

## *Supporting Information*

# **Theoretical Mechanistic Investigation of Zinc(II) Catalyzed Oxidation of Alcohols to Aldehydes and Esters**

Riffat Un Nisa<sup>a</sup>, Tariq Mahmood<sup>a</sup>, Ralf Ludwig<sup>b,c</sup>, Khurshid Ayub<sup>\*a</sup>

*<sup>a</sup> Department of Chemistry, COMSATS Institute for Information Technology, Campus  
Abbottabad, Abbottabad, Pakistan*

*<sup>b</sup> Leibniz-Institut für Katalyse e. V. an der Universität Rostock, Albert-Einstein-Str. 29a, 18059  
Rostock, Germany*

*<sup>c</sup> Department of Physical Chemistry, University of Rostock, Dr.-Lorenz-Weg 1, 18059 Rostock,  
Germany*

To Whom correspondence should be addressed:

Khurshid Ayub

E-Mail: [khurshid@ciit.net.pk](mailto:khurshid@ciit.net.pk)

Ph: +92-992-383591

Fax: +92-992-383441

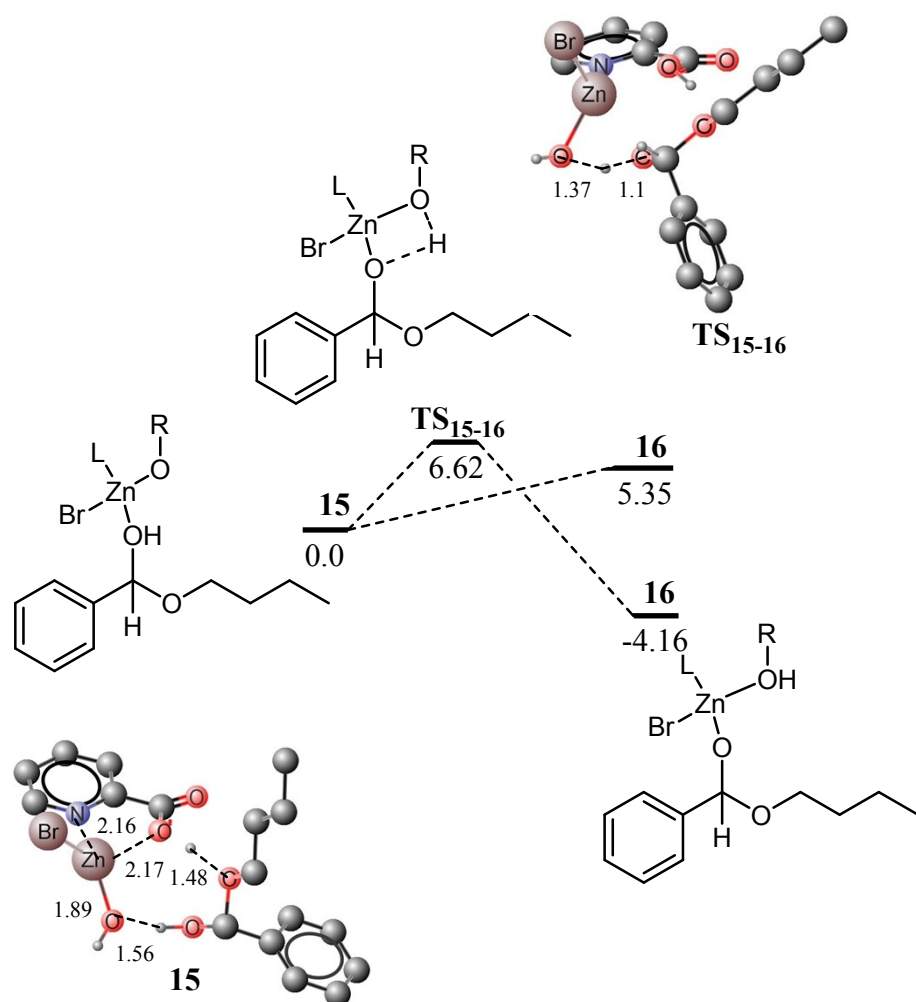


Figure S1. Energy profile for hydrogen shift between ligands, all energy values are relative to **15** at 0 kcal mol<sup>-1</sup>. All bond lengths are in Angstroms. Unnecessary hydrogen atoms are removed for clarity

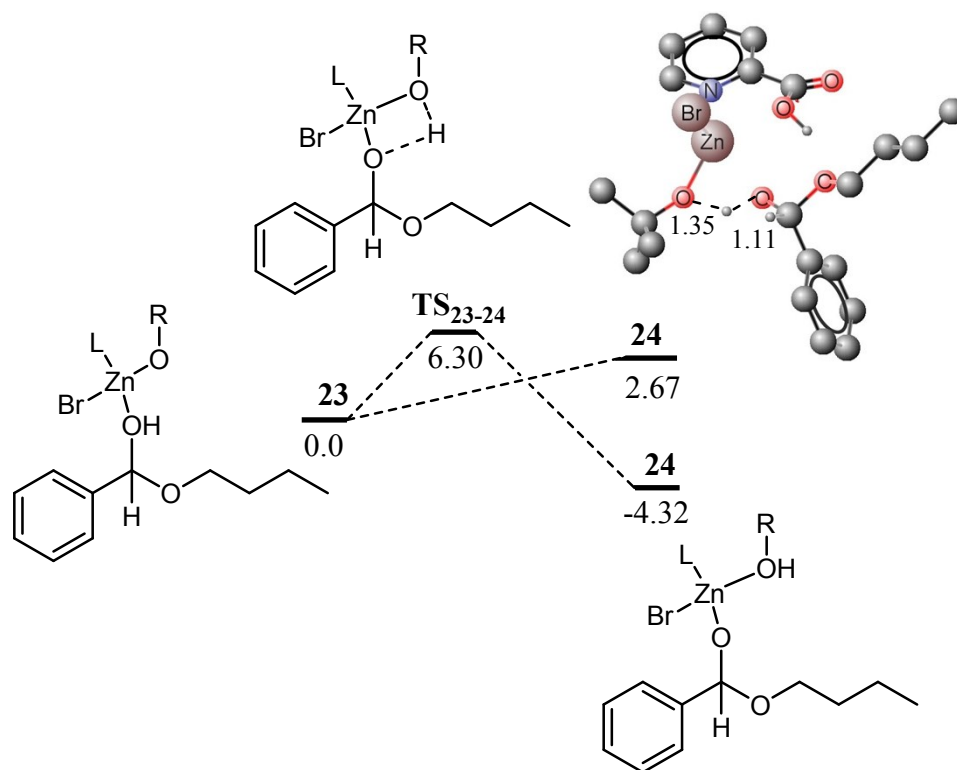


Figure S2. Energy profile for proton shift between oxy ligands, all energy values are relative to **12** at 0 kcal mol<sup>-1</sup>. All bond lengths are in Angstroms. Unnecessary hydrogen atoms are removed for clarity

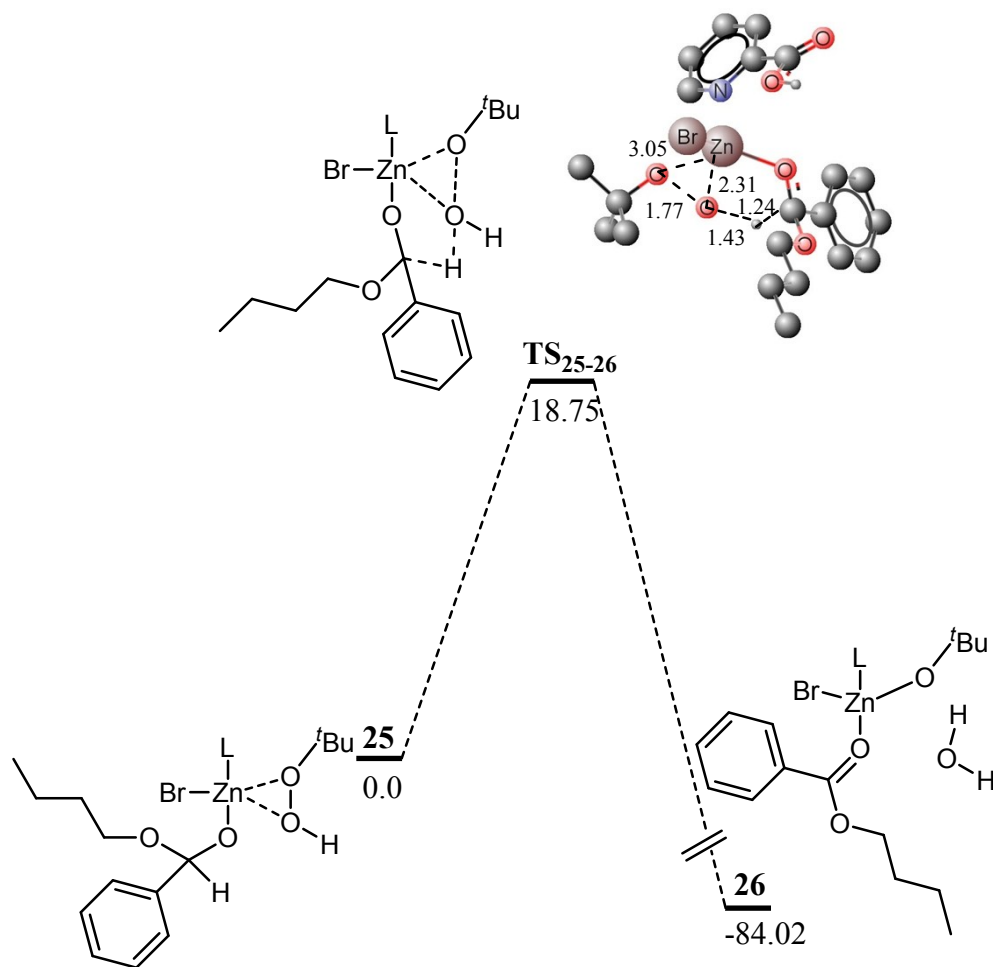


Figure S3, Energy profile for oxidation of hemiacetal to ester through TBHP coordinated to zinc catalyst, calculated at B3PW91/6-311G(d,p) with SDDALL pseudo potential for Zn and Br. All energy values are relative to **25** at 0 kcal mol<sup>-1</sup>. All bond lengths are in Angstroms. Unnecessary hydrogen atoms are removed for clarity

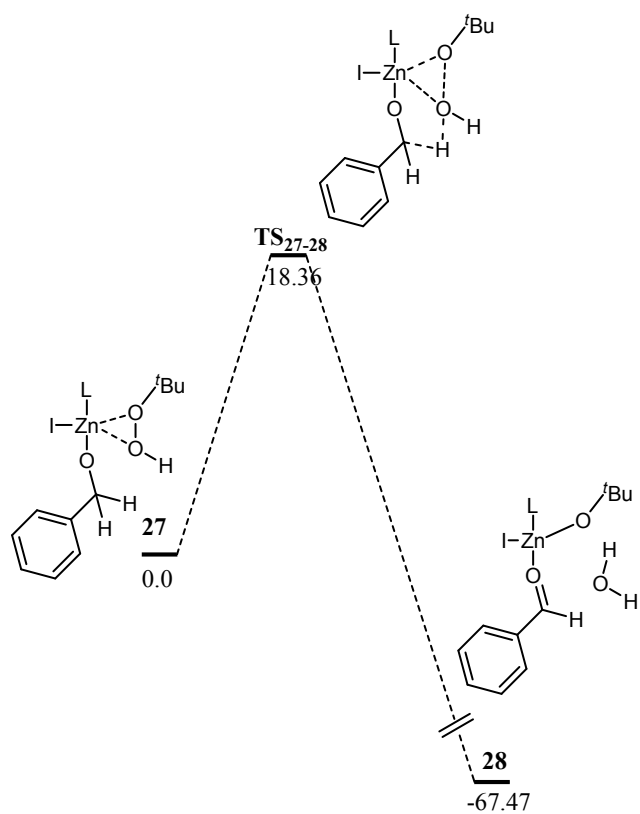


Figure S4. Energy profile for oxidation of alcohol to aldehyde through TBHP coordinated to zinc catalyst, calculated at B3PW91/6-311G(d,p) with SDDALL pseudo potential for Zn and Br. All energy values are relative to **27** at 0 kcal mol<sup>-1</sup>. Unnecessary hydrogen atoms are removed for clarity.

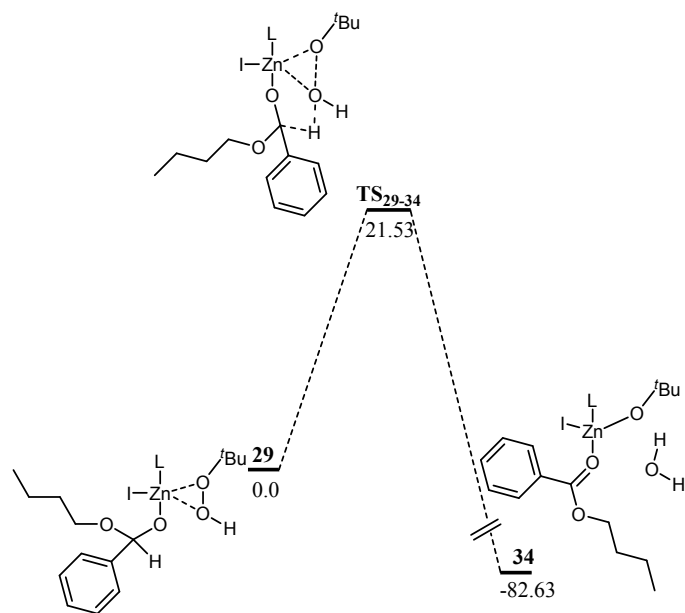


Figure S5. Energy profile for oxidation of hemiacetal to ester through TBHP coordinated to zinc catalyst, calculated at B3PW91/6-311G(d,p) with SDDALL pseudo potential for Zn and Br. All energy values are relative to **29** at 0 kcal mol<sup>-1</sup>.

