

Supplementary Information

Mechanism of Zn(OTf)₂ Catalyzed Hydroamination-Hydrogenation of Alkynes with Amines: Insight from Theory

Riffat Un Nisa, and Khurshid Ayub*^[a]

^a *Department of Chemistry, COMSATS Institute for Information Technology, Campus
Abbottabad, Abbottabad, Pakistan*

Fax = +92-992-383441 khurshid@ciit.net.pk

[a] Riffat Un Nisa, and Khurshid Ayub*
Department of Chemistry, COMSATS Institute of Information
Technology, Abbottabad 22060, Pakistan
E-mail: Khurshid@ciit.net.pk

Table 1. Total electronic, zero-point corrected and Gibbs free energies of the optimized geometries

Structure No.	Total Electronic Energy	Zero Point Corrected Energy	Gibbs Free Energy
4	-3701.964753	-3701.982249	-3702.031878
NH ₂ Ar	-287.493477	-287.499273	-287.528424
5	-3989.499094	-3989.523898	-3989.585157
TS5-6	-3989.446278	-3989.471006	-3989.531165
6	-3989.450539	-3989.475363	-3989.535155
Alkyne	-116.599877	-116.603859	-116.627038
OTfH	-961.958296	-961.966174	-961.999373
7	-3144.077357	-3144.098611	-3144.152667
TS7-8	-3145.18969	-3145.210749	-3145.264746
8	-3145.288175	-3145.308481	-3145.360149
TS8-9	-3145.256094	-3145.27568	-3145.326364
9	-3145.305039	-3145.325317	-3145.378771
10	-4107.354139	-4107.383063	-4107.447308
11	-4106.106631	-4106.137214	-4106.207062
TS11-12	-4106.029575	-4106.059366	-4106.125487
12	-4106.142856	-4106.171308	-4106.234686
TS12-13	-4106.054956	-4106.083539	-4106.148083
13	-4106.171121	-4106.200219	-4106.265323
14	-3818.609946	-3818.609946	-3818.667868
TS14-15	-4106.078613	-4106.107862	-4106.173494
15	-4106.11205	-4106.140263	-4106.204987
TS15-16	-4106.05447	-4106.08303	-4106.148133
16	-4106.15205	-4106.180482	-4106.244881
H ₂	-1.166005	-1.168366	-1.179853
17	-4106.15401	-4106.18315	-4106.248467
TS17-18	-4107.256221	-4107.286359	-4107.355126
18	-4107.312339	-4107.342536	-4107.4096
TS 17-19	-4107.272291	-4107.300975	-4107.365139
19	-4107.305637	-4107.334762	-4107.400248
TS17-20	-4107.284802	-4107.314593	-4107.38294
20	-4107.312339	-4107.342536	-4107.4096
TS 20-21	-4107.289092	-4107.318219	-4107.38349
21	-4107.354139	-4107.383063	-4107.447308

Cartesian Coordinates of the optimized geometries

4

Zn 0.00010000 -0.50086500 0.00004200

O -1.77075200 -1.32511600 -0.46242600

S	-2.51026100	-0.48046600	0.57883500
O	-3.41923100	-1.15311100	1.48392300
O	-1.37758000	0.35560000	1.18220900
C	-3.49866900	0.74185800	-0.43277000
F	-2.67041900	1.38345400	-1.26040200
F	-4.41600300	0.08624100	-1.13371700
F	-4.08140500	1.61177900	0.38373500
O	1.37794800	0.35327200	-1.18346000
S	2.51055600	-0.48145600	-0.57808900
O	1.77075300	-1.32440100	0.46435100
O	3.42009900	-1.15544400	-1.48161500
C	3.49826900	0.74278600	0.43192200
F	4.41511600	0.08837000	1.13463700
F	2.66946400	1.38583000	1.25788000
F	4.08155300	1.61126100	-0.38568500

NH₂Ar

N	2.33564200	-0.00003400	-0.07684500
C	0.93909500	-0.00004800	-0.00976500
C	0.22128900	-1.20821400	-0.00510900
C	0.22135200	1.20817600	-0.00512300
C	-1.17150000	-1.20230800	0.00328600
H	0.76276600	-2.15124600	-0.01270400
C	-1.17141800	1.20236200	0.00333000

H	0.76293600	2.15115000	-0.01274900
C	-1.88125200	0.00003900	0.00809500
H	-1.70528000	-2.14875800	0.00858500
H	-1.70514300	2.14884000	0.00866800
H	-2.96650200	0.00006100	0.01629400
H	2.77819600	-0.83562700	0.28098300
H	2.77813800	0.83578100	0.28054900

5

Zn	-0.12753000	-0.10419700	-0.11671200
N	-0.35579700	1.85609200	-0.63106600
O	1.36140000	-0.96579200	-1.22879800
S	2.33789800	-1.03508200	-0.05796900
O	3.69006400	-0.55595900	-0.29252000
O	1.55592600	-0.44455400	1.09896700
C	2.45740900	-2.85600600	0.33001700
F	1.23422000	-3.34819900	0.53094000
F	3.02900100	-3.48677100	-0.69357200
F	3.19168200	-3.02299700	1.42784900
C	0.70865400	2.79403700	-0.31053900
C	1.92744700	2.69364100	-0.98252000
C	0.51753500	3.75189000	0.68370600
C	2.96008800	3.57160800	-0.65697800
H	2.07411500	1.92901200	-1.74004700
C	1.55967500	4.62249800	1.00555000
H	-0.43462400	3.82080700	1.20386100

C	2.77987600	4.53679700	0.33541800
H	3.90952200	3.49082300	-1.17599700
H	1.41192700	5.36858800	1.77986500
H	3.58841000	5.21497100	0.58818900
O	-1.63364100	-1.01327300	0.77257200
S	-2.69893500	-0.99283600	-0.33144000
O	-2.06246100	-0.30779700	-1.49801500
O	-3.42999600	-2.23057000	-0.53419100
C	-3.92198600	0.25090000	0.32495000
F	-4.85719000	0.49645900	-0.58872300
F	-3.27525200	1.41009300	0.59763100
F	-4.48723100	-0.18984200	1.44235300
H	-0.51182300	1.81233100	-1.63953200
H	-1.24404400	2.16608800	-0.23699900

TS 5-6

Zn	0.40317700	0.28863900	-0.03002500
N	-0.77464100	1.33995800	0.95182300
O	-3.03773300	-0.72462500	0.00528700
S	-2.04767600	-1.75533300	-0.69256900
O	-2.75922000	-2.55487500	-1.66010000
O	-0.79708700	-1.06183100	-1.09088600
C	-1.59057100	-2.84228800	0.76461700
F	-0.99272400	-2.09183600	1.69091600
F	-2.68850200	-3.39128600	1.26271300
F	-0.75696600	-3.77754700	0.33216200

C	-1.78635800	2.16850500	0.48531000
C	-2.13441100	2.18468600	-0.88614800
C	-2.54443500	2.98467800	1.35715800
C	-3.18481700	2.97590500	-1.35378300
H	-1.55430700	1.59439900	-1.59348100
C	-3.58497900	3.77124400	0.87723100
H	-2.29917000	2.99386700	2.41652100
C	-3.92118300	3.77412600	-0.48071600
H	-3.41809800	2.96805900	-2.41473600
H	-4.14357700	4.38941800	1.57475100
H	-4.73581600	4.38962600	-0.84715800
H	-2.63308400	0.17375600	0.12148900
H	-0.59349600	1.47114400	1.93920400
O	1.97380100	0.57460700	-1.31541500
S	2.90632000	-0.31090500	-0.50069900
O	2.02809900	-0.78219400	0.65099900
O	3.70020700	-1.30164100	-1.20349500
C	4.09239800	0.88902000	0.29430200
F	4.88847200	0.23349300	1.13553900
F	3.39803400	1.81200100	0.96872800
F	4.82146600	1.48293700	-0.64620000
6			
Zn	0.48118400	0.37075800	-0.08485800
N	-0.54063100	1.66834300	0.77899300
O	-3.12306000	-0.69054600	-0.39738900

