

Supplementary Information

Dinuclear *versus* Mononuclear Pathways in Zinc Mediated Nucleophilic Addition: A Combined Experimental and DFT Study

Xiaotian Qi,^{1,2} Yingzi Li,¹ Guanghui Zhang,² Yang Li,¹ Aiwen Lei,^{2*}

Chao Liu,^{2*} and Yu Lan^{1*}

¹*School of Chemistry and Chemical Engineering, Chongqing University, Chongqing, 400030 (P. R. China),*

²*College of Chemistry and Molecular Sciences, Wuhan University, Wuhan, Hubei, 430072 (P. R. China).*

aiwenlei@whu.edu.cn

chao.liu@whu.edu.cn

lanyu@cqu.edu.cn

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1. Complete Reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2013.

2. Absolute Calculation Energies, Enthalpies, and Free Energies

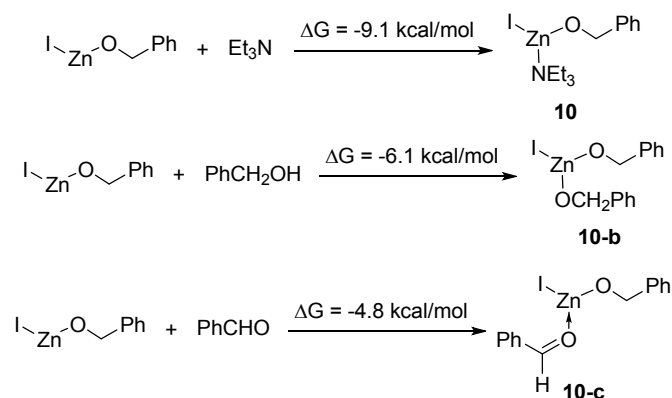


Figure S1. Calculated free energies for the combination of IZnOCH₂Ph with Et₃N, PhCH₂OH and PhCHO.

The combination of IZnOCH₂Ph with Et₃N, PhCH₂OH and PhCHO were calculated, respectively. As shown in Figure S1, the coordination free energies of these complex to generate complex **10-a**, **10-b** and **10-c** is 9.1, 6.1 and 4.8 kcal/mol exothermic, respectively. Therefore, although the coordination of IZnOCH₂Ph with

Et₃N, PhCH₂OH and PhCHO is considered, the formation of final product in monometallic mechanism is still uphill.

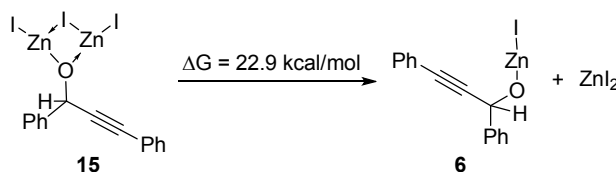


Figure S2. The dissociation of ZnI₂ from complex **15**.

As shown in Figure S2, the dissociation of ZnI₂ is calculated to be 22.9 kcal/mol endothermic. Consequently, the combination of dinuclear (step 1) and mononuclear (step 2) mechanisms is supposed to be disadvantageous.

Besides two pathways shown in the manuscript, we also calculated the pathway employing ZnI₂(Et₃N)₂ complex as the active catalytic species. When phenylacetylene is utilized to replace the ligand Et₃N, the structure of alkyne coordinated zinc complex **1-b** is shown in Figure S3. The distance between zinc and the terminal carbon of phenylacetylene is 4.97 Å, which indicates that little interaction exists between zinc and the alkyne. Moreover, as the barrier for ligand exchange is 3.1 kcal/mol, the generation of complex **1-b** is disadvantageous.

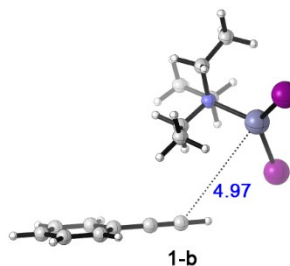


Figure S3. Optimized structure of complex **1-b**.

Subsequent deprotonation by Et₃N leads to the formation of anionic zinc complex **1-c**. As depicted in Figure S4, the barrier is calculated to be 31.9 kcal/mol endothermic. Therefore, this pathway is unfavorable thermodynamically and could be ruled out.

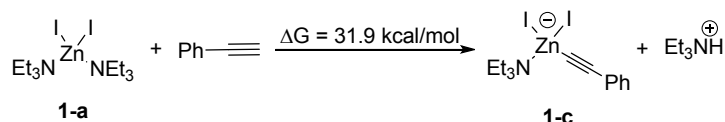


Figure S4. Calculated free energy for the generation of anionic zinc complex **1-c**.

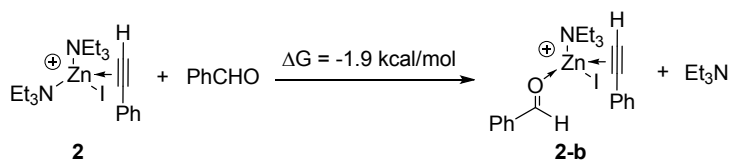


Figure S5. Calculated free energy for the ligand exchange of Et₃N by aldehyde.

It is noteworthy that a reaction pathway in which benzaldehyde coordination occurs first, followed by Zn complex as Lewis acid attacks electrophilically phenylacetylene is also possible. We have calculated the ligand exchange process shown in Figure S5, the free energy of which turns out to be 1.9 kcal/mol exothermic, which indicates the generation of complex **2-b** is possible. Thus, the pathway in which benzaldehyde coordination occurs first, followed by Zn complex as Lewis acid attacks electrophilically phenylacetylene could not be ruled out. However, both two possibilities would lead to the formation of intermediate **4**, thus the change of sequence will not affect the rate-determining step as well as the final conclusion.

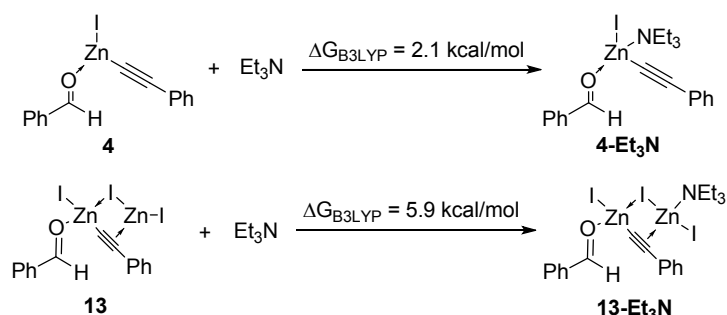


Figure S6. B3LYP calculated free energy for the formation of four-coordinated zinc complex.

In our theoretical study, the structure of compounds and transition states are optimized and determined at B3-LYP level. As the calculated results suggested the generation of four-coordinated zinc is endothermic (Figure S6), the structure of three-coordinate zinc was finally employed for solvation calculation.

Geometry	$E_{(\text{elec-B3LYP})}^{\text{a}}$	$E_{(\text{solv, M11-L})}^{\text{b}}$	$G_{(\text{corr-B3LYP})}^{\text{c}}$	$H_{(\text{corr-B3LYP})}^{\text{d}}$	IF ^e
1	-823.284478	-661.885012	0.367061	0.445723	-
2	-1131.680197	-970.296615	0.467553	0.565499	-
3	-838.863672	-677.439360	0.257163	0.333188	-

4	-892.018996	-730.597753	0.158204	0.232266	-
5-ts	-891.974400	-730.567046	0.160556	0.230371	-421.03
6	-892.008211	-730.600403	0.162234	0.232737	-
7	-1237.596229	-1076.201956	0.261928	0.351502	-
8-ts	-1237.573798	-1076.176124	0.259615	0.347708	-735.59
9	-1237.604431	-1076.203055	0.259305	0.352856	-
10	-877.247662	-715.822485	0.277978	0.355888	-
11	-1088.990635	-766.1379360	0.244696	0.342016	-
11a	-1088.983613	-766.123903	0.244908	0.342126	-
12	-796.552552	-473.6827023	0.046703	0.121106	-
13	-1142.146047	-819.2913788	0.146074	0.241086	-
14-ts	-1142.111179	-819.264404	0.149561	0.239700	-263.41
15	-1142.149820	-819.312211	0.150479	0.241894	-
16	-1487.743320	-1164.917669	0.248525	0.361855	-
17-ts	-1487.699048	-1164.876835	0.251797	0.356736	-608.78
18	-1487.719298	-1164.885564	0.248918	0.361758	-
19	-1487.755218	-1164.926213	0.250973	0.362337	-
10-b	-931.596745	-770.184334	0.202240	0.279389	-
10-c	-930.396469	-768.977867	0.179340	0.255030	-
1-a	-834.957371	-673.550121	0.365300	0.448922	-
1-b	-850.930729	-689.518126	0.257277	0.346781	-
1-c	-850.419879	-689.055254	0.252300	0.335255	-
2-b	-1184.847724	-1023.460004	0.367033	0.464140	-
4-Et3N	-1184.450364	-1023.041291	0.356001	0.453082	-
13-Et3N	-1434.575407	-1111.731900	0.347897	0.461269	-

^aThe electronic energy calculated by B3LYP in gas phase. ^bThe electronic energy calculated by M11-L in toluene solvent. ^cThe thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ^dThe thermal correction to enthalpy calculated by B3LYP in gas phase. ^eThe B3LYP calculated imaginary frequencies for the transition states.