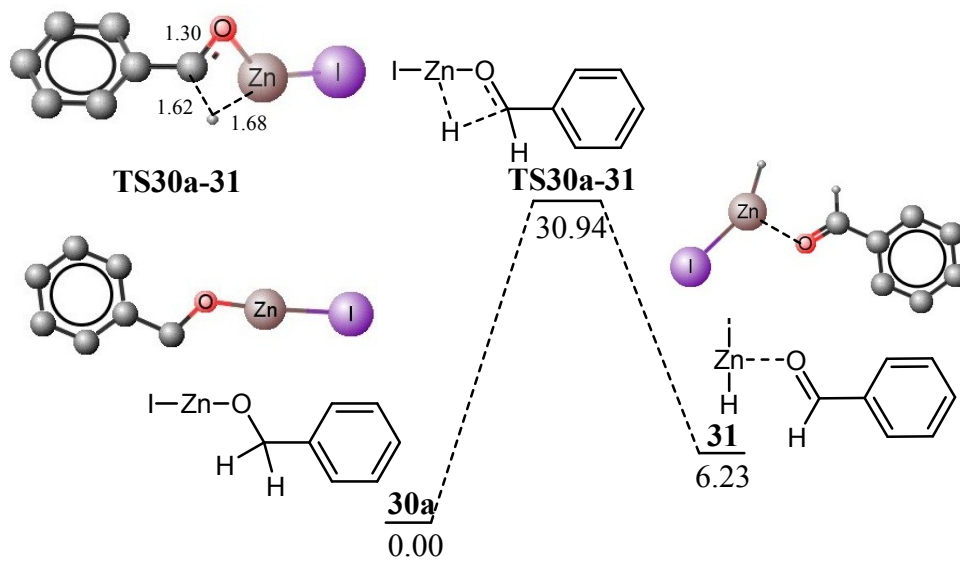


Figure S6. Energy profile for zinc mediated oxidation of alcohol to aldehyde through  $\beta$ -hydride elimination, calculated at B3PW91/6-31G\* with pseudo core potential for Zn and I. All energy values are zero point corrected and are in kcal mol<sup>-1</sup> relative to complex **30a** at 0 kcal mol<sup>-1</sup>. All bond lengths are in Angstroms. Unnecessary hydrogen atoms are removed for clarity

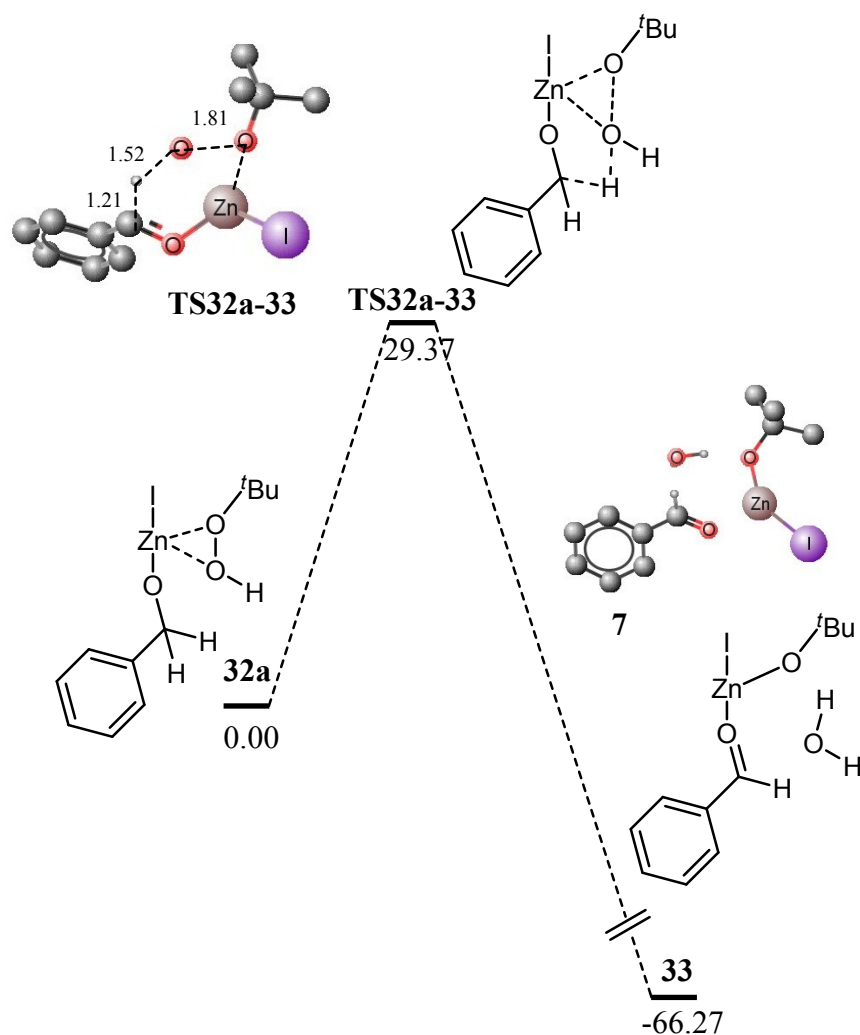


Figure S7. Energy profile for oxidation of alcohol to aldehyde through TBHP coordinated to zinc catalyst, calculated at B3PW91/6-31G\* with pseudo core potential for Zn and I. All energy values are zero point corrected and are in kcal mol<sup>-1</sup> relative to reactants at 0 kcal mol<sup>-1</sup>. All bond lengths are in Angstroms. Unnecessary hydrogen atoms are removed for clarity



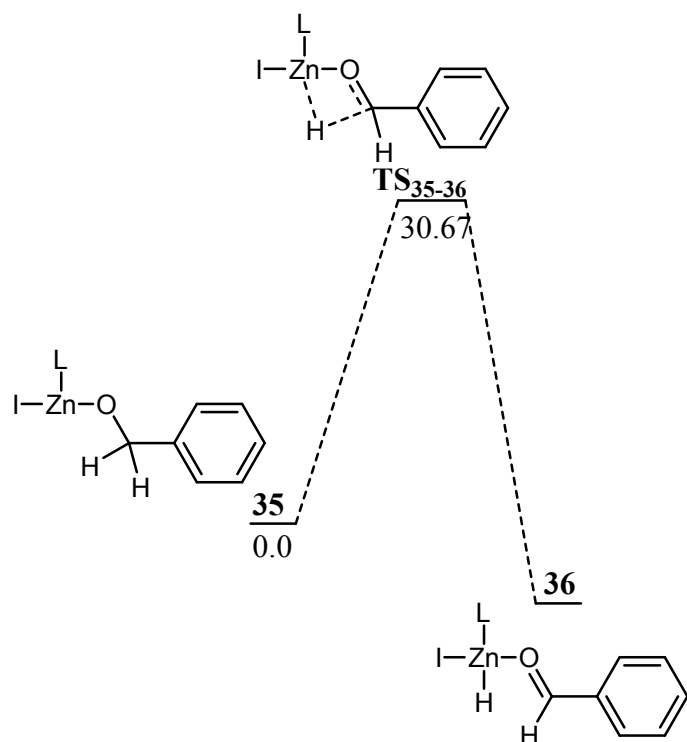


Figure S8. Energy profile for zinc mediated oxidation of alcohol to aldehyde through  $\beta$ -hydride elimination calculated at B3PW91/6-31G\* with pseudo core potential for Zn and I. All energy values are zero point corrected and are in kcal mol<sup>-1</sup> relative to complex **35** at 0 kcal mol<sup>-1</sup>.

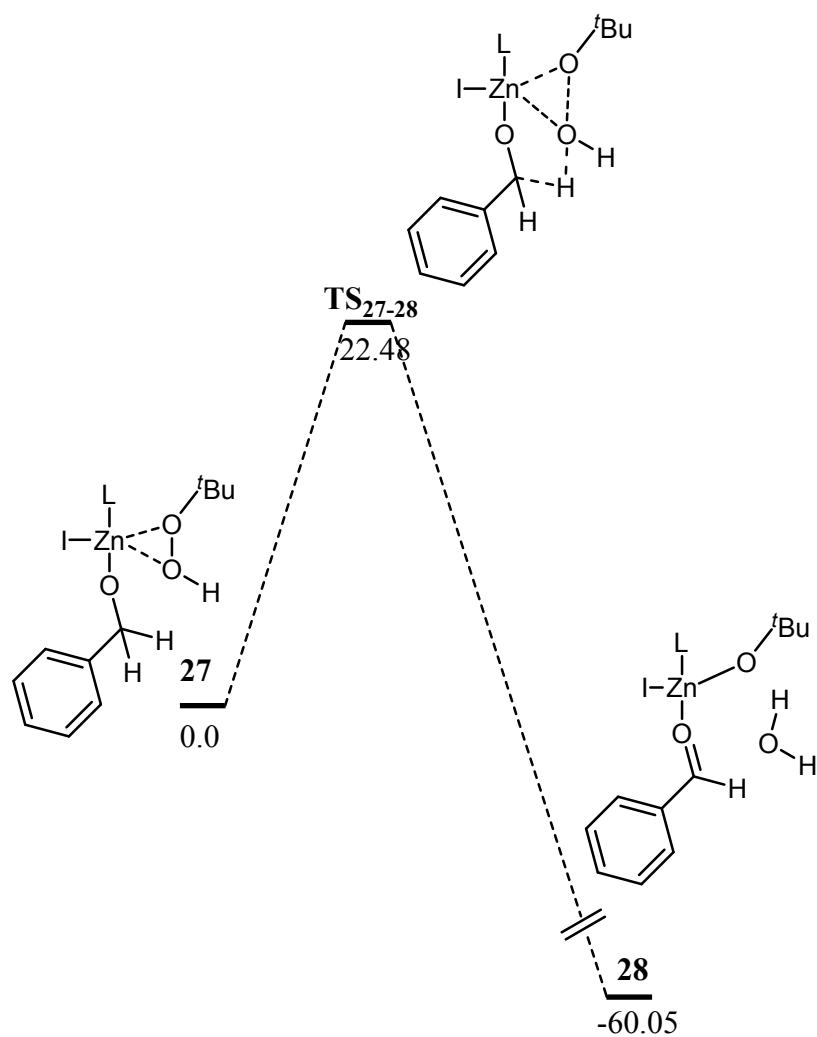


Figure S9. Energy profile for oxidation of alcohol to aldehyde through TBHP coordinated to zinc catalyst, calculated at B3PW91/6-31G\* with pseudo core potential for Zn and I. All energy values are zero point corrected, and are in kcal mol<sup>-1</sup> relative to **27** at 0 kcal mol<sup>-1</sup>.

## Comparison of geometries of **9** and **10**

The alcohol can coordinate to the metal (Zn) by replacing a halide to form complex **9** where a bidentate ligand is also attached to the metal centre. The mechanism and associated kinetic barrier for the exchange of a halide with alkoxide is beyond the scope of this study. Although the literature reveals up to 22 electron octahedral complexes of zinc[56], however, their catalytic role is not well established.

The complex **9** is an eighteen electron complex, and has a distorted tetrahedral geometry around the zinc atom. The ligand is bidentate for coordination with zinc. Br-Zn-O1, Br-Zn-N7 and Br-Zn-O8 (see Figure 2 for numbering) angles in **9** are 143.6, 105.9 and 114.6 degrees, respectively. The O1-Zn-O8 bond angle is 86.6 degrees. Zn-Br, Zn-O8, Zn-N7 and Zn-O1 bond distances are 2.32, 2.37, 2.16 and 1.85 Å, respectively. The complex **9** has another isomer **10** which is lower in energy than **9** by 19.01 kcal mol<sup>-1</sup>. A proton from carboxylic oxygen (O8) in **9** is shifted to O1 in complex **10**. The complex **10** is occasionally obtained during the optimization of complex **9**. The geometry of the complex **10** is also analyzed to explore the reasons for the higher stability over the complex **9**, and driving force for the proton shift. Probably, the higher acidity of carboxylic acid drives a proton shift to alkoxy ligand. Since in **10**, the neutral and anionic oxygens are interchanged, therefore, the angles and bond lengths are expected to change. The Br-Zn-O8 bond angle is 140.46°, which is considerably higher than 114.59° for Br-Zn-O8 in **9**. Br-Zn-O1 and Br-Zn-N7 bond angles in **10** are 109.59 and 122.38 degrees, respectively. The O1-Zn-O8 bond angle is 83.88°. The bond angles in complex **10** indicate a more distorted tetrahedral geometry of complex **10** compared to **9**. Zn-O8, Zn-O1 and Zn-N7 bond lengths are 1.96, 2.14 and 2.07 Å, respectively. The small bond distances indicate strong coordination of ligands on zinc in **10** compared to **9**, which probably illustrates the higher thermodynamic stability of the former. An additional hydrogen bonding between the OH of the alcohol and the oxygen of the acetate group imparts even higher stability to complex **10**. The O(1)-H .....O8 bond distance is 2.34 Å

