2.14408700	-0.02762300	2.88996600
H	-1.55198600	0.28902400	3.76284800
P	1.29780000	-0.05392400	0.11402000
O	0.15343600	0.28069200	-0.88674100
O	2.45676400	-1.12067200	-0.44411500
O	2.34439900	1.26069500	-0.39681300
O	1.18657600	0.24808100	1.60620600
C	3.78240600	-1.08462400	-0.11874200
C	4.25510800	-0.61717200	1.11774200
C	4.66674300	-1.60957800	-1.07136400
C	5.61494700	-0.67549500	1.39147600
H	3.55461700	-0.21489600	1.83999400
C	6.02516100	-1.67395600	-0.79669100
H	4.26774900	-1.95711500	-2.01841000
C	6.48930400	-1.20453900	0.43613300
H	6.00686300	-0.32118100	2.33698200
H	6.72682000	-2.07339100	-1.51843100
C	1.84070800	2.51343400	-0.38840300
C	1.71923400	3.19207500	-1.61484400
C	1.44452500	3.15280600	0.80397300



C	1.17354700	4.46602100	-1.66485900
H	2.03776400	2.68111900	-2.51701200
C	0.89398800	4.42606400	0.76009700
H	1.55520000	2.61804600	1.73878800
C	0.74773300	5.06952100	-0.47494400
H	1.05458600	4.99194500	-2.60431900
H	0.57242500	4.92819400	1.66465200
N	7.91836300	-1.27250400	0.73242500
O	8.66946900	-1.75259900	-0.12486900
O	8.30843600	-0.84867100	1.82581300
N	0.11640900	6.38141700	-0.52680600
O	-0.28395000	6.88257900	0.53217700
O	-0.00685200	6.93022700	-1.62977800
C	-0.75302200	-1.07578400	-3.59557200
H	-1.65510400	-0.45706600	-3.68203600
H	-0.06410000	-0.53712500	-2.93567700
H	-0.30941300	-1.18742500	-4.58841100
C	-1.87466400	2.47819600	-0.98684600
H	-2.01700800	3.54668000	-1.16656800
H	-1.23304300	2.34622000	-0.11026900
H	-1.31819600	2.04001500	-1.81860500
H	-0.37251300	0.24326900	1.90103800
O	0.25698200	-1.80131500	0.43165300
H	0.60183900	-2.45483000	-0.19596600
O	-3.33427400	0.73338400	2.80244000
H	-3.08148200	1.63462300	2.54698900
C	-1.24968000	-2.35674200	3.16390700
H	-0.62730800	-2.26801900	2.26975500
H	-0.64420000	-2.02973600	4.01822900
H	-1.50315600	-3.41124800	3.33354700
C	-3.29942600	-1.62786300	4.41507900
H	-3.52596800	-2.67659000	4.64007600
H	-2.68752900	-1.23937600	5.23684300
H	-4.23575800	-1.06192200	4.39719600
2-IM <sub>SB</sub>			
Zn	1.65094600	-0.79514800	-0.05817700
N	2.03819900	-2.27776700	1.56132500
N	3.31127600	-2.08018400	-0.86233400
N	3.33180900	0.54600400	0.13858900
O	1.35781200	0.00381600	-2.08434800
C	1.57466600	-2.21962600	2.82809100
C	1.47541300	-3.38372600	3.59824400
H	1.09373400	-3.32497100	4.61225700
C	1.87464100	-4.60299000	3.05335800

H	1.80391200	-5.51483100	3.63956300
C	2.37787900	-4.63945900	1.75366800
H	2.71285000	-5.56896600	1.30329500
C	2.43713700	-3.44753000	1.03334900
C	2.92548400	-3.42762600	-0.40585800
H	3.75964000	-4.13977300	-0.51967600
H	2.11174300	-3.76872000	-1.05000300
C	4.48182000	-1.57290100	-0.10303800
H	5.41986700	-1.98125800	-0.50463700
H	4.39708400	-1.90948500	0.93338900
C	4.51062600	-0.05836300	-0.10511100
C	5.68001100	0.66004700	-0.32639600
H	6.60981400	0.13942500	-0.53223700
C	5.61834200	2.05401200	-0.29302500
H	6.51036000	2.64831300	-0.46944100
C	4.39805900	2.67307900	-0.04396300
H	4.31627100	3.75475600	-0.01953100
C	3.25137600	1.89413400	0.16685600
C	3.64512000	-2.05831000	-2.32442200
H	4.11692400	-3.02130800	-2.57521000
H	4.40578000	-1.28659600	-2.45415700
C	2.54487600	-1.76269900	-3.37002800
C	2.05480100	-0.29812900	-3.27363800
H	1.37615600	-0.10312200	-4.11866500
P	-1.14144100	-0.39010800	-0.26462300
O	0.03028100	0.16091400	0.61516900
O	-2.20948400	-1.46279400	0.46057700
O	-2.25568400	0.90255900	0.22883100
O	-1.17305300	-0.17738300	-1.78024600
C	-3.56542200	-1.45215600	0.29919800
C	-4.17976300	-1.12108600	-0.91892800
C	-4.33000100	-1.86650800	1.39763000
C	-5.56087100	-1.20294500	-1.02873900
H	-3.56766100	-0.79759500	-1.75293100
C	-5.71075800	-1.95512400	1.28818900
H	-3.82296800	-2.10997100	2.32527600
C	-6.31592500	-1.62101400	0.07285600
H	-6.06146600	-0.95145500	-1.95569700
H	-6.32258600	-2.27030200	2.12429700
C	-1.84570800	2.17821800	0.10731500
C	-1.71240300	2.95256900	1.27610200
C	-1.55375000	2.75839100	-1.14564700
C	-1.25235900	4.25848700	1.21012000
H	-1.95110600	2.48833600	2.22697300

C	-1.09012400	4.06390700	-1.21800100
H	-1.67415900	2.15165300	-2.03415300
C	-0.92557600	4.80250400	-0.03909100
H	-1.12246500	4.85628300	2.10411900
H	-0.84863900	4.51999200	-2.17065200
N	-7.76894200	-1.71454000	-0.04849800
O	-8.41351300	-2.09172300	0.93740700
O	-8.28493200	-1.41377100	-1.13050000
N	-0.37664700	6.14802100	-0.10944100
O	-0.05359300	6.59421000	-1.21911600
O	-0.23871400	6.78294600	0.94520400
C	1.18640100	-0.86530400	3.34956200
H	2.05375900	-0.19364000	3.32698100
H	0.42481800	-0.41837400	2.70075400
H	0.81650300	-0.92361900	4.37655300
C	1.90652600	2.51565400	0.40169500
H	1.97965200	3.60312000	0.47881000
H	1.22128400	2.26096800	-0.41281100
H	1.43781500	2.11842200	1.30543200
H	0.33831300	-0.07434000	-2.17331800
O	-0.05672900	-2.00302200	-0.49133000
H	-0.30303400	-2.63024900	0.20570700
O	3.18364300	0.55303800	-3.34472100
H	2.87883100	1.45440200	-3.15512400
C	1.32961200	-2.69858000	-3.28575300
H	0.76602700	-2.57248500	-2.35822100
H	0.64139600	-2.49214300	-4.11444000
H	1.64983600	-3.74382600	-3.38455000
C	3.22216400	-1.93798400	-4.74896200
H	3.51606600	-2.98281600	-4.90285000
H	2.52383200	-1.67022500	-5.54972500
H	4.10811600	-1.30413100	-4.85063200
2-TS <sub>2SB</sub>			
Zn	1.77243100	-0.69412700	0.08135700
N	2.17048900	-2.30901400	1.50900100
N	3.40627700	-1.88870200	-0.88536800
N	3.32355500	0.64565300	0.33308300
O	1.20697300	0.03721600	-1.83611600
C	1.67791000	-2.35290800	2.76733600
C	1.56354200	-3.57550800	3.43515200
H	1.16058200	-3.60025000	4.44215900
C	1.97433900	-4.74739100	2.79922600
H	1.88681300	-5.70455800	3.30523000
C	2.51086000	-4.67712800	1.51522400

H	2.85539100	-5.56650300	0.99647300
C	2.58773200	-3.42891000	0.89886100
C	3.11923500	-3.28858300	-0.51636700
H	4.01465000	-3.91951800	-0.63951700
H	2.35917200	-3.66528200	-1.20312400
C	4.57915400	-1.37027100	-0.12817000
H	5.52003000	-1.69283800	-0.59427000
H	4.55141000	-1.79238900	0.88036200
C	4.52516400	0.13971600	-0.00880400
C	5.62675600	0.96014400	-0.21261200
H	6.58185500	0.53198100	-0.49898200
C	5.46429900	2.34033200	-0.06036500
H	6.30243900	3.01062500	-0.22748800
C	4.21953400	2.85102600	0.29508300
H	4.06217400	3.91812800	0.41135300
C	3.14511500	1.97399000	0.48947800
C	3.68385100	-1.74551700	-2.35286000
H	4.20344800	-2.65572400	-2.68938100
H	4.38815600	-0.91794200	-2.45479300
C	2.51404500	-1.45474700	-3.31857700
C	1.91413000	-0.05406000	-3.06058400
H	1.20105800	0.17843700	-3.86578700
P	-1.13172000	-1.15742900	-0.19747600
O	-0.05268600	-0.45625400	0.69614400
O	-2.40975800	-1.81434600	0.62334400
O	-2.27592100	0.60176300	0.21823300
O	-1.18161600	-0.88283900	-1.69462800
C	-3.74004900	-1.54008700	0.45004400
C	-4.29456000	-1.29347600	-0.81363400
C	-4.54558800	-1.61158900	1.59105200
C	-5.66564300	-1.11478500	-0.92832500
H	-3.64288800	-1.22250300	-1.67640500
C	-5.91835700	-1.43807200	1.47847400
H	-4.07817200	-1.79516900	2.55235400
C	-6.46709200	-1.19144100	0.21668800
H	-6.12359500	-0.91730100	-1.88962600
H	-6.56469600	-1.48505800	2.34598200
C	-1.82101400	1.77613500	-0.08750100
C	-1.73327600	2.79098000	0.91680200
C	-1.38312300	2.12879400	-1.40565400
C	-1.15068200	4.01475200	0.66035200
H	-2.11060500	2.54800600	1.90542600
C	-0.79351100	3.35048600	-1.66166400
H	-1.51486200	1.39845000	-2.19329900