3. B3LYP Geometries for All the Optimized Compounds and Transition States

1				H	3.86966000	-1.26765700	-1.37741200
Zn	-0.00309600	-0.04077200	0.00039000	H	1.06864200	2.80477200	-0.42051600
I	-0.09644300	-2.53950800	-0.00743200	C	3.21047900	2.97597200	-0.58065000
N	1.81690200	0.97961800	0.29943600	H	3.36691500	3.43872500	0.39768400
N	-1.74208400	1.11464900	-0.28780900	H	4.09634600	2.38644600	-0.83216300
C	-1.71802500	1.64450300	-1.70015600	H	3.13793000	3.78442100	-1.31546900
H	-2.70729600	2.05254800	-1.93603000	H	1.46419500	0.89841200	3.75831500
H	-1.01260900	2.48149900	-1.71475400				
C	-1.32108100	0.61891100	-2.75916600	2			
H	-0.31056000	0.21755400	-2.59814000	Zn	0.61605300	0.04023300	0.14991600
H	-2.01144400	-0.22642100	-2.81675000	I	-0.75203600	-0.36314300	-1.99752800
H	-1.31570500	1.10757400	-3.73891400	N	1.66444400	1.99077800	0.00421100
C	-2.93615000	0.20042800	-0.11538600	N	1.88177300	-1.72680600	0.69385500
H	-3.82005900	0.72626800	-0.49611600	C	3.07281500	-1.40398600	1.55236100
H	-2.76585700	-0.66391400	-0.75979600	H	3.69020300	-2.30605700	1.63683700
C	-3.18288300	-0.27665000	1.31262200	H	3.66870200	-0.66671200	1.00597000
H	-2.29966700	-0.75734300	1.74641100	C	2.78455700	-0.89741000	2.96390700
H	-3.51573000	0.52460500	1.97830600	H	2.17381000	0.00922400	2.97103400
H	-3.97451500	-1.03206600	1.28867000	H	2.29841000	-1.64947300	3.59079800
C	-1.77918000	2.26468800	0.68972900	H	3.73817900	-0.64933000	3.44169500
H	-1.68863500	1.83910800	1.69277700	C	1.04846700	-2.76138900	1.40395100
H	-0.87616800	2.85489000	0.50685200	H	1.72233600	-3.54455400	1.77793700
C	-3.00409800	3.17962600	0.62396700	H	0.61551700	-2.27353600	2.27988600
H	-2.89068200	3.96120400	1.38231900	C	-0.07189400	-3.39923300	0.58737200
H	-3.10404200	3.67749200	-0.34448600	H	-0.76348700	-2.65802100	0.17938200
H	-3.93555600	2.64938000	0.84017400	H	0.30049300	-4.00276400	-0.24450200
C	1.85083200	1.46761400	1.72660100	H	-0.63443600	-4.06728100	1.24881600
H	2.86258800	1.82628300	1.94682000	C	2.38147600	-2.23633400	-0.63835900
H	1.18285500	2.33339200	1.78207600	H	1.51016300	-2.34112300	-1.28633700
C	2.94003300	-0.00998600	0.07952300	H	2.99090200	-1.43220700	-1.06242500
H	2.72000500	-0.87855800	0.70279000	C	3.18907800	-3.53921300	-0.64029800
H	3.86531500	0.44135500	0.45765200	H	3.42868700	-3.78147200	-1.68108200
C	1.92014500	2.15461100	-0.64301500	H	4.13771200	-3.46332100	-0.10138500
H	1.77633200	1.76989000	-1.65631300	H	2.62810700	-4.38547100	-0.23325400
C	1.43818300	0.43086600	2.76868100	C	3.00810000	1.83391000	-0.65758900
H	2.10406400	-0.43524200	2.79655000	H	3.52495400	2.80032500	-0.62407300
H	0.41455400	0.06224800	2.61539200	H	3.58676500	1.14703700	-0.03191800
C	3.12757400	-0.46323500	-1.36524000	C	0.82569400	2.93007700	-0.82123900
H	2.20722300	-0.87605400	-1.79217700	H	0.63131200	2.42838600	-1.76973100
H	3.49757800	0.33234200	-2.01799600	H	1.42594400	3.82405200	-1.03684700

C	1.87152800	2.51817500	1.39909000	H	-6.67384500	1.64124400	0.52411800
H	0.90438300	2.47359600	1.90515100	H	-7.79328400	-0.52368400	0.02888400
C	2.99158600	1.34123300	-2.10362800	N	1.54007200	1.86577300	0.01527200
H	2.59803600	2.09189800	-2.79367500	C	3.04021100	1.82307500	0.01574400
H	2.40391900	0.42879300	-2.23553500	H	3.34088800	1.06746100	0.74290100
C	-0.50821600	3.33509800	-0.20221200	H	3.40718700	2.79970200	0.37093100
H	-1.13576200	2.46385600	0.00382900	C	1.05608900	2.41411200	1.32279000
H	-0.39799100	3.91932100	0.71626400	H	1.38726800	3.46186000	1.40684500
H	-1.04304600	3.95826100	-0.92632200	H	-0.03489500	2.41372600	1.28313900
H	2.53210800	1.80521400	1.90122600	C	1.08031800	2.75266400	-1.10867900
C	2.45413400	3.92890900	1.54820600	H	1.67871700	3.67738600	-1.07346800
H	3.46062000	4.02333200	1.13192700	H	1.33700900	2.24062800	-2.03907800
H	1.82058300	4.69611000	1.09469900	C	3.68744000	1.49140600	-1.32810500
H	2.52502100	4.15548600	2.61745600	H	3.58995200	2.29968300	-2.05851800
H	4.02303100	1.13157700	-2.40683800	H	4.75682600	1.32432800	-1.16156500
C	-1.81468100	0.13538900	1.73651100	H	3.28020100	0.57049100	-1.75567700
C	-3.14140800	0.06724700	1.27834300	C	-0.40497000	3.11300300	-1.13147400
C	-3.87335600	1.25742500	1.04885200	H	-0.61298200	3.62751500	-2.07624900
C	-3.75505000	-1.19046200	1.06472800	H	-1.04435600	2.22809900	-1.07652400
C	-5.18749400	1.18298900	0.60791900	H	-0.68287800	3.79551100	-0.32276700
H	-3.40093800	2.21828600	1.22429000	C	1.50347600	1.62805500	2.55524000
C	-5.06937700	-1.24890200	0.62216600	H	1.23619500	0.56663400	2.48608900
H	-3.18892900	-2.09809500	1.24532100	H	2.57943700	1.69455600	2.73683200
C	-5.78265500	-0.06603400	0.39263600	H	0.99195100	2.03598700	3.43339600
H	-5.75210400	2.09264200	0.43001100				
H	-5.54224600	-2.21099300	0.45313100	4			
H	-6.81039700	-0.11784000	0.04534700	C	-3.03788600	0.22663300	-0.00685400
C	-0.61384700	0.19768200	2.04272300	C	-1.90663300	-0.24150500	-0.01283600
H	0.02549500	0.26160400	2.90532000	Zn	-0.16656500	-0.97484800	-0.00937500
				I	1.35008300	-2.98738600	0.02036300
3				O	1.20857200	0.68208700	-0.03530300
Zn	0.65942200	-0.13206900	-0.08953900	C	2.44416000	0.64887800	0.01845100
I	2.39750400	-1.98541200	0.02016700	H	2.95594500	-0.32517700	0.08780500
C	-1.25201500	-0.12916100	-0.08385700	C	-4.35536500	0.77762000	0.00171700
C	-2.47642500	-0.18839900	-0.06000200	C	-5.48038500	-0.04691400	-0.20046200
C	-3.90258100	-0.27414600	-0.03613400	C	-4.55463700	2.15664600	0.21424600
C	-4.54864100	-1.49571800	-0.31433100	C	-6.76331100	0.49527500	-0.18948600
C	-4.69010900	0.85495500	0.26579000	H	-5.33185900	-1.10979600	-0.36426200
C	-5.93858800	-1.58032200	-0.29077900	C	-5.84074000	2.69090800	0.22486800
H	-3.94616900	-2.36853600	-0.54611300	H	-3.69065400	2.79535500	0.37066900
C	-6.07965500	0.76214900	0.28869600	C	-6.94898800	1.86389300	0.02319400
H	-4.19856000	1.79883000	0.48204600	H	-7.62172300	-0.15239900	-0.34683600
C	-6.70902100	-0.45401000	0.01052400	H	-5.97947200	3.75604700	0.39085600
H	-6.42275200	-2.52887500	-0.50731700	H	-7.95137300	2.28347000	0.03172100

