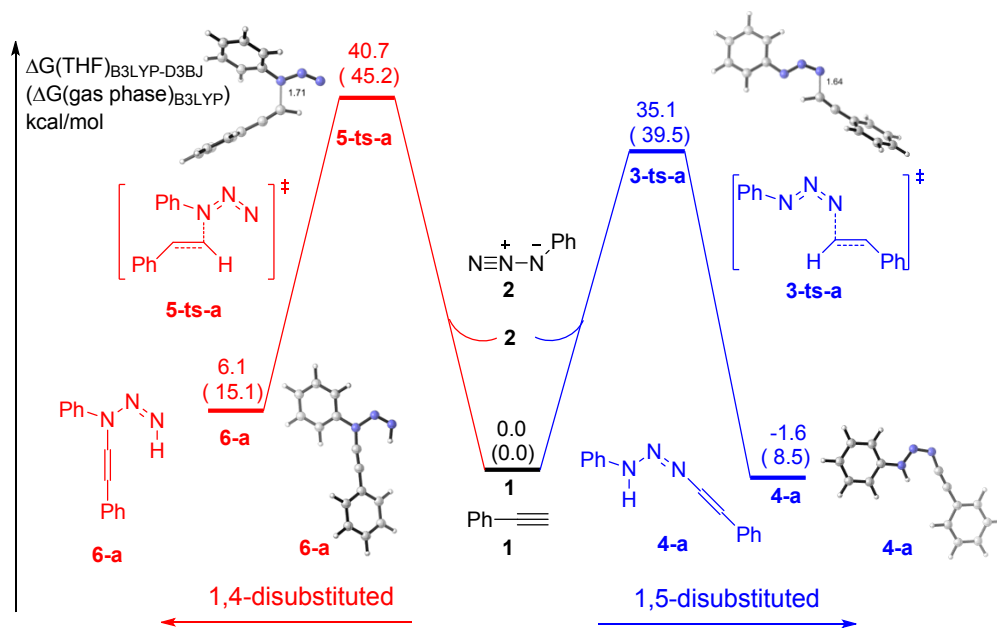


Table of contents

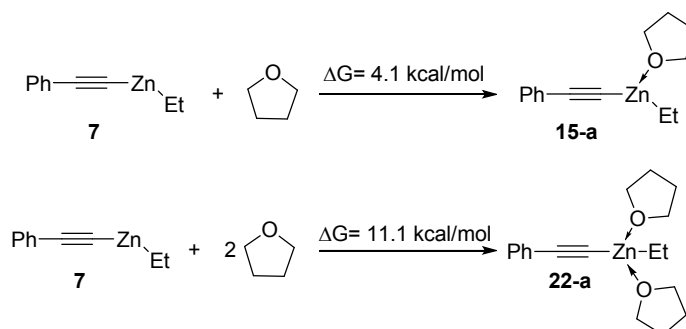
1. “Stepwise mechanism” for the uncatalytic cycloaddition of phenylacetylene and azidobenzene.	Page S2
2. The coordination of THF to Zn complex 7.	Page S2
3. Completes reference for Gaussian 09	Page S3
4. B3LYP absolute calculation energies, enthalpies, and free energies.	Page S4
5. B3LYP-D3BJ calculated single point energies in THF	Page S5
6. B3LYP geometries for all the optimized compounds and transition states.	Page S7
7. The data of distortion, interaction and total energies of the transition states by B3LYP-D3BJ method in THF solvent.	Page S20
8. The data of distortion, interaction and total energies along the reaction pathways of the dipolar cycloadditions by B3LYP-D3BJ method in THF solvent.	Page S20
9. B3LYP-D3BJ geometries for all the optimized distortion–interaction analysis compounds in THF solvent.	Page S22
10. The orbital energies of the model complex	Page S52
11. The values of proportions which represent the weight of the atomic orbitals in the ground state molecular orbitals	Page S53

1. "Stepwise mechanism" for the uncatalyzed cycloaddition of phenylacetylene and azidobenzene.



For the uncatalyzed cycloaddition of phenylacetylene and azidobenzene, although many efforts have been devoted to the stepwise mechanism, neither correct transition state nor possible intermediates are obtained. The only result about stepwise mechanism is shown in Figure S1. Two stepwise type transition states **3-ts-a** and **5-ts-a** were obtained in uncatalyzed cycloaddition, however, these transition states would lead to the generation of C-H bond cleavage products **4-a** and **6-a**, which are different from the stepwise intermediates. More importantly, the activation energy of **3-ts-a** and **5-ts-a** are 35.1 and 40.7 kcal/mol, respectively. These barriers are much higher than that in concerted pathway (27.8 and 30.1 kcal/mol, respectively). Thus, this possibility could be ruled out.

2. The coordination of THF to Zn complex 7.



As shown above, the generation of complex **15-a** with one THF coordination towards complex **7** is 4.1 kcal/mol endothermic and the formation of complex **22-a** with two THF coordination is 11.1 kcal/mol endothermic. These data indicate that the coordination ability of THF is weaker than NMA in this system.

3. Complete reference for Gaussian 09

Gaussian 09, Revision A.2, 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, **2009**.

4. B3LYP absolute calculation energies, enthalpies, and free energies.

Geometry	$E_{(\text{elec})}$	$H_{(\text{gas phase})}$	$G_{(\text{gas phase})}$	IF*
1	-308.465647	-308.349270	-308.387127	-
2	-395.934245	-395.823212	-395.863110	-
3-ts	-704.366140	-704.138246	-704.197406	-426.3
4	-704.490228	-704.256927	-704.311414	-
5-ts	-704.363565	-704.135643	-704.194428	-409.4
6	-704.495092	-704.261870	-704.317212	-
7	-614.266283	-614.088760	-614.142473	-
8	-1010.202909	-1009.912383	-1009.993978	-
9-ts	-1010.165995	-1009.877440	-1009.952947	-366.5
10	-1010.270875	-1009.978120	-1010.048074	-
11	-1010.203932	-1009.913523	-1009.993134	-
12-ts	-1010.169718	-1009.881246	-1009.953129	-219.0
13	-1010.278627	-1009.985823	-1010.056156	-
14	-265.592465	-265.487380	-265.522733	-
15	-879.876663	-879.592133	-879.665924	-
16	-1275.814107	-1275.416562	-1275.517106	-
17-ts	-1275.780872	-1275.385352	-1275.479155	-318.4
18	-1275.885992	-1275.486038	-1275.573094	-
19	-1275.814894	-1275.417385	-1275.515838	-
20-ts	-1275.778778	-1275.383208	-1275.474381	-215.6
21	-1275.893260	-1275.493277	-1275.581386	-
22	-1145.479568	-1145.088223	-1145.180255	-
23-ts	-1541.386610	-1540.884106	-1540.995104	-307.5
24	-1541.489332	-1540.982383	-1541.087969	-
25-ts	-1541.383069	-1540.880463	-1540.992246	-320.5
26	-1541.496633	-1540.880463	-1540.992246	-
27	-540.4510534	-540.2410654	-540.2943794	-
28	-806.0596197	-805.7416127	-805.8178567	-

29	-1201.995923	-1201.565945	-1201.667205	-
30-ts	-1201.964711	-1201.535603	-1201.631001	-309.7
31	-1202.073578	-1201.639849	-1201.730105	-
32	-1201.99715	-1201.567105	-1201.665614	-
33-ts	-1201.966448	-1201.537293	-1201.631789	-
34	-1202.076926	-1201.643375	-1201.736511	-248.7
3-ts-a	-704.354933	-704.127688	-704.187211	-232.0
4-a	-704.4089583	-704.1771603	-704.2367073	-
5-ts-a	-704.3458948	-704.1186578	-704.1781588	-437.7
6-a	-704.3975031	-704.1662891	-704.2261451	-
15-a	-846.7858051	-846.4836911	-846.5570321	-
22-a	-1079.301263	-1078.875051	-1078.964163	-
THF	-232.5086688	-232.3858978	-232.4210068	-

5. B3LYP-D3BJ calculated single point energies in THF

Geometry	E_{solv}
1	-308.4998506
2	-395.9685646
3-ts	-704.44316
4	-704.5771442
5-ts	-704.4398549
6	-704.5789772
7	-614.3264627
8	-1010.3019
9-ts	-1010.270751
10	-1010.385399
11	-1010.293188
12-ts	-1010.267887
13	-1010.394808

14(NMI)	-265.6286867
15	-879.9711659
16	-1275.947146
17-ts	-1275.918448
18	-1276.030305
19	-1275.950606
20-ts	-1275.916301
21	-1276.043792
22	-1145.612712
23-ts	-1541.56373
24	-1541.671476
25-ts	-1541.561171
26	-1541.689629
27	-540.4502785
28	-806.1461237
29	-1202.123182
30-ts	-1202.096926
31	-1202.208939
32	-1202.124591
33-ts	-1202.096926
34	-1202.218448
3-ts-a	-704.4304989
4-a	-704.4936797
5-ts-a	-704.4216436
6-a	-704.4804201
15-a	-846.8725841
22-a	-1079.417592
THF	-232.535419

6. B3LYP geometries for all the optimized compounds and transition states.

1							
C	-2.02218500	-0.00002100	-0.00003800	C	-0.90797200	2.68650900	-0.01639100
C	-3.22748400	0.00001000	0.00005700	C	-0.66336900	1.32734700	-0.01124500
C	-0.59433600	-0.00002100	-0.00008900	C	-1.60449600	0.20088900	-0.08791500
C	0.11933200	1.21067000	-0.00001200	C	-2.75959600	0.21264900	0.70741500
C	0.11936200	-1.21068800	-0.00000700	C	-1.40829600	-0.86518500	-0.97804300
C	1.51014400	1.20655500	0.00002000	C	-3.69384700	-0.81590800	0.61566600
H	-0.42641200	2.14762800	0.00000300	H	-2.91700000	1.02686900	1.40706000
C	1.51017500	-1.20653400	0.00001600	C	-2.34241500	-1.89294400	-1.06488600
H	-0.42635300	-2.14766300	0.00000900	H	-0.52942200	-0.88384100	-1.61269000
C	2.21001800	0.00001900	0.00001100	C	-3.48736700	-1.87302200	-0.26886400
H	2.04943700	2.14827300	0.00005400	H	-4.58102100	-0.79287900	1.24015400
H	2.04949400	-2.14823600	0.00004300	H	-2.17859100	-2.70846700	-1.76175400
H	3.29515200	0.00003100	0.00004000	H	-4.21444300	-2.67540100	-0.33928300
H	-4.29147200	0.00001700	0.00010500	C	1.57597300	0.12460400	0.09334500
2				C	2.68952800	0.06893200	-0.74477600
N	1.47280600	-0.87578800	0.00001200	C	1.33305700	-0.88516800	1.02400200
N	2.41699800	-0.08546400	0.00012300	C	3.56170800	-1.01233100	-0.65110600
N	3.37087500	0.52738600	-0.00026800	H	2.86730200	0.87286800	-1.44854500
C	0.14893900	-0.36055100	0.00005300	C	2.20526900	-1.96802100	1.10054100
C	-0.87956500	-1.30759700	-0.00009200	H	0.47656700	-0.82082900	1.68428000
C	-0.15550700	1.00529600	0.00017200	C	3.31949100	-2.03487300	0.26533200
C	-2.20504200	-0.88753900	-0.00012500	H	4.43079400	-1.05546200	-1.29899600
H	-0.62425500	-2.36119500	-0.00017900	H	2.01768700	-2.75461900	1.82371800
C	-1.48733300	1.41260000	0.00014300	H	3.99932300	-2.87771400	0.33254900
H	0.63689800	1.74726200	0.00029700	H	-1.85437100	3.20206700	-0.06550000
C	-2.51637100	0.47257900	-0.00001000	5-ts			
H	-2.99865400	-1.62752700	-0.00024000	N	0.66699200	-1.29850200	-0.30733000
H	-1.71791600	2.47300500	0.00024000	N	-0.45791900	-1.54454600	-0.14066700
H	-3.55155100	0.79677400	-0.00003200	N	1.35852700	-0.29732600	-0.65194600
3				C	-0.25454700	1.13368900	-0.57605000
N	-1.23293400	2.34578500	-0.23973600	C	-1.27841000	0.47779100	-0.35033000
N	-0.72228900	3.38680900	-0.04888300	C	-2.68548100	0.28966800	-0.09192100
N	-0.85792000	1.15129100	-0.37311700	C	-3.37508900	1.24195200	0.67920600
C	1.18393300	2.94249700	0.23456300	C	-3.39649800	-0.80407300	-0.60878600
C	1.42083700	1.73083200	0.16002400	C	-4.73754800	1.10215600	0.92161100
C	2.02807400	0.43876000	0.13318700	H	-2.83145800	2.08727700	1.08647200
C	2.59865800	-0.05563300	-1.05339200	C	-4.76196700	-0.93128800	-0.37340200
C	2.09637200	-0.34231400	1.30004700	H	-2.87117300	-1.55163300	-1.19004200
C	3.22269900	-1.29790100	-1.06677900	C	-5.43722900	0.01730800	0.39366200
H	2.54435600	0.54145500	-1.95677800	H	-5.25436600	1.84368700	1.52248500
C	2.72553600	-1.58228500	1.27809800	H	-5.29916000	-1.77977000	-0.78493300
H	1.65260900	0.03134400	2.21593900	H	-6.50077400	-0.08929100	0.58130700
C	3.28900000	-2.06549500	0.09707000	C	2.69470400	-0.14598700	-0.23030100
H	3.66087700	-1.66792500	-1.98805900	C	3.26279300	-0.88221100	0.81888400
H	2.77322600	-2.17494000	2.18582300	C	3.45571300	0.83091700	-0.88383300
H	3.77753200	-3.03425800	0.08343000	C	4.57922100	-0.64125200	1.19733500
C	-1.76100900	0.08373800	-0.22350300	H	2.67507800	-1.64124300	1.32385600
C	-3.05616400	0.22817000	0.29732300	C	4.76536100	1.07584900	-0.48307300
C	-1.30140000	-1.18767800	-0.59131700	H	3.01618100	1.38097400	-1.70883500
C	-3.87504700	-0.88744300	0.43398400	C	5.33515200	0.34052100	0.55558700
H	-3.41432400	1.21180300	0.58144600	H	5.01508200	-1.22189100	2.00402200
C	-2.12630200	-2.29706000	-0.43591800	H	5.34712100	1.83566400	-0.99474800
H	-0.30028800	-1.29149400	-0.99354200	H	6.35969200	0.52635200	0.85941400
C	-3.41691500	-2.15517300	0.07303000	H	0.37353200	1.96224700	-0.81093800
H	-4.87881200	-0.76442300	0.82859800	6			
H	-1.75955500	-3.27750100	-0.72251800	N	-0.67668600	-1.60484100	-0.36517600
H	-4.06032400	-3.02133400	0.18514900	N	-1.09731600	-0.34306000	-0.08900000
H	1.52707500	3.94197400	0.39415000	N	0.61765500	-1.59538500	-0.36256200
4				C	-0.02710400	0.47578300	0.09233800
N	1.24773400	2.50542800	0.01542400	C	1.07667900	-0.33306900	-0.08705200
N	0.27148200	3.35827700	-0.00522100	C	2.50832800	-0.02193900	-0.00707300
N	0.70609300	1.25437300	0.00987600	C	2.96227600	1.29955300	0.11196800
				C	3.45472000	-1.05609200	-0.04910700