C	-0.63954000	4.28911100	-0.62365400
H	-1.04615700	4.76092200	1.43962900
H	-0.43753500	3.60189300	-2.65461500
N	-7.91205300	-1.01351400	0.09178700
O	-8.59945200	-1.08152900	1.11782600
O	-8.37965500	-0.80551200	-1.03328000
N	0.12184900	5.48103600	-0.84965300
O	0.60928600	5.67801200	-1.98075500
O	0.30661600	6.26465100	0.10235800
C	1.26605000	-1.04900100	3.38952700
H	2.08445500	-0.32232100	3.31815200
H	0.41501700	-0.63462300	2.83755100
H	0.99949000	-1.17501900	4.44189100
C	1.76380400	2.43175300	0.84173900
H	1.72206400	3.50866900	1.01269600
H	1.06502600	2.18243100	0.03589300
H	1.39630100	1.91224400	1.73292200
H	0.22558200	-0.24235800	-1.93726200
O	-0.37080600	-2.70026400	-0.27408000
H	-0.47734700	-3.17446800	0.56565800
O	2.95722300	0.89153600	-3.03025400
H	2.56557700	1.76676800	-2.87761700
C	1.38575400	-2.49645900	-3.25648200
H	0.88200000	-2.53112300	-2.28863400
H	0.61368800	-2.26334200	-3.99842000
H	1.77866000	-3.49299200	-3.49351400
C	3.12417900	-1.45163100	-4.73797500
H	3.51348500	-2.44395700	-4.99327200
H	2.35808400	-1.19748300	-5.47880900
H	3.93502600	-0.72235100	-4.82810100
2-PC <sub>SB</sub>			
Zn	1.73549800	-0.44174800	0.36297200
N	2.18820000	-2.24208900	1.54584700
N	3.33773900	-1.49585200	-0.81586400
N	3.23404700	0.88333800	0.73456400
O	0.96978100	0.38354500	-1.36967700
C	1.74228200	-2.45711600	2.80678300
C	1.64770100	-3.75840900	3.30584800
H	1.28253500	-3.92048400	4.31472600
C	2.04279400	-4.83382100	2.50691900
H	1.97015600	-5.85041600	2.88242000
C	2.55269800	-4.58781000	1.23566700
H	2.89551600	-5.39590200	0.59674300
C	2.60745400	-3.26694300	0.78846800

C	3.13753300	-2.93945000	-0.59649700
H	4.07291300	-3.49691100	-0.76945800
H	2.41826000	-3.29677200	-1.33632700
C	4.52397700	-1.00145800	-0.05926100
H	5.45315200	-1.23662000	-0.59519100
H	4.55426200	-1.52368600	0.90163000
C	4.41333100	0.48589200	0.20915200
C	5.43005200	1.39123800	-0.04845700
H	6.36628200	1.05359400	-0.48083200
C	5.19949200	2.74460300	0.22411400
H	5.96093000	3.48412100	-0.00492800
C	3.98472000	3.14140400	0.77114600
H	3.76127200	4.18449500	0.95789900
C	3.00467200	2.17742300	1.03709000
C	3.52119700	-1.18387600	-2.27233000
H	4.03336500	-2.03721700	-2.74214300
H	4.19598000	-0.32878400	-2.32523400
C	2.27649500	-0.81433200	-3.10541300
C	1.68367700	0.53181300	-2.62118100
H	0.94047000	0.89183300	-3.34568300
P	-1.23080600	-1.17307100	0.29401300
O	-0.10584700	-0.48343300	1.08704800
O	-2.56216300	-0.86202000	1.16823200
O	-3.78120000	2.86660800	1.54849600
O	-1.36450500	-0.87938700	-1.17017900
C	-3.85587600	-1.08157200	0.70404700
C	-4.22430200	-2.29928400	0.12140000
C	-4.76990200	-0.04440800	0.89437400
C	-5.54338000	-2.48565800	-0.27670900
H	-3.48889300	-3.08316500	-0.02040600
C	-6.09046400	-0.23496100	0.49808700
H	-4.43946000	0.90710900	1.31044500
C	-6.46249700	-1.45235200	-0.07883300
H	-5.86550700	-3.41373600	-0.73207900
H	-6.82308800	0.55276600	0.62413000
C	-2.76151200	3.18037500	0.88513900
C	-1.86377300	4.24702900	1.31384300
C	-2.39675200	2.50870700	-0.35765800
C	-0.73152500	4.56378600	0.62063700
H	-2.14060300	4.78510600	2.21559000
C	-1.27030800	2.84117400	-1.05629700
H	-3.05297900	1.72083000	-0.71375700
C	-0.39303700	3.85461500	-0.57007800
H	-0.06917000	5.35517300	0.95487100

H	-1.00901600	2.32638300	-1.97271000
N	-7.85576000	-1.65659100	-0.49252700
O	-8.65953200	-0.74127900	-0.29890400
O	-8.15396100	-2.73714200	-1.01316600
N	0.82778600	4.07931700	-1.18434600
O	1.07089900	3.53048600	-2.31472100
O	1.70878900	4.78633200	-0.62415000
C	1.37733200	-1.25133400	3.62709700
H	2.18477200	-0.51114300	3.58279300
H	0.48097000	-0.77532500	3.21741100
H	1.20346400	-1.51973000	4.67211000
C	1.68084100	2.50183300	1.65989400
H	1.55337400	3.57656900	1.78130400
H	0.85509600	2.13661800	1.04074400
H	1.59409300	2.01305900	2.63834600
H	0.02881400	0.07511100	-1.49794600
O	-0.99979100	-2.79635400	0.44989300
H	-0.81613200	-3.03541000	1.37389400
O	2.69866500	1.44731800	-2.42620700
H	2.27431500	2.34661400	-2.35205800
C	1.18754400	-1.89809500	-3.10151200
H	0.77672600	-2.08906000	-2.10699600
H	0.34078700	-1.59132900	-3.72545100
H	1.57862500	-2.83678600	-3.51300800
C	2.77541100	-0.60337900	-4.55159400
H	3.20099800	-1.52925100	-4.95633900
H	1.94324200	-0.30960600	-5.20049200
H	3.53355600	0.18397300	-4.59819600

### 3-AC<sub>SB</sub>

Zn	-1.04108600	-1.10063300	0.01603700
N	-1.06029400	-0.48313500	-2.49203800
N	-3.12764100	-1.28622600	-0.84486800
N	-2.22149300	0.87087400	0.70284400
C	-0.05236500	0.01648000	-3.23372800
C	0.25015500	-0.51098300	-4.49337500
H	1.07240000	-0.09833100	-5.07027300
C	-0.51269900	-1.56910300	-4.98904600
H	-0.28424500	-2.00888000	-5.95563700
C	-1.57020700	-2.05846300	-4.22699900
H	-2.18550600	-2.88022600	-4.58136000
C	-1.81030600	-1.48256000	-2.97624400
C	-2.94075300	-2.01791600	-2.11278200
H	-3.87927500	-2.01100100	-2.69525000

H	-2.69653600	-3.04888000	-1.87135000
C	-3.62968600	0.07720900	-1.11659300
H	-4.70084600	0.05515100	-1.37226600
H	-3.09038400	0.46944100	-1.98053500
C	-3.38741100	1.01175200	0.04570300
C	-4.32758200	1.98854400	0.37202000
H	-5.25847400	2.05277700	-0.18308600
C	-4.04368500	2.86410300	1.41703400
H	-4.75166700	3.63798800	1.70023400
C	-2.84110200	2.71937800	2.09936100
H	-2.58890500	3.37569500	2.92582000
C	-1.94368700	1.70835300	1.72698400
C	-4.09930500	-1.96249300	0.05793500
H	-4.94904600	-2.31138700	-0.55236900
H	-4.48784700	-1.18435700	0.72180400
C	-3.67049900	-3.14140100	0.97198000
C	-4.97316400	-3.59178700	1.68017400
H	-5.70481200	-3.94889200	0.94746500
H	-5.43117600	-2.77607700	2.25332400
H	-4.76700100	-4.41625200	2.37089900
C	-3.07006000	-4.35003600	0.21493600
H	-2.09744600	-4.09359100	-0.21892400
H	-3.76603400	-4.68686100	-0.56472600
H	-2.92529200	-5.18648100	0.90892800
C	-2.68560600	-2.76007800	2.06168300
H	-2.80832400	-3.22964800	3.04071800
N	-1.67002000	-2.00611200	1.89726200
O	1.63181700	-6.48022500	-3.14202000
N	1.72835000	-5.31896600	-3.54515400
C	2.13174000	-4.28528700	-2.58707600
O	1.49352400	-4.97006900	-4.70802700
C	2.27703100	-4.62062000	-1.23813800
C	2.32008900	-2.98053500	-3.04963000
C	2.59710500	-3.62205700	-0.32507700
H	2.10611800	-5.63966500	-0.91530100
C	2.64638500	-1.98812900	-2.13373600
H	2.18445200	-2.75450700	-4.09858500
C	2.76800400	-2.31143900	-0.77895900
H	2.66664200	-3.82811400	0.73657200
H	2.77335900	-0.95841700	-2.44718100
O	3.07285200	-1.29378200	0.10359700
P	1.91761900	-0.72387000	1.14290900
O	0.76776300	-0.14789400	0.32360900
O	1.63190300	-1.68938400	2.25029200