C	3.28402900	1.83969000	-0.00552800	C	-0.00365200	1.61638400	0.61894400
C	4.67930600	1.68465900	0.06614300	C	-0.95841800	0.92278700	0.92420600
C	2.71840500	3.12556200	-0.09856300	C	-2.03149600	-0.03127400	1.27451000
C	5.50490700	2.80561600	0.04559600	H	-2.32004500	0.15351600	2.32325700
H	5.10610200	0.68710000	0.13745900	O	-1.53552900	-1.36133400	1.19643400
C	3.54709600	4.24018500	-0.11935200	Zn	0.12530900	-1.44786700	0.46433200
H	1.63876900	3.22260700	-0.15281900	I	2.30797800	-2.11864300	-0.42569900
C	4.93755300	4.07980200	-0.04714000	C	-3.27877000	0.17493200	0.40483000
H	6.58310500	2.69057600	0.10085600	C	-3.80498300	1.45823300	0.21012600
H	3.11897000	5.23554100	-0.19137100	C	-3.93077000	-0.92524200	-0.15717100
H	5.58112100	4.95514500	-0.06360100	C	-4.96481900	1.63881400	-0.54281400
5-ts				H	-3.30116000	2.31991600	0.64222300
C	-1.34170000	-1.01687200	-0.28023600	C	-5.09174300	-0.74290600	-0.91342800
C	-0.42947800	-0.19653000	-0.46696100	H	-3.52391300	-1.91669700	0.00735400
Zn	1.58907700	0.22704600	-0.37005700	C	-5.61168000	0.53687800	-1.10881500
I	3.75990000	-0.74073800	0.34470800	H	-5.36176200	2.63987000	-0.69016200
O	0.92555500	1.91709600	-1.07935800	H	-5.59011600	-1.60535500	-1.34867200
C	-0.34027300	1.57029900	-1.20155200	H	-6.51451800	0.67699700	-1.69730200
H	-0.67444700	1.24119400	-2.19612200	C	1.09375500	2.45954500	0.25973000
C	-2.40296100	-1.92601100	-0.05596500	C	2.06692700	2.80883000	1.21604800
C	-2.76534900	-2.86475800	-1.04822800	C	1.21071900	2.95339200	-1.05416300
C	-3.11645600	-1.90003700	1.16377100	C	3.13113300	3.63413100	0.86198400
C	-3.81424100	-3.74921400	-0.82266300	H	1.97733400	2.42802500	2.22876400
H	-2.21250800	-2.88585500	-1.98210000	C	2.27833700	3.77840100	-1.39849900
C	-4.16422100	-2.78887600	1.37808500	H	0.46096400	2.68324900	-1.79130900
H	-2.83386900	-1.17915700	1.92417500	C	3.23954400	4.12038800	-0.44356600
C	-4.51429500	-3.71281400	0.38798900	H	3.87784200	3.89771700	1.60562200
H	-4.08776700	-4.46965900	-1.58802600	H	2.36138600	4.15435400	-2.41427900
H	-4.70934000	-2.76489400	2.31718900	H	4.07163100	4.76342600	-0.71643900
H	-5.33249100	-4.40649900	0.56056900	7			
C	-1.36965100	2.37396500	-0.47788400	C	1.07701700	1.72648300	-0.35879400
C	-0.98299500	3.25701000	0.53887700	C	1.60950800	0.81157000	-0.96174800
C	-2.72089800	2.28871700	-0.84405400	C	2.16760000	-0.39974100	-1.60947100
C	-1.93908100	4.03926800	1.18536800	H	1.86948000	-0.36400500	-2.67398100
H	0.06906400	3.33306400	0.79289100	O	1.63369200	-1.56040800	-1.01747300
C	-3.67486800	3.07110100	-0.19891600	Zn	0.30291200	-1.22658100	0.22144000
H	-3.02032600	1.60360400	-1.63456400	I	-0.43062800	-1.51459800	2.61266200
C	-3.28469300	3.94657200	0.82036100	C	-2.64412100	-0.83265700	-0.44969000
H	-1.63475100	4.72630900	1.97029400	O	-1.49523700	-0.90576300	-0.90294100
H	-4.71970700	3.00371100	-0.48946800	H	-2.80430800	-0.93226400	0.63653100
H	-4.02833800	4.55822300	1.32426100	C	0.47632000	2.82785600	0.32828900
6				C	0.61079100	2.96109100	1.72434200
				C	-0.25478100	3.79874000	-0.38438400

C	0.02559500	4.03876900	2.38535400	C	-1.52723900	4.92094700	-0.38010800
H	1.17252800	2.21454600	2.27678600	C	-4.21067800	4.25995700	-0.80522100
C	-0.83182100	4.87543600	0.28460700	H	-3.64157200	2.24450300	-0.28840300
H	-0.35772100	3.69908300	-1.46076600	C	-2.43595700	5.90445800	-0.76150200
C	-0.69476400	4.99871200	1.66988100	H	-0.48432300	5.17060900	-0.21058800
H	0.13473300	4.12988900	3.46248300	C	-3.77789300	5.57781300	-0.97530900
H	-1.38956300	5.62061800	-0.27626600	H	-5.25331600	4.00306600	-0.96942000
H	-1.14664500	5.83941800	2.18921300	H	-2.09709300	6.92848300	-0.89136600
C	-3.82547600	-0.62179800	-1.27723300	H	-4.48406400	6.34799300	-1.27274600
C	-5.08323300	-0.55083700	-0.65382300	C	2.48693400	-0.59531600	-1.78297600
C	-3.72007700	-0.49179400	-2.67494200	C	3.34583800	0.45236100	-2.14946300
C	-6.22850800	-0.35055100	-1.41999900	C	3.00112800	-1.89082500	-1.62725500
H	-5.15384800	-0.65276900	0.42644600	C	4.70112000	0.20806700	-2.35929200
C	-4.86609200	-0.29235000	-3.43430400	H	2.94717800	1.45707700	-2.27241400
H	-2.73958300	-0.55159200	-3.13642800	C	4.35641600	-2.13256700	-1.83970900
C	-6.11763400	-0.22176000	-2.80739500	H	2.32477200	-2.69641300	-1.36109700
H	-7.20194000	-0.29508000	-0.94231800	C	5.20827800	-1.08516300	-2.20361400
H	-4.79349000	-0.19201800	-4.51315700	H	5.36105600	1.02188900	-2.64635200
H	-7.01081600	-0.06605300	-3.40627200	H	4.75008900	-3.13889000	-1.72641200
C	3.70373500	-0.38085900	-1.57461900	H	6.26482000	-1.27701800	-2.36985000
C	4.40923300	0.67469400	-2.16583800	C	1.92705100	0.94945500	1.56856700
C	4.40958500	-1.43078900	-0.98542900	C	2.52792100	2.20147000	1.37964900
C	5.80342500	0.68346300	-2.16177600	C	2.55443800	-0.00365600	2.38032500
H	3.86424000	1.49688800	-2.62567700	C	3.73993600	2.49831500	2.00103600
C	5.80739800	-1.42253800	-0.98183200	H	2.03675900	2.94436600	0.75752300
H	3.85158200	-2.24798000	-0.54243200	C	3.76597300	0.29754100	3.00121400
C	6.50793700	-0.36778600	-1.56773900	H	2.07553500	-0.96499000	2.52862900
H	6.34036000	1.50954800	-2.62140700	C	4.36228100	1.54677000	2.81286100
H	6.34852200	-2.24488200	-0.52019700	H	4.19625800	3.47369900	1.85542100
H	7.59492400	-0.36297300	-1.56428900	H	4.24303900	-0.44299500	3.63739100
				H	5.30546700	1.77976300	3.29961100

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C	-1.03067300	2.57402100	0.18089400
C	-0.25115500	1.70916900	0.53167900
C	0.62720500	0.59698500	0.88120400
H	1.08383100	0.30207500	-0.32009100
O	0.02142100	-0.50427900	1.30309700
Zn	-0.93219500	-1.64604100	0.09885500
I	-2.83121000	-3.22721700	0.30986200
C	1.04204900	-0.31950500	-1.55879400
O	0.20851600	-1.30809300	-1.43662700
H	0.66096300	0.59456700	-2.04845100
C	-1.95465100	3.58958700	-0.20718200
C	-3.30981000	3.26926800	-0.42391500