Table S1. Total electronic, ZP and Gibbs free energies of optimized geometries

	Total Electronic energies	Zero point corrected Energies	Gibbs Free energies
<b>9</b>	-1023.6413489	-1023.413243	-1023.462231
<b>10</b>	-1023.6707739	-1023.441686	-1023.492534
<b>TS9-11</b>	-1023.5798714	-1023.357761	-1023.411582
<b>11</b>	-1023.625379	-1023.403074	-1023.455791
<b>12</b>	-1175.1889706	-1174.932072	-1174.985423
<b>13</b>	-1175.2180724	-1174.959667	-1175.017396
<b>TS12-14</b>	-1175.1476074	-1174.896484	-1174.949307
<b>14</b>	-1175.3093404	-1175.054830	-1175.110974
<b>15</b>	-1332.5497996	-1332.180171	-1332.241867
<b>16</b>	-1332.5422416	-1332.173023	-1332.233332
<b>17</b>	-1407.6426232	-1407.268107	-1407.329977
<b>18</b>	-1407.6648356	-1407.289249	-1407.350184
<b>TS17-19</b>	-1407.6024367	-1407.233880	-1407.294924
<b>19</b>	-1407.7798845	-1407.907323	-1407.473656
<b>20</b>	-1332.4252857	-1332.058091	-1332.121050
<b>21</b>	-1332.4392739	-1332.070894	-1332.131913
<b>TS20-22</b>	-1332.3867642	-1332.024696	-1332.084288
<b>22</b>	-1332.5345974	-1332.168898	-1332.230324
<b>23</b>	-1489.7779104	-1489.296913	-1489.362924
<b>24</b>	-1489.7733672	-1489.291911	-1489.358666
<b>25</b>	-1564.8771697	-1564.392550	-1564.460749
<b>TS25-26</b>	-1564.8414904	-1564.361294	-1564.430863
<b>26</b>	-1565.004212	-1564.520052	-1564.594646
<b>27</b>	-1330.464363	-1330.097119	-1330.160833
<b>TS27-28</b>	-1330.4297375	-1330.068036	-1330.131559
<b>28</b>	-1330.5744538	-1330.208389	-1330.268362
<b>29</b>	-1562.9154081	-1562.431315	-1562.502530
<b>TS29-34</b>	-1562.8799878	-1562.400225	-1562.468208
<b>30</b>	-584.8269366	-584.703611	-584.745190
<b>30a</b>	-584.8224001	-584.699319	-584.741208
<b>TS<sub>30-31</sub></b>	-584.7699262	-584.652660	-584.692463
<b>31</b>	-584.8112696	-584.693327	-584.735689
<b>32</b>	-731.6230795	-731.556785	-731.608266
<b>32a</b>	-731.8147498	-731.548980	-731.602150
<b>TS<sub>32-33</sub></b>	-731.7757906	-731.515019	-731.567259
<b>33</b>	-731.9138416	-731.649548	-731.704889

### Cartesian coordinates of the optimized geometries

10

C	2.14799100	0.30467800	1.73824300
H	2.28218200	1.35805800	1.48016200
O	0.74864300	-0.04131600	1.58431600
Zn	-0.64549400	0.89641700	0.26459400
C	2.98138000	-0.57287700	0.85182000
C	3.65225400	-0.03755800	-0.24636500
C	3.08776500	-1.94120000	1.11469600
C	4.42800200	-0.85402000	-1.06481600
H	3.55864900	1.02122500	-0.46589500
C	3.85649400	-2.75756900	0.29633900
H	2.56324700	-2.36680700	1.96503900
C	4.53088700	-2.21354100	-0.79492200
H	4.94778900	-0.42624000	-1.91554500
H	3.93576500	-3.81821200	0.51089300
H	5.13557100	-2.85064600	-1.43195500
H	2.41499600	0.15948500	2.78914200
C	-1.71594800	-1.05683200	-1.91137800
C	-2.63830100	-1.98318500	-2.37103800
C	-3.67316600	-2.37330700	-1.52502900
C	-3.75295900	-1.82652700	-0.25204000
C	-2.79381500	-0.90147300	0.13854400
H	-0.89268600	-0.71223200	-2.52789000

H	-2.54530700	-2.38603000	-3.37231000
H	-4.41030300	-3.09559600	-1.85963000
H	-4.53063300	-2.08414300	0.45591600
N	-1.79871800	-0.53629200	-0.68269500
C	-2.82851600	-0.25995100	1.52930600
O	-1.90719000	0.62311000	1.74173700
H	0.26777900	0.06237300	2.41545400
O	-3.68828100	-0.62766800	2.30357600
Br	0.40888600	2.60592700	-0.89313000

## 9

C	-1.98964900	-0.46192800	2.02698000
H	-2.35170200	-1.49949000	1.93910400
O	-0.60060600	-0.36282600	1.88650600
Zn	0.24628600	-0.97298500	0.36471200
C	-2.75809900	0.39514900	1.04047900
C	-3.85156000	-0.10491900	0.33368400
C	-2.37295400	1.72178300	0.82250700
C	-4.55141700	0.69835100	-0.56388200
H	-4.15515700	-1.13744900	0.48338700
C	-3.06887500	2.52723200	-0.07095900
H	-1.51919200	2.11156500	1.36790200
C	-4.16277300	2.01741500	-0.76815400
H	-5.39730000	0.29018800	-1.10808800

H	-2.76489300	3.55918500	-0.22006300
H	-4.70744400	2.64567300	-1.46571200
H	-2.24942900	-0.13116300	3.04575500
C	0.91307600	1.20690700	-1.68015000
C	1.52173900	2.32975000	-2.22938000
C	2.59750100	2.90315600	-1.56511000
C	3.03647300	2.33226300	-0.37667300
C	2.37733100	1.20580500	0.09485000
H	0.06817600	0.72605700	-2.16126700
H	1.14939500	2.74090400	-3.15984400
H	3.09082300	3.78137700	-1.96643000
H	3.86969400	2.73001200	0.18888300
N	1.33195200	0.65950000	-0.53948900
C	2.84112300	0.56553700	1.36321900
O	2.28037100	-0.64838900	1.53848100
H	2.48975500	-0.97162200	2.42607000
O	3.62514700	1.05757700	2.12451100
Br	0.28954900	-2.70463100	-1.18557400

**TS<sub>9-11</sub>**

C	-1.53691800	-1.63038900	0.57798400
H	-0.84186200	-1.28630800	-0.96976900
O	-0.70402400	-1.24388800	1.45504700
Zn	0.61971800	-0.94050700	-0.18473900
C	-2.83455100	-0.92686600	0.38060700
C	-3.80105500	-1.45088100	-0.48028900

C	-3.10977200	0.23182600	1.10709100
C	-5.02514100	-0.81321700	-0.62710900
H	-3.58437900	-2.35709500	-1.03930900
C	-4.33757400	0.86671600	0.96410700
H	-2.35482100	0.60192900	1.79188700
C	-5.29406700	0.34851400	0.09472200
H	-5.77402000	-1.22198000	-1.29737600
H	-4.55471700	1.76260400	1.53686400
H	-6.25333100	0.84400600	-0.01474600
H	-1.55656300	-2.68753000	0.26805300
C	-0.14533300	1.58705200	-1.54748100
C	-0.18110700	2.91463100	-1.95490800
C	0.57735700	3.84827500	-1.26312400
C	1.33768400	3.42299400	-0.18169700
C	1.30904200	2.07996300	0.16800500
H	-0.71474600	0.81567300	-2.05544400
H	-0.79318700	3.19835100	-2.80244600
H	0.57771900	4.89157400	-1.55875600
H	1.95236200	4.09723300	0.40116700
N	0.58552700	1.17418400	-0.50818800
C	2.12199400	1.63680300	1.34656700
O	1.85777600	0.37296200	1.67533700
H	2.44811700	0.08540000	2.38543700
O	2.90103200	2.35130600	1.91854400
Br	2.62393100	-2.09381500	-0.55555300



**11**

C	-2.43101600	-0.53642200	0.12991700
H	1.57599900	1.27563100	2.73642600
O	-1.87079000	-1.47049100	0.69282500
Zn	1.42721000	1.00969500	1.22353100
C	-3.87994100	-0.43761200	-0.02719200
C	-4.41308800	0.68591800	-0.66736800
C	-4.72711000	-1.44394300	0.45375400
C	-5.78746800	0.80434900	-0.82632800
H	-3.74522300	1.46032100	-1.03289900
C	-6.09667700	-1.32198000	0.29168500
H	-4.28865000	-2.30492800	0.94586200
C	-6.62526500	-0.19878600	-0.34741200
H	-6.20578300	1.67423800	-1.32027600
H	-6.75970300	-2.09701900	0.66041500
H	-7.69944100	-0.10704400	-0.47130600
H	-1.83547800	0.29466200	-0.28767300
C	4.27309000	0.43652300	0.10983200
C	5.29398100	-0.24488800	-0.54048800
C	5.03645700	-1.51382500	-1.04395200
C	3.76940300	-2.05693100	-0.87920900
C	2.80937700	-1.30824900	-0.21100100
H	4.42808700	1.43194300	0.51303600
H	6.26727200	0.21851400	-0.64890500
H	5.81068100	-2.07120200	-1.55963900
H	3.49920700	-3.03671900	-1.25250600

N	3.05660900	-0.08481300	0.27179800
C	1.42931500	-1.87359200	-0.03575400
O	0.66842700	-1.10214600	0.74132300
H	-0.31193200	-1.37519800	0.73706200
O	1.07883400	-2.90462500	-0.54498900
Br	0.40383700	2.08041100	-0.66229400

## 12

Zn	-0.26952600	0.56192800	-0.47777800
O	0.71814400	-0.34229600	-1.78367400
C	2.07414700	-0.07801500	-1.98042600
H	2.29794000	1.00089600	-2.03687200
C	2.96683700	-0.69150200	-0.91716500
C	2.77951500	-2.02520800	-0.53677500
C	3.97112500	0.04635800	-0.28372200
C	3.58448700	-2.60747600	0.43379800
H	1.98446700	-2.59200400	-1.00991500
C	4.77786400	-0.53482900	0.69626600
H	4.12507600	1.08530500	-0.56392300
C	4.58756200	-1.86415800	1.05460700
H	3.42991900	-3.64521400	0.71241300
H	5.55028800	0.05500600	1.17930400
H	5.21198900	-2.31856200	1.81664800
O	1.08697300	0.21560400	1.35410400
H	2.01886100	0.14269300	1.07875100
O	1.09230700	1.26803100	2.32860000

C	-1.84218200	-0.46541300	1.91749700
C	-2.79306100	-1.17538800	2.64137800
C	-3.72677200	-1.94284300	1.95904700
C	-3.68622200	-1.97028200	0.57081300
C	-2.71903700	-1.21572500	-0.07662700
H	-1.08333100	0.13129300	2.41124500
H	-2.78681700	-1.12414500	3.72339700
H	-4.47574200	-2.51244200	2.49803000
H	-4.37928300	-2.55461800	-0.02128200
N	-1.80704200	-0.48442700	0.58236300
C	-2.65371700	-1.23052300	-1.57179000
O	-1.98896000	-0.15846200	-2.02897000
H	-1.68706500	-0.30775500	-2.93657300
O	-3.13538200	-2.08756800	-2.25856600
H	2.37510400	-0.50197100	-2.95313700
Br	-0.53366000	2.88664400	0.00643800
H	0.72382100	2.00968900	1.80003800

### 13

Zn	-0.55940100	0.05837700	0.45078800
O	0.89047800	1.73009600	0.37285700
C	2.18317500	1.72520300	0.99636900
H	2.15043100	1.16036600	1.93295900
C	3.17613400	1.11048800	0.04889700
C	3.24001600	1.54166400	-1.28147300

C	4.05300500	0.11601000	0.48198500
C	4.16747600	0.98667200	-2.15775600
H	2.55941000	2.31476300	-1.62394700
C	4.98849000	-0.42922900	-0.39233900
H	3.99428500	-0.24052400	1.50534100
C	5.04648700	0.00267500	-1.71284500
H	4.20726000	1.32726900	-3.18705000
H	5.66370600	-1.20308800	-0.04318200
H	5.77035300	-0.42894100	-2.39572400
O	0.61576000	-0.53143000	-1.39214300
H	1.52203400	-0.17746800	-1.37106200
O	0.80186700	-1.94962000	-1.45724400
C	-2.63627000	-1.32715200	-1.40864900
C	-3.89973600	-1.44642000	-1.96647800
C	-4.86253700	-0.49020400	-1.65611800
C	-4.53101100	0.55584500	-0.80646800
C	-3.24552100	0.60846800	-0.28391300
H	-1.84176100	-2.03411400	-1.62263600
H	-4.11920600	-2.27351500	-2.63081400
H	-5.85998300	-0.56062900	-2.07717900
H	-5.22710500	1.33800800	-0.53080400
N	-2.32819100	-0.32151800	-0.58283100
C	-2.80984500	1.74678900	0.63923100
O	-1.59529300	1.64417000	1.07071000
H	0.27018400	2.31966200	0.83295500
O	-3.60513600	2.63305300	0.87683700

H	2.46501500	2.76067000	1.22007400
Br	0.41766700	-1.65816100	1.77941500
H	0.82582100	-2.18250900	-0.50309200

**TS<sub>12-14</sub>**

Zn	0.74986500	-0.74842200	-0.05349900
O	-0.97973700	-0.27272400	-0.82107200
C	-2.00945400	-1.00839000	-0.41601900
H	-1.70219100	-1.46731000	0.69195500
C	-3.31622100	-0.31326100	-0.20680100
C	-3.38776300	1.08106300	-0.20426500
C	-4.48335200	-1.05611600	0.00071400
C	-4.60428400	1.72019700	0.00259500
H	-2.47949100	1.64388700	-0.38636500
C	-5.69763400	-0.41703000	0.21140700
H	-4.43553000	-2.14196500	-0.00652200
C	-5.76113300	0.97478200	0.21440500
H	-4.65332600	2.80449300	-0.00686500
H	-6.59768700	-1.00248300	0.36843200
H	-6.71027500	1.47536600	0.37542100
O	-0.62553500	-1.52758100	1.59385900
H	-1.02907100	-0.93128500	2.23932300
O	0.90306700	-1.37076300	2.52772300
C	1.88916200	1.35186800	1.80334000
C	2.32383100	2.59481700	2.25072700
C	2.41976700	3.64255100	1.34714700

C	2.09309200	3.40952500	0.01704300
C	1.69004900	2.13587400	-0.35607900
H	1.77211700	0.49538500	2.46201100
H	2.57403900	2.72606600	3.29662600
H	2.74677300	4.62543000	1.66819400
H	2.14692000	4.18117800	-0.74048300
N	1.57609200	1.12642300	0.52327000
C	1.38120400	1.88148400	-1.79896700
O	1.40590300	0.57339600	-2.07787900
H	1.08161900	0.42828700	-2.97753900
O	1.17138800	2.75049100	-2.60043500
H	-2.13315700	-1.98204100	-0.92834700
Br	2.12641500	-2.60737700	-0.47257900
H	1.24184400	-2.23586600	2.25747400

#### 14

Zn	-0.63118700	-0.45327100	-0.79578800
O	1.23361700	-0.39814000	0.22559600
C	2.17199000	0.25894900	-0.22727600
H	1.54504200	3.10497500	-2.49694900
C	3.52104400	0.22267600	0.32412100
C	3.84896800	-0.56588700	1.43446500
C	4.49856400	1.00374200	-0.30421500
C	5.14776700	-0.56441400	1.91361800
H	3.07536100	-1.16789000	1.89785700
C	5.79990500	0.99946600	0.18068200