O	2.78288300	0.53046400	1.76492400
C	2.95056000	1.74187900	1.14326600
C	3.28260200	1.85806000	-0.21287300
C	2.80027700	2.88120400	1.94373200
C	3.43071000	3.11981700	-0.77563900
H	3.42009800	0.96542000	-0.80883300
C	2.95573000	4.14425100	1.38732800
H	2.55638200	2.75287700	2.99258200
C	3.25917000	4.25029900	0.02692000
H	3.67817700	3.23865300	-1.82328100
H	2.83778700	5.04027500	1.98400700
N	3.39751700	5.57986500	-0.57351000
O	3.24867500	6.56401900	0.15686700
O	3.65053400	5.64750800	-1.78026000
O	-0.91454500	-1.86440600	3.05885200
C	-0.64505200	1.53745100	2.46025500
H	-0.53472900	0.50829100	2.81005400
H	0.19143700	1.75126000	1.79172400
H	-0.59259400	2.20935900	3.32162100
C	0.70911100	1.16887300	-2.63706700
H	0.09237500	2.07671400	-2.64610100
H	0.95379600	0.95277600	-1.59437500
H	1.62486400	1.38119800	-3.19837700
O	-0.50564100	-2.81962200	-0.66479100
H	0.13947100	-2.74766600	-1.38033900
H	0.03758000	-1.80716200	2.75204300
3-TS1 <sub>SB</sub>			
Zn	1.49895000	-0.65934500	-0.40696400
N	1.64094600	-2.09881100	1.47174500
N	3.26504300	-1.97708700	-0.71460700
N	3.15547100	0.73034900	-0.05269900
C	0.88618400	-2.01967700	2.58609800
C	0.43457000	-3.18191900	3.22433400
H	-0.17787400	-3.09761500	4.11673900
C	0.78173900	-4.42829700	2.71150400
H	0.43401600	-5.33791900	3.19302300
C	1.59362000	-4.49507300	1.58030700
H	1.89998500	-5.44848200	1.15931800
C	1.99474300	-3.29926500	0.98998900
C	2.85557300	-3.32277600	-0.26522300
H	3.74271100	-3.95677800	-0.09681300
H	2.27788900	-3.78843000	-1.06105900
C	4.26323600	-1.41118300	0.23071800
H	5.25618900	-1.84882400	0.04931800

H	3.95854400	-1.68476300	1.24267200
C	4.32636400	0.09962300	0.15230600
C	5.52294200	0.78775100	0.32815200
H	6.44998700	0.24386800	0.48150200
C	5.49306400	2.18285400	0.30271800
H	6.40603100	2.75522300	0.44078800
C	4.28229300	2.83073900	0.08389900
H	4.22877000	3.91363800	0.04581300
C	3.11151000	2.08136400	-0.10436500
C	3.87525000	-1.97479200	-2.07358900
H	4.58032700	-2.82010400	-2.13459400
H	4.47218900	-1.06016800	-2.13054700
C	2.99990100	-2.00106600	-3.35330800
C	2.11965000	-0.78050100	-3.54486700
H	1.92181200	-0.44973900	-4.56766800
P	-1.27485900	-0.06374300	-0.27060000
O	0.03115600	0.37569900	0.44090200
O	-2.20171800	-1.18733300	0.53434300
O	-2.26660500	1.19174300	0.47580000
O	-1.54963700	0.22268500	-1.74798900
C	-3.56132900	-1.23925200	0.54940600
C	-4.36847300	-0.74519800	-0.48907100
C	-4.13697300	-1.89040600	1.65102100
C	-5.74565200	-0.90183200	-0.41454200
H	-3.90828500	-0.24435400	-1.33246500
C	-5.51244900	-2.05057600	1.72490300
H	-3.48395300	-2.26298600	2.43313200
C	-6.30915200	-1.55308600	0.68820700
H	-6.38992500	-0.52865100	-1.20119900
H	-5.97670100	-2.54792900	2.56748300
C	-1.85658100	2.47320700	0.40060100
C	-1.55835400	3.14713000	1.60031500
C	-1.72657100	3.15172700	-0.82855000
C	-1.09811100	4.45488900	1.58002700
H	-1.67470500	2.60702000	2.53382800
C	-1.26069300	4.45858900	-0.85601700
H	-1.97446100	2.62468300	-1.74170600
C	-0.93596200	5.09840700	0.34660300
H	-0.84582100	4.97825500	2.49425200
H	-1.13916300	4.98861500	-1.79295400
N	-7.75722500	-1.72199700	0.75808400
O	-8.23055800	-2.30255700	1.74290600
O	-8.44283400	-1.27884400	-0.17027600
N	-0.39481400	6.45007900	0.31389400

O	-0.21108200	6.98211400	-0.78889800
O	-0.12742600	7.00231000	1.38955800
C	0.55285900	-0.65775200	3.13022200
H	1.24810700	0.09243700	2.75023700
H	-0.44618500	-0.35174100	2.80517500
H	0.57787300	-0.66766800	4.22552700
C	1.79311900	2.73668600	-0.38570700
H	1.88633400	3.82521700	-0.39721700
H	1.40656300	2.40307700	-1.35462800
H	1.04568000	2.44075900	0.35483600
O	-0.20957100	-1.72749800	-0.79063900
H	-0.48162600	-1.88312000	-1.70756400
C	2.07047800	-3.23425100	-3.46176000
H	1.27897200	-3.20840100	-2.70820700
H	1.58726300	-3.25545000	-4.44482300
H	2.64575500	-4.16214000	-3.35446000
C	4.00428000	-2.04112300	-4.53164000
H	4.61205400	-2.95171300	-4.49303700
H	3.47292900	-2.03671500	-5.48907500
H	4.67874400	-1.17700800	-4.51651100
N	1.49508200	-0.20343800	-2.59510700
O	0.66337600	0.82475000	-3.02403700
H	-0.20109100	0.67151400	-2.50489200
3-IM <sub>SB</sub>			
Zn	1.60588400	-0.65868800	-0.36366800
N	1.78254800	-2.08878300	1.51625000
N	3.38818900	-1.95208900	-0.68015300
N	3.23399200	0.76134500	-0.04500000
C	1.02717200	-2.01422800	2.63083100
C	0.58946800	-3.17962800	3.27290400
H	-0.02406200	-3.09941600	4.16490800
C	0.95063400	-4.42368800	2.76412800
H	0.61250300	-5.33554800	3.24819000
C	1.76397200	-4.48509400	1.63360500
H	2.08154600	-5.43635100	1.21603300
C	2.15173400	-3.28667500	1.03986500
C	3.01803500	-3.30316500	-0.21171800
H	3.92413600	-3.90569200	-0.02949700
H	2.46150500	-3.80067800	-1.00338000
C	4.38446800	-1.35493900	0.24913100
H	5.38329400	-1.77712600	0.06393200
H	4.09284100	-1.62174600	1.26685900
C	4.41925700	0.15567100	0.15244000
C	5.60365600	0.86907800	0.30736200

H	6.54325000	0.34572900	0.45552800
C	5.54488800	2.26319100	0.26888900
H	6.44763500	2.85508800	0.39080300
C	4.31888400	2.88476300	0.05889800
H	4.24311400	3.96597700	0.01207900
C	3.16104900	2.11056700	-0.10851000
C	3.98369600	-1.95315000	-2.04583200
H	4.70241600	-2.78677700	-2.10636300
H	4.56407900	-1.02916000	-2.11968500
C	3.09115400	-2.00803400	-3.31267600
C	2.19033300	-0.80229400	-3.50336200
H	1.98674800	-0.47208100	-4.52512200
P	-1.17720600	-0.15836900	-0.22088100
O	0.12134300	0.33444600	0.48063000
O	-2.10762500	-1.28129500	0.59085100
O	-2.18312000	1.09400000	0.54503600
O	-1.48346700	0.14185500	-1.69241100
C	-3.46638600	-1.27785700	0.67493000
C	-4.29892900	-0.80733000	-0.35436900
C	-4.01640500	-1.85331000	1.82958400
C	-5.67595300	-0.91170700	-0.21853100
H	-3.85529500	-0.36090400	-1.23667400
C	-5.39264800	-1.96227900	1.96555400
H	-3.34431400	-2.20887900	2.60342900
C	-6.21420700	-1.48894000	0.93732900
H	-6.33996600	-0.55489100	-0.99628800
H	-5.83805600	-2.40125700	2.84972100
C	-1.79750400	2.37926900	0.46412500
C	-1.49345300	3.06088200	1.65921700
C	-1.69707500	3.06126900	-0.76696500
C	-1.05577700	4.37586700	1.63187500
H	-1.58696800	2.51958900	2.59467100
C	-1.25389800	4.37545600	-0.80151900
H	-1.94946400	2.52939400	-1.67604900
C	-0.92174200	5.02187400	0.39600300
H	-0.79885400	4.90388800	2.54216500
H	-1.15523500	4.90709000	-1.74027900
N	-7.66303900	-1.60476000	1.07222700
O	-8.11445200	-2.11917900	2.10303300
O	-8.37130400	-1.18526000	0.14988900
N	-0.40156600	6.38025700	0.35496600
O	-0.23738400	6.91335800	-0.75089000
O	-0.12979500	6.93909300	1.42658700
C	0.67912600	-0.65470600	3.17152800