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C	1.90076500	-0.67578400	1.38140200
C	1.82023700	0.34429400	0.71789000
C	1.64894000	1.47159700	-0.13860100
O	0.78526900	1.43976500	-1.04858700
Zn	-0.60843800	-0.08224400	-1.31259800
I	0.30632200	-1.92473300	-2.75403000
C	-3.22797400	-0.18572300	-0.19383500
O	-2.01709700	0.51773700	-0.32438500
H	-3.07668100	-1.17497000	0.27376400
H	-3.68818300	-0.38450300	-1.17850200
C	1.98238500	-1.87573400	2.13475900

C	2.74181200	-1.92714000	3.32223200	H	-3.21100500	1.29347500	0.66732100
C	1.29980000	-3.02825400	1.69011200	C	-5.81172100	-1.32197900	-0.51294800
C	2.81092900	-3.11001500	4.05032300	H	-4.15495700	-2.69521400	-0.58513200
H	3.26421400	-1.03781200	3.66057000	C	-6.22466500	-0.01557400	-0.23992100
C	1.38103500	-4.20627000	2.42572300	H	-5.59816400	1.94606400	0.39819600
H	0.72509700	-2.98533600	0.77020500	H	-6.53252900	-2.06228500	-0.85141900
C	2.13271100	-4.24883300	3.60382400	H	-7.26762000	0.26563300	-0.36133400
H	3.39358500	-3.14688800	4.96605900	N	1.16080100	1.86672500	0.08466600
H	0.85732900	-5.09250000	2.08014200	C	0.76029100	2.33454700	1.45108600
H	2.19104400	-5.17097300	4.17523600	H	0.97353600	3.40842500	1.54151000
C	2.49078600	2.66760700	0.04482000	H	-0.32263200	2.19652400	1.51467400
C	3.48172200	2.71241600	1.04032700	C	2.61350700	2.13108800	-0.15549000
C	2.29150400	3.77897000	-0.79403200	H	3.16901800	1.49697100	0.53934100
C	4.26285600	3.85399400	1.19493600	H	2.83466500	3.17611700	0.10811500
H	3.63282200	1.85206900	1.68470600	C	0.26748700	2.49310900	-0.95013100
C	3.07461900	4.91654500	-0.63471300	H	0.52800200	2.04343600	-1.91247600
H	1.52238500	3.72994900	-1.55696600	C	1.43314500	1.58833000	2.60292000
C	4.05980600	4.95543800	0.35859700	H	2.51315200	1.75573100	2.64511600
H	5.02840300	3.88679900	1.96441500	H	1.25838500	0.50645300	2.55282400
H	2.92015200	5.77492900	-1.28171000	C	3.09552000	1.83997000	-1.57494800
H	4.66978600	5.84632200	0.48033600	H	2.84632700	0.81993200	-1.88414800
C	-4.23488100	0.58560100	0.64794000	H	2.69225300	2.54202500	-2.31102400
C	-4.00444300	1.91178100	1.02309300	H	4.18673700	1.92979400	-1.59746500
C	-5.43034800	-0.03047100	1.04252800	H	-0.74545900	2.15743200	-0.71443800
C	-4.95180700	2.60997900	1.77689200	C	0.31956200	4.01981200	-1.06769600
H	-3.07531400	2.38124900	0.71879500	H	-0.01891400	4.52186100	-0.15635400
C	-6.37825200	0.66463400	1.79283800	H	1.32070800	4.39065400	-1.31209000
H	-5.62001200	-1.06498500	0.75951600	H	-0.35122600	4.32838000	-1.87692500
C	-6.14138900	1.99147100	2.16378300	H	1.00638100	1.94206300	3.54751700
H	-4.75869200	3.64162500	2.06248800				
H	-7.30032500	0.17127900	2.09102100	11			
H	-6.87777900	2.53528500	2.75020300	Zn	1.43220300	0.36583800	-0.02100600
				I	3.03463500	1.42742500	-1.70011700
10				I	0.81982000	-2.41339500	-0.93174600
Zn	0.62837500	-0.21256700	0.05656000	N	2.17401000	0.23735200	2.01563900
I	2.42238800	-1.97176400	-0.09677700	C	1.68982300	1.46502800	2.73127900
C	-2.07472000	-1.15958000	0.27260600	H	0.59666200	1.41192000	2.72374000
O	-1.19807800	-0.05735200	0.22256600	C	1.55981700	-0.97642000	2.65261300
H	-1.99929100	-1.67001500	1.25025300	H	1.80932700	-1.83432100	2.02640500
H	-1.82648200	-1.92068400	-0.48538200	C	3.67250900	0.19136400	2.02091400
C	-3.52268000	-0.74019300	0.06824100	H	4.01310000	1.04807200	1.43634800
C	-3.94561300	0.56508100	0.33982200	H	4.02662400	0.33246400	3.05248300
C	-4.47089300	-1.67750600	-0.36192600	C	4.27546800	-1.07738900	1.42360200
C	-5.28583800	0.92614200	0.18547200	H	5.36217000	-0.95277200	1.37019600

H	4.07390400	-1.96964500	2.02412700	H	3.84884400	3.25532300	1.01387200
H	3.91562100	-1.25211600	0.40502500	C	4.02110800	2.39494100	-0.95233300
H	2.01637200	1.41359800	3.77830700	H	4.10602000	3.37331600	-1.43793400
C	2.13705000	2.79891600	2.13552000	H	5.03427900	2.00720800	-0.81413600
H	1.64083200	3.60480500	2.68757200	H	3.49463500	1.72649800	-1.63969400
H	3.21545400	2.95838200	2.22106400	Zn	-1.76818300	-0.05545400	0.03562300
H	1.86382100	2.89827800	1.08068000	H	1.18879500	2.10750100	1.89198200
Zn	-1.35059700	-1.09442500	-0.27683800	C	2.68919500	2.60028200	3.37116200
I	-3.69632400	-1.92535000	0.05090900	H	2.92764700	3.59366700	2.98053000
H	0.47489300	-0.84298800	2.58136800	H	1.94247900	2.73212800	4.16170300
C	1.94536900	-1.27360100	4.10606200	H	3.58903300	2.18807000	3.83879900
H	1.64143300	-0.48435500	4.80000800	C	-3.65212900	-0.04402600	0.01972700
H	1.43488200	-2.19266700	4.41349300	C	-4.87633800	-0.03641300	-0.00039100
H	3.02038600	-1.44147400	4.22514700	C	-6.30406100	-0.02832700	-0.02551600
C	-0.55915600	0.80396700	0.10136000	C	-7.03698700	-1.07874500	0.56220000
C	-1.44793300	1.66894800	0.09164800	C	-7.00343600	1.02972300	-0.63988500
C	-2.47580800	2.65034100	0.06420800	C	-8.42930900	-1.06766100	0.53337200
C	-3.25218100	2.90606400	1.21399300	H	-6.50109500	-1.89571600	1.03555100
C	-2.72387900	3.37697400	-1.11983500	C	-8.39588100	1.03359200	-0.66297000
C	-4.25576500	3.86861700	1.17467300	H	-6.44156600	1.83975000	-1.09473700
H	-3.06274900	2.33967000	2.12018200	C	-9.11314200	-0.01328100	-0.07778500
C	-3.72626100	4.34130100	-1.14513900	H	-8.98296500	-1.88422700	0.98903600
H	-2.12411400	3.17507300	-2.00160800	H	-8.92346900	1.85524100	-1.13997100
C	-4.49229600	4.58701900	-0.00143300	H	-10.19957200	-0.00776500	-0.09843600
H	-4.85578700	4.05909100	2.05958100	I	-0.07410000	1.48904800	-1.34801100
H	-3.91385200	4.90000800	-2.05723000				
H	-5.27667900	5.33825400	-0.02726100				
				12			
				Zn	1.77382800	0.36589700	-0.00005400
11a				I	4.03026000	1.40388200	-0.00007500
Zn	1.89290400	-0.05562700	-0.12739400	I	1.34757800	-2.36210600	0.00017700
I	3.29016700	-1.60655600	-1.58558700	Zn	-0.97361300	-1.03701900	-0.00003800
I	0.00110200	-1.47997000	1.39990700	I	-3.31485500	-1.89442700	-0.00013100
N	2.97615000	1.32555300	1.13642300	C	-0.15184700	0.89093300	-0.00007600
C	3.27285000	2.58247100	0.36593800	C	-1.01986300	1.77817200	-0.00001300
H	2.30840700	3.06082800	0.17170900	C	-2.03578400	2.76621200	0.00006100
C	2.09896500	1.66581000	2.30999700	C	-2.54207000	3.26162400	1.22145700
H	1.80156900	0.72556200	2.77652900	C	-2.54198900	3.26184800	-1.22128000
C	4.26198500	0.67186300	1.55330400	C	-3.53645000	4.23336900	1.21430900
H	4.77504300	0.38050000	0.63501800	H	-2.14803000	2.87656000	2.15639600
H	4.88795000	1.42167800	2.05717300	C	-3.53636400	4.23360000	-1.21402400
C	4.10186400	-0.56081200	2.43902900	H	-2.14788400	2.87696100	-2.15626400
H	5.09027600	-1.00640700	2.59283600	C	-4.03311500	4.71864300	0.00017000
H	3.68692300	-0.32802300	3.42425900	H	-3.92661300	4.61329800	2.15360400
H	3.47400000	-1.32174100	1.96461300	H	-3.92645300	4.61370500	-2.15327800