C	4.32286400	1.57974800	0.19397000	H	6.20285200	0.74910600	-0.32391100
H	2.25127900	2.11990200	0.13312400	N	-0.73764400	-2.81339900	-1.07823100
C	4.81480100	-0.77273800	0.02971200	N	0.35968200	-2.63183600	-0.55962400
H	3.11062100	-2.07902600	-0.14442000	N	1.43034500	-2.51659500	-0.20098400
C	5.25605700	0.54437400	0.15315600	C	-1.91492000	-2.53253300	-0.33288700
H	4.65498600	2.60907600	0.28496400	C	-3.12686500	-2.80762800	-0.97248900
H	5.53363100	-1.58527900	-0.00416900	C	-1.90608300	-2.00932700	0.96453600
H	6.31724000	0.76277700	0.21502000	C	-4.32580100	-2.56226700	-0.31167700
C	-2.48494100	-0.03503400	-0.01949000	H	-3.11228400	-3.21002500	-1.97895000
C	-2.93525000	1.24062800	-0.36236800	C	-3.11379300	-1.76879500	1.61474900
C	-3.38520400	-1.02066600	0.38876300	H	-0.96897100	-1.78130700	1.46203900
C	-4.29391700	1.53438600	-0.27675400	C	-4.32621300	-2.04308300	0.98341000
H	-2.23748300	1.99181500	-0.71479100	H	-5.26405100	-2.77844500	-0.81193900
C	-4.74169900	-0.71826900	0.45550700	H	-3.10275300	-1.36026700	2.61980800
H	-3.01623900	-2.00557600	0.64443900	H	-5.26300500	-1.85321400	1.49604600
C	-5.20087100	0.55793100	0.13016500	9-ts			
H	-4.64280100	2.52620700	-0.54406300	N	-0.13014900	-1.95718600	0.07130500
H	-5.44194100	-1.48429100	0.77130900	N	1.05481400	-1.90496700	0.11816600
H	-6.25915500	0.78844700	0.18941200	N	-1.04888300	-1.09338400	0.02306400
H	-0.13613200	1.51134900	0.36392400	C	1.47661600	0.00496100	0.11633700
7				C	0.44871700	0.71211400	0.06612900
C	-0.75589500	-0.07346800	-0.00002800	Zn	3.37883600	-0.17473200	0.20114500
C	0.46222900	-0.14340300	-0.00004000	C	5.31525900	-0.36837700	0.29206000
C	-2.18007800	0.00481900	-0.00001400	H	5.55231600	-0.78321600	1.27835000
C	-2.96149500	-1.16487900	-0.00003000	H	5.74819800	0.63826300	0.28056000
C	-2.82996200	1.25238000	0.00001900	C	5.94478400	-1.23283300	-0.81375000
C	-4.34982600	-1.08548700	-0.00001400	H	5.75973500	-0.82447500	-1.81160300
H	-2.46745300	-2.13013600	-0.00005400	H	7.03225600	-1.30246200	-0.69390100
C	-4.21880000	1.32363700	0.00003500	H	5.55642200	-2.25515500	-0.80799300
H	-2.23423300	2.15844700	0.00003100	C	-0.41878700	1.84903100	0.01145600
C	-4.98381100	0.15712400	0.00001900	C	-0.91962300	2.42528900	1.19216400
H	-4.93942500	-1.99674100	-0.00002500	C	-0.75612600	2.42875400	-1.22431300
H	-4.70628900	2.29335400	0.00005900	C	-1.73332300	3.55151200	1.13434900
H	-6.06740200	0.21608800	0.00003200	H	-0.66927100	1.97784800	2.14747100
Zn	2.34590700	-0.25298000	-0.00000600	C	-1.57077700	3.55479500	-1.27357300
C	4.28829900	-0.38147100	0.00012000	H	-0.37839500	1.98473400	-2.13848400
H	4.57938900	-0.97789600	0.87284900	C	-2.06286500	4.12008600	-0.09664600
H	4.57951700	-0.97822000	-0.87234300	H	-2.11343900	3.98615200	2.05322400
C	5.04871400	0.95669500	-0.00007100	H	-1.82385000	3.99188000	-2.23410700
H	4.81418000	1.56385600	0.87936800	H	-2.69981500	4.99757000	-0.13843000
H	6.13395000	0.80142600	0.00004100	C	-2.39878900	-1.49243800	-0.01019800
H	4.81431500	1.56352900	-0.87977100	C	-2.81665900	-2.83262400	0.01446200
8				C	-3.36068000	-0.47480500	-0.06949700
C	0.50413400	1.74430900	-0.05188000	C	-4.17327400	-3.13762100	-0.02002900
C	1.50994200	1.05410000	-0.01401400	H	-2.07656300	-3.62361000	0.06000100
C	-0.66651500	2.55906700	-0.09855300	C	-4.71437900	-0.79467100	-0.10287400
C	-1.94448800	1.97920800	-0.19525900	H	-3.03732100	0.55922900	-0.08853200
C	-0.56265300	3.96132900	-0.04968900	C	-5.13132600	-2.12512000	-0.07852700
C	-3.08034700	2.78060500	-0.24302800	H	-4.48292100	-4.17810100	-0.00065600
H	-2.03630500	0.89945400	-0.23042100	H	-5.44780200	0.00431800	-0.14844200
C	-1.70305800	4.75572300	-0.09744500	H	-6.18771800	-2.37057200	-0.10485400
H	0.41915700	4.41557700	0.02508100	10			
C	-2.96550900	4.16990300	-0.19454800	N	-0.80103400	-2.46200500	0.06217300
H	-4.05905700	2.31759900	-0.31887500	N	0.49221600	-2.46887200	0.02162400
H	-1.60633700	5.83614800	-0.05951100	N	-1.20657900	-1.15906100	0.04181600
H	-3.85369500	4.79238000	-0.23273700	C	0.98167200	-1.18123500	-0.02160500
Zn	3.10880000	0.03863800	0.02404100	C	-0.11678200	-0.32927700	-0.00851600
C	4.81100700	-0.90620600	0.06859800	Zn	2.88608700	-0.87236400	-0.18799200
H	4.70906600	-1.72455700	0.79075000	C	4.81311200	-0.60637100	-0.36468900
H	4.93994600	-1.39315300	-0.90534900	H	4.98750600	-0.02921000	-1.28067600
C	6.04899300	-0.05586800	0.40123000	H	5.26330800	-1.58931300	-0.54800900
H	5.97352000	0.41305900	1.38707400	C	5.50760000	0.07577700	0.82740200
H	6.96423900	-0.65992700	0.40520900	H	5.38938400	-0.49448000	1.75387800

H	6.58523300	0.18691700	0.65796600	N	-1.10082100	-0.63429000	-0.14976200
H	5.11152400	1.07859300	1.01569000	C	1.08814300	0.95594500	-0.06715900
C	-0.15770500	1.13856200	-0.10971100	C	1.92179300	-0.00186800	-0.05969400
C	0.65615500	1.91562900	0.72782000	Zn	-0.74675000	1.55225200	-0.04531900
C	-0.95219800	1.78913500	-1.06560000	C	-2.21137500	2.85625900	0.02988200
C	0.68025600	3.30364900	0.60931700	H	-2.99900500	2.44608700	0.67192400
H	1.25584800	1.42707400	1.48889400	H	-2.65682700	2.92167000	-0.97088900
C	-0.92949100	3.17584100	-1.17955100	C	-1.81754900	4.26323700	0.51061300
H	-1.58002900	1.20551600	-1.72991200	H	-1.06017300	4.72071300	-0.13347900
C	-0.11326900	3.93854300	-0.34401900	H	-2.67759400	4.94422000	0.52500000
H	1.31350000	3.88857800	1.26863000	H	-1.40628200	4.25031600	1.52479300
H	-1.54689900	3.66211800	-1.92792800	C	3.35314500	-0.29167900	-0.02940500
H	-0.09707600	5.01962000	-0.43578900	C	3.85970800	-1.59685700	-0.04229200
C	-2.60019500	-0.86830800	0.13903500	C	4.25220300	0.78813200	0.01345700
C	-3.49848100	-1.60004500	-0.63899600	C	5.23514300	-1.81495500	-0.01226600
C	-3.05926500	0.10809500	1.02343200	H	3.17698100	-2.43511700	-0.07615600
C	-4.86292700	-1.34518900	-0.53167500	C	5.62267800	0.56300500	0.04322900
H	-3.12260400	-2.36545000	-1.30669900	H	3.86555800	1.80131100	0.02317100
C	-4.42526000	0.36371500	1.11299300	C	6.12082900	-0.74069800	0.03048400
H	-2.35693900	0.65682000	1.63909900	H	5.61385600	-2.83184400	-0.02303500
C	-5.32993500	-0.36027300	0.33804300	H	6.30408700	1.40692900	0.07629700
H	-5.56171200	-1.91728900	-1.13295200	H	7.19154500	-0.91570400	0.05351000
H	-4.78182800	1.12347300	1.80052900	C	-2.42784400	-1.16056800	-0.07718200
H	-6.39377600	-0.16199500	0.41567300	C	-2.71671800	-2.36349700	0.58059500
11				C	-3.46644100	-0.42945500	-0.65988700
C	-2.45786500	0.43658100	0.03185400	C	-4.02716900	-2.82561200	0.64083700
C	-1.34949000	0.94701400	0.03674400	H	-1.91362700	-2.92929300	1.03859700
C	-3.75424000	-0.15987400	0.02341300	C	-4.77698000	-0.89492900	-0.58517800
C	-4.16158600	-1.00695400	1.06985500	H	-3.24730600	0.49613000	-1.17873500
C	-4.65143700	0.09032600	-1.03070900	C	-5.06504600	-2.09431400	0.06261500
C	-5.42694100	-1.58396400	1.05903000	H	-4.23839100	-3.76049900	1.15019400
H	-3.47577500	-1.20538600	1.88594100	H	-5.57324200	-0.31846600	-1.04477500
C	-5.91511800	-0.49052500	-1.03500500	H	-6.08624700	-2.45623300	0.11692400
H	-4.34540300	0.74307700	-1.84072300	13			
C	-6.30821600	-1.32910400	0.00818300	N	0.70019400	-2.57017100	0.27463200
H	-5.72644200	-2.23560100	1.87376300	N	1.09572800	-1.27330700	0.17499600
H	-6.59611700	-0.28765300	-1.85550100	N	-0.59415000	-2.57939500	0.27525800
H	-7.29495500	-1.78079700	0.00229000	C	0.02480400	-0.41887700	0.10487100
Zn	0.33828600	1.81429200	0.05432800	C	-1.05786900	-1.29402500	0.18170600
C	1.87268200	3.02438500	0.09268700	Zn	0.08065700	1.47441200	-0.32298600
H	2.49864300	2.75606000	0.95214700	C	0.10752200	3.36736700	-0.79096200
H	2.48522700	2.83140000	-0.79616800	H	-0.46314900	3.47986000	-1.72006100
C	1.51105000	4.51910600	0.16023900	H	1.14118000	3.62752000	-1.04698900
H	0.92862700	4.76046900	1.05454400	C	-0.43155300	4.33256000	0.27939400
H	2.40612800	5.15252000	0.18199100	H	0.13673800	4.27460800	1.21274700
H	0.91695000	4.83723800	-0.70179600	H	-0.38162900	5.37397500	-0.05900800
N	-0.20215000	-2.30569400	-0.17476000	H	-1.47763100	4.12956200	0.52735900
N	0.68665500	-1.60999000	-0.13099600	C	-2.49729200	-1.00236000	0.13971200
N	1.56763500	-0.73995800	-0.08178300	C	-3.01261200	0.21756700	0.60217200
C	2.92356600	-1.18842700	-0.06902400	C	-3.39310600	-1.95222600	-0.37435100
C	3.90948400	-0.19905100	-0.03218500	C	-4.37565300	0.49424800	0.52663200
C	3.28802000	-2.53922600	-0.09028200	H	-2.34958000	0.94300800	1.06573600
C	5.25216900	-0.56224000	-0.01700400	C	-4.75564300	-1.67894100	-0.44051900
H	3.61658500	0.84323200	-0.01635200	H	-3.00602300	-2.90308900	-0.72158100
C	4.63582800	-2.88913500	-0.07492200	C	-5.25331600	-0.45291100	0.00217800
H	2.53133400	-3.31671100	-0.11853200	H	-4.75401100	1.44256100	0.89521800
C	5.62331100	-1.90646100	-0.03819900	H	-5.43293700	-2.42560800	-0.84307000
H	6.01161200	0.21216400	0.01131200	H	-6.31644100	-0.24191900	-0.05165100
H	4.91136300	-3.93854500	-0.09171100	C	2.48462700	-0.96252300	0.13927500
H	6.67133900	-2.18544600	-0.02632100	C	2.97491000	0.13880900	0.84295900
12-ts				C	3.35101500	-1.77320400	-0.59612600
N	-0.15970900	-1.50949100	-0.12520800	C	4.33310000	0.44634700	0.78452000
N	1.03796200	-1.45345700	-0.10584000	H	2.30704500	0.72586000	1.46396200

C	4.70814700	-1.46668900	-0.63461200
H	2.95446700	-2.63121800	-1.12425100
C	5.20265600	-0.35410300	0.04656300
H	4.71109100	1.30150000	1.33479500
H	5.37994300	-2.09767900	-1.20683800
H	6.26041600	-0.11741800	0.00853300
14			
N	-1.47439100	-0.76733000	0.00001800
C	-0.19945100	-1.08511600	-0.00007800
C	-1.50207900	0.60666500	0.00014400
H	0.20183100	-2.08870200	-0.00015500
C	-0.22701700	1.11336000	-0.00007300
H	-2.43451300	1.15163000	0.00026500
H	0.15553100	2.12195000	-0.00020200
N	0.61059100	0.01609000	-0.00023400
C	2.06266800	0.03127000	0.00017300
H	2.42771300	-0.99553900	-0.00248700
H	2.44578800	0.53844000	-0.88807500
H	2.44552000	0.53382700	0.89117600
15			
C	1.93907500	0.34121000	-0.01750100
C	0.77469100	0.71086900	-0.02367700
C	3.29972400	-0.09014200	-0.00799100
C	3.90679200	-0.59023400	-1.17528300
C	4.06837000	-0.02573800	1.16936800
C	5.23300800	-1.00996900	-1.16200100
H	3.32588300	-0.64065800	-2.08979900
C	5.39389500	-0.44752300	1.17613200
H	3.61223400	0.36105000	2.07408300
C	5.98318300	-0.94177700	0.01218300
H	5.68403500	-1.39068800	-2.07331600
H	5.97046100	-0.38859300	2.09421700
H	7.01798300	-1.26903900	0.01960600
Zn	-1.05996100	1.32283500	-0.03216100
C	-2.46981700	2.71268800	-0.06097500
H	-3.11526500	2.52168400	-0.93019900
H	-3.11588400	2.55630300	0.81464900
C	-1.99584700	4.17542100	-0.09013400
H	-1.38249700	4.38627100	-0.97196600
H	-2.83155000	4.88782000	-0.10456900
H	-1.38284300	4.42148400	0.78279200
N	-2.11963500	-0.62715200	0.02227700
C	-3.42277700	-0.83987100	0.02259100
C	-1.52555600	-1.86868600	0.06126300
H	-4.18333500	-0.07424600	-0.00260900
C	-2.49403100	-2.83370500	0.08479800
H	-0.45120000	-1.96692900	0.06919500
H	-2.44005000	-3.91007700	0.11642900
N	-3.70478700	-2.16508500	0.05976900
C	-5.02831000	-2.77161100	0.07229000
H	-5.17070900	-3.35932400	0.98076100
H	-5.78032200	-1.98426100	0.04334300
H	-5.16157800	-3.41578200	-0.79848400
16			
C	-0.74368300	-1.75752200	0.51571600
C	0.27880800	-1.14703100	0.79100700
C	-1.94594800	-2.46729200	0.21674900
C	-2.29835400	-2.77511200	-1.11092000
C	-2.81331200	-2.87463000	1.24863200
C	-3.47342700	-3.46414400	-1.39385300
H	-1.64081600	-2.46427200	-1.91558000
C	-3.98647400	-3.56407700	0.95971700
H	-2.55229800	-2.64291300	2.27532900