S	-1.98965900	-1.72767800	-0.74381800
O	-2.44476000	-2.73610600	-1.67335300
O	-0.71985100	-1.01049400	-1.04303200
C	-1.73791200	-2.52667700	0.93079000
F	-1.32718600	-1.59706500	1.79558900
F	-2.87967700	-3.05793700	1.34359600
F	-0.80885900	-3.46464100	0.80312400
C	-1.75236300	2.16905800	0.39463800
C	-2.24935800	1.95768700	-0.92427000
C	-2.58680700	2.89681100	1.28292900
C	-3.48727600	2.49359200	-1.32768300
H	-1.58442600	1.53512900	-1.67626200
C	-3.81269300	3.39430700	0.87098800
H	-2.24394600	3.06945000	2.30001600
C	-4.28659200	3.19459300	-0.43590200
H	-3.81300600	2.34237200	-2.35320500
H	-4.41957600	3.94802000	1.58246500
H	-5.24815800	3.59075800	-0.74266800
H	-2.85916800	0.29305900	-0.55753500
H	-0.30029900	1.91337400	1.73171600
O	2.09165400	0.41144000	-1.35766300
S	2.96537400	-0.39905000	-0.41144100
O	2.04979900	-0.67217200	0.77319800
O	3.72412400	-1.50808700	-0.95980900
C	4.19473600	0.84041800	0.24385600

F	4.94057900	0.26987600	1.18726200
F	3.53580000	1.87999400	0.76852900
F	4.97182900	1.26569800	-0.74868500

Alkyne

C	0.00000000	0.00000000	1.42573600
H	0.00000000	0.00000000	2.49084200
C	0.00000000	0.00000000	0.21833400
C	0.00000000	0.00000000	-1.24105500
H	0.00000000	1.02177300	-1.63631100
H	0.88488100	-0.51088700	-1.63631100
H	-0.88488100	-0.51088700	-1.63631100

OTfH

O	1.25473000	1.09273100	-0.90331800
S	0.85286800	-0.14731900	0.07568800
O	1.21523000	-1.37585300	-0.59841400
O	1.26235500	0.18181600	1.43366500
C	-1.00852000	0.00965600	-0.00147400
F	-1.36233400	1.21972700	0.43554200
F	-1.42507900	-0.15520900	-1.25211900
F	-1.54159000	-0.92409600	0.78135000
H	1.50773000	1.84580400	-0.34057900

7

Zn	0.13249900	-0.02312300	-0.18376600
N	1.72097100	-0.87231500	-0.62108600
C	0.71158700	2.33482100	-0.30642700

C	1.82042300	2.62994700	-1.20605100
H	2.69726100	2.03552200	-0.92994100
H	1.55573000	2.41583700	-2.24492200
H	2.07206000	3.69205300	-1.12100200
H	1.67684500	-1.58218200	-1.34217300
O	-1.40436700	-0.57272000	1.16458500
S	-2.34331500	-0.96848900	0.03908200
O	-1.59799000	-0.56789800	-1.22168300
O	-2.94773400	-2.28829300	0.08110700
C	-3.74266800	0.25829900	0.16449000
F	-3.24596300	1.50789800	0.17114900
F	-4.41494500	0.05607600	1.29526100
F	-4.55901000	0.12234900	-0.87624100
C	3.01073600	-0.67119500	-0.16390800
C	3.27726700	0.17357300	0.93714100
C	4.11953700	-1.29604600	-0.77903800
C	4.57868200	0.38843800	1.38550500
H	2.44545800	0.64494600	1.45690400
C	5.41469200	-1.08192300	-0.31821100
H	3.94827700	-1.95546800	-1.62711200
C	5.66304800	-0.23395600	0.76447800
H	4.74248600	1.04148500	2.23900100
H	6.24132900	-1.58261600	-0.81575300
H	6.67508500	-0.06948200	1.11978200
C	-0.18562700	2.13452000	0.49278600

H	-1.00933500	2.09113800	1.17230700
---	-------------	------------	------------

TS 7-8

Zn	-0.08434700	0.35894200	0.15343900
----	-------------	------------	------------

N	1.61988900	0.33155800	-0.66869000
---	------------	------------	-------------

C	1.58810200	3.05429700	0.98022500
---	------------	------------	------------

C	2.38096200	2.76156900	0.06172300
---	------------	------------	------------

C	3.42421000	2.65032300	-0.93875500
---	------------	------------	-------------

H	3.98923900	1.71833800	-0.83075000
---	------------	------------	-------------

H	3.02107400	2.71134200	-1.95408900
---	------------	------------	-------------

H	4.12127300	3.48856200	-0.79845000
---	------------	------------	-------------

H	-0.04773800	1.42106300	1.46690500
---	-------------	------------	------------

H	1.41778100	3.88816300	1.64490600
---	------------	------------	------------

H	0.65260200	2.11128200	1.23255500
---	------------	------------	------------

H	1.65190300	0.49331100	-1.66981400
---	------------	------------	-------------

O	-1.42543200	-1.19208200	0.41643800
---	-------------	-------------	------------

S	-2.39639300	-0.64597200	-0.61884800
---	-------------	-------------	-------------

O	-1.73894900	0.63120900	-1.10587800
---	-------------	------------	-------------

O	-2.91747400	-1.56838900	-1.61301200
---	-------------	-------------	-------------

C	-3.85427200	-0.06263300	0.38737300
---	-------------	-------------	------------

F	-3.43775000	0.79163200	1.32881300
---	-------------	------------	------------

F	-4.44103800	-1.10671600	0.97012000
---	-------------	-------------	------------

F	-4.72669900	0.55386500	-0.40908800
---	-------------	------------	-------------

C	2.67119200	-0.47377400	-0.24718100
---	------------	-------------	-------------

C	2.78116100	-0.84983700	1.10988600
---	------------	-------------	------------

C	3.67703400	-0.91790500	-1.13267300
---	------------	-------------	-------------

C	3.82876700	-1.65141000	1.54767300
H	2.04173600	-0.48967200	1.82230700
C	4.72444000	-1.72161000	-0.68321000
H	3.60929900	-0.65371500	-2.18596200
C	4.81105900	-2.09702600	0.65727600
H	3.88203700	-1.92824300	2.59697600
H	5.47552800	-2.05838200	-1.39262500
H	5.62702900	-2.72256200	1.00426000

8

Zn	0.30728400	-1.57413000	-1.05602200
N	-1.60933200	-1.14869700	-0.19641200
H	-1.91342900	-3.60636900	2.14777900
C	-1.98929300	-3.07817400	1.20504600
C	-1.60607100	-1.80135600	1.10799200
H	-2.35845700	-3.63980300	0.35175900
C	-1.07763200	-0.98126300	2.24918800
H	-1.66119000	-0.06649700	2.38947900
H	-1.11843600	-1.56213800	3.17194700
H	-0.04051100	-0.68848700	2.06697500
H	0.16954600	-2.77951900	-2.01319500
O	1.73984700	-1.20560000	0.43629800
S	2.37578700	-0.05458800	-0.32057100
O	3.80461500	-0.11974300	-0.57713800
O	1.45060400	0.17919800	-1.49573000
C	2.11690400	1.42587500	0.78215800