H	1.36052600	0.10348600	2.78257200
H	-0.32661000	-0.36367300	2.85360800
H	0.71364600	-0.65993500	4.26664900
C	1.82591800	2.73515900	-0.37959300
H	1.89488900	3.82530400	-0.39805000
H	1.43644200	2.38748000	-1.34246900
H	1.09204200	2.42728500	0.36978200
O	-0.12531100	-1.75337300	-0.71415800
H	-0.41540100	-1.95717100	-1.61618900
C	2.17812800	-3.25557700	-3.39290900
H	1.39965300	-3.23366300	-2.62558700
H	1.67730900	-3.29244600	-4.36663800
H	2.76784900	-4.17460900	-3.28779900
C	4.07862200	-2.04704900	-4.50490700
H	4.70085600	-2.94773200	-4.46466500
H	3.53345500	-2.06188800	-5.45442400
H	4.73983400	-1.17264400	-4.50966900
N	1.55422100	-0.23972200	-2.55229900
O	0.70433000	0.77331700	-2.97654000
H	-0.15801700	0.60625100	-2.45185500
3-TS <sub>2SB</sub>			
Zn	1.74725500	-0.66558300	-0.45531200
N	1.87175900	-2.04420400	1.31562400
N	3.50020700	-1.97929500	-0.84472800
N	3.26401600	0.72231300	-0.14231100
C	1.15048600	-1.90132300	2.44996200
C	0.85834800	-3.01917200	3.24062600
H	0.27478700	-2.89168700	4.14664300
C	1.32218000	-4.27605200	2.86088400
H	1.09548800	-5.15021000	3.46448500
C	2.09631900	-4.39788600	1.70767400
H	2.49420100	-5.35757100	1.39113200
C	2.34368500	-3.24926900	0.96129400
C	3.15923500	-3.31816300	-0.32073000
H	4.07295100	-3.91161100	-0.15285200
H	2.57231900	-3.84183400	-1.07303200
C	4.52768100	-1.34336800	0.02704200
H	5.53021900	-1.71919900	-0.22214500
H	4.31666400	-1.63367700	1.05950100
C	4.48972100	0.16951800	-0.04783600
C	5.63784800	0.94726800	0.03462800
H	6.61417600	0.47771700	0.10107100
C	5.49770900	2.33841200	0.03374100
H	6.37439800	2.97609900	0.10172800

C	4.22917700	2.89911700	-0.06588200
H	4.08991200	3.97480000	-0.07797400
C	3.10654600	2.06509800	-0.16599500
C	4.02064600	-2.01111100	-2.23871200
H	4.73968600	-2.84208100	-2.32260100
H	4.58958500	-1.08555400	-2.36831300
C	3.04405800	-2.10149300	-3.43945100
C	2.12391800	-0.90437600	-3.57769400
H	1.88919900	-0.54440700	-4.58187900
P	-1.22873600	-0.89511600	-0.71131400
O	-0.04631000	-0.27877600	0.07748300
O	-2.36159800	-1.80729600	0.07656900
O	-2.33115600	0.64616000	0.46648000
O	-1.62999100	-0.29628500	-2.04730000
C	-3.69460700	-1.52936800	0.24320900
C	-4.47392900	-0.92768400	-0.75470200
C	-4.27072700	-1.97850900	1.43588300
C	-5.83728600	-0.77377300	-0.54748400
H	-3.99631100	-0.56619600	-1.65722000
C	-5.63491100	-1.82939400	1.64449600
H	-3.63287500	-2.43432700	2.18543100
C	-6.40796000	-1.22735400	0.64754100
H	-6.46460300	-0.30525700	-1.29567400
H	-6.10523500	-2.16515600	2.56026700
C	-1.92221000	1.87118400	0.45824900
C	-1.60615600	2.53552800	1.68733900
C	-1.74593300	2.62045400	-0.75073700
C	-1.09299500	3.81546500	1.70776900
H	-1.76839600	1.98442300	2.60915700
C	-1.22771400	3.89806800	-0.73151700
H	-2.01428300	2.13836300	-1.68375300
C	-0.87583800	4.49826400	0.49480700
H	-0.82714500	4.30101700	2.63983600
H	-1.07002000	4.45079500	-1.65068900
N	-7.84562300	-1.07437400	0.85747600
O	-8.32686600	-1.47963900	1.92278500
O	-8.51438000	-0.54974300	-0.03982600
N	-0.21122500	5.76547600	0.50386800
O	0.11796500	6.27685600	-0.58665300
O	0.05060100	6.30345600	1.59777900
C	0.68138900	-0.52669400	2.83671200
H	1.34345800	0.23881700	2.42360000
H	-0.31329300	-0.33165700	2.42294200
H	0.64572000	-0.42459500	3.92598800

C	1.71668300	2.59047900	-0.32669800
H	1.69409700	3.68095100	-0.31118400
H	1.29083100	2.24574600	-1.27540000
H	1.05192500	2.21280700	0.45821600
O	-0.37317700	-2.32179200	-1.13449200
H	-0.94452900	-2.88462700	-1.68135200
C	2.13036000	-3.35117600	-3.42823200
H	1.39128000	-3.29411100	-2.62501600
H	1.57868300	-3.41641200	-4.37268500
H	2.72797000	-4.26589000	-3.33000400
C	3.94351600	-2.15499200	-4.69772400
H	4.57340200	-3.05096000	-4.68491700
H	3.33130000	-2.19203900	-5.60464300
H	4.59612700	-1.27677000	-4.76714800
N	1.50942400	-0.36920900	-2.59741800
O	0.66059000	0.66835000	-2.98062700
H	-0.24567800	0.40516100	-2.59558500
3-PC <sub>SB</sub>			
Zn	1.05394900	-1.18388900	-0.66448400
N	1.53031500	-1.97056300	1.30323900
N	3.30989700	-0.94012600	-0.55070500
N	1.11001400	0.88672600	-0.71116700
C	0.62050800	-2.21471900	2.27718800
C	1.02913300	-2.71820200	3.51971100
H	0.27883200	-2.89942900	4.28182200
C	2.37578700	-2.93920600	3.77391500
H	2.70296800	-3.30769900	4.74173400
C	3.30392800	-2.65435600	2.77321100
H	4.36916000	-2.78706400	2.93453800
C	2.83866500	-2.18427000	1.55057100
C	3.81293700	-1.92826000	0.42210200
H	4.77901100	-1.60103600	0.83593000
H	3.99480600	-2.86799300	-0.10213600
C	3.35665100	0.41839300	0.06678500
H	4.37276800	0.82845500	0.04103500
H	3.08035800	0.33318900	1.12135300
C	2.37260200	1.36120100	-0.57586400
C	2.71257900	2.65961700	-0.91774500
H	3.72238800	3.01647300	-0.75414400
C	1.70476000	3.51575100	-1.36671200
H	1.93475500	4.54880200	-1.60461300
C	0.40341000	3.03973700	-1.45475500
H	-0.40921800	3.68761900	-1.76416700
C	0.12178800	1.71116200	-1.11715900

C	4.12344100	-0.96374900	-1.79420900
H	5.16083900	-1.22433900	-1.53554800
H	4.14485600	0.05609100	-2.18903400
C	3.63477200	-1.89424800	-2.93711400
C	2.38972100	-1.30223400	-3.56607700
H	2.41658700	-0.94783000	-4.59909300
P	-1.73999100	-2.66810100	-1.64846900
O	-0.49863900	-2.37545200	-0.81049800
O	-3.08555100	-2.43965600	-0.72406500
O	-2.18068700	0.64502400	3.27690500
O	-1.87918100	-1.94345700	-2.96495700
C	-3.67195200	-1.19065900	-0.55632400
C	-4.22218600	-0.50543700	-1.64720100
C	-3.71578600	-0.65501900	0.73185200
C	-4.77666800	0.75329900	-1.44683000
H	-4.17469600	-0.94539900	-2.63558800
C	-4.25648400	0.61177100	0.93710100
H	-3.29688200	-1.19611600	1.56874100
C	-4.77086000	1.30273400	-0.16067500
H	-5.19501600	1.31681500	-2.27160000
H	-4.21925800	1.05563000	1.92443600
C	-1.12441400	1.28734300	3.02364700
C	0.18494900	0.82430000	3.45882800
C	-1.12190200	2.53027200	2.26950600
C	1.34518500	1.47226100	3.11996400
H	0.21237200	-0.05739000	4.09072100
C	0.03889800	3.19811400	1.96847900
H	-2.08753400	2.92702500	1.96656900
C	1.29692400	2.66646600	2.35748600
H	2.30968900	1.10721100	3.45804600
H	0.02106200	4.12946800	1.41421100
N	-5.29180400	2.66295200	0.02928500
O	-5.26309000	3.14175800	1.16411500
O	-5.71854800	3.26228900	-0.96436700
N	2.49025400	3.30937500	1.98168100
O	2.44554800	4.44560000	1.45492700
O	3.58690200	2.70146100	2.13207600
C	-0.82410000	-1.92599800	2.02329500
H	-0.93685800	-1.07859500	1.34918400
H	-1.30862700	-2.78709100	1.55275200
H	-1.34063700	-1.66651600	2.94971000
C	-1.26894400	1.16351800	-1.14784500
H	-1.99293500	1.92828400	-1.43515100
H	-1.35269900	0.33823800	-1.85772200



H	-1.54349900	0.79754000	-0.15420500
O	-1.78350500	-4.27880800	-1.78078600
H	-2.51662900	-4.57272500	-2.34683900
C	3.33714600	-3.34010400	-2.48501900
H	2.52977900	-3.38448200	-1.74751600
H	3.01679800	-3.93779900	-3.34452500
H	4.23453600	-3.81136000	-2.06743200
C	4.74726700	-1.91523500	-4.00574000
H	5.65746200	-2.37464900	-3.60604900
H	4.43234900	-2.49733800	-4.87852200
H	4.99709000	-0.90326800	-4.34644100
N	1.29200000	-1.21186300	-2.92130200
O	0.28524400	-0.60096700	-3.65328800
H	-0.55828700	-1.08699800	-3.39577300