C	-4.32307600	-3.86199100	-0.36132200
H	-3.72765600	-3.69124800	-2.42459300
H	-4.64115900	-3.87110100	1.76948900
H	-5.23875100	-4.40041100	-0.58385000
Zn	1.89546200	-0.21698300	1.33686800
C	2.96564900	0.77234200	2.67864600
H	3.30637400	1.70846500	2.21493700
H	3.88140600	0.19639100	2.87394100
C	2.27014900	1.08949900	4.01313900
H	2.92252800	1.63509000	4.70824000
H	1.37551700	1.70390600	3.86924200
H	1.94563100	0.18000700	4.52908700
N	0.84442000	2.54028000	-0.32903700
N	-0.17918000	3.01101300	-0.46238900
N	-1.21085500	3.65782800	-0.63118100
C	-2.46472200	2.98722500	-0.58320400
C	-3.59151200	3.77847400	-0.82474700
C	-2.60477400	1.62205600	-0.31098400
C	-4.85695000	3.20225200	-0.79537900
H	-3.45972400	4.83456300	-1.03194500
C	-3.87836200	1.05818500	-0.28632700
H	-1.73836200	0.99792100	-0.11357200
C	-5.00662400	1.84122800	-0.52693800
H	-5.72914000	3.82023100	-0.98310300
H	-3.98077200	-0.00109200	-0.07633900
N	3.18404300	-0.53171400	-0.41925400
C	4.38417000	-0.02023300	-0.62153100
C	2.88387700	-1.26849700	-1.54241400
H	4.91914900	0.61506400	0.06776300
C	3.92483200	-1.19307900	-2.42570100
H	1.94417100	-1.79140700	-1.62628700
H	4.07536500	-1.62266300	-3.40307500
C	6.16934200	-0.01569300	-2.38878400
H	6.77855400	-0.90207800	-2.57381800
H	6.03354200	0.53057300	-3.32370700
H	6.69188400	0.62681300	-1.68139500
N	4.87983300	-0.39142800	-1.82684900
H	-5.99477200	1.39403500	-0.50485600
17-ts			
N	-0.85432600	-1.49401700	-0.97888200
N	0.29882200	-1.22150700	-1.06505800
N	-1.88501600	-0.91513500	-0.53294300
C	0.52273800	0.58690200	-0.31998500
C	-0.54623800	1.05948300	0.11299800
Zn	2.42478000	1.01742500	-0.65538400
C	3.72306800	2.29423000	-1.43958100
H	4.43614100	1.71648300	-2.04255500
H	4.31654200	2.71387600	-0.61557100
C	3.13428900	3.43607000	-2.28275600
H	2.44468700	4.05756600	-1.70273400
H	3.91012500	4.10437900	-2.67932100
H	2.57017900	3.05845100	-3.14146400
C	-1.56615800	1.87916700	0.68612000
C	-1.82338500	1.84293900	2.06880800
C	-2.30742200	2.76703900	-0.11515500
C	-2.79281900	2.66784000	2.62882200
H	-1.25880200	1.15875600	2.69244000
C	-3.27519000	3.58891000	0.45143500
H	-2.11772500	2.79701500	-1.18214600
C	-3.52346200	3.54293400	1.82410100
H	-2.98034900	2.62734700	3.69723200
H	-3.83898600	4.26794300	-0.18034200
H	-4.28037500	4.18465200	2.26342700

C	-3.12822500	-1.56827500	-0.60432800	H	5.20206300	0.99701900	-0.35273400
C	-3.33053800	-2.82706700	-1.19399400	H	6.69104100	-1.33438500	-0.24171700
C	-4.22289900	-0.89341700	-0.04418100	N	4.72820500	-2.20724600	-0.03643700
C	-4.60228200	-3.39094800	-1.21406500	C	5.05110300	-3.62294600	0.06693800
H	-2.49014900	-3.35167400	-1.63516600	H	4.12637300	-4.18780700	0.17415300
C	-5.48928200	-1.46793800	-0.07176400	H	5.56963500	-3.96372300	-0.83110900
H	-4.06469200	0.07920500	0.40785100	H	5.68068400	-3.80926200	0.93894100
C	-5.68990200	-2.71947700	-0.65466900	H	-6.77747600	-2.70072000	0.41557700
H	-4.74378400	-4.36439200	-1.67429700	19			
H	-6.32594100	-0.93203900	0.36589500	C	2.21531700	-0.64480100	0.80614300
N	3.48195300	-0.61453100	0.31046200	C	1.16533000	-0.06051500	1.02987800
C	2.95078400	-1.76394800	0.69121100	C	3.44320300	-1.32822000	0.55249600
C	4.82173100	-0.68355900	0.62639800	C	3.66168900	-1.99264900	-0.66932100
H	1.91528500	-2.03725100	0.55889000	C	4.46738500	-1.35309400	1.51795100
C	5.08870300	-1.89177900	1.20633300	C	4.86036500	-2.65548800	-0.91334500
H	5.49389400	0.13289100	0.41450100	H	2.87864400	-1.98422200	-1.41992900
H	5.99968200	-2.32288200	1.58911700	C	5.66396400	-2.01683100	1.26743300
N	3.88554100	-2.57356600	1.24079400	H	4.30874000	-0.84808600	2.46449200
C	3.66574300	-3.91604500	1.76164500	C	5.86748400	-2.67080700	0.05188100
H	4.28513700	-4.63762300	1.22658900	H	5.00851900	-3.16437300	-1.86099500
H	3.90163000	-3.95613800	2.82642000	H	6.44096100	-2.02565500	2.02570000
H	2.61896400	-4.18189300	1.62293300	H	6.80124700	-3.18959600	-0.14030600
H	-6.67918300	-3.16451800	-0.67514500	Zn	-0.50369900	0.88513500	1.37341300
18				C	-2.07577700	1.30571600	2.50779200
N	-0.75242700	-2.19889200	0.12789100	H	-2.91820200	1.58301700	1.85947600
N	0.40266200	-1.60892600	0.09534900	H	-2.39484100	0.39660900	3.03240300
N	-1.70157400	-1.22786800	0.06932500	C	-1.84123300	2.42452200	3.53997200
C	0.26585300	-0.23600100	0.01792600	H	-1.54159600	3.36605500	3.06607100
C	-1.10468500	0.00867600	0.00188700	H	-2.73840800	2.64125100	4.13538600
Zn	1.80887000	1.01160900	-0.12698100	H	-1.04779200	2.16399400	4.24820200
C	2.53373900	2.86079900	-0.24582700	N	-0.18167000	-0.62255200	-2.51813100
H	1.73464700	3.53390700	-0.57850500	N	-0.96266100	-0.71209900	-1.70237100
H	3.28551700	2.89190800	-1.04643700	N	-1.74933100	-0.68339200	-0.75526500
C	3.15083600	3.41026600	1.05415300	N	-0.28330300	2.46037700	-0.17889000
H	3.97152100	2.78372000	1.42170900	C	0.80842200	2.58639000	-0.91182500
H	3.55729700	4.42354000	0.93231400	C	-1.13006800	3.47182500	-0.57299000
H	2.41555000	3.46302500	1.86479400	H	1.67151200	1.94075700	-0.84594900
C	-1.83095700	1.28116600	-0.14712400	C	-0.53190300	4.20919600	-1.55725000
C	-1.49694200	2.37684900	0.66137100	H	-2.10310800	3.59935400	-0.12506200
C	-2.82970900	1.44577100	-1.11906300	H	-0.86218800	5.06936400	-2.11733900
C	-2.14206100	3.60123500	0.50334000	C	1.71355400	4.06480300	-2.72649900
H	-0.73133600	2.26205800	1.42068600	H	1.31947100	4.00832800	-3.74262900
C	-3.47563800	2.66871900	-1.27348700	H	2.02789500	5.08874000	-2.51709900
H	-3.09253800	0.61499500	-1.76493900	H	2.57965200	3.40917900	-2.65006600
C	-3.13550500	3.75136300	-0.46251200	N	0.70816300	3.63350300	-1.76552400
H	-1.86897900	4.43761600	1.13885900	C	-2.76040500	-1.68280100	-0.68040300
H	-4.24178700	2.77842000	-2.03452600	C	-3.64553400	-1.58946800	0.39699400
H	-3.63872600	4.70505000	-0.58541100	C	-2.89359400	-2.71721500	-1.61288800
C	-3.07437000	-1.60343600	0.15882800	C	-4.66144500	-2.52924300	0.53543100
C	-3.53499600	-2.67418500	-0.60910900	H	-3.52516000	-0.78532200	1.11307000
C	-3.93740900	-0.93258900	1.02605000	C	-3.91557800	-3.65097200	-1.46190900
C	-4.86648500	-3.06852400	-0.50922200	H	-2.20625300	-2.79969200	-2.44896600
H	-2.84613200	-3.19099700	-1.26598000	C	-4.80313400	-3.56280400	-0.39086900
C	-5.27043400	-1.32686000	1.10881600	H	-5.34474800	-2.45318900	1.37487100
H	-3.56782200	-0.11438800	1.63190400	H	-4.01373200	-4.45264400	-2.18673800
C	-5.73917300	-2.39399000	0.34397300	H	-5.59628500	-4.29402600	-0.27775400
H	-5.22274100	-3.90306100	-1.10429600	20-ts			
H	-5.94056600	-0.80318800	1.78258300	N	0.30577300	-1.68911600	-1.01347600
N	3.54213800	-0.34862500	-0.12438500	N	1.49081900	-1.48914700	-1.00050900
C	3.48724200	-1.66577000	-0.00375400	N	-0.68154100	-1.25944400	-0.31915500
C	4.87695000	-0.02526100	-0.24027800	C	1.34442700	0.09288300	0.84166800
H	2.56615400	-2.22436200	0.10001200	C	2.23899700	-0.44089000	0.11568400
C	5.62739400	-1.16640300	-0.18768000	Zn	-0.50928300	0.30871300	1.47461200

C	3.68744400	-0.46102700	-0.08765100	H	-3.00011100	-1.67686400	-2.62997500
C	4.50471100	0.23639400	0.81933100	C	-4.74067000	-0.00527100	0.39819100
C	4.29069600	-1.13867600	-1.15457300	H	-2.90717800	-0.39184300	1.45938100
C	5.88475400	0.25578200	0.65842800	C	-5.43451100	-0.14863600	-0.80161400
H	4.04570700	0.75713500	1.65268200	H	-5.34324300	-0.87764700	-2.82664000
C	5.67518500	-1.11432400	-1.31102000	H	-5.22304400	0.44978200	1.25704800
H	3.67355100	-1.68456300	-1.85547900	C	-0.76202200	2.03811700	2.61063700
C	6.47803600	-0.41969200	-0.40934800	H	0.18680800	2.50730000	2.90481300
H	6.49976300	0.79682800	1.37062900	H	-1.38152300	2.86353300	2.23383500
H	6.12669100	-1.64533100	-2.14317300	C	-1.43080400	1.42223000	3.85071600
H	7.55610600	-0.40592900	-0.53375800	H	-1.58604100	2.15781200	4.65076100
C	-1.96054400	-1.73044200	-0.72895100	H	-2.41485100	0.99955400	3.62015900
C	-2.16554800	-2.46540500	-1.90857500	H	-0.83364300	0.61040100	4.27848400
C	-3.06378200	-1.42783800	0.07768800	N	0.74814000	1.97947900	-0.40479500
C	-3.44425000	-2.88415800	-2.25964600	C	1.35887700	1.46476900	-1.45830900
H	-1.31927900	-2.70760800	-2.54016600	C	1.04949900	3.32410800	-0.40455100
C	-4.34004600	-1.85057900	-0.28429100	H	1.33707900	0.42428700	-1.74384900
H	-2.91724200	-0.87214300	0.99553600	C	1.84936800	3.61011700	-1.47535900
C	-4.54205000	-2.58017500	-1.45390800	H	0.67498900	3.98570000	0.36046900
H	-3.58200800	-3.45464300	-3.17323700	H	2.29194300	4.53083600	-1.81991700
H	-5.18019400	-1.61064100	0.35997200	C	2.83906700	2.20726200	-3.34220700
C	-1.62670700	0.16828100	3.11766500	H	3.87826600	2.48523900	-3.15994100
H	-1.28442300	0.95844100	3.80011000	H	2.80138500	1.15391900	-3.61546700
H	-2.67117900	0.42628900	2.89381100	H	2.44453000	2.80101500	-4.16832900
C	-1.57915000	-1.18299800	3.85130600	N	2.04082000	2.41321300	-2.14074200
H	-2.18900800	-1.18750400	4.76483400	H	-6.45730000	0.20339100	-0.88613900
H	-1.94115400	-2.00464000	3.22416200	22			
H	-0.55888000	-1.44497800	4.15001200	C	-2.41465700	-0.09970700	0.38895100
N	-1.17753700	2.00872700	0.25477600	C	-1.22157100	-0.06113400	0.65851800
C	-0.60401500	2.42374300	-0.85916600	C	-3.81073700	-0.13001400	0.09321000
C	-2.24877100	2.84536300	0.47032800	C	-4.37035100	-1.16242400	-0.68434000
H	0.27293500	1.98481800	-1.30996500	C	-4.67203000	0.87673700	0.57196900
C	-2.31221300	3.77217300	-0.53308700	C	-5.73169400	-1.18467200	-0.97061100
H	-2.89356400	2.72398200	1.32619700	H	-3.72219500	-1.94915600	-1.05560600
H	-2.99418900	4.58518500	-0.72340400	C	-6.03248700	0.85007300	0.28284600
C	-0.91060300	4.20699900	-2.59984400	H	-4.25640700	1.67598700	1.17599900
H	-0.71021400	5.25768300	-2.38367300	C	-6.57102800	-0.17902200	-0.49038400
H	-0.01514700	3.76130700	-3.03061900	H	-6.14049800	-1.99252000	-1.57042700
H	-1.72235600	4.13576500	-3.32575200	H	-6.67694300	1.63633100	0.66479200
N	-1.25460700	3.49288800	-1.37833300	H	-7.63302600	-0.19841900	-0.71403000
H	-5.53719800	-2.91069400	-1.73242300	Zn	0.69775600	0.03168000	1.11970000
21				C	2.00104100	0.06564500	2.64988200
N	-1.10484100	-2.65492400	-1.15303100	H	3.02932200	0.11022500	2.25365400
N	0.14775500	-2.85468300	-0.91639800	H	1.87298500	1.01076200	3.19603700
N	-1.45986200	-1.51272300	-0.48813800	C	1.90329500	-1.10113600	3.64868000
C	-0.40546700	-0.95758100	0.19005200	H	2.04896500	-2.07301400	3.16132700
C	0.62144600	-1.85771700	-0.09903500	H	2.64269700	-1.04054500	4.46082100
Zn	-0.37446700	0.82779400	1.08922500	H	0.91653800	-1.14138800	4.12178300
C	2.03210700	-1.83508500	0.31307300	N	1.27143100	1.78606300	-0.17750800
C	2.46163000	-1.12473800	1.44478200	C	2.36422500	2.51855400	-0.10582700
C	2.99580400	-2.53579700	-0.43178800	C	0.47521300	2.37672400	-1.13080900
C	3.80640700	-1.09182000	1.80510500	H	3.19629000	2.34086000	0.55881600
H	1.73446700	-0.61842200	2.07298100	C	1.10974700	3.47798700	-1.63805700
C	4.33818800	-2.51018000	-0.06549800	H	-0.49775500	1.97306900	-1.36444100
H	2.67317200	-3.10656600	-1.29500100	H	0.82057100	4.19891100	-2.38606900
C	4.75351200	-1.78284600	1.05058300	N	2.32099000	3.56137100	-0.97566300
H	4.11177000	-0.53864300	2.68801200	C	3.33805600	4.58492900	-1.15688800
H	5.06440100	-3.06322100	-0.65367500	H	2.93754200	5.57162100	-0.91625100
H	5.80057600	-1.76462900	1.33583600	H	4.17443000	4.37690800	-0.49048200
C	-2.80258400	-1.05191300	-0.58675300	H	3.70279700	4.58703600	-2.18591500
C	-3.49466400	-1.20417800	-1.79089600	N	1.47738300	-1.55713600	-0.28709900
C	-3.43042500	-0.46498500	0.51338400	C	2.64683200	-2.16223500	-0.24396100
C	-4.80851100	-0.75607000	-1.89015800	C	0.76463500	-2.17228700	-1.28928900