F	0.81012300	1.56796400	1.05330600
F	2.77919200	1.25659600	1.92602600
F	2.55404900	2.52501800	0.16978400
C	-2.29502900	0.14851700	-0.27224200
C	-1.70115600	1.19771700	-0.96974700
C	-3.56129000	0.30253000	0.30007300
C	-2.38017300	2.41237400	-1.09158200
H	-0.71550000	1.07551000	-1.40472500
C	-4.22930600	1.51986100	0.18026500
H	-4.01485200	-0.52641100	0.83588000
C	-3.63991100	2.57699000	-0.51715700
H	-1.91621300	3.22979200	-1.63453500
H	-5.21126200	1.64007800	0.62761500
H	-4.16199600	3.52420200	-0.61078300
H	-2.09654800	-1.77762200	-0.83694500

TS 8-9

Zn	0.01827100	-1.09322300	-0.24979800
N	-1.68646100	-0.65706200	0.62305100
H	-2.64091600	-3.06130200	1.81478000
C	-1.81129600	-3.05028600	1.09614800
C	-2.05748000	-1.89731200	0.13777900
H	-1.77727800	-4.01002700	0.57545300
C	-3.25437100	-2.09136200	-0.77216700
H	-3.34115900	-1.29128800	-1.50818900
H	-3.17751100	-3.05229300	-1.28467600

H	-4.16939800	-2.10278200	-0.16991700
H	-0.92216100	-2.34350300	-0.92182800
O	1.89830800	-1.32326000	0.57260300
S	2.52787100	-0.39031700	-0.44948200
O	3.73732900	-0.82231800	-1.12475000
O	1.34185400	0.03632600	-1.31290300
C	2.95232300	1.14718600	0.52119500
F	3.88170500	0.85600800	1.42708100
F	3.40757200	2.08235300	-0.30895700
F	1.85366600	1.59550100	1.13633200
C	-2.37670000	0.52286500	0.26959700
C	-3.73786400	0.70616400	0.57946900
C	-1.67910300	1.59679100	-0.31065900
C	-4.38037400	1.90481100	0.27931900
H	-4.27974300	-0.08723500	1.08411100
C	-2.32460000	2.79704100	-0.60236500
H	-0.61894600	1.48980800	-0.52371700
C	-3.68081800	2.95681000	-0.31666400
H	-5.43122200	2.02330600	0.52832700
H	-1.76219100	3.60884200	-1.05442000
H	-4.18341700	3.89225600	-0.54166200
H	-0.88960400	-2.91157900	1.66642400
9			
Zn	0.03064600	-0.01680600	-0.39230500
N	-1.64702100	-0.69481200	-0.19172800

H	-3.01534000	-2.57633000	1.55864500
C	-2.05413200	-2.82835900	1.10520200
C	-1.84471900	-2.15625100	-0.26494300
H	-2.01216600	-3.91785900	0.99940400
C	-2.89941700	-2.57362100	-1.30291100
H	-2.66323800	-2.13826700	-2.27834400
H	-2.91085700	-3.66355200	-1.40705600
H	-3.90670700	-2.25304200	-1.02847200
O	1.82632500	-0.66386700	-1.16526300
S	2.55588700	0.55476900	-0.61787400
O	3.44363700	1.28443000	-1.50160700
O	1.43014000	1.33428900	0.06784000
C	3.57814100	-0.10254900	0.79932000
F	4.51985000	-0.91059200	0.32376400
F	4.13519000	0.91280600	1.45021600
F	2.78023900	-0.78354800	1.62890600
C	-2.66792800	0.23015200	0.04813700
C	-3.94146800	-0.06913300	0.57592700
C	-2.40718100	1.58888800	-0.24404200
C	-4.87750800	0.94081200	0.80440700
H	-4.20450200	-1.08744600	0.82617400
C	-3.33448600	2.59146000	0.00380900
H	-1.45293300	1.85745400	-0.70308100
C	-4.58972600	2.27650400	0.53115000
H	-5.84678200	0.66886700	1.21402000

H	-3.08136800	3.62078800	-0.23390800
H	-5.32398400	3.05328800	0.71718700
H	-1.26744400	-2.52354800	1.80272900
H	-0.88687300	-2.54301700	-0.64014300
10			
Zn	-0.22549500	-0.37100000	0.00435800
N	0.59306600	1.23301700	0.94628100
C	-0.75258800	0.79402200	2.98093400
C	-0.20914700	1.88826900	2.06285700
H	-1.19877000	1.24957400	3.86928200
C	-1.30439000	2.79334100	1.50916300
H	-2.00532500	2.23653100	0.88368700
H	-1.86573800	3.22221600	2.34417200
H	-0.89336400	3.61786500	0.92313200
H	0.03544400	0.11035300	3.31195100
H	-1.53121900	0.20531500	2.48544000
H	1.33767400	0.71803300	1.42367600
O	-1.93108000	-1.46544000	0.38750900
O	1.09869400	-1.42956800	-1.06275300
S	-2.69630200	-0.91494500	-0.80695200
O	-3.19544200	-1.85788300	-1.79153500
O	-1.82875500	0.23194900	-1.28899500
C	-4.20181400	-0.10894100	-0.05660700
F	-4.82826800	0.61342200	-0.98303400
F	-5.01837900	-1.04768300	0.41197300

F	-3.83695000	0.69605400	0.95343100
S	1.79848600	-2.19478600	0.06252400
O	1.24983600	-1.62342400	1.33773400
O	1.88124700	-3.63670800	-0.08942500
C	3.54531900	-1.55159900	-0.02011000
F	3.54012100	-0.22017300	0.17927900
F	4.28016400	-2.12298400	0.93346000
F	4.07807900	-1.80848500	-1.21077700
H	0.50539500	2.50601700	2.62322900
C	1.24779100	2.18981800	0.05142400
C	2.46448900	2.76488200	0.42694100
C	0.65549600	2.52350900	-1.16790100
C	3.09202500	3.67506900	-0.42258600
H	2.92660700	2.49252000	1.37218400
C	1.28734600	3.43991700	-2.01033900
H	-0.29112900	2.07896600	-1.45790900
C	2.50321500	4.01573500	-1.64150100
H	4.04204600	4.11278000	-0.13260000
H	0.82760600	3.69506500	-2.95973800
H	2.99387500	4.72242900	-2.30328300

11

Zn	-0.31378100	-0.48454500	-0.22190900
N	-0.23937700	1.31627400	0.70304600
H	0.16397200	1.22311200	1.64306600
C	0.74635000	1.71218000	3.86550500

C	1.03807200	0.54029100	3.95824100
C	1.39241300	-0.87038600	4.08493600
H	1.53979200	-1.33049600	3.10316300
H	2.31764900	-0.98073700	4.66008400
H	0.60275200	-1.42198200	4.60547600
O	-1.95962100	-1.60700400	0.21652700
O	1.02885000	-1.19623500	-1.54969500
S	1.87485700	-1.96463500	-0.53863900
S	-2.90527000	-0.93407900	-0.77061100
C	-4.06573400	0.01663600	0.33496600
C	3.51848400	-1.08581200	-0.57111300
F	3.33926400	0.21891200	-0.32952000
F	4.31052900	-1.59804200	0.37147500
F	4.08568100	-1.23770900	-1.76436500
F	-4.79350500	-0.81490000	1.07141400
F	-3.34532900	0.80812800	1.16404800
F	-4.86374600	0.78949700	-0.39721700
O	-2.07424900	0.13692800	-1.42904200
O	-3.73311200	-1.79318800	-1.59695500
O	2.14779500	-3.36270500	-0.81935600
O	1.26836500	-1.59981200	0.79741700
H	-1.22054100	1.56623200	0.83228800
H	0.50687000	2.75113400	3.85947000
C	0.43852300	2.37652800	-0.03260300
C	1.70023900	2.80666500	0.37747300