H	4.21990500	1.59736400	-1.17057600
C	6.12058100	0.21811400	1.28719100
H	5.41289000	-1.17174900	2.77226400
H	6.56340000	1.59942100	-0.30201700
H	7.13755900	0.21371800	1.66605400
O	1.89418300	2.25050300	-2.75947000
H	1.10796900	1.65068600	-2.71140600
O	-0.20023400	0.62063900	-2.32906800
C	-2.29537600	1.98780400	-0.75349600
C	-3.26582700	2.93899600	-0.45944800
C	-3.93216200	2.86778400	0.75566600
C	-3.60042900	1.85008900	1.64071800
C	-2.60801600	0.94870000	1.27940100
H	-1.74273800	1.95955500	-1.69083900
H	-3.49335800	3.71239200	-1.18345700
H	-4.70125200	3.58851900	1.01119800
H	-4.08778000	1.72977700	2.59997000
N	-1.96886300	1.01186400	0.10167400
C	-2.26191400	-0.14475400	2.24236300
O	-1.13103200	-0.76515900	1.90290700
H	-1.01974200	-1.54364600	2.46564900
O	-2.92773600	-0.41168200	3.20792700
H	2.02207200	0.92600900	-1.08955300
Br	-1.50711700	-2.63695100	-0.95289900
H	-0.39356000	0.11235600	-3.12068800

**15**

H	0.64389400	-1.06769000	1.74621000
O	-0.73032300	-0.51184900	2.27884800
O	1.47798700	-1.39188700	1.28633000
Zn	-1.91316200	0.20885800	1.01794500
C	2.33626600	-0.35588900	1.10175300
H	2.32417300	0.36700200	1.93400500
C	3.73782300	-0.85652900	0.85540500
C	4.78980900	-0.46641400	1.67825200
C	3.97983300	-1.73984600	-0.19831400
C	6.07663000	-0.95183800	1.45643600
H	4.60319400	0.21619400	2.50282000
C	5.26202800	-2.22247600	-0.42093200
H	3.15508700	-2.04330200	-0.83357300
C	6.31360600	-1.82973300	0.40583200
H	6.89064400	-0.64446300	2.10481200
H	5.44492100	-2.90988900	-1.24054800
H	7.31475900	-2.20958100	0.22970100
C	2.50515200	1.66614200	-0.27884600
H	2.32365600	2.30098400	0.60053200
H	3.58710100	1.51394700	-0.37028200
C	1.95318400	2.31512600	-1.53375300
H	2.09445200	1.62678000	-2.37476700
H	0.87293900	2.46456800	-1.42195600
C	2.62484000	3.65360300	-1.83663200
H	2.49625800	4.32812200	-0.98110500



C	2.07434200	4.31911300	-3.09408300
H	2.57197900	5.27293100	-3.28938200
H	2.21774900	3.68308100	-3.97326600
H	1.00208900	4.51678900	-2.99970700
H	3.70563100	3.50115500	-1.94607200
O	1.88001500	0.39755500	-0.08171900
C	-2.13788200	-1.66628700	-1.28767300
C	-4.07722900	-1.70236700	-0.04097200
C	-4.65122200	-2.63950000	-0.89003700
C	-3.91679500	-3.09850700	-1.97658400
C	-2.63572000	-2.60355200	-2.18165700
H	-4.61307200	-1.30632200	0.81491100
H	-5.65552300	-2.99641400	-0.69659200
H	-4.33769900	-3.83091600	-2.65659000
H	-2.01091800	-2.91940600	-3.00755800
N	-2.84400800	-1.23208600	-0.23527300
C	-0.75380900	-1.11230500	-1.47860500
O	0.01135800	-1.54642200	-2.29609000
O	-0.50795800	-0.09985200	-0.64624900
H	0.49960700	0.10403600	-0.51116900
Br	-3.28394800	2.10063600	1.09442400
H	-0.82359800	-0.16383900	3.16679000

**16**

H	-0.75179500	-2.60345000	-0.87923000
O	-1.71559300	-2.66846400	-0.73572800

O	0.38868900	-1.16441800	-0.32881600
Zn	-1.35680800	-0.71407000	0.40546500
C	1.58498300	-0.86248900	0.20128900
H	1.67342800	-1.10340700	1.27756700
C	2.72386600	-1.50933300	-0.55886100
C	3.63231500	-2.34025300	0.09022500
C	2.84912000	-1.30099000	-1.93373700
C	4.65808900	-2.96005400	-0.62089700
H	3.53426100	-2.50953000	1.15926600
C	3.87322800	-1.91296100	-2.64305000
H	2.13525000	-0.65665500	-2.43480000
C	4.78024500	-2.74568700	-1.98821700
H	5.35893900	-3.60913600	-0.10589400
H	3.96709800	-1.74466900	-3.71126200
H	5.57857600	-3.22508800	-2.54545900
C	2.84668100	1.14106300	0.89859300
H	2.70495400	0.88514300	1.95902800
H	3.77411600	0.66575800	0.55836200
C	2.92031800	2.64457600	0.71125400
H	3.01088500	2.86041800	-0.35893700
H	1.97939200	3.09953200	1.04184200
C	4.08740600	3.26993500	1.47352400
H	3.99733700	3.03043300	2.54040400
C	4.16382100	4.78337400	1.29806300
H	5.00746000	5.20621200	1.85050200
H	4.28617300	5.05354100	0.24452600

H	3.25215400	5.26965200	1.65903300
H	5.02703800	2.81448900	1.13727400
O	1.75863800	0.62151200	0.13275300
C	-2.44271700	1.59245400	-1.15701200
C	-3.89022500	-0.20415000	-1.20585800
C	-4.80885900	0.50886600	-1.96455300
C	-4.50829800	1.81570000	-2.32949700
C	-3.29857700	2.36637200	-1.92775500
H	-4.06511700	-1.23147300	-0.90845900
H	-5.73869700	0.03995300	-2.26283900
H	-5.20545900	2.39605100	-2.92392700
H	-2.99577800	3.37090100	-2.19530600
N	-2.73519800	0.33201300	-0.80654700
C	-1.10288700	2.12989100	-0.73398600
O	-0.59635000	3.08511600	-1.26086900
O	-0.58047100	1.41312500	0.25519300
H	0.45135600	1.27503400	0.21318600
Br	-2.22170800	-1.30521700	2.51491700
H	-1.82153000	-3.29596600	-0.01251100

## 17

Zn	0.88527100	-0.02535400	0.51915300
O	-0.87197700	-0.06341300	-0.10966100
C	-1.84537200	0.86069700	0.20611400
H	-1.91248200	1.01420800	1.30318300
C	-1.59111500	2.20248700	-0.45874000

C	-1.75747100	2.34435100	-1.83836400
C	-1.11622300	3.28651800	0.28124000
C	-1.45177900	3.54650100	-2.46353700
H	-2.13663700	1.50166500	-2.40450000
C	-0.79819800	4.49247700	-0.34780000
H	-0.99729300	3.18833600	1.35718100
C	-0.96519600	4.62283900	-1.72248900
H	-1.59037400	3.64797700	-3.53534900
H	-0.42760900	5.32672800	0.23893600
H	-0.72246800	5.55909800	-2.21405100
O	1.56920200	1.86086400	-0.58515400
H	0.85577700	2.52411600	-0.53022000
O	2.70425100	2.52682600	-0.01721300
C	-3.54903300	-0.77335900	0.35783000
H	-2.87429700	-1.59826500	0.09662200
H	-3.53093100	-0.66171100	1.45582300
C	-4.95959100	-1.06855900	-0.11546300
H	-5.60125700	-0.21605200	0.13564600
H	-4.95151300	-1.14127300	-1.20929400
C	-5.52949500	-2.34998500	0.48797600
H	-4.87081500	-3.19255600	0.24161000
H	-5.52462700	-2.27112100	1.58263400
C	-6.94515800	-2.65764800	0.00941700
H	-7.32887700	-3.57908800	0.45682400
H	-7.63481900	-1.84878600	0.27106900
H	-6.97679000	-2.77784600	-1.07823400

O	-3.10889300	0.42563400	-0.24994300
C	3.15036800	-0.58330900	-1.41663300
C	3.96188200	-1.27406200	-2.30926400
C	3.76681000	-2.63609500	-2.48433600
C	2.77409300	-3.26840200	-1.74723900
C	2.01932800	-2.51103800	-0.86313300
H	3.26431300	0.48265000	-1.26094800
H	4.72752100	-0.73764000	-2.85650800
H	4.37837000	-3.19977900	-3.18006100
H	2.56869100	-4.32791800	-1.83265400
N	2.19262400	-1.18868800	-0.70767200
C	0.97249600	-3.20301900	-0.04883200
O	0.54144200	-2.42914600	0.95778500
H	-0.20765900	-2.85779900	1.39421200
O	0.58614000	-4.31939400	-0.26042300
H	2.68188300	2.18305000	0.90227600
Br	1.96359900	0.62486000	2.54289500

## 18

Zn	0.07399800	-1.10550500	-0.47533500
O	-1.03445900	0.61126100	-1.50822500
C	-1.47820500	1.84982600	-0.96206800
H	-1.64298000	2.54078400	-1.80427500
C	-2.77445400	1.59649900	-0.22566000
C	-3.09811000	2.34470800	0.90915400
C	-3.67757000	0.64226500	-0.70175000
C	-4.30967700	2.13473500	1.56188300

H	-2.39436500	3.08249300	1.27512100
C	-4.88671100	0.43977300	-0.04715100
H	-3.42078700	0.05072800	-1.57223900
C	-5.20608800	1.18520500	1.08413600
H	-4.55116700	2.71616700	2.44538100
H	-5.57792900	-0.30854000	-0.41968000
H	-6.14956700	1.02245100	1.59437800
O	-0.81696100	-0.34261800	1.42762000
H	-1.55491600	0.28375000	1.32691900
O	-1.38196400	-1.41168000	2.19493800
C	0.56955600	3.02761500	-0.71388800
H	1.12297600	2.29631400	-1.31577300
H	0.20313200	3.81946300	-1.38359400
C	1.47243300	3.60544900	0.35576500
H	0.91025000	4.34317300	0.94025600
H	1.75290400	2.80313700	1.04722700
C	2.72865100	4.24493800	-0.23447400
H	3.27452600	3.49525500	-0.81883500
H	2.43961000	5.03307000	-0.94099500
C	3.64826600	4.83224200	0.83145600
H	4.53874900	5.28121500	0.38337000
H	3.14001500	5.60906000	1.41187300
H	3.98287800	4.06110400	1.53250800
O	-0.55097900	2.39749000	-0.08232700
C	2.03621800	-2.15080100	1.72915300
C	3.30424300	-2.38559100	2.23996600

C	4.40924900	-1.92945000	1.52704700
C	4.21241000	-1.24591600	0.33508500
C	2.91246500	-1.05389700	-0.11387500
H	1.13754700	-2.46907200	2.24650400
H	3.41764800	-2.91475400	3.17848800
H	5.41259700	-2.10197000	1.90209600
H	5.02537000	-0.85131200	-0.26133500
N	1.85565800	-1.50521800	0.57342000
C	2.62110100	-0.28503800	-1.39848400
O	1.37232400	-0.26749900	-1.73509100
H	-0.25922800	0.75284300	-2.07823300
O	3.54257900	0.25904800	-1.97547700
H	-1.63446800	-2.04396100	1.48630000
Br	-1.38083800	-2.96809000	-0.67310400

**TS<sub>17-19</sub>**

Zn	-0.48340800	-0.86864600	-0.12205900
O	0.47462300	0.57033800	0.74686300
C	1.31432900	1.28589400	0.01354900
H	1.13325700	0.88896200	-1.14787200
C	1.04881700	2.77130000	-0.07564700
C	-0.18189800	3.27681500	0.34068000
C	2.00517800	3.64273600	-0.60246100
C	-0.45473200	4.63641700	0.23553000
H	-0.90648700	2.59388500	0.76774400
C	1.73050500	5.00052300	-0.70700000

H	2.96548200	3.24877800	-0.91353500
C	0.49928600	5.50142300	-0.29096700
H	-1.41084500	5.02308400	0.57386300
H	2.48136000	5.67221800	-1.11045900
H	0.28750800	6.56259700	-0.37220400
O	0.36461400	0.07021800	-2.01924800
H	-0.00070700	0.83021000	-2.49083300
O	-0.71349600	-0.93574700	-3.04204200
C	3.08437900	-0.27984500	0.32393100
H	2.58980700	-0.75218800	1.17845100
H	2.77498800	-0.82032300	-0.58130700
C	4.59145600	-0.30431600	0.47969700
H	5.04705200	0.18871900	-0.38708800
H	4.86268800	0.29251100	1.35841300
C	5.14105500	-1.72248100	0.62032900
H	4.67491200	-2.20932900	1.48560200
H	4.84621700	-2.31604400	-0.25343600
C	6.65847600	-1.75813200	0.77243000
H	7.02469000	-2.78369500	0.87248600
H	7.15438400	-1.31190200	-0.09560200
H	6.98125800	-1.20202000	1.65856000
O	2.67123800	1.08235000	0.22249400
C	-3.17752600	-0.39503100	-1.38154200
C	-4.52687000	-0.07568800	-1.49380800
C	-5.25755700	0.19404800	-0.34645200
C	-4.61910200	0.12223000	0.88574000



C	-3.27499200	-0.21786600	0.91843900
H	-2.54454200	-0.61563600	-2.24066600
H	-4.98410000	-0.04070200	-2.47538500
H	-6.30944100	0.45127100	-0.40495400
H	-5.13064500	0.31580500	1.82010700
N	-2.56235400	-0.45855200	-0.19506600
C	-2.59905700	-0.32857300	2.24877100
O	-1.42970700	-0.97564500	2.15109900
H	-0.96094600	-0.92977000	2.99595700
O	-3.06138800	0.09205200	3.27345200
H	-0.22310000	-1.75159200	-2.86738300
Br	0.10709700	-3.12545300	-0.41861400