H	3.44658600	-1.93411100	0.44446500	C	-2.60484200	4.44989100	-1.59359700
C	1.52705200	-3.15797200	-1.85512100	H	-2.66561100	5.36736100	-1.00582800
H	-0.24553900	-1.86762900	-1.51417400	H	-1.57882100	4.32380700	-1.93623800
H	1.33096900	-3.85652600	-2.65293900	H	-3.26077400	4.53404500	-2.46226600
C	3.86426600	-4.02969900	-1.40673100	N	-2.97530700	3.30083000	-0.78018600
H	3.58159000	-5.06906900	-1.22876000	H	8.04550900	-1.71542200	-0.03910300
H	4.23204800	-3.92795300	-2.42959900	24			
H	4.66681300	-3.76470700	-0.71930700	N	1.30407900	-2.08511900	0.13794300
N	2.73315200	-3.14446600	-1.17871500	N	0.13492300	-1.51067600	0.12830100
23-ts				N	2.23087600	-1.09725600	0.08420600
N	2.01388000	-1.84085100	0.57614600	C	0.24025800	-0.13107200	0.07206000
N	0.84240200	-1.93483300	0.74375700	C	1.60688000	0.13198600	0.04322500
N	2.82139200	-0.90108100	0.31475800	Zn	-1.40209500	1.07094300	-0.05358700
C	0.05333700	-0.14279200	0.58483900	C	-1.86443600	3.01308300	-0.32081900
C	0.91177300	0.71370300	0.29736000	H	-1.80911800	3.19741700	-1.40403900
Zn	-1.89071500	-0.47139200	1.13518500	H	-1.06197900	3.63330700	0.09949600
C	-2.77082700	-0.93715700	2.87607300	C	-3.21401700	3.53425800	0.20216500
H	-2.79340200	-0.03588100	3.50377900	H	-3.26645500	3.49306700	1.29644700
H	-2.11102400	-1.63508700	3.40688500	H	-3.40878900	4.58050000	-0.07589800
C	-4.18302800	-1.54063900	2.79898400	H	-4.06258100	2.94936100	-0.17504100
H	-4.20238300	-2.46292900	2.20749200	C	2.31361900	1.41559100	-0.10130900
H	-4.59576000	-1.79157200	3.78682100	C	3.32745200	1.59498000	-1.05525800
H	-4.90262200	-0.85721200	2.32956400	C	1.94558200	2.50934500	0.69510800
C	1.60919600	1.91647600	-0.03081700	C	3.95728100	2.82746600	-1.20136200
C	1.89695200	2.24646400	-1.36996800	H	3.61513300	0.76786400	-1.69530200
C	1.98472100	2.82623900	0.97634600	C	2.57435300	3.74294600	0.54563500
C	2.53516200	3.44139500	-1.68678300	H	1.15973900	2.38590800	1.43141400
H	1.63157100	1.54335500	-2.15229300	C	3.58524200	3.90662700	-0.40003300
C	2.62287400	4.01928700	0.65295300	H	4.73539700	2.94726700	-1.94887800
H	1.77511100	2.57872600	2.01085000	H	2.27238000	4.57787500	1.17006500
C	2.90143700	4.33414800	-0.67793200	H	4.07491500	4.86828200	-0.51663400
H	2.75751900	3.67301200	-2.72409900	C	3.60914400	-1.44885900	0.17132900
H	2.90930000	4.70505300	1.44431500	C	4.09094100	-2.50704900	-0.60171300
H	3.40533400	5.26280400	-0.92615000	C	4.46109600	-0.76841800	1.04269100
C	4.19376100	-1.18855600	0.23363400	C	5.42891700	-2.79114000	-0.50275400
C	4.75861100	-2.45505000	0.46170800	H	3.41206600	-3.03173700	-1.26270200
C	5.03974200	-0.11710300	-0.09209100	C	5.80068800	-1.13992500	1.12480900
C	6.13450200	-2.63512700	0.36049400	H	4.07730800	0.04168400	1.65044200
H	4.11372400	-3.28747800	0.72105600	C	6.28924900	-2.19473900	0.35521600
C	6.41368000	-0.30980600	-0.18851600	H	5.80020500	-3.70375900	-1.10265900
H	4.60310200	0.86067200	-0.26289500	H	6.46098300	-0.60722900	1.80134500
C	6.97307200	-1.56833800	0.03552200	N	-2.64572100	0.10361300	1.58764400
H	6.55506200	-3.62012700	0.54109900	C	-2.34782200	-1.08522500	2.07911300
H	7.05255200	0.53162700	-0.43952700	C	-3.76889800	0.52492300	2.26403400
N	-2.53689300	-1.79371300	-0.51830300	H	-1.52073500	-1.69706100	1.74681100
C	-1.76989200	-2.75499100	-0.99878100	C	-4.14360500	-0.42702300	3.17283900
C	-3.74771300	-1.91161600	-1.16164900	H	-4.22842200	1.47718500	2.05465000
H	-0.74978900	-2.93860300	-0.69509200	H	-4.95407100	-0.46961000	3.88296100
C	-3.69945600	-2.95851400	-2.04105300	N	-3.22740500	-1.45451000	3.04535400
H	-4.56671600	-1.24143700	-0.95338700	C	-3.19967400	-2.69250900	3.80782300
H	-4.43116200	-3.36678800	-2.71967200	H	-3.06760000	-2.48688600	4.87204200
N	-2.42916600	-3.49137500	-1.92798900	H	-4.12518000	-3.25368700	3.66368000
C	-1.89682200	-4.62912900	-2.66275000	H	-2.36408800	-3.30039200	3.46331600
H	-2.47658500	-5.52917600	-2.44958000	N	-2.54138500	-0.06098200	-1.65103300
H	-1.91560200	-4.43473700	-3.73676700	C	-2.32242900	-1.32347900	-1.96461000
H	-0.86538700	-4.79640000	-2.35586400	C	-3.50277000	0.39049700	-2.52499100
N	-2.82639400	1.35739400	0.26211000	H	-1.60868500	-1.96440900	-1.46583600
C	-2.20355700	2.21532600	-0.52313400	C	-3.86439400	-0.62088700	-3.37339300
C	-4.05808700	1.91092100	0.53083500	H	-3.86269000	1.40687700	-2.48887900
H	-1.20104300	2.09726100	-0.90384000	H	-4.57048100	-0.66529800	-4.18727600
C	-4.16927200	3.11517700	-0.10936700	C	-3.11780800	-3.02998300	-3.62571700
H	-4.76945200	1.41637300	1.17356200	H	-2.83956200	-2.96173700	-4.67934100
H	-4.96255100	3.84468000	-0.14428700	H	-2.39792600	-3.66890300	-3.11579600

H	-4.10812000	-3.48306300	-3.54544100
N	-3.10260900	-1.71481900	-3.00552100
H	7.33284300	-2.48338000	0.42588000
25-ts			
N	-1.30874800	2.87148800	-0.08176100
N	-0.22530200	3.28890900	0.11278800
N	-1.79297700	1.74835500	-0.41870500
C	0.45926700	0.73328000	-0.49101700
C	1.06302700	1.80063900	-0.21068500
Zn	0.01365300	-1.17887200	-0.94423600
C	2.35366800	2.44116400	-0.03071000
C	3.40059600	2.16560300	-0.92952800
C	2.60683900	3.31559700	1.03859500
C	4.65820400	2.73673500	-0.75487700
H	3.20991600	1.50974100	-1.77189600
C	3.86843200	3.87855700	1.21287900
H	1.80320300	3.55630400	1.72379600
C	4.90081800	3.59304500	0.31957300
H	5.44852100	2.51929900	-1.46719900
H	4.04298900	4.55139100	2.04708300
H	5.88022600	4.04176400	0.45242900
C	-3.18695700	1.60180400	-0.52564500
C	-4.11450400	2.57838700	-0.12300200
C	-3.66029800	0.38968300	-1.05020800
C	-5.47957600	2.33855000	-0.24687800
H	-3.75699900	3.52205000	0.27457400
C	-5.02776600	0.16156600	-1.16495500
H	-2.94612600	-0.35831500	-1.37379300
C	-5.94841800	1.13042500	-0.76411000
H	-6.18253500	3.10669700	0.06189300
H	-5.37491100	-0.77948200	-1.58049400
C	-0.57210200	-2.26336500	-2.52568000
H	-0.54670600	-3.33091800	-2.25802000
H	-1.63014800	-2.05618600	-2.73618500
C	0.24293700	-2.05021500	-3.81339700
H	-0.10473300	-2.67346700	-4.64976200
H	0.19504800	-1.01014100	-4.15342200
H	1.30485200	-2.28173300	-3.66862600
N	-1.19089500	-1.74879500	0.81560300
C	-1.61766100	-0.89757300	1.72869400
C	-1.79667100	-2.95149000	1.10091500
H	-1.35186400	0.14701500	1.77099200
C	-2.59431100	-2.81177100	2.20328300
H	-1.62610400	-3.82728800	0.49460400
H	-3.22695600	-3.50779100	2.73044200
C	-3.17699400	-0.84584700	3.69365200
H	-4.25081000	-0.82684800	3.49910000
H	-2.98742100	-1.37081100	4.63155000
H	-2.82152400	0.17924500	3.78711400
N	-2.47062700	-1.49281500	2.59791300
N	1.94076100	-2.05096100	-0.18324900
C	2.87096300	-1.37614200	0.46508100
C	2.45180200	-3.31358400	-0.37828800
H	2.79965300	-0.34113700	0.76235800
C	3.70533300	-3.39063000	0.16533500
H	1.89234400	-4.07254000	-0.90258100
H	4.42350000	-4.19338900	0.21591800
C	5.18052900	-1.72547800	1.38396700
H	5.30665800	-2.27433700	2.31938200
H	6.05012300	-1.89517700	0.74691500
H	5.11411300	-0.66101200	1.60426300
N	3.96453700	-2.14350000	0.70165800
H	-7.01407900	0.95082800	-0.86105800

26			
N	-0.71505800	-3.12399200	-1.15480800
N	0.57181100	-3.12212500	-1.19143400
N	-1.09157300	-2.06842500	-0.35915900
C	-0.01497600	-1.35980500	0.12465700
C	1.04837800	-2.08759100	-0.42119600
Zn	-0.08368800	0.42798800	1.12858300
C	2.50081100	-1.91336900	-0.26687100
C	3.05698200	-1.33868400	0.88586700
C	3.37528200	-2.34804000	-1.27767300
C	4.43479100	-1.18154500	1.01502200
H	2.40540300	-1.03032600	1.69572100
C	4.75297900	-2.19524800	-1.14556800
H	2.95875100	-2.81929800	-2.16086200
C	5.29145300	-1.60562100	-0.00082300
H	4.84059000	-0.74089000	1.92069200
H	5.40994600	-2.54520700	-1.93667500
H	6.36615300	-1.49342700	0.10545600
C	-2.47865500	-1.91013200	-0.09096300
C	-3.41026700	-2.22882200	-1.08459400
C	-2.91670000	-1.47091500	1.15940400
C	-4.77132600	-2.09214500	-0.82567600
H	-3.05799300	-2.59731200	-2.04000800
C	-4.28015900	-1.32478000	1.40368900
H	-2.19507800	-1.25641500	1.93793200
C	-5.21347100	-1.63308800	0.41538300
H	-5.48919100	-2.35003300	-1.59824000
H	-4.61109200	-0.98234400	2.37885100
C	-0.17938800	1.07686100	3.03437300
H	-0.13473000	2.17698600	3.04281500
H	-1.17358600	0.84019200	3.43999400
C	0.88933500	0.53201000	3.99856100
H	0.78560800	0.91997500	5.02193500
H	0.85058600	-0.56059200	4.07227500
H	1.90414500	0.78617100	3.66988900
N	-1.67503500	1.56999200	0.03034800
C	-2.16078800	1.35948500	-1.17679000
C	-2.36426000	2.64883000	0.53469400
H	-1.85439200	0.57307500	-1.84897800
C	-3.27346300	3.08577100	-0.38958000
H	-2.16387900	3.02953600	1.52366000
H	-3.99300000	3.88860000	-0.37264400
C	-3.91294600	2.29812400	-2.71193300
H	-4.96849700	2.11489200	-2.50344400
H	-3.80419200	3.26908600	-3.19865500
H	-3.55266600	1.52435200	-3.38849600
N	-3.13444900	2.25309200	-1.48351500
N	1.49835400	1.62980700	0.11596100
C	2.13280300	1.36630100	-1.00997800
C	2.07955500	2.77018500	0.62209500
H	1.94894100	0.51761800	-1.64976900
C	3.07480500	3.18932000	-0.21780900
H	1.74893700	3.20433700	1.55253800
H	3.75539300	4.02432200	-0.17178700
C	4.02998400	2.27262000	-2.37970600
H	3.97214900	3.21164900	-2.93316100
H	5.05105300	2.12239700	-2.02510300
H	3.77104000	1.45248100	-3.04751200
N	3.09895200	2.28327900	-1.26105500
H	-6.27530300	-1.52920500	0.61418900
27			
C	0.91224900	0.68424900	-0.00004800
C	-0.25731200	0.34470600	-0.00005500