C	-0.17579000	2.92885600	-1.15861200
C	2.35085000	3.80601100	-0.34757500
H	2.16667300	2.36610000	1.25343400
C	0.48346600	3.92954700	-1.87174700
H	-1.15038000	2.57108800	-1.47704600
C	1.74547500	4.37108800	-1.47001600
H	3.33270500	4.14199100	-0.02899400
H	0.00728600	4.36035100	-2.74685700
H	2.25452400	5.14860600	-2.03054300

TS 11-12

Zn	-0.19384400	-0.33886700	-0.08268900
N	0.08418100	1.31081200	0.91243400
H	0.16782800	1.37043100	1.91917500
H	-1.47348900	0.56281900	2.24002400
C	-1.22859700	-0.09303400	3.10419400
C	-0.03618500	-0.50842200	3.31433800
H	-2.07830400	-0.36219900	3.73692400
C	1.20896700	-1.11820800	3.68314200
H	1.68074800	-1.55962200	2.79383700
H	1.88685400	-0.41803900	4.18005100
H	0.99815200	-1.95498400	4.37231500
O	-1.87051200	-1.46451500	0.30356300
O	1.16902700	-0.92353000	-1.49025600
S	1.98010500	-1.88206700	-0.63613000
S	-2.68733000	-0.95879700	-0.88068500

C	-4.00091500	0.08424900	-0.06770800
C	3.57920400	-0.96955400	-0.34878000
F	3.32731600	0.22961100	0.19729900
F	4.34543500	-1.66912200	0.49458900
F	4.22682900	-0.79722900	-1.49818300
F	-4.78958500	-0.68223900	0.68844900
F	-3.42671700	1.01334500	0.72059000
F	-4.73382500	0.70092800	-0.99154100
O	-1.79272900	0.02653100	-1.57615600
O	-3.39649900	-1.95165900	-1.67008100
O	2.33927100	-3.16237900	-1.22204300
O	1.30725900	-1.86852000	0.71153400
C	0.59950500	2.43658600	0.31604400
C	0.65678300	2.53425300	-1.09824400
C	1.05201800	3.54185000	1.08209700
C	1.13308600	3.68659600	-1.70479900
H	0.30761500	1.70701700	-1.70751200
C	1.53323800	4.68518800	0.46216900
H	1.02145600	3.47992400	2.16752600
C	1.57712200	4.76824100	-0.93485900
H	1.16183500	3.74401300	-2.78845200
H	1.87764500	5.51892000	1.06678800
H	1.95434700	5.66432900	-1.41687500
12			
Zn	-0.09418200	-0.58094000	0.05630700

N	-0.38988000	1.33764200	0.71445400
H	-0.85460400	1.32109700	4.09796800
C	-1.06860500	1.30201400	3.03619900
C	-0.08454900	1.45563600	2.14830900
H	-2.09686100	1.12347000	2.73945300
C	1.35771400	1.68588100	2.48788400
H	1.98777600	0.88727700	2.08698600
H	1.71966600	2.63323800	2.07622000
H	1.48137200	1.71088700	3.57158100
O	-1.69042200	-1.75950600	0.50001000
O	1.38370700	-1.27533100	-1.17751400
S	-2.54314400	-1.40128300	-0.71299100
S	2.20008700	-1.92071100	-0.06056300
O	-3.11484000	-2.49981800	-1.47041100
O	-1.76024800	-0.33867200	-1.43315400
O	2.57261600	-3.31452500	-0.21797300
O	1.48106000	-1.49719800	1.20092600
C	3.78968600	-0.94621600	-0.05626600
C	-3.98124000	-0.48109700	0.03504700
F	-3.51961600	0.58959100	0.72954200
F	-4.65404600	-1.26428800	0.87031500
F	-4.78975300	-0.03980600	-0.92298800
F	4.55787800	-1.34630600	0.95403600
F	3.51542100	0.36047700	0.09332700
F	4.43004700	-1.12520800	-1.20839500

H	-1.40836000	1.36025800	0.62662700
C	0.11398000	2.44273700	-0.12315500
C	-0.26676100	3.75211500	0.18137000
C	0.92435600	2.17572200	-1.22274000
C	0.17447700	4.80134300	-0.62239900
H	-0.89821800	3.94471200	1.04403000
C	1.36130700	3.23283600	-2.02475600
H	1.21772600	1.15938800	-1.46359900
C	0.98971200	4.54281700	-1.72705600
H	-0.12144400	5.81897500	-0.38748200
H	1.99057000	3.02406200	-2.88388200
H	1.33108100	5.36079900	-2.35360900

TS 12-13

Zn	-0.19099500	-0.55513600	0.05803100
N	-0.08438000	1.32426100	0.85156800
H	-0.78406000	0.71488500	3.94166400
C	-0.78057500	1.19044300	2.96293900
C	0.36694500	1.32874100	2.17987300
H	-1.52894800	1.97952000	2.85057400
C	1.80173200	1.29830600	2.58207500
H	2.46624600	1.46279900	1.73486500
H	2.01353700	2.02046500	3.37489500
H	2.01404900	0.29583800	2.97508600
O	-1.86866300	-1.50048600	0.74588400
O	1.18160800	-1.38121200	-1.19795800

S	-2.68951300	-1.29807500	-0.52406600
S	2.05398300	-2.00891800	-0.11733800
O	-3.36695500	-2.45894300	-1.07357300
O	-1.79145900	-0.48541500	-1.42250900
O	2.40882500	-3.40861800	-0.26903700
O	1.42338900	-1.55564800	1.17658800
C	3.64944200	-1.05009900	-0.23610300
C	-4.02851900	-0.11263800	0.00424000
F	-3.47421000	1.01443000	0.48563900
F	-4.77458400	-0.66657500	0.95768100
F	-4.79233200	0.19750900	-1.04036700
F	4.43818800	-1.36060200	0.79279500
F	3.39281000	0.26979800	-0.20166400
F	4.26647600	-1.33868200	-1.37771800
H	-1.21965600	1.01997100	1.60308800
C	0.36099700	2.35986700	-0.04058700
C	0.43474100	2.11139000	-1.41744100
C	0.67159200	3.63449600	0.45326300
C	0.84747900	3.12104900	-2.28292900
H	0.16908700	1.13917700	-1.81951100
C	1.09653800	4.63596100	-0.41758900
H	0.56397500	3.84228600	1.51410100
C	1.18641200	4.38202100	-1.78706300
H	0.90481100	2.91902700	-3.34762000
H	1.34151800	5.61877700	-0.02692500