H	-4.81068400	5.47722600	0.00021700	C	-1.12562500	3.27676600	-1.35214600
				C	-2.31073800	4.03188700	-1.19124000
13				C	-0.09504100	3.76970400	-2.18568300
Zn	0.95125200	1.06994400	-0.24280800	C	-2.45395300	5.24889600	-1.84736000
I	2.46749400	3.06929100	-0.61123600	H	-3.10054700	3.64530700	-0.55495700
I	0.42587100	-0.65619400	-2.51470300	C	-0.24958800	4.98962400	-2.83411000
Zn	-1.51545200	-0.74406100	-0.73417600	H	0.81114800	3.18526900	-2.31082600
I	-3.40700800	-2.37305700	-0.49582900	C	-1.42586800	5.72849600	-2.66647400
C	-0.90917500	0.86999000	0.47989400	H	-3.36576200	5.82568400	-1.72422200
C	-1.92439600	1.21697600	1.10021300	H	0.54385200	5.36653600	-3.47244400
C	-3.09639000	1.59565700	1.81063200	H	-1.54255000	6.68001100	-3.17759900
C	-3.42507700	0.96295600	3.02759500	C	-2.60936500	-0.11911000	4.17044600
C	-3.93520400	2.60992900	1.30301800	C	-3.18030300	1.11688700	4.48643600
C	-4.57298500	1.33939400	3.71750500	C	-2.69823900	2.28382600	3.88634800
H	-2.77787500	0.18119400	3.41177200	C	-1.65473800	2.21161000	2.96613500
C	-5.07813600	2.98068900	2.00404800	C	-1.08079500	0.97374000	2.64478000
H	-3.67637300	3.09429600	0.36685100	C	-1.56057800	-0.19282400	3.25522700
C	-5.39839000	2.34661000	3.20841600	H	-2.97883700	-1.02582000	4.64077800
H	-4.82641400	0.84759900	4.65196900	H	-3.99693300	1.17126900	5.20096900
H	-5.72169400	3.76237600	1.61149600	H	-3.13524300	3.24652300	4.13635900
H	-6.29378100	2.63735800	3.75069200	H	-1.28181200	3.11705000	2.49210800
C	4.12672400	-3.56458900	2.76668500	H	-1.09751000	-1.14542500	3.01916200
C	5.51191200	-3.41574800	2.92025500	C	0.05861500	0.91518400	1.68243300
C	6.16520200	-2.27757400	2.43868700	H	0.56792300	1.87457800	1.54452500
C	5.43170800	-1.28203000	1.79922800	O	0.80124400	-0.15552400	1.69682400
C	4.04151300	-1.42499200	1.64382200				
C	3.38919400	-2.57389600	2.13143100	15			
H	3.63148000	-4.45458700	3.14313000	Zn	2.29146900	-0.05481500	-0.52861600
H	6.08391600	-4.19406500	3.41789500	I	4.20270200	-1.58153600	-0.94061000
H	7.23866700	-2.17106500	2.56123100	I	1.76866600	2.53864600	-0.66846900
H	5.92645400	-0.39210200	1.41776900	Zn	-0.52228000	1.25567300	0.13046400
H	2.31614200	-2.66748500	1.99917400	I	-2.64675700	2.35656000	0.77010500
C	3.30202200	-0.36758400	0.97049300	O	0.43994900	-0.41110800	-0.02700400
H	3.87900200	0.49491100	0.59968900	C	-0.10443900	-1.72452600	0.33751900
O	2.07480200	-0.39147100	0.80000700	H	0.55054900	-2.45784600	-0.14931800
				C	-1.45228000	-1.84705300	-0.21143900
14-ts				C	-2.56501700	-1.93653000	-0.68924800
Zn	2.24644300	-0.51516100	0.47405700	C	-3.87457800	-2.04612800	-1.24939400
I	4.59269800	0.32046000	0.47295200	C	-5.00039600	-1.61677700	-0.51991800
I	1.03721700	-2.10728100	-1.26368500	C	-4.05438200	-2.58481700	-2.53837800
Zn	-1.30942900	-0.88808600	-0.55702200	C	-6.27431000	-1.72395700	-1.07212500
I	-3.41692000	-2.21587900	-0.76834200	H	-4.86254900	-1.19959400	0.47251400
C	-0.84294000	0.98099700	-0.04144600	C	-5.33245600	-2.69002000	-3.08110900
C	-0.97631100	2.04160600	-0.68143000	H	-3.18696300	-2.91550000	-3.10125600

C	-6.44400100	-2.26026800	-2.35128900	H	1.11993200	-2.80010500	2.75677600
H	-7.13657000	-1.38781200	-0.50322700	C	4.51194900	-2.54714000	2.88279400
H	-5.46175200	-3.10707500	-4.07588900	H	5.63674900	-0.78024900	2.36894200
H	-7.43954100	-2.34224000	-2.77861400	H	3.12328400	-4.13837600	3.33287600
C	-0.01615700	-1.91910900	1.84222200	H	5.39147800	-3.13270500	3.13655600
C	-1.01843500	-1.45053800	2.70197500	C	-3.52653700	0.63982600	-0.11084300
C	1.12324100	-2.52766500	2.38439000	H	-4.14304100	-0.10273300	0.42154100
C	-0.87357500	-1.57589100	4.08399400	O	-2.33029500	0.39362600	-0.32156400
H	-1.91744700	-1.00238600	2.28801500	C	-4.17865500	1.87121200	-0.52909000
C	1.26559800	-2.65621700	3.76687300	C	-5.54616400	2.04134300	-0.24875900
H	1.90024000	-2.90367800	1.72237000	C	-3.46341200	2.87808500	-1.20606600
C	0.26823700	-2.17763500	4.61891800	C	-6.19561000	3.20779100	-0.64281600
H	-1.65662600	-1.21041100	4.74256200	H	-6.08951900	1.25793600	0.27413900
H	2.15185100	-3.13327800	4.17588000	C	-4.11700900	4.03993600	-1.59562400
H	0.37680400	-2.27879000	5.69522500	H	-2.40852400	2.72863000	-1.41211400
16				C	-5.48034500	4.20348800	-1.31479000
Zn	-1.32030300	-1.39575000	0.16813600	H	-7.25152800	3.34320000	-0.42978500
I	-2.76149900	-2.68721600	1.80429200	H	-3.57262100	4.82106000	-2.11758000
I	-0.46132500	-2.04636600	-2.34539000	H	-5.98676600	5.11411700	-1.62285500
Zn	1.47414700	-0.62822300	-1.11760900	17-ts			
I	3.47786500	0.43812600	-2.13951600	Zn	-2.17238600	0.47964300	-0.83151000
O	0.50948600	-0.74713500	0.54846700	I	-4.46341800	0.96557300	0.07816300
C	0.98139300	-0.27544100	1.83978000	I	-1.72114700	-2.04338000	-1.92012100
H	0.19209900	-0.53865100	2.55713600	Zn	-0.10530700	-1.91506800	0.11236600
C	1.12581900	1.18256200	1.81603100	I	1.28669900	-3.57215100	1.34742100
C	1.22088200	2.39142100	1.76194900	O	-0.54681500	-0.03459500	0.64547300
C	1.34216500	3.81426500	1.69809900	C	0.34287800	0.85850100	1.07555100
C	2.10883100	4.41848300	0.68219100	H	0.20268800	1.91257800	0.07334500
C	0.69888100	4.63066700	2.64857800	C	1.72560200	0.58337200	0.80306900
C	2.22431400	5.80543300	0.62288900	C	2.88261100	0.37996400	0.48118100
H	2.60699700	3.79117300	-0.05100100	C	4.24389700	0.14478000	0.13360100
C	0.82294900	6.01647300	2.58255800	C	4.72923900	-1.17105400	-0.00481100
H	0.10929400	4.16687400	3.43356400	C	5.11279300	1.23489000	-0.07508200
C	1.58413900	6.60798400	1.57090200	C	6.06341400	-1.38448600	-0.34033700
H	2.81872900	6.26074200	-0.16451100	H	4.05799900	-2.00782400	0.16112800
H	0.32495800	6.63649000	3.32309600	C	6.44339800	1.00648300	-0.41368600
H	1.67933200	7.68932900	1.52274200	H	4.73090800	2.24649900	0.01854000
C	2.24321900	-1.03364800	2.23190000	C	6.92160800	-0.30035800	-0.54475400
C	3.52012000	-0.47107000	2.12982900	H	6.43449900	-2.40024400	-0.44177200
C	2.11077500	-2.35980000	2.67022700	H	7.10919700	1.84932800	-0.57598900
C	4.64988500	-1.22706000	2.45263100	H	7.96165000	-0.47364300	-0.80670600
H	3.62870200	0.55915600	1.80554800	C	-0.00397500	1.67099000	2.28071700
C	3.23815400	-3.11305600	2.99202600	C	0.93444200	2.56307700	2.82808900