Zn	-2.06720800	-0.17673700	-0.00004900	H	-3.80921300	1.63126200	2.42511400
C	-3.93543600	-0.72887700	-0.00005600	C	-2.29108200	1.52312400	3.96596100
H	-4.09023100	-1.37466100	-0.87262100	H	-2.99362100	1.55853800	4.80977200
H	-4.09014700	-1.37498600	0.87228200	H	-1.45102300	0.89445700	4.27908200
C	-4.97082000	0.41012500	0.00021200	H	-1.89372700	2.53562700	3.84036300
H	-4.87457400	1.05413100	-0.87910200	N	-0.72292300	-2.37089200	0.97649500
H	-5.99621100	0.02186400	0.00019100	N	0.21857700	-2.56512500	0.37664900
H	-4.87448300	1.05379600	0.87976100	N	1.14959400	-2.85422000	-0.37451200
C	2.32192400	1.06489500	-0.00004900	C	2.47466100	-2.52324400	0.01480900
H	2.52651900	1.69408400	0.87539400	C	3.49571900	-2.99660300	-0.81496800
H	2.52653300	1.69402700	-0.87553000	C	2.78710900	-1.76572700	1.14890000
C	3.28268600	-0.14144100	-0.00000200	C	4.82306400	-2.71987700	-0.50479800
H	3.07083200	-0.76441300	0.87597800	H	3.23403600	-3.57859200	-1.69153700
H	3.07087200	-0.76445400	-0.87596300	C	4.12011100	-1.49835100	1.44946600
C	4.75614500	0.27514800	0.00002000	H	1.99909600	-1.36920100	1.77998400
H	4.95698900	0.90500000	0.87581500	C	5.14308900	-1.97231200	0.62898200
H	4.95703800	0.90492800	-0.87581600	H	5.61081700	-3.09210500	-1.15184600
C	5.71449000	-0.91824300	0.00009900	H	4.35648900	-0.90826100	2.32899100
H	5.56540200	-1.54865200	-0.88210500	N	-3.12034300	0.22379700	-0.57892200
H	6.75878800	-0.59336800	0.00010700	C	-4.39437500	-0.11136800	-0.50301900
H	5.56536100	-1.54856300	0.88236000	C	-2.75599800	0.06119400	-1.89592400
28				H	-4.99392400	-0.09789100	0.39458200
C	2.08537100	-0.15917700	-0.68141800	C	-3.83377700	-0.37801500	-2.61418600
C	1.00233600	0.35593700	-0.46142100	H	-1.74814700	0.27189200	-2.21820700
Zn	-0.68374100	1.22566100	-0.11683500	H	-3.95642600	-0.62078700	-3.65756000
C	-1.85991600	2.78944500	0.19540700	C	-6.23479800	-0.92160000	-2.00977100
H	-2.65431300	2.77208100	-0.56464200	H	-6.69689900	-0.26046100	-2.74500000
H	-2.37783000	2.63795000	1.15341800	H	-6.23300700	-1.94298400	-2.39454300
C	-1.18572700	4.17176100	0.19483200	H	-6.82502200	-0.89372200	-1.09475600
H	-0.69271200	4.38275600	-0.75959500	N	-4.87816400	-0.48551800	-1.71335600
H	-1.89812600	4.98854100	0.37361300	H	6.17919100	-1.75894300	0.86921300
H	-0.41437100	4.24765900	0.96802700	C	2.19177400	1.48401900	-1.19447300
N	-2.04266800	-0.54520400	-0.02210000	H	2.85130500	0.62371400	-1.02269500
C	-3.34595900	-0.56184100	0.18527300	H	2.01388200	1.51125900	-2.27786600
C	-1.65822100	-1.85870500	-0.16686200	C	2.92037700	2.77471000	-0.77076500
H	-3.96765800	0.30701600	0.33975900	H	2.25324800	3.62894900	-0.93245500
C	-2.75333600	-2.66864300	-0.04307600	H	3.10951100	2.73740100	0.30793000
H	-0.62553200	-2.11253400	-0.34879100	C	4.23560500	2.99071500	-1.52433800
H	-2.86946900	-3.73948900	-0.09196700	H	4.03632400	3.02024400	-2.60328500
N	-3.82933900	-1.82882400	0.18231600	H	4.89330400	2.12717600	-1.36391200
C	-5.21459100	-2.23058400	0.37852100	C	4.96405600	4.27064600	-1.10702600
H	-5.30591700	-2.87431900	1.25514400	H	5.21327100	4.25750800	-0.04111900
H	-5.82403100	-1.34116000	0.53320500	H	5.89780200	4.40114000	-1.66203600
H	-5.58687900	-2.76201000	-0.49907400	H	4.34693000	5.15679600	-1.28695600
C	3.40029000	-0.75213600	-0.92448400	30-ts			
H	3.30279100	-1.83994800	-1.03988100	N	0.88003500	-1.29803000	0.88839200
H	3.79265300	-0.38677500	-1.88270500	N	-0.24839100	-0.95591200	1.02399000
C	4.42427900	-0.45194200	0.18795400	N	1.87614800	-0.86407000	0.23383300
H	4.03093400	-0.82129300	1.14190900	C	-0.49492000	0.68998500	-0.04511800
H	4.51818300	0.63404400	0.29889700	C	0.54787000	1.02554300	-0.63441200
C	5.79888200	-1.06985600	-0.08300900	Zn	-2.35125700	1.22100800	0.36878400
H	5.69327700	-2.15567000	-0.20446800	C	-3.56386000	2.63928300	1.04037600
H	6.18339600	-0.69694000	-1.04095800	H	-4.19567700	2.19543500	1.82128600
C	6.81750500	-0.77866400	1.02153900	H	-4.25495500	2.90534400	0.22862900
H	7.78906600	-1.23082700	0.80126400	C	-2.89019000	3.91103500	1.57975200
H	6.97522700	0.29758400	1.14423200	H	-2.28182900	4.40556000	0.81548700
H	6.48211000	-1.17185600	1.98661700	H	-3.61905300	4.65147300	1.93538700
29				H	-2.22231900	3.69268300	2.41901600
C	0.92549700	1.27122800	-0.49333100	C	3.10158600	-1.54407100	0.36021900
C	-0.12349500	1.11763300	0.10968100	C	3.34942700	-2.56069300	1.29871900
Zn	-1.78619300	0.89624100	1.06954300	C	4.13599100	-1.15775300	-0.50512900
C	-2.94348100	1.00102400	2.67492200	C	4.59835800	-3.17014800	1.35716700
H	-3.35990200	0.00028500	2.85722800	H	2.55990300	-2.86242700	1.97783600

C	5.38253400	-1.77173200	-0.43517300	C	4.93055400	-3.50777700	-0.67930900
H	3.94850400	-0.37773200	-1.23446200	H	3.99719100	-4.06734600	-0.64227600
C	5.62452300	-2.78262700	0.49456500	H	5.40127700	-3.67174700	-1.65040600
H	4.77203700	-3.95366900	2.08881200	H	5.59197000	-3.87382300	0.10808900
H	6.16916400	-1.45899100	-1.11506500	H	-6.86588200	-2.42319600	0.51803900
H	6.59714100	-3.26031200	0.54760000	C	-1.83588700	1.41938900	0.46046000
N	-3.50565200	-0.51920700	-0.23088900	H	-2.59660600	1.37117700	1.24653600
C	-4.87121800	-0.62673100	-0.38212100	H	-1.10130000	2.15789600	0.79490000
C	-3.00648800	-1.71189400	-0.50604100	C	-2.49084100	1.91274600	-0.84437700
C	-5.18664500	-1.90292800	-0.75537300	H	-1.72347600	1.97250400	-1.62493700
H	-5.52517100	0.21399900	-0.21230800	H	-3.22183400	1.17265600	-1.19092900
H	-1.95977400	-1.96842200	-0.45519900	C	-3.17689200	3.27295000	-0.68685600
H	-6.12930500	-2.37993300	-0.97010800	H	-3.94013900	3.20602700	0.09880100
C	-3.81019400	-3.99022500	-1.17892000	H	-2.44455900	4.00959200	-0.33336100
H	-4.18753800	-4.18368900	-2.18442200	C	-3.82094700	3.77480600	-1.98109600
H	-2.74865900	-4.23093600	-1.14955400	H	-3.07857900	3.89000800	-2.77724200
H	-4.33524800	-4.62873100	-0.46657000	H	-4.58411000	3.07827200	-2.34289000
N	-3.98652600	-2.58696400	-0.83043500	H	-4.30311100	4.74619500	-1.83811300
C	1.56925200	1.72812500	-1.41424300	32			
H	1.04944800	2.45027500	-2.05971000	C	2.29732200	-1.35730600	0.76458200
H	2.07163300	1.03095100	-2.09264700	C	1.37082000	-0.60083900	1.00409300
C	2.60920000	2.47623400	-0.56037400	Zn	-0.12028000	0.56413300	1.44277300
H	2.08650800	3.17779800	0.09928900	C	-1.50579100	1.24121500	2.69404700
H	3.11275700	1.75864600	0.09426700	H	-2.30486600	1.73226800	2.12174100
C	3.63843400	3.22889300	-1.40874300	H	-1.98373800	0.39097800	3.19691600
H	3.12145000	3.93553300	-2.07057700	C	-0.97516200	2.21928100	3.75926500
H	4.15436800	2.52125200	-2.07050600	H	-0.51067000	3.10422400	3.30964600
C	4.67099300	3.98173100	-0.56640500	H	-1.76664000	2.58285700	4.42872600
H	5.39339500	4.50976800	-1.19560200	H	-0.21354300	1.75404900	4.39367800
H	4.19187200	4.72405300	0.07967900	N	-0.19831200	-1.63966600	-2.14338800
H	5.23183300	3.29894400	0.07923600	N	-0.99058400	-1.35269600	-1.38712500
31				N	-1.74331900	-0.96227300	-0.49236900
N	-0.82836100	-2.08881500	-0.01316100	N	0.12849900	2.06098900	-0.19651900
N	0.33687900	-1.51929400	-0.03615700	C	1.13369200	2.00378800	-1.05008600
N	-1.74522700	-1.10508000	0.20737700	C	-0.61134600	3.16725700	-0.54702400
C	0.23377900	-0.15377700	0.16072600	H	1.90185200	1.24462000	-1.04400500
C	-1.12075500	0.11061700	0.31880300	C	-0.03636000	3.77718400	-1.62800100
Zn	1.78170100	1.08898600	0.19022900	H	-1.49937400	3.44746600	-0.00231100
C	2.49604300	2.93775500	0.39151300	H	-0.30819500	4.65541700	-2.19158000
H	1.67847700	3.65895100	0.26754800	C	2.02026300	3.27779600	-3.02361100
H	3.17929900	3.13809300	-0.44554400	H	1.50847200	3.25814400	-3.98739600
C	3.22107700	3.22322400	1.72051600	H	2.50344200	4.24761900	-2.89164700
H	4.06615000	2.54522200	1.88555500	H	2.78427700	2.50179100	-3.01782400
H	3.62141500	4.24495700	1.77147900	N	1.08017800	3.02366100	-1.94165300
H	2.55546500	3.10316500	2.58221100	C	-3.11520700	-1.33311000	-0.55419000
C	-3.12601900	-1.44653700	0.29487500	C	-3.92799200	-0.87564100	0.48713600
C	-3.72781600	-2.13525400	-0.75923300	C	-3.66173700	-2.11073900	-1.58143300
C	-3.86148200	-1.12336400	1.43585100	C	-5.28130700	-1.19597300	0.49569600
C	-5.07178500	-2.48857000	-0.67297800	H	-3.48827300	-0.27922200	1.27757600
H	-3.13623800	-2.39205500	-1.62988800	C	-5.01853500	-2.42411500	-1.55985200
C	-5.20920200	-1.46858000	1.50870900	H	-3.03683500	-2.47297900	-2.39176400
H	-3.37551600	-0.62679400	2.26780300	C	-5.83444200	-1.96979000	-0.52515500
C	-5.81754100	-2.15032500	0.45592400	H	-5.90628500	-0.83939900	1.30793800
H	-5.53775200	-3.02642400	-1.49214700	H	-5.43659500	-3.02872100	-2.35831100
H	-5.77913400	-1.21748500	2.39731000	H	-6.89026600	-2.21824800	-0.51310100
N	3.49728000	-0.23727000	-0.14894400	C	3.41418500	-2.26614700	0.50376100
C	3.41415300	-1.55095700	-0.29240100	H	3.19967700	-2.86491000	-0.39129300
C	4.83413400	0.08100700	-0.25425700	H	3.49660500	-2.98596700	1.32866100
H	2.48343400	-2.10384700	-0.26388100	C	4.76802300	-1.55261500	0.32199400
C	5.55759100	-1.05967000	-0.46287000	H	4.68766900	-0.84179000	-0.50941400
H	5.18011800	1.09945400	-0.17324600	H	4.97685700	-0.95312300	1.21519500
H	6.61400300	-1.23092600	-0.59384700	C	5.92527000	-2.52142300	0.06242700
N	4.63934500	-2.09471400	-0.48488900	H	5.70303800	-3.12421000	-0.82737600