1-RC<sub>LB</sub>

Zn	-0.58758800	-1.14995300	0.56220400
N	-2.22372400	0.34957900	0.30441200
N	-1.84531900	-1.88928600	-1.19540400
N	-1.79217700	-2.64424600	1.51872600
O	0.90453600	-2.29049600	0.24879900
C	-2.71108700	1.19381800	1.23696800
C	-3.64020600	2.17958700	0.88840000
H	-4.01771900	2.85315300	1.64944300
C	-4.05896600	2.29125400	-0.43501000
H	-4.76748000	3.06219800	-0.72428900
C	-3.56748200	1.39208900	-1.38083300
H	-3.89199700	1.42915200	-2.41597600
C	-2.65345800	0.42621500	-0.96821200
C	-2.12173500	-0.63019800	-1.91503500
H	-2.83578000	-0.78294800	-2.74048000
H	-1.17832200	-0.27827100	-2.34197900
C	-3.05798500	-2.43938400	-0.54401300
H	-3.63424300	-3.06857400	-1.23717400
H	-3.70861900	-1.61150000	-0.25022700
C	-2.70255300	-3.21787200	0.70950400
C	-3.28547300	-4.44250300	1.02384800
H	-4.01133600	-4.88937900	0.35186500
C	-2.90529300	-5.07811600	2.20738900
H	-3.34222500	-6.03463600	2.47987100
C	-1.94321000	-4.48729000	3.02269200
H	-1.60905800	-4.97111100	3.93454200
C	-1.38327000	-3.26167000	2.64429100
C	-1.21377100	-2.92593900	-2.06994100

H	-1.56964000	-2.77244300	-3.10195000
H	-1.61505300	-3.89057100	-1.74180800
C	0.32463300	-3.05712000	-2.05619800
C	0.83401100	-3.37440900	-0.61740600
H	1.84331400	-3.81238200	-0.72006300
P	1.01970600	1.38998900	0.36802900
O	0.55833700	1.23527500	-1.04828900
O	2.63600300	1.62491000	0.50784700
O	0.65729400	2.87571600	1.01701300
O	0.54839600	0.35229700	1.38827900
C	3.59462200	0.78056900	-0.00619900
C	3.39522100	-0.59566300	-0.16125200
C	4.81284400	1.38414100	-0.34400700
C	4.43124900	-1.36677500	-0.67787400
H	2.45448400	-1.08147500	0.10169500
C	5.84777900	0.61115900	-0.85226400
H	4.92573300	2.45396600	-0.20498200
C	5.64364100	-0.76256500	-1.01968100
H	4.30245200	-2.43382300	-0.81217400
H	6.79790800	1.05303200	-1.12538800
C	-0.38122500	3.68223700	0.65888700
C	-0.79215500	3.86999200	-0.67082900
C	-1.00827400	4.37714500	1.70569200
C	-1.86148600	4.71521200	-0.93735900
H	-0.29160000	3.33241800	-1.46549600
C	-2.06773700	5.23158400	1.43800600
H	-0.64993400	4.22365700	2.71783800
C	-2.49844100	5.37787300	0.11560300
H	-2.21113200	4.86269300	-1.95172800
H	-2.57361400	5.76717800	2.23202600
N	6.72394100	-1.58285100	-1.56804100
O	7.79584400	-1.03031500	-1.83872300
O	6.51194600	-2.78867600	-1.73661500
N	-3.66888200	6.20492000	-0.16569200
O	-4.17218600	6.84094100	0.76645000
O	-4.11362900	6.20898300	-1.31996800
C	0.64818200	-4.26816800	-2.95399400
H	0.24660300	-4.14001600	-3.96710700
H	1.73248800	-4.39572300	-3.04098300
H	0.23466300	-5.19813300	-2.54124600
C	1.02489400	-1.80858800	-2.60740300
H	0.67566100	-1.57671000	-3.62267000
H	0.87096200	-0.93325900	-1.97353900
H	2.10715400	-1.97463300	-2.65614300

C	-2.23796300	1.00581500	2.65167500
H	-2.52188900	0.00789700	3.00873300
H	-1.14648900	1.06773800	2.69352400
H	-2.67585300	1.75275900	3.31853400
C	-0.27453300	-2.59052700	3.40355000
H	0.61998300	-2.56873700	2.76658700
H	-0.52988900	-1.54814100	3.62541000
H	-0.04793700	-3.10878200	4.33875800
H	0.19117400	-4.18668800	-0.21119100
1-TS <sub>LB</sub>			
Zn	-1.40005300	-0.83361500	0.35486900
N	-3.13756400	0.27767200	0.05007300
N	-2.60027400	-2.28496400	-0.76750900
N	-1.52869000	-2.26349700	1.84814200
O	0.42261500	-1.64925900	-0.44386100
C	-3.35716700	1.49095000	0.61732200
C	-4.37590900	2.31620100	0.13725600
H	-4.52114600	3.29890600	0.57238300
C	-5.16819500	1.87913500	-0.92241900
H	-5.94291700	2.52725500	-1.31977300
C	-4.95263800	0.61332500	-1.46756200
H	-5.55981700	0.23915100	-2.28647800
C	-3.91391800	-0.16039700	-0.95765600
C	-3.57973300	-1.51545700	-1.56704500
H	-4.50260800	-2.09840200	-1.71202800
H	-3.15898800	-1.35132200	-2.55747000
C	-3.30528800	-2.95591100	0.35799000
H	-3.81112300	-3.86900300	0.01416700
H	-4.07729400	-2.26582700	0.71695300
C	-2.37699000	-3.25826400	1.51740200
C	-2.41003100	-4.45319600	2.22485200
H	-3.09641000	-5.24246800	1.93584400
C	-1.53904400	-4.60555800	3.30774700
H	-1.53959800	-5.52622500	3.88400900
C	-0.66452000	-3.57453600	3.63484200
H	0.02810600	-3.67330900	4.46389400
C	-0.66354500	-2.39700400	2.87460500
C	-1.84817300	-3.29104800	-1.58544100
H	-2.56500500	-3.76156400	-2.27701400
H	-1.52443200	-4.07219000	-0.88897300
C	-0.59299700	-2.82611000	-2.37861000
C	0.62748600	-2.63712300	-1.44615800
H	1.49696300	-2.36370100	-2.05249600
P	1.14792900	-0.01570900	-0.52185600

O	1.40800800	0.13248400	-1.98420900
O	2.41401300	-0.44513700	0.44456700
O	1.90578400	2.09351100	-0.15219000
O	-0.02095000	0.50973600	0.36018700
C	3.72362800	-0.05529700	0.33662200
C	4.28194000	0.51709000	-0.81528100
C	4.51247300	-0.31704700	1.46463800
C	5.63770400	0.81821500	-0.82784400
H	3.65029700	0.73945000	-1.66488700
C	5.86690200	-0.01764400	1.45178200
H	4.04397800	-0.75208700	2.34119700
C	6.42058800	0.54657000	0.29896200
H	6.09535600	1.26617700	-1.70128700
H	6.49461700	-0.21029100	2.31281600
C	0.94290700	2.94127600	-0.28016000
C	0.11215400	2.98695700	-1.45499100
C	0.59915600	3.83558300	0.78830200
C	-1.05870300	3.70718300	-1.47424000
H	0.40306600	2.36987300	-2.29759300
C	-0.57759800	4.55117800	0.77275400
H	1.26012700	3.86433800	1.64935200
C	-1.44450600	4.45695800	-0.33916100
H	-1.71676700	3.68614800	-2.33565400
H	-0.87522200	5.16012800	1.61897900
N	7.84849500	0.85549700	0.27357400
O	8.51514100	0.61526200	1.28770900
O	8.32351700	1.33876000	-0.75960500
N	-2.74690500	5.01684800	-0.27718800
O	-3.15774900	5.48434800	0.81194000
O	-3.48399500	4.96956200	-1.28781300
C	-0.24090200	-3.99041000	-3.32965000
H	-1.03770500	-4.15433800	-4.06432000
H	0.67820000	-3.76612400	-3.88126300
H	-0.08446500	-4.92974200	-2.78400900
C	-0.82926400	-1.55506800	-3.20979100
H	-1.63367200	-1.70594300	-3.94160000
H	-1.06187000	-0.68734400	-2.58623000
H	0.08151300	-1.28826100	-3.75068500
C	-2.46345400	1.88859100	1.75445000
H	-2.49735800	1.12708700	2.54531500
H	-1.42834300	1.97019900	1.40824100
H	-2.76457800	2.85170600	2.17108300
C	0.29836200	-1.27225900	3.12251900
H	1.09379800	-1.28986800	2.36785600

H	-0.19268800	-0.29993000	3.02117900
H	0.75022900	-1.34902600	4.11476600
H	0.84361100	-3.58403100	-0.93105100
1-PC <sub>LB</sub>			
Zn	-0.85633600	-0.36054900	0.32579100
N	-2.30821200	0.99883600	0.57600200
N	-2.43172900	-1.48575500	-0.62856000
N	-0.96059400	-1.88564500	1.75913300
O	0.73851500	-2.32105600	-0.90492000
C	-2.24273700	2.05702600	1.41202900
C	-3.33021400	2.92740600	1.50869500
H	-3.26481100	3.78774000	2.16527800
C	-4.46452300	2.70129300	0.73317000
H	-5.30096300	3.39082200	0.76858600
C	-4.51337500	1.59492400	-0.11701500
H	-5.36313900	1.42054700	-0.76621100
C	-3.40291700	0.76679600	-0.18354300
C	-3.32635300	-0.40622200	-1.14261500
H	-4.33324800	-0.79929600	-1.33890000
H	-2.93453800	-0.03392800	-2.09024700
C	-3.05718300	-2.11226700	0.57453500
H	-3.79245500	-2.87169300	0.27963300
H	-3.59975800	-1.33154700	1.11741400
C	-2.01730500	-2.69144900	1.50913200
C	-2.15094700	-3.93214500	2.11486500
H	-3.00593400	-4.56159400	1.89045300
C	-1.16246300	-4.34072500	3.01681800
H	-1.23462400	-5.30694600	3.50751200
C	-0.08808900	-3.50001800	3.27646700
H	0.69273600	-3.78949900	3.97215500
C	0.00250900	-2.26149900	2.62271100
C	-2.19520700	-2.56669300	-1.65054000
H	-3.14273100	-2.69224500	-2.19424400
H	-2.03069200	-3.48999800	-1.08607200
C	-1.03727800	-2.44485600	-2.68001200
C	0.29619200	-2.98064300	-2.10674300
H	1.07556700	-2.90234600	-2.87056200
P	1.69944000	-0.99258600	-0.98436800
O	2.13860800	-0.65742500	-2.36080800
O	2.93174200	-1.49947100	-0.01595800
O	1.65186100	3.18332800	-0.18068700
O	0.91749900	0.03643500	-0.12927000
C	3.86912100	-0.63949000	0.52686200
C	3.76526800	0.75904000	0.49388400