## 19

Zn	-0.67368700	-0.93505500	-0.34371900
O	0.52675200	0.65449700	0.28491600
C	1.65808900	1.13569200	0.29515000
H	1.44094600	1.44567700	-3.03699400
C	1.87322900	2.59871900	0.39168300
C	0.77809000	3.41801100	0.67313700
C	3.13584900	3.16276300	0.19623100
C	0.94617900	4.79254300	0.76646500
H	-0.19237200	2.95949200	0.82177000
C	3.29730100	4.53906900	0.28327500
H	3.97450900	2.51818200	-0.03416600
C	2.20534600	5.35398200	0.57028200

H	0.09640900	5.42803400	0.99174700
H	4.27632300	4.97827900	0.12477400
H	2.33579600	6.42901800	0.63990900
O	1.85151700	0.68025000	-2.63090400
H	1.12206500	0.01763900	-2.56974900
O	-0.14396100	-1.05847700	-2.17604100
C	2.69252700	-0.98910800	0.06790300
H	2.12618200	-1.43792600	0.88853700
H	2.15392300	-1.14960900	-0.86803300
C	4.10839100	-1.51503200	-0.00094600
H	4.63727200	-0.99461300	-0.80683100
H	4.62842600	-1.27541800	0.93407800
C	4.14161900	-3.02341200	-0.24376700
H	3.58192500	-3.53424300	0.54846600
H	3.61756100	-3.25058700	-1.17972500
C	5.56123900	-3.57744400	-0.30802100
H	5.55806500	-4.65602200	-0.48715800
H	6.13372600	-3.10800700	-1.11436900
H	6.09975800	-3.39830200	0.62816700
O	2.76944700	0.44200000	0.28766000
C	-2.84481200	0.10245000	-2.03677000
C	-4.06768500	0.54278000	-2.53025700
C	-5.06520600	0.90226100	-1.63572300
C	-4.80241700	0.81846300	-0.27471400
C	-3.54713100	0.39192300	0.13887900
H	-2.02450800	-0.22933900	-2.67117900

H	-4.22618700	0.58813100	-3.60119900
H	-6.03430900	1.23826000	-1.98829200
H	-5.53884500	1.07143800	0.47747300
N	-2.58561100	0.03177400	-0.72532100
C	-3.28200900	0.31853900	1.61123600
O	-1.97785000	0.25222700	1.88185400
H	-1.86771700	0.06149300	2.82377200
O	-4.15410800	0.33773600	2.43983500
H	0.00166700	-1.96931500	-2.44029000
Br	-0.72276200	-2.80577400	1.10929400

## 20

Zn	-0.80378000	-0.07862700	-0.94226000
O	0.06150600	-1.73662300	-1.15047900
C	1.31294600	-1.92476400	-1.72409000
H	1.58803900	-1.13344500	-2.44173600
C	2.43950400	-2.04553900	-0.71084100
C	2.16086600	-2.37049000	0.61861400
C	3.77310100	-1.86306900	-1.08819100
C	3.19029900	-2.50852300	1.54968700
H	1.12458700	-2.53346700	0.89721000
C	4.80066100	-2.00661900	-0.16341500
H	4.00613400	-1.60603000	-2.11842600
C	4.51301700	-2.32792100	1.16184600
H	2.95635600	-2.76808500	2.57772900
H	5.83067200	-1.86095000	-0.47393900

H	5.31574700	-2.43757800	1.88360800
O	1.06998700	0.65858400	0.21558900
H	1.52605100	-0.12480100	0.57365500
O	1.16334700	1.62820600	1.27394700
C	2.20823700	2.59706400	0.97033000
C	1.89579400	3.31901700	-0.33231200
H	2.64781100	4.09032500	-0.52109600
H	1.89535400	2.62406400	-1.17275400
H	0.91296700	3.79300000	-0.28819600
C	3.56218000	1.89881800	0.92979300
H	4.35947700	2.63064100	0.77530000
H	3.75479700	1.37277700	1.86859700
H	3.60708800	1.17859900	0.11032400
C	2.10120500	3.53096000	2.17211000
H	2.86375000	4.30965500	2.09601000
H	1.12105800	4.01267900	2.20454600
H	2.25729800	2.98386400	3.10519000
C	-1.98665400	1.01640500	1.66347300
C	-2.75371600	1.08566600	2.82069800
C	-3.61743600	0.04126000	3.12057100
C	-3.69229000	-1.03789100	2.24937700
C	-2.91006600	-1.01706300	1.10375300
H	-1.27955700	1.79480700	1.40196900
H	-2.66260400	1.94637600	3.47220000
H	-4.22385500	0.06494100	4.01933600
H	-4.33740300	-1.88859600	2.42996200

N	-2.06426800	-0.01533200	0.81995400
C	-2.96542200	-2.16737800	0.14713200
O	-2.60946600	-1.77862500	-1.08519000
H	-2.28666500	-2.53881600	-1.59136000
O	-3.28848700	-3.28068500	0.45705700
H	1.30819800	-2.86322500	-2.30721600
Br	-1.40258400	1.77637000	-2.24546800

## 21

Zn	0.51065900	0.08744600	0.81337700
O	-0.17161600	-1.52670600	0.13104500
C	0.60546000	-2.70150400	0.12561500
H	0.06159700	-3.47695500	-0.43077000
C	1.93799600	-2.44209300	-0.53758000
C	2.02948300	-2.36533100	-1.93080200
C	3.06604500	-2.13292700	0.22527400
C	3.21105200	-1.97123200	-2.54718400
H	1.15638200	-2.60096800	-2.53176300
C	4.25314300	-1.73105200	-0.38622500
H	3.01067700	-2.18825200	1.30855800
C	4.32621200	-1.64135400	-1.77465300
H	3.26729300	-1.91617600	-3.62958600
H	5.11926800	-1.49051900	0.22170000
H	5.24971500	-1.33355900	-2.25418100
O	-2.55323000	-0.85482600	0.93236600
H	-1.74229600	-1.29175900	0.54669100
O	-3.30523700	-0.50362100	-0.24293500

C	-4.45462400	-1.36763800	-0.36395500
C	-5.35849300	-1.20514700	0.85456800
H	-6.25043400	-1.83138800	0.76019900
H	-4.82336300	-1.49354600	1.76057200
H	-5.67587900	-0.16367400	0.95634300
C	-4.01099200	-2.81647800	-0.54472800
H	-4.87512600	-3.46408300	-0.71844600
H	-3.33429100	-2.90273500	-1.39913300
H	-3.49268500	-3.17148100	0.34805900
C	-5.12169200	-0.83352700	-1.62747500
H	-6.03321100	-1.39847600	-1.83850300
H	-5.38830100	0.21920300	-1.50383100
H	-4.44996700	-0.92358900	-2.48481100
C	-1.61931100	2.11588800	0.11116900
C	-2.19323700	3.23428700	-0.48435700
C	-1.47339700	3.93592800	-1.43957600
C	-0.20202500	3.49168600	-1.78427800
C	0.30016500	2.36951400	-1.14403700
H	-2.15296200	1.51585400	0.83939500
H	-3.19322700	3.53478900	-0.19684700
H	-1.89575300	4.81254000	-1.91816400
H	0.40615700	3.98404600	-2.53245100
N	-0.39171500	1.70078700	-0.20775200
C	1.65300800	1.86117000	-1.53037000
O	2.01016800	0.80120300	-0.78262700
H	2.84829900	0.41032000	-1.08600300

O	2.32907500	2.32912000	-2.40276700
H	0.77347400	-3.08473200	1.14365900
Br	1.44773800	0.77039300	2.83666200

**TS<sub>20-22</sub>**

Zn	0.55940500	0.31573000	-0.82400900
O	-1.34476300	0.54356500	-1.09374000
C	-2.03602200	-0.59380500	-1.12066200
H	-1.37050000	-1.41912900	-0.45805200
C	-3.39660600	-0.58937600	-0.51061100
C	-3.81725800	0.48259600	0.28012800
C	-4.26423800	-1.66896900	-0.71166900
C	-5.08071400	0.47440600	0.85820900
H	-3.14390300	1.32188900	0.41095800
C	-5.52477700	-1.67809800	-0.13029400
H	-3.94618500	-2.50304300	-1.33173400
C	-5.93649000	-0.60582200	0.65855200
H	-5.40370300	1.31613100	1.46265600
H	-6.19111400	-2.51845300	-0.29564900
H	-6.92307700	-0.61050500	1.11017200
O	-0.23112300	-1.67833200	0.23597400
H	-0.64180200	-1.51697700	1.09612500
O	1.30349400	-1.91635000	1.24296900
C	1.68493400	-3.26464400	1.18266200
C	1.96653200	-3.70600700	-0.25345200
H	2.33566100	-4.73607900	-0.27908400

H	1.05121600	-3.65031400	-0.84606600
H	2.70676000	-3.05023100	-0.71520200
C	0.63110100	-4.16037300	1.84175900
H	0.96476500	-5.20137800	1.88572600
H	0.42722100	-3.81990600	2.86146200
H	-0.29945400	-4.12782800	1.26954900
C	2.98956400	-3.29285100	2.00648400
H	3.38406500	-4.31341300	2.03230700
H	3.73726000	-2.63912400	1.55272400
H	2.80471800	-2.96497300	3.03273100
C	1.51155300	0.98316000	1.98425200
C	1.75412700	1.72737200	3.13444100
C	1.45707000	3.08171600	3.14089200
C	0.93559400	3.65538100	1.98810600
C	0.74163300	2.85199200	0.87411400
H	1.70159800	-0.08682700	1.93654800
H	2.16544000	1.23530400	4.00767100
H	1.62855000	3.68493700	4.02564700
H	0.67920400	4.70523300	1.92306300
N	1.01319500	1.53581900	0.87300000
C	0.21172600	3.48830500	-0.37314100
O	0.42470800	2.71552500	-1.44380200
H	-0.02609900	3.09183400	-2.21234600
O	-0.31221500	4.56849300	-0.40167100
H	-2.00811400	-1.15263100	-2.07579000
Br	2.30873700	-0.23543500	-2.26287400



22

Zn	-1.00817900	-0.09761100	0.45369900
O	1.13361700	-0.27376900	0.21013100
C	1.78915500	-1.08274700	-0.44621400
H	-0.23546600	-1.75031800	-3.49892000
C	3.24510700	-1.17283400	-0.36658800
C	3.98724900	-0.33670900	0.47770800
C	3.89498200	-2.12613700	-1.15855800
C	5.36550500	-0.45928300	0.52648300
H	3.46719800	0.39798600	1.08149600
C	5.27724400	-2.24604800	-1.10586000
H	3.30715800	-2.76657800	-1.80922200
C	6.00901000	-1.41352500	-0.26368300
H	5.94579400	0.18449200	1.17842500
H	5.78424800	-2.98511900	-1.71624800
H	7.08931100	-1.50692800	-0.22042500
O	-0.13059200	-2.13126500	-2.62508400
H	-0.81474300	-1.67645700	-2.06469400
O	-1.89305400	-0.92574400	-1.02445700
C	-3.05171600	-1.75267900	-0.90684900
C	-2.68223200	-3.07292400	-0.22374200
H	-3.54370100	-3.74625300	-0.16240000
H	-1.89203400	-3.57461100	-0.78945000
H	-2.32162700	-2.88792100	0.79187800
C	-3.55282100	-2.02841800	-2.32994600

H	-4.44017200	-2.66876500	-2.32232800
H	-3.81454900	-1.09035000	-2.83055900
H	-2.77445500	-2.52826700	-2.91253800
C	-4.13697500	-1.02316900	-0.11126500
H	-5.05110500	-1.62183000	-0.04285500
H	-3.79545900	-0.81506500	0.90705100
H	-4.38906500	-0.07401400	-0.59565100
C	-1.46883400	1.87193400	-1.75881500
C	-1.32361600	2.90764500	-2.67536200
C	-0.44556700	3.94232700	-2.38875300
C	0.24947500	3.91150400	-1.18669200
C	0.02130900	2.85930600	-0.31024500
H	-2.08942200	0.99844100	-1.94034700
H	-1.88642300	2.88476900	-3.60107500
H	-0.29960600	4.75886200	-3.08758500
H	0.95881600	4.67927700	-0.90438200
N	-0.81655800	1.84808000	-0.59108100
C	0.74938300	2.85920100	0.99950600
O	0.09554100	2.13971000	1.90446000
H	0.61335300	2.07324200	2.71848600
O	1.77619900	3.45879500	1.19114200
H	1.28346200	-1.76109200	-1.15220200
Br	-1.33011100	-0.64280600	2.73211100

**23**

H	-0.65201800	-1.64652900	0.19614700
---	-------------	-------------	------------

O	0.76217600	-1.78531100	-0.50981400
O	-1.52000600	-1.48374400	0.68091500
Zn	1.80289800	-0.21926700	-0.46462900
C	1.07962800	-2.91675000	-1.31371300
C	-2.40174300	-0.83722100	-0.12627600
H	-2.33604400	-1.15595000	-1.17923100
C	2.57206000	-3.23564900	-1.18236300
H	2.82324400	-3.41640400	-0.13268200
H	2.84915300	-4.12370000	-1.75906700
H	3.17717900	-2.39984600	-1.55351900
C	0.25298500	-4.09602100	-0.79467000
H	0.49259900	-4.29193400	0.25396500
H	-0.81565700	-3.87482700	-0.85814600
H	0.45097800	-5.00333500	-1.37345200
C	0.73157700	-2.62347600	-2.77609000
H	-0.33377600	-2.39301800	-2.87001200
H	1.30095200	-1.76225900	-3.13829300
H	0.95378700	-3.47789700	-3.42374200
C	-3.81220700	-0.98955800	0.38644400
C	-4.80932400	-1.53152900	-0.41859100
C	-4.11866900	-0.59713000	1.69081800
C	-6.10524300	-1.68382900	0.06964700
H	-4.57254300	-1.84327300	-1.43223800
C	-5.40979900	-0.74758800	2.17737700
H	-3.33651100	-0.17833400	2.31418600
C	-6.40632300	-1.29134000	1.36798700