H	5.99770900	-3.23189700	0.89548600	C	-2.51787700	-2.41587400	-1.42870600
C	7.27078200	-1.81598700	-0.12253100	C	-1.80419700	-2.25655400	0.87762700
H	8.07797000	-2.53109300	-0.30617200	C	-3.74935700	-2.90703900	-1.00567200
H	7.24492600	-1.12405400	-0.97085000	H	-2.29470300	-2.29654600	-2.48131400
H	7.54107400	-1.23494000	0.76497500	C	-3.04631600	-2.73363400	1.29099800
33-ts				H	-1.03022900	-2.05123200	1.60836100
N	0.58291700	-1.76238400	-0.89701600	C	-4.02399800	-3.05990400	0.35347500
N	1.75108000	-1.72978100	-0.61235300	H	-4.50047900	-3.16760100	-1.74452600
N	-0.47282800	-1.24987000	-0.37504200	H	-3.23990900	-2.86651900	2.35044500
C	1.38844700	-0.30339200	1.33997100	C	0.26327500	0.89379400	3.22898100
C	2.34273600	-0.89074100	0.75318100	H	0.74007700	1.88061000	3.30633700
Zn	-0.52763300	0.04026700	1.63888300	H	-0.75634000	1.04154400	3.61095000
C	-1.67789400	-1.49811900	-1.08856700	C	1.00833200	-0.10632200	4.12857100
C	-1.71266100	-2.13527700	-2.34088300	H	1.04106600	0.21759900	5.17707600
C	-2.88283300	-1.06855300	-0.51883700	H	0.53852000	-1.09566500	4.11884400
C	-2.92447700	-2.33390700	-2.99346400	H	2.04535400	-0.24987500	3.80856600
H	-0.78813000	-2.47570900	-2.79135400	N	-1.03224900	2.06449700	0.32801400
C	-4.09037800	-1.27169100	-1.18155200	C	-1.23265200	2.14643600	-0.97587500
H	-2.87261500	-0.58577500	0.45055300	C	-1.68399700	3.14283900	0.88463200
C	-4.12287300	-1.90369400	-2.42300100	H	-0.85183600	1.45127800	-1.70859900
H	-2.93007500	-2.83200800	-3.95840500	C	-2.27995000	3.87463300	-0.10468000
H	-5.01228700	-0.93586100	-0.71691500	H	-1.67930200	3.31614500	1.94921000
C	-1.95626400	-0.19484100	3.00952900	H	-2.87395000	4.77408700	-0.07922000
H	-1.68632600	0.43751400	3.86686600	C	-2.40021600	3.63385900	-2.62630100
H	-2.90781800	0.21677800	2.64557500	H	-2.01210300	4.62634500	-2.86073100
C	-2.17867900	-1.63556700	3.50075100	H	-2.00667600	2.92295000	-3.35127500
H	-2.95048500	-1.70077400	4.27968600	H	-3.48888600	3.64446000	-2.69931200
H	-2.48969300	-2.30151200	2.68895600	N	-1.98386500	3.22788800	-1.29037800
H	-1.26408600	-2.06414600	3.92371300	H	-4.98764900	-3.43850900	0.67786500
N	-0.87155200	1.92721100	0.55917000	C	2.84643600	0.23818400	-1.12779000
C	-0.26313300	2.31087800	-0.54683300	H	3.03378400	0.70330700	-2.10290500
C	-1.79608100	2.90504700	0.84793000	H	2.71015700	1.05975000	-0.41414100
H	0.52055800	1.76565000	-1.04970900	C	4.08074900	-0.58790200	-0.72461500
C	-1.73448800	3.88575800	-0.10319100	H	3.90065800	-1.04720700	0.25541900
H	-2.43734700	2.83486400	1.71233200	H	4.19402100	-1.41654700	-1.43233200
H	-2.28617500	4.80310900	-0.23152000	C	5.37091000	0.23602900	-0.67967900
C	-0.33079600	4.20971400	-2.18856400	H	5.24919300	1.06716800	0.02721300
H	0.03398900	5.20535600	-1.93064100	H	5.53955300	0.69837400	-1.66067400
H	0.47421200	3.65524100	-2.66885000	C	6.59921000	-0.58934500	-0.28882100
H	-1.16163600	4.29952300	-2.89042100	H	6.77017200	-1.40593100	-0.99733500
N	-0.74998400	3.49499300	-0.99135500	H	7.50551300	0.02316200	-0.26630100
H	-5.06543200	-2.06291700	-2.93624800	H	6.47924800	-1.03704900	0.70300000
C	3.81270700	-1.13559300	0.77858800	3-ts-a			
H	3.98074700	-2.20101600	0.58914400	N	1.26238600	-0.79400300	0.71726400
H	4.18580700	-0.92208400	1.78395200	N	0.07285500	-1.05937000	0.76295600
C	4.58103400	-0.30140500	-0.25963400	N	1.87687700	0.18587400	0.19209000
H	4.15343500	-0.48628200	-1.25088700	C	-0.76115300	0.04714500	-0.12058900
H	4.42747200	0.76335200	-0.04652800	C	-2.00469200	0.13992400	-0.15555600
C	6.08017300	-0.61593700	-0.27687500	C	-3.40187400	0.11962500	-0.12794100
H	6.22339700	-1.68219100	-0.49096200	C	-4.11380100	0.88216500	0.82918400
H	6.50051900	-0.45002000	0.72306900	C	-4.12845000	-0.66196800	-1.05839800
C	6.85477500	0.21775200	-1.30010500	C	-5.49960300	0.85360200	0.85299800
H	6.76618000	1.28890000	-1.09148200	H	-3.55994400	1.48197500	1.54210500
H	7.91990800	-0.03075200	-1.29560600	C	-5.51445100	-0.67445100	-1.02716700
H	6.48156000	0.04895000	-2.31529300	H	-3.58581900	-1.24884700	-1.79044800
34				C	-6.20330200	0.07956400	-0.07353400
N	0.22980300	-2.01659300	-2.10251600	H	-6.03752300	1.43652600	1.59297800
N	1.36048700	-1.40853900	-2.26773300	H	-6.06374900	-1.27580200	-1.74368200
N	-0.28933700	-1.57481000	-0.91806300	H	-7.28790700	0.06358700	-0.05199500
C	0.52992400	-0.65193700	-0.30839700	C	3.27361000	0.12302300	0.05740900
C	1.58679800	-0.57186000	-1.20633500	C	4.03994000	-1.02305700	0.32606000
Zn	0.13194800	0.44585000	1.30455900	C	3.91440800	1.28473700	-0.39553400
C	-1.54333100	-2.08152400	-0.48352300	C	5.41859200	-0.99308700	0.14826500

H	3.54816000	-1.92288600	0.67822500	H	0.41142500	2.99054300	-1.49319100
C	5.29327000	1.29991800	-0.57757100	H	2.10578600	4.07649800	-0.03638400
H	3.31630500	2.16634000	-0.59982200	H	0.80266400	-3.00587100	0.36926200
C	6.05492900	0.16340500	-0.30593800	6-a			
H	6.00150200	-1.88331300	0.36417900	N	1.59873500	-2.34738300	0.13117700
H	5.77548400	2.20651400	-0.92954800	N	0.67598000	-3.15950900	0.21569800
H	7.13078800	0.17775200	-0.44496300	N	1.29275400	-0.96252500	0.05922900
H	0.07334800	0.62738400	-0.55331700	C	0.02102000	-0.54341000	0.03478600
4-a				C	-1.16311200	-0.28698400	0.02397100
N	1.42372900	-1.89364100	-0.00072500	C	-2.54298300	0.06922900	0.02133400
N	0.22772800	-2.33973100	-0.00085900	C	-3.46591600	-0.63983900	-0.76870900
N	1.60952700	-0.57950500	-0.00013900	C	-3.00330100	1.13938500	0.81032100
C	-0.82055100	-1.50352800	-0.00055100	C	-4.81160500	-0.29019000	-0.76099400
C	-1.85750700	-0.86776500	-0.00035500	H	-3.11793400	-1.46074600	-1.38594100
C	-3.09662700	-0.17105500	-0.00014900	C	-4.34809600	1.49192700	0.79915800
C	-3.14216100	1.23607500	-0.00244700	H	-2.29840800	1.68545800	1.42726400
C	-4.31004400	-0.88658900	0.00230400	C	-5.25696100	0.77746400	0.01840900
C	-4.36155800	1.90302700	-0.00231700	H	-5.51386100	-0.84855600	-1.37124800
H	-2.21409300	1.79735900	-0.00437300	H	-4.68951200	2.32231500	1.40854800
C	-5.52524600	-0.21221500	0.00246700	H	-6.30682500	1.05128300	0.01753600
H	-4.28293000	-1.97037700	0.00407400	C	2.40516100	-0.06953400	-0.02250700
C	-5.55650300	1.18280400	0.00014200	C	3.68624600	-0.49958000	0.33728100
H	-4.38065900	2.98801300	-0.00413300	C	2.20251600	1.24231700	-0.45803500
H	-6.45199200	-0.77670000	0.00439100	C	4.75389100	0.38895700	0.25122100
H	-6.50705300	1.70604100	0.00023700	H	3.84008500	-1.51464700	0.67604800
C	2.89267800	-0.00755400	0.00009900	C	3.28034600	2.12130100	-0.52938500
C	4.04977300	-0.79451700	-0.00085500	H	1.20926000	1.57102700	-0.74106400
C	2.99406800	1.38801200	0.00135900	C	4.56111400	1.70143800	-0.17849000
C	5.29464700	-0.17413900	-0.00053800	H	5.74544800	0.04877200	0.53173100
H	3.96360400	-1.87307400	-0.00181200	H	3.11252000	3.13830100	-0.86860100
C	4.24701400	1.99308000	0.00164000	H	5.39882700	2.38799900	-0.23720900
H	2.09534600	1.99850700	0.00213500	H	-0.26181500	-2.71016900	0.23005200
C	5.40450300	1.21692500	0.00070200	15-a			
H	6.18928100	-0.78832300	-0.00128900	C	1.66694100	-0.46499000	-0.02393900
H	4.31504700	3.07596900	0.00262100	C	0.46962500	-0.70287200	-0.04365500
H	6.38061700	1.68957600	0.00093200	C	3.06563900	-0.18116400	0.00113500
H	0.79103500	0.02779000	0.00027100	C	3.75826400	-0.08861900	1.22258400
5-ts-a				C	3.78381500	0.01222800	-1.19338100
N	2.82761200	-1.95252900	-0.11115000	C	5.12115700	0.18846900	1.24510300
N	3.04438200	-3.05203500	0.18398100	H	3.21470900	-0.23929300	2.14885100
N	1.77193600	-1.20557600	-0.32439800	C	5.14676700	0.28894800	-1.16364300
C	0.35116200	-2.02887200	0.15597200	H	3.26030900	-0.06028900	-2.14039400
C	-0.76899500	-1.48584600	0.18525800	C	5.82174500	0.37886600	0.05387300
C	-1.97137500	-0.76476300	0.16665400	H	5.63926900	0.25466300	2.19677400
C	-2.81196900	-0.78649000	-0.97257800	H	5.68496300	0.43372100	-2.09524300
C	-2.38271100	-0.00736700	1.28961100	H	6.88523500	0.59421700	0.07415800
C	-4.00400100	-0.07599400	-0.98257200	Zn	-1.39684700	-1.14208200	-0.04178600
H	-2.51489100	-1.37125200	-1.83627900	C	-3.07785500	-2.15840200	0.01210700
C	-3.57806500	0.69629800	1.26516000	H	-3.65876100	-1.80604800	0.87460800
H	-1.74941300	0.01660900	2.16923000	H	-3.66790900	-1.87121700	-0.86802900
C	-4.39514900	0.66891200	0.13236600	C	-2.94513300	-3.68958900	0.07001300
H	-4.63602500	-0.10475700	-1.86452000	H	-2.39682700	-4.01939100	0.95804800
H	-3.87698600	1.27217500	2.13522600	H	-3.92238800	-4.18849300	0.09513400
H	-5.32900700	1.22087700	0.11947200	H	-2.40786100	-4.08663500	-0.79698700
C	1.90287000	0.21278600	-0.24317100	C	-1.38786900	2.19402900	-0.38763000
C	2.85180400	0.81812800	0.58711100	O	-2.20753600	1.01585400	-0.17899400
C	1.02822400	0.99698900	-0.99721400	C	-2.14298000	3.32550300	0.30043200
C	2.92859000	2.20604900	0.64745400	H	-1.29470900	2.36665400	-1.46570400
H	3.52693600	0.20494200	1.17389500	C	-3.56167400	1.40077400	0.16938300
C	1.09667800	2.38533500	-0.90904700	C	-3.60679700	2.92704400	0.05680700
H	0.30837900	0.52056100	-1.65081100	H	-1.89069000	4.30562100	-0.10951400
C	2.04786700	2.99467600	-0.09313800	H	-1.91857400	3.33846500	1.37139000
H	3.67403500	2.67160600	1.28387400	H	-4.24998300	0.89049800	-0.50663200

H	-3.75795300	1.05830100	1.18961700
H	-3.92085000	3.22903800	-0.94684100
H	-4.30150900	3.37292100	0.77149600
H	-0.40063300	1.98152900	0.01966000
22-a			
C	-1.99683300	0.02634800	0.46983800
C	-0.78130200	0.00419500	0.59440100
C	-3.41664500	0.05042500	0.32039600
C	-4.15802200	-1.14542300	0.27585600
C	-4.11264300	1.26933200	0.21426400
C	-5.54102700	-1.12017600	0.12829000
H	-3.63486000	-2.09151000	0.36296100
C	-5.49578400	1.28855600	0.06701200
H	-3.55475100	2.19866800	0.25330200
C	-6.21720700	0.09540400	0.02239500
H	-6.09421900	-2.05389000	0.09794900
H	-6.01365200	2.23956600	-0.01158200
H	-7.29637600	0.11280300	-0.09135900
Zn	1.13789400	-0.05630300	0.89592000
C	2.75547100	-0.27100600	2.01984900
H	3.64391000	-0.29325800	1.37428000
H	2.86450000	0.64129800	2.62177000
C	2.77025000	-1.48969400	2.95964900
H	2.69727200	-2.43630100	2.41181500
H	3.68538700	-1.54508200	3.56444100
H	1.92857900	-1.47180700	3.65946300
C	0.61556000	-1.97841000	-1.86220000
O	1.63623600	-1.45852000	-0.99421500
C	0.60577100	-3.48920500	-1.59785100
H	0.88693400	-1.75299300	-2.90258500
C	2.71588300	-2.40377600	-1.03585900
C	2.05537900	-3.79360800	-1.13179300
H	0.32063900	-4.05602700	-2.48675800
H	-0.11099200	-3.72767400	-0.80965500

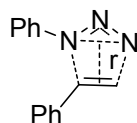
H	3.33539400	-2.19418700	-1.91753200
H	3.31842000	-2.25294100	-0.14157600
H	2.59095100	-4.43587000	-1.83431100
H	2.05741300	-4.29717900	-0.16338900
H	-0.31233800	-1.46849500	-1.61041100
C	0.81317600	2.51759600	-1.26204800
O	1.67256700	1.84874300	-0.32605100
C	2.93993700	2.52249300	-0.37483000
C	2.61555300	4.01009100	-0.62959400
C	1.12792800	4.00406900	-1.07224300
H	1.05650200	2.17860300	-2.27834400
H	-0.20879300	2.22723800	-1.02555800
H	3.44827200	2.32859200	0.56852900
H	3.53805700	2.09663600	-1.19002800
H	2.75477500	4.60777900	0.27292400
H	3.27045400	4.42551200	-1.39860400
H	0.49203900	4.42459100	-0.29025200
H	0.95656300	4.57996500	-1.98415300
THF			
C	-1.17256000	0.41804900	0.08848000
O	-0.03891600	1.21114700	-0.26552300
C	1.10693600	0.50693700	0.20117800
C	0.82382700	-0.96336000	-0.12679600
C	-0.71453900	-1.06115900	0.02928800
H	-1.50730200	0.68582400	1.10026700
H	-1.97178300	0.66191600	-0.61287000
H	1.98023500	0.92137400	-0.30435000
H	1.22695000	0.65583600	1.28581800
H	1.12148900	-1.17799400	-1.15602000
H	1.36319300	-1.65232300	0.52736800
H	-1.16763100	-1.59278700	-0.80971600
H	-0.99581900	-1.59382200	0.94079300

7. The data of distortion, interaction and total energies of the transition states by B3LYP-D3BJ method in THF solvent

	$\Delta E_{dis}(\text{azide})$	$\Delta E_{dis}(\text{alkyne})$	ΔE_{dist}	ΔE_{int}	ΔE^\ddagger
9-ts	29.9	-14.6	15.3	26.6	29.9
12-ts	40.9	-23.9	17.0	30.6	40.9
17-ts	28.0	-14.6	13.4	26.5	28.0
20-ts	39.6	-24.9	14.7	29.6	39.6
23-ts	25.7	-14.7	11.0	28.7	25.7
25-ts	29.6	-17.0	12.6	29.9	29.6

8. The data of distortion, interaction and total energies along the reaction pathways of the dipolar cycloadditions by B3LYP-D3BJ method in THF solvent.