H	1.50663700	5.16580000	-2.46617800
13			
Zn	0.07031600	-0.57995000	-0.08064700
N	-0.12443200	1.17062700	0.86662300
H	0.85586500	-0.40732500	2.93289800
C	-0.14447500	0.03467200	2.99335000
C	-0.20465600	1.28132800	2.15190900
H	-0.37075700	0.24997900	4.03867000
C	-0.33829900	2.58891500	2.87639100
H	-0.26486400	3.45423800	2.22009700
H	-1.30221000	2.61370100	3.39850200
H	0.43488100	2.64443600	3.65071100
O	-1.33109700	-2.01405300	0.43639300
O	1.66136900	-0.82413900	-1.30953500
S	-2.27891400	-1.68538000	-0.70872800
S	2.56174400	-1.55805100	-0.32056400
O	-2.82752100	-2.79285400	-1.47074600
O	-1.59977900	-0.55860300	-1.44647700
O	3.20189700	-2.77612200	-0.78505400
O	1.77384400	-1.58842600	0.96089700
C	3.93702500	-0.34114900	0.00164400
C	-3.72571300	-0.87316500	0.14312700
F	-3.28363400	0.11770000	0.94602000
F	-4.37771700	-1.76223800	0.88831700
F	-4.55258200	-0.35175300	-0.76019300

F	4.81141600	-0.86571400	0.85767100
F	3.43090500	0.78514200	0.54253300
F	4.55337900	-0.03096900	-1.13596200
H	-0.84983100	-0.71594000	2.62453600
C	-0.22507300	2.31794400	-0.00312500
C	0.92738100	2.83133000	-0.60427100
C	-1.48237900	2.85290100	-0.29928200
C	0.81709900	3.90767900	-1.48511000
H	1.89293500	2.39078500	-0.38394000
C	-1.57906400	3.92687600	-1.18373500
H	-2.36965000	2.41300400	0.14277000
C	-0.43194100	4.45875200	-1.77455500
H	1.71217900	4.31054500	-1.94860700
H	-2.55521300	4.34115700	-1.41583500
H	-0.51211500	5.29199100	-2.46545300

14

Zn	0.02185500	-0.00463100	0.12578300
C	0.15709300	1.94379200	1.20388900
C	-0.12873700	2.43646300	0.12644900
C	-0.47983300	3.03701500	-1.15370300
H	0.37467000	3.02500200	-1.83654100
H	-1.30744400	2.48897600	-1.61203900
H	-0.78592800	4.07521400	-0.99026200
O	-1.50111300	-1.17697600	0.76151900
O	1.54880400	-0.54822800	-1.09545000

S	-2.42834500	-0.89480100	-0.41724500
S	2.48404900	-0.99302600	0.02699000
O	-3.03943900	-2.03225400	-1.07873400
O	-1.65424900	0.10161400	-1.25374200
O	3.11747300	-2.29185400	-0.10352600
O	1.70496000	-0.68678300	1.28785800
C	3.84793200	0.27859100	-0.00593000
C	-3.81294000	0.10346000	0.33433400
F	-3.30218500	1.17009900	0.96578700
F	-4.48553300	-0.64215600	1.20521200
F	-4.63156600	0.52067200	-0.63027000
F	4.67634900	0.07054500	1.01476100
F	3.31750400	1.50543300	0.10149700
F	4.51530000	0.19053000	-1.15340700
H	0.45038700	1.69878100	2.20359900

TS 14-15

Zn	-0.91730600	-0.84985100	0.36990500
N	1.20269000	1.48017700	-0.28221800
C	-0.31174700	0.07285200	2.07027900
C	0.51960000	1.00814800	2.12922500
C	1.43629100	2.05331600	2.53090800
H	2.46245200	1.84301000	2.21850300
H	1.14331500	3.03313700	2.14559500
H	1.40697700	2.08832100	3.62942600
O	-2.85758500	-1.02996300	-0.09194100

O	0.52160000	-1.34916200	-1.04322400
S	-3.03238200	0.26434400	-0.88656800
S	0.75711700	-2.76135600	-0.51169000
O	-3.75089500	0.16778500	-2.14494700
O	-1.67839900	0.91584000	-0.86754000
O	0.80283900	-3.84022200	-1.48153200
O	-0.17456200	-2.87563500	0.66615600
C	2.46630400	-2.64350000	0.22638800
C	-4.07738500	1.31381400	0.24531500
F	-3.47684800	1.42526100	1.43961300
F	-5.27325800	0.75386600	0.41060800
F	-4.22166000	2.53039000	-0.28121100
F	2.77700000	-3.77608700	0.84908100
F	2.51106100	-1.62919300	1.10737700
F	3.35582200	-2.40106900	-0.73912000
C	2.34536500	2.27605400	-0.47834400
C	3.62137600	1.68910900	-0.42515400
C	2.23582400	3.66465900	-0.65112900
C	4.76014300	2.48110700	-0.55410000
H	3.70874500	0.61368000	-0.29272200
C	3.38271300	4.44675700	-0.77677600
H	1.25143900	4.12317900	-0.70366500
C	4.64988600	3.86269700	-0.72840800
H	5.73975000	2.01342800	-0.52156900
H	3.28278200	5.51865800	-0.92005500

H	5.53996500	4.47503100	-0.83023200
H	-0.80867500	-0.40731300	2.90899000
H	0.34267900	1.86869900	-0.65964600
H	1.31189500	0.52891000	-0.62627100

15

Zn	-0.69592100	-1.19462700	0.62326500
N	0.66941900	1.56574900	0.17548100
C	-0.16618200	0.14103600	1.94125500
C	0.40038700	1.31079500	1.66001900
C	0.73772400	2.46194800	2.55878800
H	1.80464200	2.70814300	2.54463800
H	0.19226800	3.37104600	2.27727400
H	0.45770600	2.20170100	3.58071700
O	-2.31582000	-1.21286400	-0.43287700
O	1.02819100	-0.98400600	-0.99774300
S	-2.87726500	0.10443600	-0.98341400
S	1.35698400	-2.42817800	-0.71676300
O	-3.52373400	-0.04114900	-2.27776600
O	-1.91514600	1.22048100	-0.80457300
O	1.62022900	-3.29977900	-1.84695100
O	0.33650500	-2.91059000	0.30006300
C	2.94436000	-2.32784000	0.25652400
C	-4.22280300	0.46529600	0.25256000
F	-3.70237900	0.51625600	1.48960400
F	-5.15140600	-0.48908600	0.21482200

F	-4.78629300	1.64308900	-0.02469000
F	3.24364500	-3.50932500	0.78631000
F	2.81520200	-1.42237600	1.24328900
F	3.93324500	-1.93183000	-0.54883300
C	1.68704400	2.55238200	-0.20007400
C	3.02880600	2.18231800	-0.12200900
C	1.29812900	3.81546200	-0.63500600
C	4.00333800	3.11115900	-0.48392600
H	3.30065300	1.18337200	0.20663500
C	2.28365800	4.73580600	-0.99601700
H	0.24530800	4.07389800	-0.70201600
C	3.63217100	4.38599400	-0.91805300
H	5.05154300	2.83532100	-0.43302700
H	1.99373800	5.72242900	-1.34229800
H	4.39475800	5.10413500	-1.20196300
H	-0.38589500	-0.00052900	2.99881000
H	-0.24911000	1.76271200	-0.26822900
H	0.94086600	0.65276800	-0.23411600

TS 15-16

Zn	-0.04590700	-1.08626100	0.15017300
N	0.93390200	2.06888900	0.67216100
C	-0.07610400	0.36346900	1.70453600
C	0.29393900	1.62741900	1.92684200
C	0.18979600	2.53628300	3.10532600
H	1.18437500	2.82871100	3.46298000