C	-1.27806700	1.56219400	2.85839500	C	0.50017400	1.47591300	-0.70170900
C	0.59963900	3.33422200	3.93722000	C	-0.49503700	2.52504600	-0.92427700
H	1.92302600	2.64159400	2.38576200	C	-0.11906000	3.88340200	-0.92826100
C	-1.60526800	2.33701400	3.97046500	C	-1.84080100	2.16631900	-1.14771400
H	-2.00252200	0.87141000	2.44319200	C	-1.07322000	4.86659600	-1.15876300
C	-0.67141300	3.22380000	4.51037600	H	0.91748000	4.15433500	-0.75526900
H	1.33095000	4.01767700	4.35917500	C	-2.78924000	3.15826600	-1.37320300
H	-2.59176300	2.24362800	4.41483000	H	-2.13621500	1.12200800	-1.11959300
H	-0.93003800	3.82486300	5.37761500	C	-2.40671800	4.50417300	-1.38149200
C	-0.21490100	2.51068000	-0.95423900	H	-0.78313600	5.91298200	-1.16503500
H	-0.82282600	3.26980400	-0.42533600	H	-3.82535800	2.87849100	-1.53652700
O	-0.87658700	1.62103500	-1.67304100	H	-3.15131900	5.27535500	-1.55962200
C	1.05317000	3.06178400	-1.52542200	C	1.84333900	1.81212100	-0.39847300
C	1.63462800	4.20232200	-0.95029100	C	3.00918300	2.03594100	-0.11435100
C	1.68518900	2.43348900	-2.60756700	C	4.36435100	2.28846600	0.21435200
C	2.82846100	4.71402300	-1.45688200	C	4.78387900	3.59373500	0.55002700
H	1.14334600	4.69363100	-0.11293400	C	5.29983300	1.23100000	0.20924900
C	2.87704800	2.94881600	-3.11442900	C	6.11392500	3.83080300	0.87777700
H	1.22077500	1.55799200	-3.04912300	H	4.05968300	4.40217600	0.55507600
C	3.45147000	4.08729300	-2.54078000	C	6.62838600	1.48370000	0.53431800
H	3.26638900	5.60569800	-1.01649500	H	4.97250200	0.23182600	-0.05977100
H	3.35793100	2.46510100	-3.96012300	C	7.03584800	2.77866700	0.86969400
H	4.37753900	4.49016700	-2.94207400	H	6.43474100	4.83453200	1.13998300
				H	7.34766500	0.67031600	0.52717900
18				H	8.07433500	2.96921100	1.12543000
Zn	-1.81990000	-0.85164300	1.41769200	Zn	1.19693200	-1.45048100	-0.82192200
I	-0.94693800	0.36739400	3.43200500	I	3.19484300	-1.74782300	-2.29218400
I	-0.15688700	-3.02314500	0.69935500				
O	-3.15321900	-0.80299900	0.16107000	19			
C	-4.41905200	-0.25031000	0.45055100	Zn	0.33858300	-0.55419500	-0.61062500
H	-5.05820400	-1.00232300	0.94711900	I	1.38673200	-2.66125900	-1.56366500
H	-4.35897000	0.60425600	1.14577000	I	-0.09294400	-0.02983100	2.08145900
C	-5.12490800	0.21325200	-0.81488300	Zn	-2.31926900	0.58295300	0.71558000
C	-6.13470000	1.18333500	-0.74606600	I	-4.31363900	1.88661500	1.44464600
C	-4.80324700	-0.33693700	-2.06128500	O	-1.56440800	-0.09961600	-0.91766400
C	-6.81261400	1.59256100	-1.89633500	C	-2.32327100	-0.45017100	-2.09300600
H	-6.39203100	1.62215900	0.21665300	H	-1.62836900	-0.92503200	-2.79609200
C	-5.47686600	0.07437300	-3.21387900	C	-3.46847000	-1.38189400	-1.77325800
H	-4.01647300	-1.08249600	-2.11314100	C	-3.21542700	-2.70642900	-1.38133800
C	-6.48359900	1.03912000	-3.13669700	C	-4.79440100	-0.93732700	-1.84533600
H	-7.59369900	2.34563900	-1.82474700	C	-4.26880600	-3.56253000	-1.06383700
H	-5.21470000	-0.36103100	-4.17514000	H	-2.18960400	-3.06445500	-1.33223200
H	-7.00723100	1.35830300	-4.03412400	C	-5.85131900	-1.79564700	-1.53146500
O	0.15283000	0.25552300	-0.77546800	H	-5.00080900	0.08660000	-2.14801400

C	-5.58954500	-3.10850800	-1.13882000	C	5.70285900	-1.69999900	0.76671900
H	-4.06096500	-4.58632100	-0.76443200	H	4.16053700	-2.55775300	2.00245200
H	-6.87504500	-1.43636000	-1.59083600	C	5.99159900	-0.99552100	-0.40296100
H	-6.40993600	-3.77767200	-0.89350500	H	5.16641500	-0.06311000	-2.16459700
C	2.39230800	1.66120100	-0.98546000	H	6.50526000	-1.99548800	1.43802500
O	1.23852400	1.20937200	-1.20348600	H	7.01942400	-0.74261300	-0.64989000
C	2.75318800	3.00680000	-1.46996500	C	0.46670000	5.48233900	-0.72863000
C	4.03962200	3.53411300	-1.26267000	C	0.05831700	4.20762000	-1.12848700
C	1.78689400	3.77176500	-2.14854400	C	-0.75371300	3.42810400	-0.29723500
C	4.35464500	4.80756500	-1.72741700	C	-1.14821100	3.93945800	0.94815400
H	4.78295900	2.94156300	-0.73901200	C	-0.73628700	5.20792100	1.35104600
C	2.10701900	5.04355100	-2.60977800	C	0.07075400	5.98278700	0.51178600
H	0.79802300	3.35381100	-2.30101600	H	1.09490300	6.07934800	-1.38384100
C	3.38971000	5.56254400	-2.40028800	H	0.37040500	3.81745300	-2.09486800
H	5.34930800	5.21229900	-1.56598500	H	-1.77409700	3.33603700	1.60078100
H	1.35972900	5.63384300	-3.13169600	H	-1.04666700	5.59582200	2.31734700
H	3.63630600	6.55703600	-2.76175400	H	0.38862400	6.97313500	0.82603400
H	-2.70038100	0.46906100	-2.55814100	C	-1.19100500	2.05068900	-0.72440000
C	3.35084400	0.88951800	-0.27411100	H	-0.86973900	1.83773800	-1.75079200
C	4.12736200	0.17152400	0.33375700	O	-0.67793400	1.03046200	0.17164700
C	5.00854600	-0.68578500	1.04074200	H	0.30074900	1.04913400	0.20136800
C	6.26542400	-0.21799100	1.47929400	H	-2.27604000	1.93078800	-0.67148300
C	4.62381900	-2.01765900	1.30834100				
C	7.11686500	-1.06809300	2.17614600	10-c			
H	6.55594200	0.80700300	1.27098600	Zn	-0.24267700	-0.82733400	0.01377500
C	5.48708000	-2.85785200	2.00452800	I	0.97116300	-3.02537200	0.02728000
H	3.66106900	-2.37373400	0.95585300	C	-3.05874000	-0.40773100	-0.04108900
C	6.72950600	-2.38631400	2.43922900	O	-1.76632600	0.15196900	0.00110200
H	8.08297100	-0.70598700	2.51514000	H	-3.23324800	-1.07725800	0.82010400
H	5.19056400	-3.88243900	2.20804900	H	-3.20479600	-1.02678900	-0.94267500
H	7.39848400	-3.04708400	2.98345900	C	-4.13081800	0.67204600	-0.02649100
				C	-3.82110300	2.00038700	0.27767300
10-b				C	-5.46316400	0.33361300	-0.29899300
Zn	-0.81661400	-1.09029900	0.12156300	C	-4.82470700	2.97222400	0.31079100
I	-3.08227700	-2.05826200	-0.12336900	H	-2.78726700	2.25859400	0.47969600
C	1.89940600	-2.03715100	0.55773600	C	-6.46690400	1.30121400	-0.26377400
O	1.00422500	-0.99028200	0.23835400	H	-5.71664200	-0.69690700	-0.54356000
H	1.64801800	-2.95214100	-0.00609300	C	-6.15007700	2.62776600	0.04211500
H	1.83624200	-2.30167000	1.62519500	H	-4.56882600	4.00268400	0.54682500
C	3.33054300	-1.64568100	0.23594200	H	-7.49535200	1.02190800	-0.47970100
C	3.63050000	-0.93823200	-0.93533000	H	-6.93003300	3.38460300	0.06714600
C	4.38004800	-2.01750300	1.08357500	C	5.71973400	2.35918900	-0.05333100
C	4.94947100	-0.61349000	-1.25221500	C	4.78474900	1.32812100	-0.03209500
H	2.81884300	-0.63931100	-1.59221600	C	3.41084000	1.62726300	-0.02327400