H	-6.87615000	-2.10969700	-0.56421500
H	-5.64265900	-0.44234500	3.19243900
H	-7.41460600	-1.40860600	1.75168700
C	-2.67019900	1.39080400	-1.12456100
H	-2.39549400	1.00873500	-2.11826000
H	-3.75725100	1.30112700	-1.01375600
C	-2.23714100	2.83532700	-0.96388000
H	-2.47439400	3.16001300	0.05553900
H	-1.14868800	2.90320000	-1.07500500
C	-2.91217900	3.75925900	-1.97654600
H	-2.68055000	3.41788900	-2.99292500
C	-2.48576500	5.21564400	-1.82095600
H	-2.98334700	5.85593100	-2.55438400
H	-2.73371000	5.59543000	-0.82481800
H	-1.40604000	5.32839100	-1.95925500
H	-4.00118100	3.68302200	-1.86869100
O	-2.04114900	0.59155400	-0.12115400
C	1.93846800	0.77349900	2.34828200
C	3.96423400	-0.14496400	1.74573800
C	4.50738800	0.13801600	2.99218200
C	3.71101300	0.76199100	3.94464400
C	2.40103400	1.08750300	3.61851200
H	4.54901100	-0.62290400	0.96722500
H	5.53613400	-0.12775600	3.20334300
H	4.10648800	0.99506500	4.92710800
H	1.72847200	1.57531800	4.31273900

N	2.70382600	0.16186900	1.43515600
C	0.52857100	1.11962000	1.96096300
O	-0.27833100	1.53448700	2.74760700
O	0.31021900	0.92086100	0.65994000
H	-0.69142500	0.86891200	0.39748900
Br	3.07133800	0.95680300	-2.04220100

## 24

H	-1.11997700	-1.81786800	-0.78735300
O	-2.05385200	-1.60390100	-0.59643400
O	0.38133000	-0.81708400	-0.23680300
Zn	-1.12714000	0.17301400	0.49008500
C	-2.72273100	-2.79932700	-0.11676500
C	1.62715400	-0.88191200	0.26450100
H	1.66037200	-1.06054000	1.35590100
C	-4.09716600	-2.34564500	0.35325900
H	-4.66073700	-1.90891500	-0.47679400
H	-4.66794400	-3.19436900	0.73833600
H	-4.00062400	-1.60547700	1.15178700
C	-2.83190400	-3.77108500	-1.29021200
H	-3.36300500	-3.30395700	-2.12342600
H	-1.83909600	-4.07025500	-1.64052600
H	-3.37134000	-4.67638000	-0.99694900
C	-1.92221400	-3.40930800	1.03104900
H	-0.91814000	-3.68833400	0.69760300
H	-1.82968700	-2.69816800	1.85514400

H	-2.41544900	-4.31135800	1.40468600
C	2.46377800	-1.92706300	-0.44580000
C	3.01876500	-2.99322200	0.25581300
C	2.65340000	-1.84497400	-1.82674100
C	3.75508300	-3.97207400	-0.40917300
H	2.87151300	-3.06134800	1.33038900
C	3.39082800	-2.81589000	-2.49041800
H	2.21857500	-1.01202300	-2.36814600
C	3.94257800	-3.88367900	-1.78308900
H	4.18164000	-4.80059000	0.14709800
H	3.53798500	-2.74393400	-3.56349000
H	4.51757600	-4.64222800	-2.30434500
C	3.48731500	0.63031500	0.80317300
H	3.29335200	0.51090200	1.87947000
H	4.20195900	-0.14545500	0.50269400
C	4.04818000	2.00875500	0.50851800
H	4.17986800	2.11106600	-0.57427400
H	3.31845400	2.77036600	0.80757400
C	5.37376500	2.25938200	1.22521200
H	5.23327300	2.13534600	2.30622000
C	5.94637900	3.64500700	0.94328400
H	6.89483100	3.79817600	1.46558800
H	6.12849300	3.78713400	-0.12656300
H	5.25727800	4.43112100	1.26745700
H	6.10029700	1.49503400	0.92286000
O	2.27345300	0.44505000	0.07626400

C	-1.47121100	2.54764500	-1.33974700
C	-3.43511100	1.36217300	-1.11610400
C	-4.11174200	2.25215100	-1.93924000
C	-3.41569100	3.32369700	-2.48520800
C	-2.06739400	3.46967200	-2.18894800
H	-3.92768400	0.50163100	-0.67969300
H	-5.16396600	2.09888900	-2.14654200
H	-3.91601800	4.03321600	-3.13517700
H	-1.46301900	4.27114100	-2.59484400
N	-2.14274000	1.51110200	-0.81846700
C	-0.00650300	2.65393700	-1.01592100
O	0.75930700	3.28771000	-1.69392300
O	0.29676500	1.96449300	0.07622500
H	1.22545100	1.51982700	0.06305700
Br	-1.95314900	0.34993500	2.68633300

## 25

Zn	0.31270300	-0.87131900	0.55358800
O	-1.13837900	-0.16445900	-0.42033600
C	-1.79646700	1.01028800	-0.16280400
H	-1.65948800	1.33023500	0.89062300
C	-1.34715900	2.15568900	-1.06576600
C	-0.60649100	1.90628000	-2.22003800
C	-1.68517800	3.47280400	-0.75042600
C	-0.20093600	2.95739300	-3.04239300
H	-0.37963400	0.87513100	-2.46981400

C	-1.28151900	4.52203500	-1.56734900
H	-2.27650200	3.67019500	0.13871000
C	-0.53432300	4.26702400	-2.71597000
H	0.36738000	2.75021500	-3.94395400
H	-1.55084900	5.54197200	-1.31139000
H	-0.21954000	5.08627000	-3.35425200
O	1.35729400	1.19510400	0.27648000
H	1.02358900	1.61522000	-0.53701800
O	2.76608800	1.48033000	0.26264400
C	3.05838200	2.60496900	1.14232400
C	2.62620500	2.28773100	2.56657900
H	2.93178200	3.09570600	3.23736500
H	1.54313000	2.17784100	2.63163800
H	3.08102900	1.35634200	2.90986900
C	2.39051100	3.86452800	0.60395100
H	2.66547600	4.72763400	1.21595600
H	2.70248700	4.05919800	-0.42567700
H	1.30227400	3.77438800	0.62796300
C	4.57693400	2.68479500	1.02025600
H	4.94545500	3.52819800	1.60881200
H	5.04544600	1.77253300	1.39714800
H	4.87696300	2.83248900	-0.02018800
C	3.03839200	-1.58162700	-0.60215100
C	4.00507500	-2.19661000	-1.38924600
C	3.61021000	-3.13776100	-2.32996600
C	2.25948200	-3.43695900	-2.45263900



C	1.36148700	-2.79501100	-1.61222300
H	3.29473600	-0.81720300	0.12214100
H	5.04714600	-1.92906700	-1.26264000
H	4.34141000	-3.63059100	-2.96123400
H	1.88453700	-4.15065400	-3.17548200
N	1.74049000	-1.87801700	-0.70929500
C	-0.10074500	-3.09141300	-1.72866800
O	-0.73631200	-2.81909200	-0.58006600
H	-1.67726400	-2.66841300	-0.75180500
O	-0.61960400	-3.51784100	-2.72269600
Br	0.82562900	-1.42979400	2.76712300
C	-3.84343500	0.04462600	0.53952600
H	-3.42544900	-0.96995600	0.49080400
H	-3.67707300	0.41511100	1.56511100
C	-5.32464700	0.02480900	0.21514000
H	-5.44797300	-0.31352400	-0.82051300
H	-5.70601300	1.05209700	0.25337500
C	-6.13058700	-0.86753500	1.15668400
H	-5.72690900	-1.88776600	1.12672500
H	-5.99962200	-0.52082600	2.18957000
C	-7.61794000	-0.90135500	0.81733900
H	-7.78281000	-1.27962300	-0.19697300
H	-8.17198000	-1.54531800	1.50671100
H	-8.05853100	0.09971600	0.87051600
O	-3.19136900	0.89004900	-0.38814200

**TS<sub>25-26</sub>**

Zn	0.44200100	-0.57078600	-0.63894100
O	-0.42981300	1.14194200	-0.90376900
C	-1.25009900	1.56357800	0.04778000
H	-1.08217000	0.76922200	0.98241900
C	-0.94305000	2.90686000	0.66964200
C	0.31128200	3.48378800	0.47467500
C	-1.87973800	3.56013200	1.47449300
C	0.62688800	4.69879500	1.07344900
H	1.02030800	2.97879100	-0.17051100
C	-1.56256700	4.77377500	2.07148900
H	-2.85777200	3.11540100	1.61497900
C	-0.30762100	5.34559200	1.87582300
H	1.60142000	5.14631700	0.90549400
H	-2.29838400	5.27838100	2.68936400
H	-0.06232300	6.29403400	2.34257000
O	-0.31979700	-0.30269700	1.53191500
H	0.19588500	0.31005400	2.07341300
O	0.74538200	-1.60935100	2.21282000
C	-0.01353700	-2.40102500	3.09265600
C	-1.22703100	-3.01242500	2.39327100
H	-1.75047600	-3.70491600	3.05963600
H	-1.92320600	-2.22396700	2.09926400
H	-0.91782500	-3.54581500	1.49269000
C	-0.43046900	-1.59603400	4.32678700
H	-0.94492500	-2.22714700	5.05742200

H	0.44787600	-1.15650500	4.80894300
H	-1.11213900	-0.79128900	4.03957500
C	0.97849600	-3.51150300	3.49223100
H	0.49584900	-4.19682300	4.19584400
H	1.29008600	-4.07472400	2.61031500
H	1.86257700	-3.08572200	3.97388100
C	-3.06034000	0.28673900	-0.83522100
H	-2.58556100	0.18273000	-1.81588700
H	-2.75640900	-0.57697100	-0.22667700
C	-4.56941700	0.35209000	-0.95872900
H	-5.00416600	0.46851100	0.04108400
H	-4.83593900	1.25354500	-1.52284800
C	-5.15376900	-0.88358500	-1.64033600
H	-4.70896900	-0.99378700	-2.63676100
H	-4.86262300	-1.78084200	-1.08091800
C	-6.67328600	-0.83001000	-1.76343100
H	-7.06491300	-1.72375800	-2.25713900
H	-7.14834700	-0.75927900	-0.77956400
H	-6.99321000	0.03933000	-2.34700300
O	-2.61426500	1.48819200	-0.21021700
C	3.15967500	-0.62125500	0.71313900
C	4.51152900	-0.38535500	0.94058300
C	5.24833400	0.30360900	-0.01069100
C	4.61010900	0.72684300	-1.16951000
C	3.26298400	0.43764300	-1.33227000
H	2.53512500	-1.14210800	1.43472000

H	4.96532000	-0.74030700	1.85812200
H	6.30254200	0.50720700	0.14171900
H	5.12328200	1.26948100	-1.95333700
N	2.54375900	-0.21467800	-0.40281600
C	2.59765200	0.87192600	-2.60174000
O	1.44037400	0.23206300	-2.79139200
H	0.97907700	0.61104500	-3.55228400
O	3.06762500	1.67819900	-3.35805600
Br	-0.10024400	-2.69490300	-1.45558700

## 26

Zn	-1.99370100	-0.38209100	-0.29318300
O	1.63306200	0.31828800	-0.01222800
C	2.67492200	0.86453400	-0.29889600
H	-1.48515900	1.54763100	-2.07576300
C	2.80634800	2.32189300	-0.56922400
C	1.63862500	3.08655600	-0.62821100
C	4.04941400	2.93153700	-0.75631500
C	1.71750700	4.45146900	-0.87212200
H	0.67938400	2.59842800	-0.49545200
C	4.12203800	4.29842200	-0.99284800
H	4.94899700	2.33003100	-0.71428600
C	2.95746600	5.05928400	-1.05112500
H	0.80855700	5.04134100	-0.92615400
H	5.08809700	4.77137200	-1.13468500
H	3.01675400	6.12638900	-1.24005500

O	-1.62718400	1.71453400	-1.13850600
H	-2.60543700	1.67337700	-0.99185400
O	-3.64413000	0.57490400	-0.08219900
C	-4.95627200	0.08953200	-0.27877300
C	-5.24214900	-0.05241400	-1.77880300
H	-6.25695500	-0.41833400	-1.96796200
H	-5.13378400	0.91742200	-2.27509900
H	-4.53391200	-0.75055700	-2.23465000
C	-5.91780600	1.10735000	0.34419000
H	-6.96369700	0.81154100	0.21315300
H	-5.71736900	1.20678100	1.41506100
H	-5.77598200	2.08732300	-0.12094600
C	-5.11887900	-1.26914500	0.41184700
H	-6.13768900	-1.65815100	0.31388900
H	-4.43762900	-2.00401800	-0.03219700
H	-4.88627500	-1.17963000	1.47738300
C	3.79769100	-1.21064400	-0.19059700
H	3.36911200	-1.40956300	0.79495900
H	3.13140500	-1.65393900	-0.93681900
C	5.20941200	-1.74234800	-0.31393200
H	5.61040100	-1.47097300	-1.29724000
H	5.84393700	-1.25051600	0.43264600
C	5.26786700	-3.25783000	-0.12836300
H	4.84079900	-3.52170900	0.84657600
H	4.62987900	-3.73987500	-0.87920700
C	6.68489800	-3.81284600	-0.23398600

H	6.69821900	-4.89795500	-0.10019800
H	7.12434900	-3.59350800	-1.21222800
H	7.33919500	-3.37637300	0.52744500
O	3.84113500	0.21472900	-0.40692900
C	-1.64977800	1.25023100	2.10012800
C	-1.13768000	1.83253400	3.25277900
C	-0.11327300	1.19018200	3.93321900
C	0.35089800	-0.02574400	3.44995000
C	-0.22403300	-0.54811500	2.30089100
H	-2.46163500	1.69102800	1.53137500
H	-1.54136800	2.77619600	3.59934800
H	0.31403000	1.62410900	4.83062500
H	1.14009600	-0.58341600	3.93784100
N	-1.19406900	0.08539500	1.62639500
C	0.23493600	-1.88379000	1.81123800
O	-0.67955400	-2.43727300	1.01112600
H	-0.30789200	-3.21944500	0.57961000
O	1.27265200	-2.40049500	2.13263400
Br	-1.35570500	-1.75918300	-2.10148200