H	-0.34407700	3.45496000	2.83929000
H	-0.34238500	2.04706500	3.92292100
O	-1.76119200	-2.15858800	0.97458400
O	1.64000200	-0.48795200	-1.25967700
S	-2.51468300	-1.97495900	-0.31963400
S	2.40288200	-1.70064600	-0.80656800
O	-3.21751800	-3.10890300	-0.89212700
O	-1.54029200	-1.22324000	-1.22009300
O	3.04048600	-2.55168700	-1.79507400
O	1.49375500	-2.38599000	0.21129900
C	3.77754100	-1.00175300	0.24283500
C	-3.81182800	-0.69374300	0.07355200
F	-3.22894400	0.38582700	0.62623900
F	-4.69338600	-1.19334000	0.93747000
F	-4.43768200	-0.32241800	-1.04081100
F	4.40498500	-1.97107700	0.90039500
F	3.26653500	-0.13012200	1.13984500
F	4.64461900	-0.34766200	-0.52979800
C	0.40675300	3.19711000	-0.05167600
C	1.28366300	4.11506700	-0.63313400
C	-0.97571400	3.33610100	-0.21145500
C	0.77550200	5.17850200	-1.37826300
H	2.35711800	3.99604800	-0.50962100
C	-1.47212600	4.40789500	-0.95182000
H	-1.65239600	2.60594900	0.22033400

C	-0.60239800	5.33085700	-1.53585300
H	1.45979500	5.88846300	-1.83202400
H	-2.54482800	4.51476000	-1.07880200
H	-0.99619200	6.16058000	-2.11392900
H	-0.54161800	-0.27004800	2.45970600
H	0.51723600	0.73507000	0.49614000
H	1.95047700	2.11048300	0.74524400

16

Zn	0.47503100	-1.03722400	-0.41149000
N	-1.45809200	1.61071000	-1.01201300
C	-0.09258300	-0.01612200	-2.10636700
C	-0.30753400	1.29479600	-1.61095900
C	0.76781700	2.33812300	-1.71222400
H	0.34381800	3.34282900	-1.74840400
H	1.42837700	2.27080000	-0.84368500
H	1.36970800	2.15856100	-2.60395100
O	2.27749000	-1.62816800	0.15504200
O	-1.11012400	-0.99193400	0.97299500
S	2.81364000	-0.39826500	0.89176600
S	-1.57811600	-2.40170700	0.65949700
O	3.48387500	-0.65249700	2.15559400
O	1.72838300	0.62951900	0.83300800
O	-1.84702500	-3.29344600	1.77360000
O	-0.67037500	-2.87686500	-0.44593800
C	-3.22317800	-2.12510900	-0.17500600

C	4.11722600	0.23020800	-0.28195500
F	3.55843500	0.48038800	-1.48169300
F	5.08124400	-0.67264800	-0.43505200
F	4.63754400	1.36540700	0.18819000
F	-3.65427100	-3.24638700	-0.74115300
F	-3.09389300	-1.18227100	-1.14614000
F	-4.11974500	-1.68906100	0.70561200
C	-1.73566000	2.78231500	-0.22683200
C	-2.82524700	3.58355500	-0.57691800
C	-0.96381500	3.07290500	0.90232900
C	-3.13814100	4.69499200	0.20479200
H	-3.41467700	3.33807800	-1.45514700
C	-1.27962900	4.19429300	1.66954400
H	-0.14338800	2.41972100	1.18282000
C	-2.36347300	5.00368800	1.32461300
H	-3.98374900	5.32012100	-0.06411700
H	-0.68438700	4.42360300	2.54763300
H	-2.60829900	5.87010500	1.93104800
H	-0.98546600	-0.58577300	-2.36318100
H	-2.15339900	0.87187700	-0.96105500
H	0.70248800	-0.10220600	-2.84174600
17			
Zn	0.07031600	-0.57995000	-0.08064700
N	-0.12443200	1.17062700	0.86662300
H	0.85586500	-0.40732500	2.93289800

C	-0.14447500	0.03467200	2.99335000
C	-0.20465600	1.28132800	2.15190900
H	-0.37075700	0.24997900	4.03867000
C	-0.33829900	2.58891500	2.87639100
H	-0.26486400	3.45423800	2.22009700
H	-1.30221000	2.61370100	3.39850200
H	0.43488100	2.64443600	3.65071100
O	-1.33109700	-2.01405300	0.43639300
O	1.66136900	-0.82413900	-1.30953500
S	-2.27891400	-1.68538000	-0.70872800
S	2.56174400	-1.55805100	-0.32056400
O	-2.82752100	-2.79285400	-1.47074600
O	-1.59977900	-0.55860300	-1.44647700
O	3.20189700	-2.77612200	-0.78505400
O	1.77384400	-1.58842600	0.96089700
C	3.93702500	-0.34114900	0.00164400
C	-3.72571300	-0.87316500	0.14312700
F	-3.28363400	0.11770000	0.94602000
F	-4.37771700	-1.76223800	0.88831700
F	-4.55258200	-0.35175300	-0.76019300
F	4.81141600	-0.86571400	0.85767100
F	3.43090500	0.78514200	0.54253300
F	4.55337900	-0.03096900	-1.13596200
H	-0.84983100	-0.71594000	2.62453600
C	-0.22507300	2.31794400	-0.00312500

C	0.92738100	2.83133000	-0.60427100
C	-1.48237900	2.85290100	-0.29928200
C	0.81709900	3.90767900	-1.48511000
H	1.89293500	2.39078500	-0.38394000
C	-1.57906400	3.92687600	-1.18373500
H	-2.36965000	2.41300400	0.14277000
C	-0.43194100	4.45875200	-1.77455500
H	1.71217900	4.31054500	-1.94860700
H	-2.55521300	4.34115700	-1.41583500
H	-0.51211500	5.29199100	-2.46545300

TS 17-18

Zn	0.44367500	-0.87873300	-0.56724300
N	-0.74556200	2.34088300	-0.38466200
C	1.53914600	3.09590100	-0.48698800
C	0.10287300	3.25169900	-0.06535300
H	1.90881200	4.02764900	-0.93205200
C	-0.20884700	4.48887700	0.74421300
H	-1.20516700	4.46234100	1.18721000
H	0.53872300	4.60090700	1.53819100
H	-0.13084900	5.38183400	0.11076600
H	1.66752000	2.28109700	-1.20102600
H	2.16294400	2.87972800	0.38796000
H	-0.40491300	0.82690000	-1.46843900
H	-0.31990600	0.20257300	-1.94317900
O	2.24292400	-0.46288600	-0.71063900

O	-0.55874500	-2.58840300	-1.08345400
S	-1.31946300	-2.60737400	0.23770900
S	3.12973800	-0.43213700	0.58094400
O	-1.34192800	-3.83284800	1.00925700
O	-0.81161900	-1.33554800	0.92691200
O	2.63546100	0.57908800	1.51913400
O	3.43304300	-1.77698300	1.05667800
C	-3.08664700	-2.20581000	-0.22414000
C	4.68579400	0.25407200	-0.18370300
F	-3.62470500	-3.25287200	-0.83968400
F	-3.77219100	-1.92715700	0.88246700
F	-3.10207400	-1.14851700	-1.03816900
F	5.13979700	-0.56787300	-1.12772200
F	5.60605700	0.38577300	0.77205600
F	4.43978400	1.45360500	-0.72385800
C	-2.12980800	2.44659900	-0.07466300
C	-2.70750900	1.54362000	0.82856000
C	-2.94590500	3.36888400	-0.74605700
C	-4.08033000	1.58365100	1.07181600
H	-2.07848600	0.82118000	1.33899000
C	-4.31886200	3.39757500	-0.50053200
H	-2.50000800	4.04887400	-1.46671400
C	-4.89150200	2.50801400	0.41020200
H	-4.51571100	0.88202000	1.77801000
H	-4.94114500	4.11728800	-1.02571000