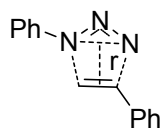
8.1 The data of distortion, interaction and total energies along the reaction pathways of the the dipolar cycloadditions for the formation of 1,5-disubstituted product by B3LYP-D3BJ method in THF solvent.



Step	r	$\square E^\ddagger$	$\square E^\ddagger_{dist}$	$\square E^\ddagger_{int}$
1	3.20	-1.72	2.35	-4.07
2	3.06	-0.82	2.87	-3.68
3	2.90	0.65	3.65	-3.00
4	2.74	3.10	5.14	-2.03

5	2.63	5.27	6.72	-1.45
6	2.55	7.08	8.40	-1.31
7	2.47	9.06	10.89	-1.83
8	2.38	10.98	14.37	-3.39
9	2.25	13.05	21.63	-8.58
10	2.17	13.35	27.95	-14.60
11	2.14	13.00	29.75	-16.75
12	2.07	11.81	35.65	-23.84
13	1.98	8.61	44.68	-36.06
14	1.89	4.32	54.81	-50.50
15	1.76	-0.76	68.66	-69.43
16	1.69	-3.95	76.77	-80.72
17	1.61	-7.89	86.15	-94.03

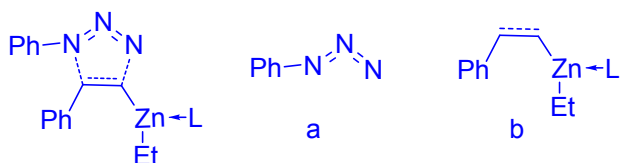
8.2 The data of distortion, interaction and total energies along the reaction pathways of the the dipolar cycloaddition for the formation of 1,4-disubstituted product by B3LYP-D3BJ method in THF solvent.



Step	r	ΔE^\ddagger	ΔE^\ddagger_{dist}	ΔE^\ddagger_{int}
1	3.21	-6.81	1.08	-7.89
2	3.10	-6.31	1.42	-7.73
3	2.97	-5.18	2.18	-7.36

4	2.85	-3.31	3.35	-6.66
5	2.73	-0.41	5.37	-5.77
6	2.61	3.27	8.53	-5.26
7	2.55	5.23	10.60	-5.37
8	2.46	8.39	14.72	-6.33
9	2.37	11.48	20.32	-8.83
10	2.31	13.33	25.10	-11.77
11	2.23	14.63	32.58	-17.95
12	2.16	14.70	39.58	-24.88
13	2.11	14.38	44.88	-30.50
14	2.07	13.93	49.10	-35.17
15	2.03	13.44	51.63	-38.19
16	1.96	11.78	56.95	-45.17
17	1.85	8.79	63.84	-55.05
18	1.78	5.31	70.48	-65.16
19	1.64	-1.25	82.57	-83.82

9. B3LYP-D3BJ geometries for all the optimized distortion – interaction analysis compounds in THF solvent.



The distortion-interaction analysis was used to shed light on the regioselectivity for the cycloaddition of ethyl(phenylethynyl)zinc and azidobenzene with one imidazole ligand. Intrinsic reaction coordinate (IRC) calculations of transition state **17-ts** and **20-ts** were performed, and every geometry on the reaction coordinate is separated to azidobenzene part (a) and ethyl(phenylethynyl)zinc part (b), which is shown in the figure above. The data in section 9.1 and 9.2 of SI represent the structural information of every point in distortion-interaction curves (Figure 8). 9.1 corresponds to transition state 17-ts, and 9.2 corresponds to transition state 20-ts. Moreover, the label “a” stands for the geometry of azidobenzene part, and “b” stands for the geometry of ethyl(phenylethynyl)zinc part.

9.1 B3LYP-D3BJ geometries for 17-ts

1				C	-4.71258900	-3.48254200	-1.21559200
N	-0.97742800	-1.58143300	-0.99277600	H	-2.60597700	-3.46474100	-1.65611800
N	0.03676100	-1.97357900	-1.31799800	C	-5.57884000	-1.53859800	-0.08272100
N	-1.98286900	-1.01263600	-0.58512800	H	-4.13275000	0.00650300	0.36468600
C	0.71273600	1.06342700	-0.06926600	C	-5.78716600	-2.79540300	-0.65304200
C	-0.35091200	1.50185800	0.34302300	H	-4.86549900	-4.45892600	-1.66429100
Zn	2.55750300	1.07694100	-0.65466000	H	-6.40984800	-0.99607100	0.35615400
C	3.87694700	2.22953200	-1.58303200	N	3.53540300	-0.62811500	0.29077000
H	4.47658400	1.63483100	-2.28413300	C	2.96737100	-1.75019800	0.69418200
H	4.59152700	2.59606400	-0.83234600	C	4.87161300	-0.73614500	0.60629200
C	3.24885600	3.42758400	-2.31685600	H	1.92152500	-1.99232300	0.58512900
H	2.65596200	4.05329700	-1.64208600	C	5.10002800	-1.94121100	1.20922400
H	4.00133900	4.08011900	-2.78019200	H	5.56901600	0.05418700	0.37751600
H	2.57333200	3.10440100	-3.11572000	H	5.99674500	-2.39466400	1.59988800
C	-1.54235500	2.10798900	0.83718600	N	3.87591900	-2.58292500	1.25706000
C	-1.89917400	1.99675500	2.19343200	C	3.61820100	-3.91005900	1.79841400
C	-2.34919800	2.89593000	-0.00496600	H	4.21036600	-4.65833000	1.26902700
C	-3.00645400	2.67381700	2.69414900	H	3.86114800	-3.94293700	2.86186000
H	-1.28463400	1.39034300	2.84987100	H	2.56256100	-4.14548100	1.67178700
C	-3.45611300	3.56954300	0.50082500	H	-6.77898100	-3.23470000	-0.66077600
H	-2.08348900	2.98596500	-1.05236500	1a			
C	-3.78602500	3.46874400	1.85313600	N	-0.97742800	-1.58143300	-0.99277600
H	-3.25804800	2.58754300	3.74688100	N	0.03676100	-1.97357900	-1.31799800
H	-4.05916000	4.18366200	-0.16102200	N	-1.98286900	-1.01263600	-0.58512800
H	-4.64284600	4.00544700	2.24809300	C	-3.23689200	-1.66546300	-0.63646300
C	-3.23689200	-1.66546300	-0.63646300	C	-3.43654800	-2.92546900	-1.21110000
C	-3.43654800	-2.92546900	-1.21110000	C	-4.31084300	-0.96949800	-0.07218900
C	-4.31084300	-0.96949800	-0.07218900	C	-4.71258900	-3.48254200	-1.21559200

H	-2.60597700	-3.46474100	-1.65611800	H	2.54008600	4.02478900	-1.65072500
C	-5.57884000	-1.53859800	-0.08272100	H	3.93673200	4.11691300	-2.72175000
H	-4.13275000	0.00650300	0.36468600	H	2.57313100	3.07784300	-3.12769100
C	-5.78716600	-2.79540300	-0.65304200	C	-1.56103900	2.05773900	0.80390100
H	-4.86549900	-4.45892600	-1.66429100	C	-1.89642500	1.95974100	2.16620700
H	-6.40984800	-0.99607100	0.35615400	C	-2.35647300	2.86766200	-0.02742600
H	-6.77898100	-3.23470000	-0.66077600	C	-2.96461900	2.68254800	2.68650500
1b				H	-1.29098100	1.33335200	2.81219800
C	0.71273600	1.06342700	-0.06926600	C	-3.42434600	3.58705600	0.49821700
C	-0.35091200	1.50185800	0.34302300	H	-2.10740900	2.94427200	-1.07996600
Zn	2.55750300	1.07694100	-0.65466000	C	-3.72646900	3.50771500	1.85844200
C	3.87694700	2.22953200	-1.58303200	H	-3.19787100	2.61056900	3.74450200
H	4.47658400	1.63483100	-2.28413300	H	-4.01664800	4.22208600	-0.15347800
H	4.59152700	2.59606400	-0.83234600	H	-4.55008000	4.08287800	2.26938700
C	3.24885600	3.42758400	-2.31685600	C	-3.21569600	-1.64921700	-0.62485100
H	2.65596200	4.05329700	-1.64208600	C	-3.41315500	-2.90651300	-1.20580600
H	4.00133900	4.08011900	-2.78019200	C	-4.29144100	-0.95620800	-0.05973600
H	2.57333200	3.10440100	-3.11572000	C	-4.68919700	-3.46347500	-1.21616100
C	-1.54235500	2.10798900	0.83718600	H	-2.58075600	-3.44295700	-1.65086100
C	-1.89917400	1.99675500	2.19343200	C	-5.55918700	-1.52502400	-0.07639000
C	-2.34919800	2.89593000	-0.00496600	H	-4.11455600	0.01786200	0.38178900
C	-3.00645400	2.67381700	2.69414900	C	-5.76548300	-2.77912600	-0.65337500
H	-1.28463400	1.39034300	2.84987100	H	-4.84096000	-4.43779700	-1.66971400
C	-3.45611300	3.56954300	0.50082500	H	-6.39155300	-0.98465200	0.36258600
H	-2.08348900	2.98596500	-1.05236500	N	3.51955100	-0.62900200	0.30147700
C	-3.78602500	3.46874400	1.85313600	C	2.96241600	-1.75883200	0.69829500
H	-3.25804800	2.58754300	3.74688100	C	4.85561300	-0.72310000	0.62122700
H	-4.05916000	4.18366200	-0.16102200	H	1.91991000	-2.01179500	0.58288700
H	-4.64284600	4.00544700	2.24809300	C	5.09544500	-1.92817500	1.21955200
N	3.53540300	-0.62811500	0.29077000	H	5.54467000	0.07614000	0.39818300
C	2.96737100	-1.75019800	0.69418200	H	5.99584900	-2.37339600	1.61118500
C	4.87161300	-0.73614500	0.60629200	N	3.87831100	-2.58363300	1.26066500
H	1.92152500	-1.99232300	0.58512900	C	3.63433600	-3.91718000	1.79238500
C	5.10002800	-1.94121100	1.20922400	H	4.23557800	-4.65519300	1.25881600
H	5.56901600	0.05418700	0.37751600	H	3.87590700	-3.95490200	2.85597800
H	5.99674500	-2.39466400	1.59988800	H	2.58156300	-4.16336300	1.66236400
N	3.87591900	-2.58292500	1.25706000	H	-6.75714900	-3.21863200	-0.66608200
C	3.61820100	-3.91005900	1.79841400	2a			
H	4.21036600	-4.65833000	1.26902700	N	-0.95350000	-1.54360600	-0.98348300
H	3.86114800	-3.94293700	2.86186000	N	0.07425400	-1.90100000	-1.31076700
H	2.56256100	-4.14548100	1.67178700	N	-1.96487100	-0.99489900	-0.56558300
2				C	-3.21569600	-1.64921700	-0.62485100
N	-0.95350000	-1.54360600	-0.98348300	C	-3.41315500	-2.90651300	-1.20580600
N	0.07425400	-1.90100000	-1.31076700	C	-4.29144100	-0.95620800	-0.05973600
N	-1.96487100	-0.99489900	-0.56558300	C	-4.68919700	-3.46347500	-1.21616100
C	0.67887800	0.99773400	-0.11321800	H	-2.58075600	-3.44295700	-1.65086100
C	-0.38566800	1.43263500	0.29881100	C	-5.55918700	-1.52502400	-0.07639000
Zn	2.52970700	1.05481100	-0.65929300	H	-4.11455600	0.01786200	0.38178900
C	3.83905400	2.25856800	-1.53405700	C	-5.76548300	-2.77912600	-0.65337500
H	4.49613700	1.69222600	-2.20660300	H	-4.84096000	-4.43779700	-1.66971400
H	4.50116400	2.65516200	-0.75101100	H	-6.39155300	-0.98465200	0.36258600
C	3.19328400	3.42910700	-2.29637100	H	-6.75714900	-3.21863200	-0.66608200
2b				C	-1.56103900	2.05773900	0.80390100
C	0.67887800	0.99773400	-0.11321800	C	-1.89642500	1.95974100	2.16620700
C	-0.38566800	1.43263500	0.29881100	C	-2.35647300	2.86766200	-0.02742600
Zn	2.52970700	1.05481100	-0.65929300	C	-2.96461900	2.68254800	2.68650500
C	3.83905400	2.25856800	-1.53405700	H	-1.29098100	1.33335200	2.81219800
H	4.49613700	1.69222600	-2.20660300	C	-3.42434600	3.58705600	0.49821700
H	4.50116400	2.65516200	-0.75101100	H	-2.10740900	2.94427200	-1.07996600
C	3.19328400	3.42910700	-2.29637100	C	-3.72646900	3.50771500	1.85844200
H	2.54008600	4.02478900	-1.65072500	H	-3.19787100	2.61056900	3.74450200
H	3.93673200	4.11691300	-2.72175000	H	-4.01664800	4.22208600	-0.15347800
H	2.57313100	3.07784300	-3.12769100	H	-4.55008000	4.08287800	2.26938700

N	3.51955100	-0.62900200	0.30147700
C	2.96241600	-1.75883200	0.69829500
C	4.85561300	-0.72310000	0.62122700
H	1.91991000	-2.01179500	0.58288700
C	5.09544500	-1.92817500	1.21955200
H	5.54467000	0.07614000	0.39818300
H	5.99584900	-2.37339600	1.61118500
N	3.87831100	-2.58363300	1.26066500
C	3.63433600	-3.91718000	1.79238500
H	4.23557800	-4.65519300	1.25881600
H	3.87590700	-3.95490200	2.85597800
H	2.58156300	-4.16336300	1.66236400

3

N	-0.92711800	-1.50364600	-0.97094600
N	0.12315900	-1.79898100	-1.28424300
N	-1.95136300	-0.97964400	-0.55027100
C	0.64951600	0.93509900	-0.14937000
C	-0.41989900	1.35920100	0.25833400
Zn	2.49912000	1.03910400	-0.66024000
C	3.80323800	2.27495800	-1.49401300
H	4.49876100	1.72496000	-2.14118900
H	4.42635400	2.68972100	-0.68858500
C	3.15660900	3.42767600	-2.28203000
H	2.47029900	4.01137600	-1.66023100
H	3.89806900	4.13006800	-2.68658400
H	2.57131200	3.05965400	-3.13119100
C	-1.57959000	2.00130900	0.77171600
C	-1.89286700	1.91663300	2.13937000
C	-2.36147500	2.83124800	-0.05135500
C	-2.92035100	2.68364400	2.67642800
H	-1.29690200	1.27181300	2.77589700
C	-3.38870100	3.59479300	0.49145700
H	-2.12812800	2.89369900	-1.10840400
C	-3.66281200	3.53643100	1.85871500
H	-3.13547100	2.62689500	3.73920300
H	-3.96916000	4.24968700	-0.15117600
H	-4.45219800	4.14851000	2.28338800
C	-3.19780800	-1.63543800	-0.61633600
C	-3.39486300	-2.89101700	-1.20082000
C	-4.27449700	-0.94304600	-0.05105600
C	-4.67161000	-3.44642300	-1.21419400
H	-2.56140100	-3.42614100	-1.64551400
C	-5.54249800	-1.51009500	-0.07107800
H	-4.09736600	0.02973900	0.39292200
C	-5.74843400	-2.76266300	-0.65149900
H	-4.82379800	-4.41958600	-1.67018800
H	-6.37520000	-0.97005300	0.36769100
N	3.50277000	-0.62674500	0.31191700
C	2.95478100	-1.76253500	0.70405700
C	4.83964800	-0.71155500	0.62988200
H	1.91440800	-2.02272100	0.58709500
C	5.08969200	-1.91763300	1.22194000
H	5.52202100	0.09423500	0.40982100
H	5.99402400	-2.35777800	1.61027000
N	3.87766000	-2.58275100	1.26134800
C	3.64427300	-3.92082400	1.78609300
H	4.25275700	-4.65102400	1.24999000
H	3.88418700	-3.96198100	2.84995500
H	2.59388300	-4.17540800	1.65286600
H	-6.74030200	-3.20165700	-0.66705300