C	2.97679900	2.96696000	-0.03621900	C	-2.54492100	-0.41554900	1.60009200
C	3.91477400	3.99112600	-0.05766900	H	-2.72132300	-0.99101900	0.69009800
C	5.28306500	3.68716100	-0.06612000	C	-0.48227100	2.77045300	2.27189900
H	6.78161200	2.13323400	-0.06017900	H	-1.10295900	3.59118700	1.90214300
H	5.10917200	0.29032400	-0.02228300	H	0.35130600	2.64787800	1.57665400
H	1.91173000	3.17551400	-0.02990500	C	-3.22060800	1.16316400	-0.84164800
H	3.58914600	5.02694500	-0.06822200	H	-2.50645300	0.68305700	-1.51494500
H	6.01215700	4.49260000	-0.08303900	H	-3.99646100	0.43429500	-0.58869300
C	2.45603900	0.52925500	-0.00236500	H	-3.69938800	1.98107000	-1.39119900
H	2.86484100	-0.49440800	0.00287500	H	-1.89758600	-1.03069500	2.23352100
O	1.22798200	0.69080000	0.00875800	C	-3.87782600	-0.17829500	2.32289600
1-a				H	-3.76319400	0.31455600	3.29304600
Zn	-0.00008500	-0.00004700	-0.06784600	H	-4.57983200	0.40756300	1.72214000
I	0.83630700	2.06187400	-1.46356500	H	-4.34203000	-1.15355200	2.50702400
N	-1.73790200	0.79055000	1.21488300	H	-0.08231300	3.07709000	3.24534300
N	1.73760400	-0.79079600	1.21496100	I	-0.83602500	-2.06174200	-1.46392200
C	1.28235900	-1.48308300	2.46324800	1-b			
H	2.16075200	-1.71386200	3.08166000	Zn	1.69493400	-0.13722800	-0.03736200
H	0.68728800	-0.75685400	3.02624000	I	1.12995100	-2.61162700	-0.19068500
C	0.48169400	-2.77080800	2.27169500	N	0.49887600	1.04550500	-1.37361200
H	-0.35405700	-2.64697300	1.57931000	C	-0.87499500	1.10729800	-0.76901000
H	1.10116700	-3.59096600	1.89867900	H	-1.49741100	1.77650300	-1.37711500
H	0.08461800	-3.07906800	3.24581600	H	-1.30403600	0.10391700	-0.84278200
C	2.53417700	-1.75574300	0.38562700	C	-0.91809000	1.56014100	0.68880900
H	3.27857500	-2.23927100	1.03633600	H	-0.31900600	0.91332200	1.34167700
H	1.83923800	-2.52807200	0.05203700	H	-0.57797900	2.59031200	0.82867500
C	3.22118000	-1.16250500	-0.84113000	H	-1.95355900	1.49413700	1.03705200
H	2.50736900	-0.68191000	-1.51444100	C	1.06729100	2.42744900	-1.50566700
H	3.99708700	-0.43391900	-0.58750100	H	0.32222200	3.06683600	-1.99986700
H	3.70002100	-1.98020800	-1.39092800	H	1.20425000	2.80939200	-0.49200900
C	2.54439900	0.41540500	1.60041600	C	2.39859800	2.50740200	-2.24924400
H	2.72110900	0.99076800	0.69041600	H	3.14874700	1.84049800	-1.81207200
H	1.89680700	1.03061800	2.23352800	H	2.30305600	2.28135700	-3.31549700
C	3.87709200	0.17831100	2.32366600	H	2.78466800	3.52823800	-2.16082600
H	4.34132500	1.15359600	2.50757000	C	0.44248400	0.31993100	-2.68912000
H	3.76215000	-0.31417300	3.29396200	H	1.47199100	0.20056900	-3.03737000
H	4.57921000	-0.40783200	1.72331300	H	0.07100300	-0.68446200	-2.47063800
C	-1.28233700	1.48231600	2.46336300	C	-0.40522600	0.96488500	-3.78990800
H	-2.16046900	1.71234200	3.08241600	H	-0.33673400	0.34106000	-4.68764700
H	-0.68667900	0.75597200	3.02557300	H	-1.46299600	1.03029900	-3.51866700
C	-2.53419700	1.75584900	0.38571600	H	-0.05616300	1.96692000	-4.05941900
H	-1.83914700	2.52836400	0.05282000	I	3.34310200	1.09189600	1.43687100
H	-3.27892600	2.23905800	1.03629000	C	-3.97168000	-1.10761300	0.57791400

C	-2.96280700	-1.77822300	0.56138700	C	-4.84412700	-1.24092100	-0.35671600
H	-2.07110700	-2.36751500	0.55288400	C	-6.23307500	1.17749300	-0.33542700
C	-5.16247400	-0.31549400	0.60178500	H	-4.28905500	2.11411300	-0.30388200
C	-6.03397800	-0.29955400	-0.50428300	C	-6.23720200	-1.23502900	-0.37151100
C	-5.48071000	0.45991300	1.73374700	H	-4.29676900	-2.17885700	-0.36981800
C	-7.19176500	0.47446000	-0.47543800	C	-6.94122600	-0.02751900	-0.36021200
H	-5.79386000	-0.90042500	-1.37609900	H	-6.77008100	2.12367500	-0.32916300
C	-6.64037200	1.23151400	1.75388900	H	-6.77749600	-2.17913300	-0.39396300
H	-4.81457700	0.44328300	2.59100100	H	-8.02864800	-0.02548900	-0.37266300
C	-7.49844500	1.24204500	0.65123400				
H	-7.85799200	0.47728200	-1.33383800	2-b			
H	-6.87639300	1.82402200	2.63356900	Zn	0.00150600	0.67260500	-0.12812700
H	-8.40301700	1.84360200	0.67071500	I	0.21271300	-0.78851500	1.93497700
				N	0.47054000	2.74431400	-0.01922000
1-c				C	-0.73847000	3.52195700	0.43289600
Zn	0.51312000	0.03722700	-0.27668100	H	-0.45664600	4.57881800	0.51024900
I	1.75721100	-1.96255500	-1.58470300	H	-1.47544400	3.43522500	-0.36991200
N	1.06628000	-0.49134000	1.95417700	C	1.58943900	2.92911200	0.96912200
C	2.44388000	-1.04409300	2.07859200	H	1.24815900	2.49909300	1.91257700
H	2.61583300	-1.36008100	3.12127400	H	1.73541100	4.00450400	1.13296800
H	2.47680600	-1.93719300	1.44839100	C	0.85236200	3.19302500	-1.40615800
C	3.57449800	-0.10823600	1.65600400	H	1.64522900	2.52704300	-1.75406600
H	3.44176500	0.24313300	0.63055800	C	-1.36107200	3.06994900	1.75156400
H	3.66785800	0.76520300	2.30949700	H	-0.70228800	3.22790100	2.60944800
H	4.51851800	-0.66445800	1.70749700	H	-1.65139800	2.01499600	1.73719100
C	0.91807800	0.71529900	2.81312000	C	2.91032400	2.27422600	0.57605400
H	1.29947900	0.49517200	3.82600700	H	2.79689000	1.19938700	0.39620800
H	1.56233800	1.48496500	2.38270900	H	3.36803700	2.73366000	-0.30523400
C	-0.50001100	1.27690300	2.90943200	H	3.61296900	2.38767400	1.40778200
H	-0.92855800	1.45195700	1.91946900	H	-0.02344000	3.00273600	-2.03524900
H	-1.17809400	0.61879100	3.46357100	C	1.29844600	4.64934500	-1.56954800
H	-0.45976000	2.23594300	3.43929100	H	0.51406000	5.36602400	-1.31136400
C	0.07277400	-1.55925100	2.26456000	H	2.18884000	4.88445100	-0.97867400
H	-0.91564000	-1.16753000	2.01597700	H	1.55392700	4.81324500	-2.62182200
H	0.26581600	-2.36984200	1.55389800	H	-2.26597300	3.66253900	1.92357000
C	0.06543300	-2.11916800	3.69549000	C	1.71859000	-0.86510400	-1.78524800
H	-0.73029700	-2.86967000	3.77390700	C	2.77420100	-1.68662600	-1.34449700
H	1.00641500	-2.61076200	3.96366700	C	4.11086300	-1.22901100	-1.42817600
H	-0.13836400	-1.34578700	4.44461900	C	2.49971100	-2.97934800	-0.83981200
I	1.55404500	2.48980800	-0.68066100	C	5.14766500	-2.05406300	-1.01293800
C	-2.68777100	-0.03280500	-0.30864600	H	4.31409300	-0.23978600	-1.82569900
C	-1.45962900	-0.02283400	-0.29235200	C	3.54763000	-3.79089200	-0.42393600
C	-4.11419500	-0.03267100	-0.32964600	H	1.47213400	-3.32010900	-0.77516800
C	-4.84012600	1.17849700	-0.32024900	C	4.86645500	-3.33051300	-0.51058700