**27**

Zn	-0.77256000	-0.06527200	-0.75064400
O	0.26626300	-1.42400400	-1.54162000
C	1.45762800	-1.22303000	-2.22839000
H	1.55224100	-0.20739500	-2.64812200
C	2.69673900	-1.50105500	-1.39381100

C	2.60813400	-2.28131000	-0.23889400
C	3.94954300	-1.01126300	-1.77420700
C	3.74443200	-2.56623800	0.51830000
H	1.63557100	-2.67742100	0.03528000
C	5.08390300	-1.29889800	-1.02431400
H	4.03448700	-0.39888900	-2.66837000
C	4.98570000	-2.07688900	0.12790700
H	3.65867400	-3.18124700	1.40901200
H	6.04891300	-0.91022700	-1.33463600
H	5.87170200	-2.29932500	0.71344700
O	1.12342900	0.52718500	0.49786800
H	1.69917000	-0.25849200	0.53305700
O	1.21409300	1.08425600	1.82037700
C	2.14349400	2.20664600	1.82699000
C	1.65431300	3.29874500	0.88652900
H	2.33362000	4.15521700	0.91983300
H	1.60808900	2.93441100	-0.14053100
H	0.65510200	3.63706300	1.16957200
C	3.54202100	1.72138900	1.46578100
H	4.25908800	2.54192800	1.55303300
H	3.85764400	0.91674700	2.13524000
H	3.57824400	1.35467600	0.43784800
C	2.06722200	2.64268300	3.28687200
H	2.73704500	3.49052200	3.44894900
H	1.05251400	2.95363400	3.54677400
H	2.36908500	1.83045600	3.95266600

C	-1.77425100	-0.00629000	2.13616800
C	-2.40030800	-0.41207600	3.30889300
C	-3.07313400	-1.62615100	3.32847500
C	-3.10212900	-2.39551100	2.17223900
C	-2.47265600	-1.90565200	1.03719500
H	-1.20926500	0.91662000	2.08129900
H	-2.34851000	0.21788000	4.18865600
H	-3.56618700	-1.97148500	4.23052300
H	-3.59722500	-3.35738000	2.12513800
N	-1.81293100	-0.73772900	1.02016600
C	-2.47338500	-2.71347000	-0.22322800
O	-2.33159200	-1.92015600	-1.29416400
H	-1.93789400	-2.41753600	-2.02680700
O	-2.58387800	-3.90781300	-0.25196600
I	-1.75948100	2.14665900	-1.47748600
H	1.49758700	-1.90594700	-3.09589600

**TS<sub>27-28</sub>**

Zn	0.81488300	0.73856300	-0.53730600
O	-0.83293600	1.64132700	-0.32223700
C	-1.94829300	1.05552100	-0.77229100
H	-1.94991200	-0.13634700	-0.35656800
C	-3.23566400	1.63743000	-0.30344900
C	-3.26116300	2.55675800	0.74820000
C	-4.44171100	1.25186600	-0.89974200
C	-4.46935200	3.07938300	1.19363700



H	-2.31950600	2.85916700	1.19160700
C	-5.64790000	1.77188800	-0.45096600
H	-4.42940300	0.54019000	-1.72085000
C	-5.66571700	2.68776800	0.59899000
H	-4.47909000	3.79912900	2.00614500
H	-6.57665200	1.46795600	-0.92281200
H	-6.60810200	3.09701800	0.94797200
O	-1.59827300	-1.22561600	0.25543900
H	-2.07105500	-1.02341700	1.07350200
O	-1.07400400	-2.73077200	1.21655900
C	-1.49795000	-3.86797900	0.51962800
C	-0.86620200	-3.94100900	-0.87249400
H	-1.14667800	-4.86465600	-1.38853600
H	-1.19634600	-3.09294000	-1.47541900
H	0.22376600	-3.90192400	-0.79945000
C	-3.02691100	-3.91802600	0.43075700
H	-3.37080000	-4.84219700	-0.04394200
H	-3.46460900	-3.85801800	1.43151600
H	-3.39006300	-3.07239500	-0.15727500
C	-0.98772800	-5.03388500	1.39158200
H	-1.28490000	-5.98968500	0.94825100
H	0.10244900	-5.00781800	1.46264100
H	-1.40774600	-4.96817100	2.39822800
C	1.31961400	-0.95726200	1.89165500
C	1.87983100	-1.34842800	3.10583300
C	2.77861200	-0.50894100	3.74519200

C	3.09183500	0.71182700	3.15678700
C	2.49043300	1.03455000	1.95086900
H	0.59822200	-1.59453500	1.37863000
H	1.59648900	-2.30513800	3.52741600
H	3.23021600	-0.79333500	4.68919600
H	3.78260900	1.41548100	3.60390300
N	1.62488700	0.21602900	1.32923900
C	2.81359700	2.34422800	1.31423100
O	2.13495700	2.51573400	0.15699200
H	2.37663500	3.36322300	-0.24190500
O	3.57483600	3.15510500	1.75957800
I	1.96863700	-0.25946700	-2.52659100
H	-1.96260000	0.81069200	-1.84957200

## 28

Zn	-0.67785600	-0.36622000	-0.05461400
O	1.37013400	0.47786800	0.24051200
C	2.38862200	-0.05639700	-0.18104400
H	1.12430300	0.24327700	-3.90875000
C	3.73453700	0.35635800	0.21337700
C	3.92733300	1.34660400	1.18451300
C	4.83530700	-0.25574500	-0.39339500
C	5.21326900	1.71634100	1.54192000
H	3.05815400	1.80042400	1.64724600
C	6.12293600	0.12169100	-0.03648800
H	4.67288400	-1.01774500	-1.14947400

C	6.30933300	1.10530500	0.93074600
H	5.37018800	2.47768800	2.29830400
H	6.97927500	-0.34806700	-0.50756100
H	7.31525200	1.39805500	1.21374800
O	1.47270100	0.21379500	-3.01564700
H	0.80739400	-0.33149000	-2.51707100
O	-0.30230500	-1.23918300	-1.68678000
C	-0.51829200	-2.60545100	-1.99326000
C	0.43271200	-3.48867200	-1.17681600
H	0.28464400	-4.55201000	-1.39269000
H	1.47313200	-3.23919700	-1.40794200
H	0.26943000	-3.33389500	-0.10575600
C	-0.23938000	-2.78379700	-3.48989300
H	-0.37054500	-3.82414800	-3.80312200
H	-0.92125900	-2.15853600	-4.07413400
H	0.78630800	-2.47998500	-3.71776700
C	-1.97046000	-2.98462700	-1.68737500
H	-2.18269600	-4.02408100	-1.95803900
H	-2.17441200	-2.86754500	-0.61776400
H	-2.65089900	-2.33375700	-2.24353700
C	-0.41011500	2.34931100	-1.36855800
C	-0.63397700	3.68723400	-1.67541100
C	-1.82486100	4.28107900	-1.28459000
C	-2.77342200	3.50390700	-0.63306400
C	-2.48530200	2.16807000	-0.39011100
H	0.50100200	1.84667000	-1.67782500

H	0.12671200	4.24344100	-2.21005300
H	-2.02029100	5.32709600	-1.49405300
H	-3.73171000	3.89596800	-0.31651200
N	-1.31224400	1.60470000	-0.71950500
C	-3.54647200	1.32009300	0.23723500
O	-3.34442500	0.01975100	-0.01153000
H	-3.95487400	-0.49671800	0.53458600
O	-4.47931900	1.76170600	0.85204200
I	-1.06910100	-1.09705700	2.36160900
H	2.31686200	-0.88703100	-0.89763800

## 29

Zn	0.30544600	-0.84061200	0.13917400
O	-1.13804200	0.02608000	-0.72079200
C	-1.90556100	1.02876800	-0.18185800
H	-1.76877700	1.09644700	0.91693600
C	-1.59208400	2.39669500	-0.78108900
C	-0.82520600	2.51059300	-1.93932400
C	-2.07900600	3.55604800	-0.17518500
C	-0.53940300	3.76445300	-2.47938500
H	-0.48254600	1.59975600	-2.41918000
C	-1.79518700	4.80637900	-0.71064900
H	-2.69126700	3.47091200	0.71757000
C	-1.02086900	4.91448900	-1.86463100
H	0.05107100	3.84009800	-3.38729500
H	-2.17947100	5.70077400	-0.23032800

H	-0.80022800	5.89115300	-2.28307300
O	1.22402900	1.30248700	0.34109000
H	0.83342300	1.84521800	-0.36751500
O	2.60236500	1.70885800	0.37133500
C	2.81571800	2.66568600	1.44981800
C	2.47762500	2.02889400	2.79046400
H	2.66927000	2.73708200	3.60143500
H	1.42701600	1.73784300	2.82820300
H	3.08319100	1.13584000	2.96054300
C	2.00072200	3.92710700	1.19061300
H	2.22484500	4.68212300	1.94870600
H	2.23757800	4.34544200	0.20874200
H	0.92926000	3.72066300	1.23308200
C	4.31117200	2.93346600	1.31308700
H	4.62242300	3.65728800	2.07000200
H	4.88508700	2.01548700	1.46071400
H	4.54560000	3.34106100	0.32672400
C	-3.82891200	-0.26770400	0.30292900
H	-3.34685800	-1.20749800	0.00064500
H	-3.63186600	-0.13667300	1.38002000
C	-5.32135600	-0.32782400	0.03968700
H	-5.76874700	0.62707100	0.33954200
H	-5.48058300	-0.41800400	-1.04128400
C	-6.00952500	-1.47974400	0.76835000
H	-5.54985400	-2.42923600	0.46646600
H	-5.83068000	-1.38811600	1.84694200

C	-7.51142200	-1.53752400	0.50636900
H	-7.97923800	-2.37088600	1.03836200
H	-8.00502100	-0.61625500	0.83221900
H	-7.72224500	-1.66364500	-0.56053400
O	-3.28760200	0.82219000	-0.42059500
C	3.18158000	-1.21509800	-0.78940400
C	4.26233600	-1.59091800	-1.57821100
C	4.02417100	-2.22607200	-2.78940200
C	2.71136800	-2.46700400	-3.17409500
C	1.69102800	-2.08003800	-2.31777000
H	3.31509800	-0.69225700	0.15007300
H	5.26990800	-1.37929500	-1.24141200
H	4.84755200	-2.52752500	-3.42750200
H	2.45790000	-2.94428600	-4.11242200
N	1.91973500	-1.45866900	-1.15065100
C	0.26330500	-2.30393300	-2.70798800
O	-0.51950700	-2.36601200	-1.62113100
H	-1.42301900	-2.08738500	-1.83693500
O	-0.11264300	-2.40172700	-3.84271000
I	0.65373400	-1.94546200	2.38430900

**TS<sub>29-34</sub>**

Zn	0.38349200	-0.52895400	-0.51278500
O	-0.37221300	1.19624300	-0.99527100
C	-1.09735900	1.81750900	-0.07614300
H	-0.95066900	1.14232900	0.95069300

C	-0.63676200	3.19500400	0.34486900
C	0.63709000	3.63385000	-0.01298300
C	-1.45190200	4.01977700	1.12429900
C	1.09173800	4.88206000	0.39942400
H	1.25039600	2.99564800	-0.63785900
C	-0.99554500	5.26551500	1.53604200
H	-2.44638000	3.68138900	1.39046500
C	0.27853600	5.69960600	1.17752500
H	2.07981800	5.22102400	0.10454900
H	-1.63742200	5.90307000	2.13548700
H	0.63261300	6.67367600	1.49906700
O	-0.23943900	0.10676400	1.62466500
H	0.35912900	0.75068800	2.02718600
O	0.75290800	-1.16712100	2.46234500
C	0.01592000	-1.68512500	3.54121000
C	-1.31271200	-2.28378300	3.08088800
H	-1.83619400	-2.75550200	3.91820100
H	-1.95272200	-1.49937300	2.67155800
H	-1.14420900	-3.02906200	2.30146500
C	-0.20079400	-0.61743300	4.61745700
H	-0.68998900	-1.03717900	5.50126100
H	0.75722500	-0.18771100	4.92505800
H	-0.83655000	0.18358700	4.23135600
C	0.93817000	-2.79993400	4.07398600
H	0.46285900	-3.29146400	4.92856000
H	1.11810500	-3.54354300	3.29493200

H	1.89635200	-2.38685600	4.39963100
C	-3.05851700	0.63551700	-0.74604800
H	-2.65290700	0.39925000	-1.73486300
H	-2.79464200	-0.19306300	-0.07364300
C	-4.56082900	0.82714900	-0.80017800
H	-4.92766500	1.05945800	0.20657700
H	-4.77927300	1.70246700	-1.42302800
C	-5.28611800	-0.39975000	-1.34946400
H	-4.91346800	-0.62100100	-2.35698500
H	-5.03696600	-1.27550300	-0.73807100
C	-6.80058400	-0.22266300	-1.39420800
H	-7.29440400	-1.11289300	-1.79361800
H	-7.20742900	-0.03769000	-0.39475000
H	-7.08191400	0.62556400	-2.02668100
O	-2.47452500	1.84460600	-0.26620700
C	3.15455700	-0.56867600	0.74471500
C	4.52300100	-0.37178000	0.89769500
C	5.24964500	0.17670700	-0.14828100
C	4.58456000	0.50125600	-1.32372400
C	3.22172900	0.25490300	-1.40781300
H	2.53693400	-0.97247400	1.54319500
H	4.99750700	-0.64494600	1.83259800
H	6.31641200	0.34806300	-0.05512400
H	5.08878100	0.93397600	-2.17855900
N	2.51342700	-0.25936100	-0.38816000
C	2.52343800	0.57727800	-2.69272200



O	1.35815100	-0.06996300	-2.79192700
H	0.87305300	0.25421000	-3.56350400
O	2.97651400	1.30752700	-3.53186600
I	-0.38113000	-2.87864800	-1.02486200