H	-5.96104200	2.53111200	0.59844700
18			
Zn	0.02695200	-2.17560300	-0.19778700
N	0.32908800	1.95271900	1.11432600
C	-0.40484600	0.91104300	3.15006400
C	-0.45746900	2.01214800	2.14514600
H	-0.37467200	1.33096200	4.15956400
C	-1.46255500	3.09907400	2.30775600
H	-1.23381000	3.98393300	1.71614500
H	-2.41041500	2.67766100	1.94497700
H	-1.58427400	3.36052900	3.36065000
H	0.44602100	0.24825800	2.98977300
H	-1.32105400	0.31415100	3.05404300
H	0.88661200	1.08649900	1.00546000
H	-0.08348800	-3.64993600	0.19304800
O	-1.26609500	-0.78910500	-0.74971900
O	1.39401300	-0.68649200	0.80188600
S	-2.41366600	-0.49655700	0.21490100
O	-2.75339900	0.93483200	0.24805100
O	-2.22989300	-1.17829200	1.50835900
C	-3.84790600	-1.34368200	-0.61482600
F	-4.94229400	-1.20656400	0.13830600
F	-4.06909500	-0.79695600	-1.81280200
F	-3.57937700	-2.64273000	-0.76850700
S	2.33106000	-0.68278300	-0.39914700

O	1.67412600	-1.52678800	-1.44711300
O	2.83859400	0.63388000	-0.77375400
C	3.79955300	-1.67684600	0.17117400
F	3.40663300	-2.89499500	0.54512800
F	4.67858000	-1.77846700	-0.82474800
F	4.37402900	-1.06135600	1.20868600
C	0.41334900	2.91101900	0.03196900
C	-0.16036000	2.58929600	-1.19739200
C	1.11215200	4.10246800	0.22926000
C	-0.03889100	3.50035900	-2.24658500
H	-0.69391800	1.65366700	-1.31845500
C	1.22060400	5.00406400	-0.82908200
H	1.57396500	4.31090300	1.18924100
C	0.64520200	4.70344500	-2.06486500
H	-0.48193700	3.26419300	-3.20852600
H	1.76246200	5.93379600	-0.68827100
H	0.73597600	5.40486700	-2.88833400

TS 17-19

Zn	-0.33497600	-0.32469500	-0.51370800
N	0.31057500	1.40251800	-1.01582900
C	0.90531400	1.55786900	-2.23168000
H	2.68043200	0.46385700	-1.69665200
H	2.23350900	1.11975600	-2.22099300
C	1.16923600	2.96568500	-2.75575300
H	1.62097500	3.61595000	-2.00884000

H	1.81204600	2.93355000	-3.63798700
H	0.20474800	3.39890800	-3.04595300
C	0.38344100	0.60954700	-3.30543100
H	0.39336000	-0.43342600	-2.97548200
H	-0.64813700	0.88421100	-3.54990500
H	0.98568100	0.67543200	-4.21401300
O	-2.05415400	-1.29222700	-1.17465200
O	3.19921200	-0.30333600	-0.84453900
S	-2.62105400	-1.38290300	0.23123500
S	2.59224400	-1.65962400	-0.48038100
O	-3.16799900	-2.65148600	0.67527100
O	-1.55477600	-0.72090100	1.09340000
O	3.33068200	-2.81613700	-0.95061000
O	1.10937500	-1.68621100	-0.75628000
C	-4.02627100	-0.15653000	0.23258900
C	2.67826200	-1.61030700	1.38504700
F	-4.49556500	-0.01035200	1.46886300
F	-3.58279400	1.02934300	-0.21346500
F	-4.99549500	-0.58725400	-0.57016700
F	1.91626500	-0.60054900	1.82393400
F	3.93353200	-1.42513600	1.77672800
F	2.21411700	-2.75729500	1.86900300
C	0.54543500	2.30969000	0.06182200
C	1.83044500	2.76674300	0.39754800
C	-0.54169800	2.69536700	0.86044600

C	2.01308000	3.60943100	1.49406100
H	2.68982800	2.44691000	-0.18200500
C	-0.34954400	3.53126100	1.95892800
H	-1.53537100	2.33783600	0.61081300
C	0.92665200	3.99777300	2.27863000
H	3.01359100	3.95313900	1.74017800
H	-1.20337100	3.82101000	2.56414300
H	1.07352100	4.65093100	3.13306000

19

Zn	-0.57336100	-0.16998100	0.52820300
N	-0.03180300	-1.96914100	0.48945500
C	-0.62963700	-2.93189600	1.42551600
C	-1.54745200	-3.92995900	0.70057000
H	-1.01515800	-4.45826500	-0.09495100
H	-1.94426300	-4.67573900	1.39807400
H	-2.39224200	-3.40175800	0.24551800
C	-1.40167800	-2.17298600	2.50734000
H	-0.74529800	-1.49113400	3.06107800
H	-2.22536100	-1.59401100	2.07306600
H	-1.84107200	-2.86433400	3.23195500
O	-2.21093400	0.86040500	1.16651800
O	3.20366700	-0.00349500	0.48635500
S	-2.50790900	1.46769000	-0.20200300
S	2.47057000	1.28266600	1.02715600
O	-2.83271500	2.88150700	-0.25762800

O	-1.38824600	0.94540200	-1.07789700
O	3.11467100	1.74420900	2.23465900
O	0.99979400	1.08912300	1.01106600
C	-4.01389600	0.53033800	-0.77691000
C	2.78171500	2.51347600	-0.34795000
F	-4.28963000	0.85808100	-2.03677400
F	-3.76661700	-0.78435800	-0.70537200
F	-5.05166900	0.82434900	0.00265800
F	2.31756600	1.99832600	-1.48822100
F	4.08566600	2.73617800	-0.45152600
F	2.14253100	3.63888700	-0.06300100
C	1.00243800	-2.34741300	-0.32444400
C	1.67244500	-3.60041900	-0.25373100
C	1.49270600	-1.42911600	-1.30607400
C	2.73290800	-3.89758100	-1.09974700
H	1.35420200	-4.34555100	0.46423900
C	2.54614900	-1.76656300	-2.17155600
H	0.91839200	-0.52739300	-1.51821800
C	3.19352800	-2.99157800	-2.06445400
H	3.21584100	-4.86665600	-1.00368400
H	2.85332700	-1.04531100	-2.92432300
H	4.01953100	-3.24643500	-2.71892600
H	2.64513500	-0.55417300	-0.17653600
H	0.17197300	-3.48970800	1.93218000

TS 17-20

Zn	-0.70577900	-0.17425800	0.55501200
N	0.05789700	1.59175500	0.97458200
C	0.82271500	0.82979900	3.13483500
C	0.72416300	1.86137600	2.05142600
C	1.45720100	3.14931700	2.27802600
H	1.30521500	3.87275100	1.47937200
H	1.15283100	3.58217700	3.23621300
H	2.52755800	2.92292100	2.35515900
O	-2.08058800	-0.24390500	-0.94587500
O	3.07092300	-0.51833600	1.34710000
S	-3.25570000	-0.49420500	-0.00738200
S	3.04635900	-0.57634000	-0.12511200
O	-4.44555900	0.31858200	-0.18858800
O	-2.61576500	-0.52765900	1.36931600
O	3.59687000	0.55792700	-0.87110700
O	1.66098400	-0.99639400	-0.65023100
C	4.08448400	-2.05209500	-0.58394700
C	-3.73784100	-2.26526300	-0.34013400
F	-2.66487200	-3.04829700	-0.19576500
F	-4.20296600	-2.37271600	-1.58153100
F	-4.67665300	-2.63627200	0.52749300
F	4.09587900	-2.21503400	-1.90771200
F	3.58418800	-3.15287400	-0.01161600
F	5.33484100	-1.86544600	-0.15267100
C	-0.07856100	2.54831200	-0.10484800