C	4.94311800	-1.27323000	1.16623000
C	4.75072800	1.51737200	1.12080800
H	2.93655400	1.28158900	0.02268700
C	5.92224000	-0.51457900	1.79149700
H	4.99358500	-2.35708900	1.15661300
C	5.81270800	0.87927200	1.76550400
H	4.68273100	2.59850900	1.11196300
H	6.76153400	-0.98104300	2.29204300
C	0.56565200	3.27769300	-0.81249900
C	0.22363300	2.39711300	-1.92203800
C	-0.44791700	4.26330700	-0.46553400
C	-1.03095600	2.38995500	-2.47232300
H	0.99516000	1.72467800	-2.28182000
C	-1.69707100	4.25799200	-1.03169000
H	-0.18389800	4.99138400	0.29673800
C	-2.03558000	3.27784300	-2.00170200
H	-1.27992500	1.72327700	-3.28907800
H	-2.45681400	4.96939300	-0.72732500
N	6.83563800	1.68327100	2.43959300
O	7.75581200	1.08835500	3.01321800
O	6.72645700	2.91135600	2.40574500
N	-3.36239600	3.12247400	-2.42355300
O	-4.23763400	3.94747700	-2.05970300
O	-3.67590600	2.10272800	-3.10535200
C	-1.39528000	-3.40627000	-3.83728500
H	-2.29253800	-3.06110500	-4.36207600
H	-0.57972500	-3.44787300	-4.56706800
H	-1.58095800	-4.42699800	-3.47918600
C	-0.87816400	-1.02752300	-3.24223000
H	-1.78456700	-0.70990100	-3.76957800
H	-0.66283500	-0.29295400	-2.46476300
H	-0.03915200	-0.98523300	-3.94142600
C	-0.97446100	2.21728000	2.20153400
H	-0.85162300	1.37218400	2.89281000
H	-0.10121300	2.25091200	1.53854000
H	-0.98485800	3.13858100	2.78785400
C	1.17463900	-1.34874600	2.84241200
H	2.03328500	-1.70483300	2.26402000
H	0.96867000	-0.33099500	2.50637300
H	1.46093200	-1.33181200	3.89859900
H	0.18122800	-4.03267400	-1.82377400
2-RC <sub>LB</sub>			
Zn	-0.57991800	-1.23525200	0.53132500
N	-2.23301200	0.31189300	0.29713400

N	-1.83426400	-1.92816900	-1.18859500
N	-1.79734600	-2.63488000	1.54739200
O	0.92956300	-2.38956900	0.19680500
C	-2.71286700	1.16599000	1.22353200
C	-3.62850900	2.16228000	0.86862800
H	-3.99896300	2.84484200	1.62512800
C	-4.04175700	2.27321600	-0.45678800
H	-4.73939900	3.05198900	-0.75146500
C	-3.55913400	1.36353000	-1.39706300
H	-3.87953300	1.40018100	-2.43359500
C	-2.65838300	0.38833900	-0.97577700
C	-2.13247100	-0.67641800	-1.91661900
H	-2.85752800	-0.84750400	-2.72835300
H	-1.20007700	-0.32290500	-2.36455200
C	-3.04618100	-2.48334900	-0.53390900
H	-3.59637400	-3.14276500	-1.21842000
H	-3.71821900	-1.65931000	-0.27895600
C	-2.71187200	-3.21753200	0.75183600
C	-3.32849800	-4.41286200	1.11014900
H	-4.05473200	-4.87205000	0.44730100
C	-2.97129500	-5.01122000	2.31842000
H	-3.42834200	-5.94915000	2.62070300
C	-2.00723900	-4.40794800	3.12429300
H	-1.69586300	-4.86205800	4.05928500
C	-1.41991900	-3.21018100	2.70562000
C	-1.21132800	-2.96738500	-2.07240600
H	-1.59414900	-2.82092100	-3.09477300
H	-1.57995400	-3.93197500	-1.72145100
C	0.32723100	-3.07145600	-2.11388700
C	0.90969900	-3.41117600	-0.70680100
H	1.94687900	-3.76459200	-0.86265000
P	0.99494600	1.32718400	0.37869800
O	0.54248900	1.20395700	-1.04275700
O	2.60540500	1.59726600	0.52918100
O	0.58514300	2.77185400	1.08175000
O	0.55734900	0.24018200	1.36364300
C	3.58020100	0.77744300	0.00572100
C	3.40461200	-0.59961800	-0.17061600
C	4.78906000	1.40536300	-0.31990000
C	4.45369700	-1.34706100	-0.69522400
H	2.47315400	-1.10126600	0.08615200
C	5.83781700	0.65632000	-0.83590200
H	4.88420900	2.47472700	-0.16517200
C	5.65685100	-0.71787100	-1.02365800

H	4.34278400	-2.41399700	-0.84619000
H	6.78157800	1.11724700	-1.09946300
C	-0.40756200	3.62466400	0.69856600
C	-0.78041400	3.83794500	-0.63804400
C	-1.03396600	4.33212800	1.73737200
C	-1.81679200	4.71889700	-0.91993600
H	-0.28129000	3.29172000	-1.42747500
C	-2.05986300	5.22149700	1.45432800
H	-0.70382300	4.15856500	2.75583000
C	-2.45691300	5.39166600	0.12424700
H	-2.13830700	4.88584300	-1.94060500
H	-2.56528800	5.76705400	2.24180800
N	6.75322300	-1.51284000	-1.57885100
O	7.81512300	-0.93771600	-1.84065100
O	6.56281000	-2.72003200	-1.76050000
N	-3.59250200	6.26061000	-0.17555000
O	-4.09850500	6.90014700	0.75264100
O	-4.00539600	6.29575200	-1.34070300
O	0.13982200	-4.54461800	-0.21324600
H	0.41177300	-4.65154300	0.71121000
C	0.64552800	-4.23873700	-3.07215200
H	0.27299900	-4.03156300	-4.08330000
H	1.72948800	-4.38199500	-3.14304600
H	0.20534900	-5.17708300	-2.72091600
C	1.00213600	-1.79591100	-2.63581000
H	0.63840300	-1.55019600	-3.64208700
H	0.84212700	-0.93480400	-1.98469000
H	2.08653800	-1.94267600	-2.70259200
C	-2.24704700	0.97609600	2.64086700
H	-2.58969700	0.00396700	3.01705400
H	-1.15397700	0.97599100	2.68117500
H	-2.63868900	1.75913600	3.29511200
C	-0.31553700	-2.52272400	3.45954200
H	0.59020800	-2.51037800	2.83947100
H	-0.57327200	-1.47659900	3.65782000
H	-0.09865700	-3.02126700	4.40775600
2-TS <sub>LB</sub>			
Zn	-1.42201600	-0.81287200	0.32161100
N	-3.15722200	0.27768300	0.01667000
N	-2.61220900	-2.29761300	-0.76884100
N	-1.51054000	-2.21039600	1.84236000
O	0.38936100	-1.65455400	-0.53277300
C	-3.38084000	1.49470900	0.57459300
C	-4.41641200	2.30302400	0.10164000



H	-4.56250800	3.29060400	0.52525200
C	-5.22433700	1.84036100	-0.93535100
H	-6.01582900	2.47245700	-1.32569900
C	-5.00667000	0.56866500	-1.46608800
H	-5.62794300	0.17518000	-2.26510600
C	-3.94835700	-0.18596700	-0.96836400
C	-3.61176500	-1.54754900	-1.56217900
H	-4.53239300	-2.13942900	-1.68293100
H	-3.20896900	-1.39596800	-2.56238300
C	-3.28817300	-2.95684600	0.38128100
H	-3.79183400	-3.87953400	0.06179000
H	-4.05842200	-2.26837000	0.74735700
C	-2.33055600	-3.23269000	1.52291600
C	-2.31085900	-4.42999000	2.22580300
H	-2.97323600	-5.24170700	1.94360800
C	-1.41581100	-4.55732900	3.29176200
H	-1.37203700	-5.48112900	3.86122100
C	-0.57672400	-3.49536800	3.61292500
H	0.12918900	-3.57115400	4.43322100
C	-0.63094800	-2.31523900	2.85957500
C	-1.87482900	-3.31954400	-1.58302100
H	-2.60150200	-3.79504100	-2.25938700
H	-1.53253200	-4.08827700	-0.88601700
C	-0.63632400	-2.86818600	-2.40496300
C	0.60123700	-2.66662800	-1.49411300
H	1.45790600	-2.38120900	-2.11706100
P	1.14701200	-0.04429600	-0.58614000
O	1.43187300	0.14085700	-2.03673900
O	2.40206600	-0.51139500	0.37641600
O	1.97542600	2.10566400	-0.14845500
O	-0.01008200	0.50525200	0.28801300
C	3.71122000	-0.09614100	0.31157400
C	4.29729600	0.46588700	-0.83027000
C	4.46311500	-0.32996900	1.46898600
C	5.64874400	0.78590800	-0.80310000
H	3.68963400	0.66989700	-1.70180200
C	5.81378800	-0.01225400	1.49589700
H	3.97126700	-0.75530100	2.33755700
C	6.39660800	0.54150300	0.35305400
H	6.12906100	1.22773500	-1.66739800
H	6.41524800	-0.18180300	2.38019100
C	1.01421200	2.95337500	-0.25290900
C	0.19610800	3.04211900	-1.43617000
C	0.65084900	3.80601600	0.84555200