**Structure 30**

C	-2.25436800	-1.98032800	0.00138700
H	-2.74104000	-2.41338100	-0.88333200
O	-0.88547700	-2.33894200	-0.00116600
Zn	0.32121500	-1.00104700	0.00000500
C	-2.44297500	-0.48331700	0.00076000
C	-2.48241900	0.22974200	-1.20386200
C	-2.48000600	0.23094800	1.20475300
C	-2.55003500	1.61929100	-1.20470100
H	-2.46906100	-0.31496200	-2.14390600
C	-2.54760900	1.62051800	1.20437400
H	-2.46487500	-0.31283400	2.14531500
C	-2.58059300	2.31627600	-0.00047600
H	-2.58420500	2.15855000	-2.14553600
H	-2.57985700	2.16070600	2.14474300
H	-2.63327500	3.39973700	-0.00096900
H	-2.73776900	-2.41209100	0.88854700
I	2.25821700	0.47468700	-0.00017100

**30a**

Zn	0.94805200	0.03802300	0.00045500
O	-0.82564300	0.19360600	0.00111600

C	-1.74845100	-0.87144300	0.00080200
H	-1.61537000	-1.51484700	0.88438300
H	-1.61474300	-1.51499000	-0.88257900
C	-3.17179400	-0.35926200	0.00024600
C	-3.45468900	1.00303000	0.00027300
C	-4.22884500	-1.27225400	-0.00027300
C	-4.77494600	1.44684700	-0.00021400
H	-2.62999800	1.70539200	0.00067600
C	-5.54552400	-0.83028200	-0.00075500
H	-4.02016400	-2.33944900	-0.00030000
C	-5.82348300	0.53468800	-0.00072600
H	-4.98300300	2.51226400	-0.00018800
H	-6.35707600	-1.55098400	-0.00115600
H	-6.85148400	0.88195500	-0.00110400
I	3.37211000	0.02307900	-0.00034800

### **TS30a-31**

C	-1.47031100	-1.11331100	0.58158600
H	-0.66882000	-1.07609000	-0.83275300
O	-0.66882600	-0.63485300	1.48245300
Zn	0.66629900	-0.49931000	0.00634900
C	-2.70106500	-0.38166800	0.19669200
C	-3.67592300	-1.00799500	-0.58380100
C	-2.90657200	0.92021300	0.65651300
C	-4.84249200	-0.33285900	-0.91372400
H	-3.51453900	-2.02378200	-0.93413100
C	-4.07702800	1.59152500	0.32993300

H	-2.14924500	1.37826200	1.28283700
C	-5.04225400	0.96857000	-0.45795700
H	-5.59860800	-0.81886800	-1.52074200
H	-4.24120000	2.60095000	0.69155900
H	-5.95524900	1.49606900	-0.71370000
H	-1.56291700	-2.20558500	0.48346200
I	2.96879400	0.31774200	-0.17664300

**31**

C	-1.71580500	0.80486400	-0.00001300
H	0.78125500	2.67163600	0.00000300
O	-0.68113400	0.15068300	-0.00006800
Zn	1.28620400	1.21447100	-0.00004200
C	-3.04996800	0.21526500	-0.00000100
C	-4.16665900	1.05811700	0.00007200
C	-3.21634800	-1.17618700	-0.00006300
C	-5.44408600	0.51532500	0.00008100
H	-4.02696100	2.13521400	0.00012000
C	-4.49258100	-1.71266400	-0.00005300
H	-2.33564200	-1.80863400	-0.00011800
C	-5.60395300	-0.86776300	0.00001800
H	-6.31272100	1.16417300	0.00013600
H	-4.62997200	-2.78829200	-0.00010200
H	-6.60215000	-1.29313300	0.00002500
H	-1.66269400	1.90913600	0.00004500
I	2.97713600	-0.61606500	0.00002700

**32**

Zn	0.24676400	0.10538600	-0.37888300
O	-0.30785600	-1.43505600	-1.24980700
C	-1.64312800	-1.64275200	-1.64844200
H	-1.74797700	-2.70581500	-1.91078800
C	-2.66181400	-1.29150200	-0.58646800
C	-2.40352600	-1.55463100	0.76221000
C	-3.88127100	-0.70861900	-0.93417600
C	-3.34284700	-1.23680400	1.73827600
H	-1.46453100	-2.01923700	1.04933200
C	-4.82372100	-0.39654800	0.03972300
H	-4.09020800	-0.48781000	-1.97733300
C	-4.55587400	-0.65790400	1.37986800
H	-3.12676000	-1.44574300	2.78099900
H	-5.76374500	0.06382900	-0.24680000
H	-5.28697700	-0.40688500	2.14112000
H	-1.86856100	-1.07282200	-2.56065000
O	1.20959000	-2.49181100	0.51795900
H	0.57907500	-2.37265600	-0.25145600
O	1.77767300	-1.16761100	0.53866100
C	3.21974800	-1.24078700	0.25170500
C	3.43376000	-1.81169200	-1.14253300
H	4.50233900	-1.83880700	-1.37155600
H	3.04262700	-2.82788100	-1.20716700
H	2.93821700	-1.19776300	-1.89961000
C	3.86368000	-2.09952200	1.33126800
H	4.94385200	-2.14761900	1.16997000
H	3.67747600	-1.67275000	2.31948300
H	3.46196100	-3.11279400	1.30631200

C	3.67307700	0.20797500	0.35146100
H	4.75799900	0.25086000	0.22729800
H	3.22207000	0.83100900	-0.42497700
H	3.42106500	0.63070500	1.32627100
I	0.27727100	2.52307800	0.06007900

**32a**

Zn	0.24773100	-0.10550700	0.37902900
O	-0.30793400	1.43466900	1.24959800
C	-1.64321500	1.64227300	1.64842700
H	-1.74795800	2.70527100	1.91104900
C	-2.66197200	1.29132700	0.58647400
C	-2.40377200	1.55462900	-0.76217600
C	-3.88151200	0.70866200	0.93423400
C	-3.34327100	1.23718200	-1.73817600
H	-1.46464900	2.01896200	-1.04929900
C	-4.82415400	0.39697000	-0.03960500
H	-4.09036400	0.48770500	1.97737800
C	-4.55640400	0.65851400	-1.37972700
H	-3.12726200	1.44622200	-2.78089500
H	-5.76424900	-0.06323900	0.24694900
H	-5.28765400	0.40782100	-2.14094400
H	-1.86852000	1.07210400	2.56049500
O	1.20965900	2.49203600	-0.51728800
H	0.57865000	2.37237500	0.25174800
O	1.77774000	1.16780500	-0.53850300
C	3.21974300	1.24085300	-0.25178900
C	3.43409200	1.81116100	1.14264700
H	4.50274600	1.83846500	1.37129600

H	3.04263000	2.82717900	1.20786600
H	2.93903500	1.19671200	1.89962700
C	3.86355000	2.10004700	-1.33109300
H	4.94380600	2.14758900	-1.17023000
H	3.67672900	1.67394600	-2.31948100
H	3.46223700	3.11345900	-1.30537000
C	3.67303500	-0.20789400	-0.35229600
H	4.75804000	-0.25086800	-0.22892600
H	3.22254700	-0.83116900	0.42425400
H	3.42035600	-0.63027900	-1.32708600
I	0.27697200	-2.52312200	-0.06021300

### TS32a-33

Zn	-0.56976600	-0.38572200	0.11942400
O	1.24580100	-0.98946400	0.14428400
C	2.11260300	-0.50823100	-0.75373800
H	1.75469100	0.62204900	-1.03068100
C	3.53528500	-0.38802800	-0.31235900
C	3.87855800	-0.53729500	1.03297600
C	4.53705900	-0.10551600	-1.24736200
C	5.20227000	-0.40668800	1.43454600
H	3.09573700	-0.77760200	1.74322600
C	5.85844800	0.02745500	-0.84420400
H	4.27619100	0.00667400	-2.29651000
C	6.19423900	-0.12089600	0.49992200
H	5.46401800	-0.53436200	2.47995900
H	6.62941200	0.24267200	-1.57668200
H	7.22717600	-0.01971000	0.81614500

H	2.03062100	-0.94809200	-1.76568900
O	0.59332200	1.48373800	-0.56072200
H	1.13951200	1.75149900	0.19253700
O	-0.84391900	1.66863400	0.53021900
C	-1.78511500	2.64071900	0.08766400
C	-2.24714900	2.35161100	-1.33738100
H	-2.97844400	3.09762900	-1.66003500
H	-1.39552400	2.38832400	-2.02098800
H	-2.71381900	1.36562700	-1.40373900
C	-1.13926500	4.01888700	0.19985500
H	-1.85025900	4.80256700	-0.07473000
H	-0.80056800	4.20028700	1.22304700
H	-0.27988000	4.08513000	-0.47210000
C	-2.94590000	2.49290700	1.08665500
H	-3.71678500	3.23145200	0.84634700
H	-3.38356900	1.49501400	1.02423900
H	-2.59946700	2.66760400	2.10735400
I	-2.67875300	-1.70184700	-0.03215300

### 33

Zn	0.94838900	-0.08459900	0.04067100
O	-1.05027500	-0.65498700	0.09777100
C	-1.96023600	0.12597500	0.39451700
H	-1.47289300	1.97761000	-2.26644000
C	-3.36774300	-0.21615200	0.24661900
C	-3.75610300	-1.49083800	-0.18504800
C	-4.33267900	0.75148800	0.54489700
C	-5.10228200	-1.79188100	-0.30773700
H	-2.99040600	-2.22420600	-0.41163400

C	-5.67999800	0.44618500	0.41616200
H	-4.01637100	1.74213500	0.85439800
C	-6.06211500	-0.82432700	-0.00716800
H	-5.41131000	-2.77792000	-0.63685900
H	-6.43207200	1.19438300	0.64037600
H	-7.11587600	-1.06396100	-0.10592200
H	-1.72424500	1.10386400	0.82791000
O	-1.61621000	2.16097800	-1.33554400
H	-0.72066300	2.13022700	-0.92651000
O	0.68073800	1.74441400	0.00934700
C	1.72505600	2.71087700	0.11774400
C	2.59512100	2.39899100	1.33677100
H	3.38409200	3.14560100	1.47018400
H	1.98193500	2.38168400	2.24241300
H	3.07881700	1.42141600	1.22737100
C	1.04663600	4.07182300	0.29044400
H	1.78419900	4.87674900	0.36124400
H	0.38703900	4.27970700	-0.55633100
H	0.44017600	4.07664000	1.20023200
C	2.57040800	2.69482500	-1.15869800
H	3.36441500	3.44738800	-1.12697800
H	3.03982400	1.71470500	-1.29496700
H	1.94125600	2.89765200	-2.03021000
I	2.48792500	-2.01982500	-0.01871700

901599

C	-2.00728000	-0.52217000	-1.89006700
H	-2.25479200	0.54273900	-1.91413500
O	-0.60008400	-0.68119000	-1.59337600



Zn	0.65192000	0.61951500	-0.43302000
C	-2.82454900	-1.23566700	-0.85327200
C	-3.71522000	-0.53272500	-0.04441400
C	-2.70498600	-2.61875500	-0.69363100
C	-4.48571100	-1.20143600	0.90282600
H	-3.79917100	0.54429600	-0.14958900
C	-3.46736100	-3.28587300	0.25556300
H	-2.00720100	-3.17141200	-1.31529600
C	-4.36266800	-2.57739500	1.05429500
H	-5.17615500	-0.64387000	1.52671700
H	-3.36891900	-4.36030600	0.37058100
H	-4.96141000	-3.09909100	1.79364700
H	-2.18861500	-0.94691800	-2.88248800
I	-0.61584800	2.56382600	0.48588500
C	1.86302100	-0.88848400	2.01180100
C	2.84754900	-1.66472700	2.60235700
C	3.90906400	-2.10916700	1.81865000
C	3.95202900	-1.76457600	0.47518600
C	2.93077400	-0.98159600	-0.04639800
H	1.01643200	-0.51056500	2.57497000
H	2.78087500	-1.91145700	3.65504200
H	4.69470000	-2.71674500	2.25526300
H	4.74675800	-2.07542400	-0.19126700
N	1.91067000	-0.56213200	0.71608400
C	2.92181600	-0.56939900	-1.52093800
O	1.93937600	0.20099500	-1.86083000
H	-0.06846900	-0.66958900	-2.40103100
O	3.80505500	-0.99519700	-2.23680200

901623

C	1.85424000	-0.89241800	-2.30040000
H	1.80649300	-1.99385200	-2.33988100
O	0.58323800	-0.30979800	-2.21990200
Zn	-0.43941700	-0.51373600	-0.69306400
C	2.73905400	-0.49203300	-1.13794100
C	2.87016500	-1.32015800	-0.01971800
C	3.37623600	0.75251600	-1.12159000
C	3.61819100	-0.91903400	1.08602300
H	2.38632600	-2.29322600	-0.01843200
C	4.13004000	1.15507500	-0.02474000
H	3.28013300	1.40495200	-1.98459000
C	4.25209000	0.31978200	1.08505600
H	3.71540100	-1.58056700	1.94106800
H	4.63297900	2.11733100	-0.03684400
H	4.84946100	0.62790400	1.93740700
H	2.32694400	-0.56149700	-3.23725300
I	-1.41724700	-2.26638800	0.82601900
C	0.52372800	1.64959900	1.23630300
C	0.57873600	2.86299300	1.91390200
C	-0.38584400	3.82540700	1.65112500
C	-1.37277500	3.54890000	0.71275300
C	-1.35274500	2.31325600	0.08158300
H	1.26300700	0.87354300	1.40659200
H	1.37060500	3.03831300	2.63184300
H	-0.37042400	4.77978100	2.16555900
H	-2.15029200	4.25769900	0.45720800
N	-0.42686100	1.38099700	0.34138100
C	-2.39911600	2.00582300	-0.93863600

O	-2.25390700	0.76325900	-1.44454200
O	-3.26517000	2.76273200	-1.27616600
H	-2.93128200	0.60553000	-2.11686000