C	0.93570700	2.69908600	-1.05464100
C	-1.27966000	3.25520600	-0.21473200
C	0.74091300	3.58880800	-2.11294900
H	1.85321200	2.12334500	-0.97849700
C	-1.45694900	4.14240200	-1.27557200
H	-2.06348700	3.10985100	0.52250500
C	-0.44752700	4.31116900	-2.22508900
H	1.52562600	3.70849700	-2.85328400
H	-2.38754700	4.69449900	-1.36064600
H	-0.59099900	4.99737500	-3.05387900
H	0.84525800	1.30116300	4.12017900
H	-0.00887200	0.12086800	3.10545700
H	0.11853000	-1.61067000	0.89166400
H	0.76566700	-1.39822100	0.28823000
H	1.75805600	0.27493900	2.99205800

20

Zn	0.02695200	-2.17560300	-0.19778700
N	0.32908800	1.95271900	1.11432600
C	-0.40484600	0.91104300	3.15006400
C	-0.45746900	2.01214800	2.14514600
H	-0.37467200	1.33096200	4.15956400
C	-1.46255500	3.09907400	2.30775600
H	-1.23381000	3.98393300	1.71614500
H	-2.41041500	2.67766100	1.94497700
H	-1.58427400	3.36052900	3.36065000

H	0.44602100	0.24825800	2.98977300
H	-1.32105400	0.31415100	3.05404300
H	0.88661200	1.08649900	1.00546000
H	-0.08348800	-3.64993600	0.19304800
O	-1.26609500	-0.78910500	-0.74971900
O	1.39401300	-0.68649200	0.80188600
S	-2.41366600	-0.49655700	0.21490100
O	-2.75339900	0.93483200	0.24805100
O	-2.22989300	-1.17829200	1.50835900
C	-3.84790600	-1.34368200	-0.61482600
F	-4.94229400	-1.20656400	0.13830600
F	-4.06909500	-0.79695600	-1.81280200
F	-3.57937700	-2.64273000	-0.76850700
S	2.33106000	-0.68278300	-0.39914700
O	1.67412600	-1.52678800	-1.44711300
O	2.83859400	0.63388000	-0.77375400
C	3.79955300	-1.67684600	0.17117400
F	3.40663300	-2.89499500	0.54512800
F	4.67858000	-1.77846700	-0.82474800
F	4.37402900	-1.06135600	1.20868600
C	0.41334900	2.91101900	0.03196900
C	-0.16036000	2.58929600	-1.19739200
C	1.11215200	4.10246800	0.22926000
C	-0.03889100	3.50035900	-2.24658500
H	-0.69391800	1.65366700	-1.31845500

C	1.22060400	5.00406400	-0.82908200
H	1.57396500	4.31090300	1.18924100
C	0.64520200	4.70344500	-2.06486500
H	-0.48193700	3.26419300	-3.20852600
H	1.76246200	5.93379600	-0.68827100
H	0.73597600	5.40486700	-2.88833400

TS 20-21

Zn	0.03728400	-1.17084200	0.41166600
N	0.86245500	2.22537200	1.11698900
C	1.05456000	1.25868700	3.31572100
C	0.22799600	1.69573100	2.14185700
H	1.17269300	2.12741500	3.97926000
C	-1.25014200	1.86347400	2.30069700
H	-1.76062700	1.83401800	1.33706600
H	-1.63672500	1.06554200	2.93385300
H	-1.45812700	2.82171800	2.79351200
H	2.04500700	0.91209500	3.01744500
H	0.55248700	0.46651500	3.86816400
H	1.85041700	1.99591900	1.04144400
H	0.01202600	-0.35822200	1.74957400
O	-1.42714400	-2.17070000	-0.42466200
O	1.43304200	-0.52611900	-1.06161900
S	-2.44223500	-1.11912400	-0.88487800
O	-3.05560500	-1.38639200	-2.17777300
O	-1.87263800	0.22676100	-0.61383100

C	-3.79437700	-1.31522200	0.38034200
F	-4.75161800	-0.40755900	0.16214700
F	-4.32506800	-2.53561800	0.32049500
F	-3.29817500	-1.11950600	1.61619200
S	2.43154000	-1.62697500	-0.76147100
O	1.79690000	-2.46604700	0.30927600
O	3.07268200	-2.28666800	-1.88623700
C	3.79668200	-0.70072200	0.10979200
F	3.27135600	0.10015300	1.07820200
F	4.65086400	-1.53882700	0.68571900
F	4.44620600	0.08208700	-0.75184400
C	0.31369000	2.96890700	0.01030000
C	0.56623800	2.53133200	-1.29118700
C	-0.39396400	4.14909500	0.25485200
C	0.07384700	3.27986700	-2.35907500
H	1.10771700	1.60751900	-1.46184900
C	-0.88197800	4.88491800	-0.82319400
H	-0.54241500	4.49968900	1.27049500
C	-0.65086800	4.45022200	-2.12938400
H	0.25002600	2.93584100	-3.37276200
H	-1.43350200	5.80150100	-0.64030400
H	-1.03365000	5.02469300	-2.96694700
21			
Zn	-0.22549500	-0.37100000	0.00435800
N	0.59306600	1.23301700	0.94628100

C	-0.75258800	0.79402200	2.98093400
C	-0.20914700	1.88826900	2.06285700
H	-1.19877000	1.24957400	3.86928200
C	-1.30439000	2.79334100	1.50916300
H	-2.00532500	2.23653100	0.88368700
H	-1.86573800	3.22221600	2.34417200
H	-0.89336400	3.61786500	0.92313200
H	0.03544400	0.11035300	3.31195100
H	-1.53121900	0.20531500	2.48544000
H	1.33767400	0.71803300	1.42367600
O	-1.93108000	-1.46544000	0.38750900
O	1.09869400	-1.42956800	-1.06275300
S	-2.69630200	-0.91494500	-0.80695200
O	-3.19544200	-1.85788300	-1.79153500
O	-1.82875500	0.23194900	-1.28899500
C	-4.20181400	-0.10894100	-0.05660700
F	-4.82826800	0.61342200	-0.98303400
F	-5.01837900	-1.04768300	0.41197300
F	-3.83695000	0.69605400	0.95343100
S	1.79848600	-2.19478600	0.06252400
O	1.24983600	-1.62342400	1.33773400
O	1.88124700	-3.63670800	-0.08942500
C	3.54531900	-1.55159900	-0.02011000
F	3.54012100	-0.22017300	0.17927900
F	4.28016400	-2.12298400	0.93346000

F	4.07807900	-1.80848500	-1.21077700
H	0.50539500	2.50601700	2.62322900
C	1.24779100	2.18981800	0.05142400
C	2.46448900	2.76488200	0.42694100
C	0.65549600	2.52350900	-1.16790100
C	3.09202500	3.67506900	-0.42258600
H	2.92660700	2.49252000	1.37218400
C	1.28734600	3.43991700	-2.01033900
H	-0.29112900	2.07896600	-1.45790900
C	2.50321500	4.01573500	-1.64150100
H	4.04204600	4.11278000	-0.13260000
H	0.82760600	3.69506500	-2.95973800
H	2.99387500	4.72242900	-2.30328300