C	-0.98184500	3.74978600	-1.43942100
H	0.50150200	2.46011400	-2.29867800
C	-0.53206800	4.50979900	0.84487100
H	1.30408800	3.81010700	1.71308500
C	-1.38870400	4.44904600	-0.27848300
H	-1.63179700	3.75531800	-2.30727200
H	-0.84412500	5.08346900	1.71045300
N	7.82179900	0.86964600	0.36972300
O	8.45693900	0.65256900	1.40843100
O	8.32306200	1.34434400	-0.65435400
N	-2.70030500	4.97917300	-0.20286300
O	-3.13338800	5.37933700	0.90633800
O	-3.42756200	4.97218200	-1.22235900
O	0.85794100	-3.88094600	-0.80975900
H	1.61236700	-3.72400500	-0.21992500
C	-0.31790900	-4.02305600	-3.37939600
H	-1.12164100	-4.13785000	-4.11594600
H	0.60754100	-3.81206400	-3.92615300
H	-0.18603700	-4.97132800	-2.85079200
C	-0.86011700	-1.58148700	-3.21661400
H	-1.65830600	-1.72546100	-3.95513800
H	-1.10005400	-0.72002200	-2.58733700
H	0.05283000	-1.30838300	-3.75146800
C	-2.48021400	1.90749200	1.70097400
H	-2.53933200	1.17313300	2.51611400
H	-1.44138900	1.95414100	1.35954200
H	-2.75895600	2.89103100	2.08419400
C	0.28309400	-1.15117800	3.11190100
H	1.08464200	-1.13046800	2.36425200
H	-0.24985000	-0.20121400	3.01139500
H	0.73162800	-1.21015100	4.10698800
2-PC <sub>LB</sub>			
Zn	-0.89941700	-0.45029000	0.25894900
N	-2.37205300	0.86464600	0.56503500
N	-2.48539200	-1.64637300	-0.59786200
N	-0.86949600	-1.93188800	1.73500700
O	0.63203900	-2.45079400	-1.00781800
C	-2.29343100	1.93491600	1.38467500
C	-3.39315400	2.78496900	1.51367500
H	-3.31932000	3.65537000	2.15594500
C	-4.55248900	2.52562900	0.78656900
H	-5.39972800	3.20031900	0.84487600
C	-4.61589800	1.40294100	-0.04075300
H	-5.48986300	1.19949600	-0.64811900

C	-3.49374700	0.59356100	-0.13945800
C	-3.43852600	-0.60074300	-1.07357500
H	-4.44458700	-1.02326600	-1.20158200
H	-3.11206200	-0.24141500	-2.05153600
C	-3.00247100	-2.27330400	0.65665400
H	-3.73623400	-3.05592700	0.42747100
H	-3.51965900	-1.49964200	1.23320200
C	-1.87166300	-2.81050500	1.50815000
C	-1.86141900	-4.08650900	2.05174000
H	-2.67153200	-4.77701600	1.84192600
C	-0.77938900	-4.45512100	2.85808300
H	-0.73173700	-5.45184900	3.28682800
C	0.23366300	-3.53618100	3.10434600
H	1.08010000	-3.79254600	3.73285300
C	0.16866100	-2.25858800	2.52997100
C	-2.29738000	-2.74056700	-1.61788400
H	-3.26682600	-2.87006600	-2.11822000
H	-2.09962300	-3.65930100	-1.06188200
C	-1.19127900	-2.62633300	-2.69960100
C	0.16536300	-3.15942700	-2.17149400
H	0.92386900	-3.06037500	-2.95673000
P	1.62277800	-1.14357000	-1.11999200
O	2.10211100	-0.88145900	-2.49788900
O	2.81129400	-1.64815100	-0.09607800
O	1.54571400	3.05004900	-0.36691400
O	0.84254800	-0.06658300	-0.32897300
C	3.70669300	-0.79371300	0.51771900
C	3.63598400	0.60597000	0.44832900
C	4.70037800	-1.43283900	1.27218100
C	4.56674400	1.35874300	1.16037000
H	2.86720500	1.13382400	-0.11027900
C	5.62611600	-0.67963600	1.97989500
H	4.73034900	-2.51744300	1.28698200
C	5.54524900	0.71518700	1.92090000
H	4.51998300	2.44057600	1.12744700
H	6.40189100	-1.15087800	2.57043800
C	0.43878400	3.13203200	-0.96419500
C	0.06981000	2.24571200	-2.06018900
C	-0.57468500	4.10644700	-0.58679000
C	-1.20470100	2.21543200	-2.56207500
H	0.83857800	1.58551700	-2.44711300
C	-1.84416400	4.07989800	-1.10586100
H	-0.29380500	4.84188900	0.16226900
C	-2.20435700	3.08897900	-2.05636200

H	-1.47413800	1.53981100	-3.36494700
H	-2.60243500	4.78171500	-0.77675000
N	6.50730700	1.51408300	2.68511300
O	7.35115500	0.91364600	3.36091500
O	6.42431000	2.74274400	2.62045300
N	-3.54480700	2.90907800	-2.42435900
O	-4.41689100	3.72576100	-2.03649900
O	-3.86819300	1.87775700	-3.08286900
O	0.00065300	-4.49718300	-1.77751800
H	0.85275100	-4.82039100	-1.44405600
C	-1.61231100	-3.56085800	-3.85815300
H	-2.50456100	-3.16462400	-4.35479300
H	-0.81432700	-3.62400500	-4.60604800
H	-1.82327600	-4.57399900	-3.50505900
C	-1.01906400	-1.20732900	-3.25523400
H	-1.93253700	-0.88301500	-3.76455200
H	-0.78683600	-0.47177600	-2.48417500
H	-0.19667600	-1.17054100	-3.97503700
C	-0.99862400	2.12655900	2.12254200
H	-0.82681000	1.28472800	2.80704500
H	-0.15294100	2.17981400	1.42613100
H	-1.00742600	3.04831500	2.70821100
C	1.20591000	-1.20862600	2.81253900
H	2.18998800	-1.65474500	2.97753900
H	1.28924900	-0.49449400	1.99190500
H	0.93241700	-0.65409700	3.71992200

### 3-RC<sub>LB</sub>

Zn	-1.55696100	-0.41475000	-0.40208500
N	-2.63042800	-0.57645700	-2.42560700
N	-3.73895600	-0.47886100	0.10638100
N	-1.95526500	1.39267100	0.82043200
C	-2.16169800	-0.34474700	-3.67677600
C	-2.94273500	-0.64496100	-4.80245500
H	-2.53682100	-0.45435000	-5.79020800
C	-4.21896600	-1.17083200	-4.64741800
H	-4.83264400	-1.40033500	-5.51386400
C	-4.70094500	-1.38325100	-3.35823100
H	-5.69651600	-1.77894400	-3.18298900
C	-3.87375300	-1.08312800	-2.27992900
C	-4.33796100	-1.38448800	-0.87133500
H	-5.43859900	-1.38430000	-0.82249500
H	-3.99117100	-2.39153300	-0.62826400
C	-4.17761200	0.91625000	-0.05350600

H	-5.18321400	1.07523800	0.36918100
H	-4.24009200	1.13366800	-1.12509600
C	-3.19331500	1.87697400	0.59817300
C	-3.56038800	3.16566200	0.96867300
H	-4.56623900	3.52626100	0.77508700
C	-2.60862200	3.96900200	1.60217100
H	-2.84807900	4.98873000	1.88907500
C	-1.35981700	3.43499800	1.89906500
H	-0.61979900	4.02440900	2.43009600
C	-1.05658500	2.12145100	1.51300900
C	-3.86915900	-0.91450300	1.51927400
H	-4.92340600	-0.81958200	1.83002700
H	-3.30287900	-0.18216000	2.09617800
C	-3.37662600	-2.33277000	1.93091300
C	-3.00452700	-2.21641700	3.43636600
H	-3.85168900	-1.84073000	4.02639900
H	-2.15382600	-1.54028200	3.57321800
H	-2.72382000	-3.19603900	3.83705300
C	-4.52558400	-3.37113000	1.83331200
H	-4.89329000	-3.50700500	0.81236700
H	-5.37263300	-3.06897600	2.46131500
H	-4.18168200	-4.34883300	2.18706600
C	-2.16403900	-2.87760600	1.20051300
H	-1.88331300	-3.90864300	1.42634800
N	-1.35381900	-2.22892100	0.41211100
O	2.69240700	6.18381100	2.13288600
N	1.75988600	5.78784500	1.42949600
C	1.98048600	4.62228500	0.57505900
O	0.63423900	6.30478900	1.42127100
C	3.14147400	3.86079500	0.74358100
C	1.00208400	4.27594700	-0.36290200
C	3.29812600	2.70083300	-0.00734700
H	3.88464200	4.16718400	1.46970600
C	1.17174200	3.12429700	-1.11719900
H	0.12272600	4.89700600	-0.47649800
C	2.30161300	2.31676700	-0.91544500
H	4.16821600	2.06475500	0.11206900
H	0.42293300	2.80760000	-1.83168300
O	2.45950900	1.15712800	-1.61737300
P	1.55515000	-0.21269100	-1.27812700
O	0.15656800	0.34021900	-0.97652300
O	1.83671200	-1.20259200	-2.34224800
O	2.15906000	-0.58823700	0.20744300
C	3.04986800	-1.60957800	0.45582500