H	6.17464700	-1.70913100	-1.07904500	C	3.72259200	4.25572700	1.33349000
H	3.34154200	-4.78178100	-0.03212700	H	2.50253600	2.58983700	1.97462900
H	5.68135000	-3.97094000	-0.18597600	C	4.29066300	4.91226700	0.23353600
C	0.77484700	-0.11742900	-2.06998600	H	4.53435500	4.94431900	-1.91060300
H	0.13164200	0.25388200	-2.84720800	H	3.88196900	4.64073200	2.33649400
C	-5.40546200	-2.70836100	-0.24531400	H	4.89013600	5.80491600	0.39031900
C	-5.91595700	-1.73964700	-1.11591100	N	0.25070300	-1.99854900	1.84302300
C	-5.12830900	-0.64858500	-1.46356500	C	-0.84127400	-1.59111000	2.78761400
C	-3.82168300	-0.52295000	-0.94423600	H	-1.78416000	-1.68922600	2.24803000
C	-3.31581200	-1.50559500	-0.06652700	H	-0.85425300	-2.30721100	3.62606300
C	-4.11024600	-2.59039800	0.27849400	C	0.10296900	-3.45317700	1.51745200
H	-6.02046400	-3.56039700	0.03005500	H	0.88340800	-3.69913000	0.79588000
H	-6.92037000	-1.83807900	-1.51500600	H	0.29420500	-4.03448200	2.43487600
H	-5.51496000	0.11222400	-2.13733800	C	1.57551900	-1.76370600	2.50124100
H	-2.31773300	-1.40699700	0.34644800	H	1.54977900	-2.23605400	3.49770100
H	-3.72861400	-3.34611000	0.95800400	H	1.66744900	-0.68717500	2.65070600
C	-3.05851700	0.63661800	-1.35044000	C	-0.74750700	-0.16506400	3.32858900
H	-3.58741400	1.33499000	-2.02113300	H	0.09390400	-0.02191300	4.01294700
O	-1.89211800	0.93795200	-1.04154700	H	-0.67965400	0.56463200	2.51720600
4-Et3N				H	-1.66537100	0.04877700	3.88713700
C	-2.82255400	0.61773100	-0.15613100	C	-1.24629300	-3.85306800	0.92140100
C	-1.73737400	0.05236800	-0.07443000	H	-2.07068700	-3.77652500	1.63586700
Zn	-0.02603100	-0.84927000	-0.00216000	H	-1.49243000	-3.25284400	0.03930100
I	1.19013900	-1.97799800	-2.02650900	H	-1.18364900	-4.89774500	0.59820100
O	1.42306300	0.75593600	0.48904000	C	2.80257500	-2.25477300	1.73502300
C	1.94945600	1.42468400	-0.40542000	H	2.82782100	-1.86344800	0.71456700
H	1.82695800	1.11386400	-1.45591000	H	3.69764300	-1.90120900	2.25959000
C	-4.09015100	1.26984100	-0.26143200	H	2.86375400	-3.34548000	1.68388700
C	-5.03693000	0.84950400	-1.21805800	13-Et3N			
C	-4.42380500	2.34560000	0.58639600	Zn	1.03211200	0.49112700	-0.95520500
C	-6.27280100	1.48416100	-1.31866700	I	2.12087700	2.11139700	-2.61364900
H	-4.78618100	0.02347300	-1.87659900	I	0.05218200	-1.92770300	-1.84169200
C	-5.66125100	2.97648300	0.47953700	Zn	-1.47638700	-0.81218100	0.21761600
H	-3.69950500	2.67689500	1.32473800	I	-1.80515800	-2.29427100	2.29560900
C	-6.59127200	2.54924500	-0.47185800	C	-0.43881200	0.98936800	0.40033300
H	-6.99053100	1.14702300	-2.06223500	C	-0.58571200	1.97066200	1.13866200
H	-5.90124800	3.80508500	1.14115100	C	-0.75090500	3.08733800	2.00592100
H	-7.55602700	3.04292000	-0.55336100	C	-0.47788600	2.95891700	3.38423200
C	2.75144800	2.62327700	-0.16345300	C	-1.18737500	4.32938100	1.49936600
C	3.32175800	3.28654200	-1.26239800	C	-0.64578900	4.04973200	4.23218100
C	2.95505800	3.11400800	1.13895900	H	-0.14290700	2.00105400	3.76966400
C	4.09180400	4.43008000	-1.06282700	C	-1.34244100	5.41606800	2.35496000
H	3.15815600	2.90061800	-2.26566400	H	-1.39037900	4.42676800	0.43744300

C	-1.07535700	5.27786200	3.72037800
H	-0.43897200	3.94421700	5.29328900
H	-1.67238500	6.37198000	1.95837400
H	-1.20086300	6.12788600	4.38541600
C	5.40973600	-2.20625700	2.78445400
C	6.76179000	-2.03608800	2.45778500
C	7.13727000	-1.27030300	1.35011200
C	6.15717200	-0.67110900	0.56346600
C	4.79960700	-0.83666700	0.88819900
C	4.42697300	-1.60915400	2.00493500
H	5.13022700	-2.80628900	3.64527500
H	7.52622000	-2.50583400	3.07080200
H	8.18721500	-1.14496000	1.10343500
H	6.43388700	-0.07452300	-0.30253900
H	3.37315100	-1.72909000	2.23552400
C	3.79300500	-0.20126800	0.04790200
H	4.14749300	0.36982000	-0.82571600
O	2.57801200	-0.27412000	0.27100800
N	-3.40687000	-0.32913500	-0.70889800
C	-4.15586000	0.29390000	0.42874400
H	-4.40858800	-0.52085600	1.11332200
H	-3.44279800	0.93300300	0.96200500
C	-3.09478300	0.61479200	-1.83014200
H	-2.83297100	1.56908600	-1.36288200
H	-2.18426500	0.24308100	-2.31035000
C	-3.93980300	-1.65936000	-1.14980100
H	-3.37821600	-1.92672300	-2.05023200
C	-4.14197200	0.83145500	-2.92975700
H	-3.74553800	1.57507500	-3.63105900
H	-4.32333200	-0.08366000	-3.50143700
H	-5.09899600	1.20133700	-2.55480800
C	-5.40061100	1.13905100	0.12789700
H	-5.82506700	1.46583900	1.08465300
H	-5.15582800	2.04143700	-0.44103400
H	-6.17655600	0.59090000	-0.41068300
H	-3.65638200	-2.38295800	-0.37774800
C	-5.44572100	-1.81127000	-1.39938900
H	-5.62704800	-2.83422200	-1.74971200
H	-6.02453800	-1.67987700	-0.47989100
H	-5.83426300	-1.12568200	-2.15603500