C	2.80900500	-2.91920000	0.02407100
C	4.17352300	-1.28830200	1.22445700
C	3.71850200	-3.91359300	0.36435300
H	1.91331400	-3.13722500	-0.54199800
C	5.08020600	-2.28280600	1.57067300
H	4.31555600	-0.26176300	1.54619900
C	4.84197800	-3.58777600	1.13167300
H	3.56087600	-4.93821700	0.05146500
H	5.95886300	-2.06458200	2.16461700
N	5.79220700	-4.64204100	1.49469900
O	6.76806300	-4.33260300	2.18785500
O	5.57264000	-5.78849900	1.09227600
O	-0.29332900	-2.81511400	-0.07802000
C	0.23483700	1.47223600	1.92111500
H	0.28128500	0.43005100	1.60831500
H	1.09236300	1.98961600	1.48581700
H	0.33902600	1.52373900	3.01186800
C	-0.79152700	0.23674100	-3.85220800
H	-0.63577700	1.07575300	-3.17141200
H	-0.02021100	-0.50498000	-3.61659300
H	-0.64620500	0.57264700	-4.88253000
3-TS <sub>LB</sub>			
Zn	1.79921600	-0.34201000	-0.00758700
N	2.06974900	-0.99688800	1.97863700
N	3.78057400	-1.37656400	-0.12573100
N	3.04011000	1.30486100	-0.37595800
C	1.35513600	-0.57175600	3.04526200
C	1.48667900	-1.22510100	4.27870400
H	0.89837300	-0.88061400	5.12233300
C	2.36194300	-2.29573300	4.40705100
H	2.47045800	-2.80590800	5.35978200
C	3.11229800	-2.70138000	3.30083500
H	3.81724800	-3.52431000	3.36553500
C	2.92701800	-2.03153900	2.09922100
C	3.63491800	-2.48090800	0.83234500
H	4.59851100	-2.95371000	1.07648800
H	2.99973700	-3.23620300	0.36752800
C	4.70357800	-0.33116900	0.35080800
H	5.74928000	-0.57953900	0.11500700
H	4.62105700	-0.28103300	1.44172900
C	4.35329500	1.03996200	-0.20258000
C	5.33381300	1.99287700	-0.44837100
H	6.38148400	1.74442800	-0.31132100
C	4.93647800	3.26525400	-0.86477300

H	5.67761400	4.03420200	-1.06271100
C	3.58263900	3.53652800	-1.02589600
H	3.24244900	4.51597600	-1.34427200
C	2.63358600	2.53459900	-0.77995000
C	4.11539800	-1.74089600	-1.52392600
H	5.17804600	-2.02904300	-1.58353200
H	4.01188400	-0.80701000	-2.08599200
C	3.30617500	-2.84109800	-2.26345200
C	3.51066900	-2.56001900	-3.77891900
H	4.57936600	-2.54855500	-4.02573500
H	3.07563300	-1.59635700	-4.06411400
H	3.03597900	-3.33958200	-4.38352100
C	3.86411700	-4.26146400	-1.98564800
H	3.77802000	-4.56223900	-0.93901300
H	4.92197200	-4.31162800	-2.26806100
H	3.32516600	-5.00355100	-2.58420900
C	1.81330300	-2.84329400	-2.02638300
H	1.23074000	-3.58955500	-2.57174900
N	1.18463000	-2.00774500	-1.28711500
O	-1.30155700	6.02063300	-1.55068200
N	-1.42325400	5.73958700	-0.34072900
C	-1.77118300	4.39773600	0.01951500
O	-1.22237200	6.57409500	0.56205200
C	-2.06148100	3.45397900	-0.98546000
C	-1.75406600	4.00764900	1.37187400
C	-2.26239100	2.13231300	-0.65110800
H	-2.10220000	3.78195000	-2.01791900
C	-1.95814000	2.68357200	1.70419300
H	-1.55629500	4.75396400	2.13283900
C	-2.16343200	1.67896400	0.70486900
H	-2.45831700	1.39877500	-1.42432000
H	-1.93620600	2.36362600	2.74136300
O	-2.21522900	0.42641300	1.03665600
P	-0.99201700	-1.05518500	-0.08269500
O	-0.04302900	0.15120700	-0.31060500
O	-0.96467200	-1.91287700	1.13987200
O	-2.26513500	-1.09263500	-1.11899800
C	-3.58957700	-1.24048900	-0.79597700
C	-4.04266900	-1.78235000	0.41484500
C	-4.49036900	-0.84974700	-1.79395700
C	-5.40790800	-1.93500400	0.61539400
H	-3.32889500	-2.05348600	1.18196600
C	-5.85563700	-1.00298000	-1.59438800
H	-4.10160900	-0.43064400	-2.71575900

C	-6.30284100	-1.54813800	-0.38786600
H	-5.78862100	-2.34656400	1.54190400
H	-6.57119700	-0.70664300	-2.35111400
N	-7.73835500	-1.71957200	-0.17201400
O	-8.50985100	-1.37138700	-1.07341900
O	-8.11333200	-2.20678200	0.90030500
O	-0.16863700	-2.14025900	-1.29542400
C	0.42689000	0.58586600	2.86796200
H	0.81760200	1.30446100	2.14205500
H	-0.53832600	0.23777100	2.47556900
H	0.25616900	1.09901500	3.81839700
C	1.16574400	2.78271200	-0.94279200
H	0.71616200	2.05921100	-1.62826000
H	0.63143100	2.64347800	0.00272000
H	0.96982200	3.79426200	-1.30397700
3-PC <sub>LB</sub>			
Zn	0.85614000	-0.68949300	0.27725300
N	1.66933200	-1.30015500	2.18448200
N	3.05344700	-0.38024800	-0.09097900
N	0.83688400	1.13496500	-0.76512800
C	0.94856800	-1.59031300	3.30132300
C	1.57408100	-1.58548600	4.55715900
H	0.97899200	-1.80687400	5.43560200
C	2.92517100	-1.29018700	4.67209500
H	3.40339600	-1.25856600	5.64631200
C	3.66019600	-1.05197700	3.51287300
H	4.72465800	-0.84617500	3.54827200
C	2.99956700	-1.08837400	2.29080800
C	3.79974400	-1.00946600	1.00650000
H	4.75165200	-0.48953000	1.18696100
H	4.04796100	-2.03110900	0.72215700
C	3.09791600	1.09827400	0.08571000
H	4.09018900	1.49699100	-0.16036700
H	2.91284500	1.33008300	1.13747700
C	2.03248600	1.76536000	-0.74235200
C	2.26314500	2.95633100	-1.41388400
H	3.21849400	3.45649100	-1.31325200
C	1.20725200	3.53155200	-2.11868600
H	1.34032200	4.48382000	-2.62072000
C	-0.01555100	2.87464500	-2.15618100
H	-0.85719700	3.29323100	-2.69620900
C	-0.18961100	1.67014800	-1.46351300
C	3.57659400	-0.71540400	-1.44228200
H	4.66608900	-0.55299000	-1.44532300



H	3.14739100	0.03154400	-2.11435700
C	3.32121000	-2.10000000	-2.10199200
C	3.95525900	-1.99743600	-3.51283900
H	5.03044700	-1.80862400	-3.43778200
H	3.50575300	-1.18964000	-4.09915400
H	3.82012600	-2.93217700	-4.06487900
C	3.97543600	-3.29794900	-1.36714100
H	3.46921400	-3.52911200	-0.42710700
H	5.03435000	-3.09575000	-1.17266100
H	3.91787800	-4.19717400	-1.98846500
C	1.86433900	-2.46804600	-2.28281000
H	1.60359800	-3.15207400	-3.09338500
N	0.95294200	-2.09928000	-1.47507300
O	1.76576600	5.20791200	0.51676700
N	1.91338300	4.20483900	1.24369800
C	0.78164600	3.46726600	1.64948400
O	3.05506700	3.78248600	1.56420500
C	-0.49295900	3.74470500	1.09483600
C	0.92926000	2.38784400	2.54928500
C	-1.55091800	2.90338400	1.32993600
H	-0.59247300	4.61129400	0.45162300
C	-0.12995600	1.55173100	2.80104500
H	1.88457600	2.24936300	3.04478300
C	-1.41754300	1.69913500	2.13464400
H	-2.52354600	3.09332200	0.88510200
H	-0.03782700	0.76410900	3.53729100
O	-2.33316300	0.84210400	2.24176600
P	-1.15798600	-2.79402800	-0.30412800
O	-0.94484500	-1.43558100	0.37281100
O	-0.77210600	-4.05843700	0.36124900
O	-2.67489300	-2.84936700	-0.88970300
C	-3.52151200	-1.75284600	-0.97049400
C	-3.76629900	-0.93051200	0.13268100
C	-4.14648000	-1.52736400	-2.20013200
C	-4.60579800	0.16804000	-0.01280700
H	-3.24683800	-1.07336500	1.06963100
C	-5.00849800	-0.44570200	-2.34074200
H	-3.93864800	-2.19541700	-3.02837900
C	-5.21753700	0.39563200	-1.24541800
H	-4.74008600	0.85335700	0.81377900
H	-5.50543700	-0.23428900	-3.27895500
N	-6.08258400	1.57043600	-1.40987100
O	-6.62105000	1.73830000	-2.50685100
O	-6.21529500	2.32522500	-0.44669900

O	-0.31462500	-2.61228300	-1.78568000
C	-0.50573600	-1.93583500	3.19396700
H	-1.09815100	-1.10874600	2.78600000
H	-0.63739900	-2.79480200	2.53099400
H	-0.89586600	-2.18621300	4.18289400
C	-1.49479900	0.94239000	-1.46498800
H	-1.38864500	-0.03789000	-1.93785500
H	-1.83077200	0.76717300	-0.44259400
H	-2.26094500	1.50674200	-1.99859200