3a

N	-0.92711800	-1.50364600	-0.97094600
N	0.12315900	-1.79898100	-1.28424300

N	-1.95136300	-0.97964400	-0.55027100
C	-3.19780800	-1.63543800	-0.61633600
C	-3.39486300	-2.89101700	-1.20082000
C	-4.27449700	-0.94304600	-0.05105600
C	-4.67161000	-3.44642300	-1.21419400
H	-2.56140100	-3.42614100	-1.64551400
C	-5.54249800	-1.51009500	-0.07107800
H	-4.09736600	0.02973900	0.39292200
C	-5.74843400	-2.76266300	-0.65149900
H	-4.82379800	-4.41958600	-1.67018800
H	-6.37520000	-0.97005300	0.36769100
H	-6.74030200	-3.20165700	-0.66705300

3b

C	0.64951600	0.93509900	-0.14937000
C	-0.41989900	1.35920100	0.25833400
Zn	2.49912000	1.03910400	-0.66024000
C	3.80323800	2.27495800	-1.49401300
H	4.49876100	1.72496000	-2.14118900
H	4.42635400	2.68972100	-0.68858500
C	3.15660900	3.42767600	-2.28203000
H	2.47029900	4.01137600	-1.66023100
H	3.89806900	4.13006800	-2.68658400
H	2.57131200	3.05965400	-3.13119100
C	-1.57959000	2.00130900	0.77171600
C	-1.89286700	1.91663300	2.13937000
C	-2.36147500	2.83124800	-0.05135500
C	-2.92035100	2.68364400	2.67642800
H	-1.29690200	1.27181300	2.77589700
C	-3.38870100	3.59479300	0.49145700
H	-2.12812800	2.89369900	-1.10840400
C	-3.66281200	3.53643100	1.85871500
H	-3.13547100	2.62689500	3.73920300
H	-3.96916000	4.24968700	-0.15117600
H	-4.45219800	4.14851000	2.28338800
N	3.50277000	-0.62674500	0.31191700
C	2.95478100	-1.76253500	0.70405700
C	4.83964800	-0.71155500	0.62988200
H	1.91440800	-2.02272100	0.58709500
C	5.08969200	-1.91763300	1.22194000
H	5.52202100	0.09423500	0.40982100
H	5.99402400	-2.35777800	1.61027000
N	3.87766000	-2.58275100	1.26134800
C	3.64427300	-3.92082400	1.78609300
H	4.25275700	-4.65102400	1.24999000
H	3.88418700	-3.96198100	2.84995500
H	2.59388300	-4.17540800	1.65286600

4

N	-0.90349500	-1.46744700	-0.95773300
N	0.18057500	-1.66937100	-1.23966800
N	-1.94165100	-0.96846700	-0.53979500
C	0.62131700	0.86897000	-0.18313400
C	-0.45255900	1.28338200	0.22065500
Zn	2.46658500	1.02833400	-0.65709900
C	3.76873400	2.28212300	-1.46363500
H	4.48419100	1.73459500	-2.09115500
H	4.36958900	2.70539300	-0.64582000
C	3.13527800	3.42653500	-2.27375900
H	2.43878300	4.01643600	-1.66931100
H	3.88388900	4.12480700	-2.67217400
H	2.56452900	3.05056600	-3.12931200
C	-1.59109300	1.94976600	0.74332600
C	-1.88220200	1.87876300	2.11567700
C	-2.35779600	2.79816300	-0.07349400

C	-2.87730500	2.67817800	2.66449300	H	-2.13667500	2.84924700	-1.13376700
H	-1.29357100	1.22003300	2.74467900	C	-3.60683600	3.54810300	1.85316700
C	-3.35253000	3.59409600	0.48158400	H	-3.07747000	2.63369300	3.73071900
H	-2.13667500	2.84924700	-1.13376700	H	-3.92294900	4.26434900	-0.15409200
C	-3.60683600	3.54810300	1.85316700	H	-4.37153300	4.18451200	2.28692000
H	-3.07747000	2.63369300	3.73071900	N	3.48837200	-0.62401400	0.31872000
H	-3.92294900	4.26434900	-0.15409200	C	2.94743900	-1.76434600	0.70708700
H	-4.37153300	4.18451200	2.28692000	C	4.82600600	-0.70234200	0.63445100
C	-3.18388900	-1.62399800	-0.61054900	H	1.90849500	-2.02916000	0.58968200
C	-3.38188700	-2.87835900	-1.19680300	C	5.08388600	-1.90948100	1.22105800
C	-4.26083300	-0.93076900	-0.04519800	H	5.50344100	0.10821700	0.41665900
C	-4.65922500	-3.43198000	-1.21098500	H	5.99130800	-2.34615200	1.60606100
H	-2.54769800	-3.41256400	-1.64120700	N	3.87557500	-2.58155100	1.25957800
C	-5.52927100	-1.49590100	-0.06645900	C	3.64878400	-3.92195200	1.78092600
H	-4.08303200	0.04129200	0.39994200	H	4.26216500	-4.64771300	1.24435600
C	-5.73576200	-2.74783800	-0.64800500	H	3.88693900	-3.96436800	2.84515400
H	-4.81244900	-4.40454600	-1.66789700	H	2.60002600	-4.18196400	1.64522300
H	-6.36169600	-0.95534600	0.37223400	5			
N	3.48837200	-0.62401400	0.31872000	N	-0.89253200	-1.45890900	-0.95419400
C	2.94743900	-1.76434600	0.70708700	N	0.21264800	-1.57807300	-1.20412800
C	4.82600600	-0.70234200	0.63445100	N	-1.93672900	-0.96374300	-0.53608200
H	1.90849500	-2.02916000	0.58968200	C	0.60252300	0.82323700	-0.20559900
C	5.08388600	-1.90948100	1.22105800	C	-0.47304900	1.23494600	0.19853500
H	5.50344100	0.10821700	0.41665900	Zn	2.44876500	1.02349800	-0.65390800
H	5.99130800	-2.34615200	1.60606100	C	3.75013000	2.28416400	-1.45056800
N	3.87557500	-2.58155100	1.25957800	H	4.47036300	1.73291600	-2.06961300
C	3.64878400	-3.92195200	1.78092600	H	4.34487500	2.70917600	-0.62925600
H	4.26216500	-4.64771300	1.24435600	C	3.12796200	3.42690100	-2.27148700
H	3.88693900	-3.96436800	2.84515400	H	2.43148100	4.02477100	-1.67487700
H	2.60002600	-4.18196400	1.64522300	H	3.88340800	4.11808200	-2.66929800
H	-6.72789200	-3.18614300	-0.66445500	H	2.56032500	3.04922500	-3.12832500
4a				C	-1.59331100	1.92473100	0.72939100
N	-0.90349500	-1.46744700	-0.95773300	C	-1.87251700	1.86267400	2.10428200
N	0.18057500	-1.66937100	-1.23966800	C	-2.35110800	2.78388900	-0.08380200
N	-1.94165100	-0.96846700	-0.53979500	C	-2.85529800	2.67389700	2.65757300
C	-3.18388900	-1.62399800	-0.61054900	H	-1.28790600	1.19767600	2.73040700
C	-3.38188700	-2.87835900	-1.19680300	C	-3.33333000	3.59171900	0.47590400
C	-4.26083300	-0.93076900	-0.04519800	H	-2.13621800	2.82979700	-1.14557800
C	-4.65922500	-3.43198000	-1.21098500	C	-3.58216600	3.54817500	1.84856000
H	-2.54769800	-3.41256400	-1.64120700	H	-3.04908400	2.63392700	3.72515200
C	-5.52927100	-1.49590100	-0.06645900	H	-3.89948900	4.26792500	-0.15725500
H	-4.08303200	0.04129200	0.39994200	H	-4.33930200	4.19149500	2.28535300
C	-5.73576200	-2.74783800	-0.64800500	C	-3.17708400	-1.61601600	-0.60712100
H	-4.81244900	-4.40454600	-1.66789700	C	-3.37503500	-2.86991400	-1.19412800
H	-6.36169600	-0.95534600	0.37223400	C	-4.25479100	-0.92294100	-0.04187500
H	-6.72789200	-3.18614300	-0.66445500	C	-4.65152300	-3.42400500	-1.20900100
4b				H	-2.53953800	-3.40239800	-1.63802500
C	0.62131700	0.86897000	-0.18313400	C	-5.52290900	-1.48868600	-0.06413600
C	-0.45255900	1.28338200	0.22065500	H	-4.07805300	0.04891700	0.40406500
Zn	2.46658500	1.02833400	-0.65709900	C	-5.72863000	-2.74055000	-0.64608000
C	3.76873400	2.28212300	-1.46363500	H	-4.80422100	-4.39650500	-1.66634100
H	4.48419100	1.73459500	-2.09115500	H	-6.35590500	-0.94876900	0.37434200
H	4.36958900	2.70539300	-0.64582000	N	3.48155100	-0.62273100	0.32084800
C	3.13527800	3.42653500	-2.27375900	C	2.94379900	-1.76524800	0.70730200
H	2.43878300	4.01643600	-1.66931100	C	4.81950100	-0.69812600	0.63596200
H	3.88388900	4.12480700	-2.67217400	H	1.90549400	-2.03193900	0.58952500
H	2.56452900	3.05056600	-3.12931200	C	5.08075500	-1.90571100	1.22022000
C	-1.59109300	1.94976600	0.74332600	H	5.49482200	0.11455700	0.41950600
C	-1.88220200	1.87876300	2.11567700	H	5.98948200	-2.34075300	1.60399000
C	-2.35779600	2.79816300	-0.07349400	N	3.87412300	-2.58091600	1.25796700
C	-2.87730500	2.67817800	2.66449300	C	3.64973600	-3.92198800	1.77855800
H	-1.29357100	1.22003300	2.74467900	H	4.26499500	-4.64632400	1.24221900
C	-3.35253000	3.59409600	0.48158400	H	3.88710000	-3.96439300	2.84297000

H	2.60159800	-4.18401200	1.64192800	H	2.55816200	3.04950800	-3.12814900
H	-6.72055300	-3.17932000	-0.66298500	C	-1.59302400	1.91109000	0.72158700
5a				C	-1.86559000	1.85501200	2.09804700
N	-0.89253200	-1.45890900	-0.95419400	C	-2.34568800	2.77700600	-0.08911000
N	0.21264800	-1.57807300	-1.20412800	C	-2.84312500	2.67127300	2.65344200
N	-1.93672900	-0.96374300	-0.53608200	H	-1.28402700	1.18631000	2.72305400
C	-3.17708400	-1.61601600	-0.60712100	C	-3.32248300	3.58998400	0.47271900
C	-3.37503500	-2.86991400	-1.19412800	H	-2.13510000	2.81985900	-1.15186600
C	-4.25479100	-0.92294100	-0.04187500	C	-3.56988400	3.54668800	1.84561300
C	-4.65152300	-3.42400500	-1.20900100	H	-3.03412200	2.63270900	3.72155700
H	-2.53953800	-3.40239800	-1.63802500	H	-3.88693900	4.26843100	-0.15953100
C	-5.52290900	-1.48868600	-0.06413600	H	-4.32497700	4.19161500	2.28354200
H	-4.07805300	0.04891700	0.40406500	C	-3.17237400	-1.60946200	-0.60455800
C	-5.72863000	-2.74055000	-0.64608000	C	-3.37013400	-2.86336200	-1.19200900
H	-4.80422100	-4.39650500	-1.66634100	C	-4.25141600	-0.91763300	-0.03966200
H	-6.35590500	-0.94876900	0.37434200	C	-4.64559500	-3.41867300	-1.20771200
H	-6.72055300	-3.17932000	-0.66298500	H	-2.53341500	-3.39422100	-1.63541200
5b				C	-5.51908700	-1.48464700	-0.06290400
C	0.60252300	0.82323700	-0.20559900	H	-4.07662300	0.05422700	0.40707500
C	-0.47304900	1.23494600	0.19853500	C	-5.72378900	-2.73650600	-0.64511200
Zn	2.44876500	1.02349800	-0.65390800	H	-4.79700800	-4.39124200	-1.66543400
C	3.75013000	2.28416400	-1.45056800	H	-6.35278200	-0.94555400	0.37536200
H	4.47036300	1.73291600	-2.06961300	N	3.47771900	-0.62203700	0.32162600
H	4.34487500	2.70917600	-0.62925600	C	2.94169200	-1.76589300	0.70689600
C	3.12796200	3.42690100	-2.27148700	C	4.81587500	-0.69580700	0.63663800
H	2.43148100	4.02477100	-1.67487700	H	1.90380500	-2.03373000	0.58837800
H	3.88340800	4.11808200	-2.66929800	C	5.07884900	-1.90359300	1.21970900
H	2.56032500	3.04922500	-3.12832500	H	5.49014300	0.11798200	0.42106400
C	-1.59331100	1.92473100	0.72939100	H	5.98822200	-2.33769700	1.60299900
C	-1.87251700	1.86267400	2.10428200	N	3.87314300	-2.58051700	1.25683100
C	-2.35110800	2.78388900	-0.08380200	C	3.64994500	-3.92187700	1.77726500
C	-2.85529800	2.67389700	2.65757300	H	4.26615600	-4.64557000	1.24116900
H	-1.28790600	1.19767600	2.73040700	H	3.88691600	-3.96403500	2.84177200
C	-3.33333000	3.59171900	0.47590400	H	2.60211600	-4.18489800	1.64020700
H	-2.13621800	2.82979700	-1.14557800	H	-6.71533700	-3.17611400	-0.66250900
C	-3.58216600	3.54817500	1.84856000	N	-0.88782600	-1.46028500	-0.95419600
H	-3.04908400	2.63392700	3.72515200	N	0.23111200	-1.51417000	-1.17793700
H	-3.89948900	4.26792500	-0.15725500	N	-1.93287100	-0.95924400	-0.53379300
H	-4.33930200	4.19149500	2.28535300	C	-3.17237400	-1.60946200	-0.60455800
N	3.48155100	-0.62273100	0.32084800	C	-3.37013400	-2.86336200	-1.19200900
C	2.94379900	-1.76524800	0.70730200	C	-4.25141600	-0.91763300	-0.03966200
C	4.81950100	-0.69812600	0.63596200	C	-4.64559500	-3.41867300	-1.20771200
H	1.90549400	-2.03193900	0.58952500	H	-2.53341500	-3.39422100	-1.63541200
C	5.08075500	-1.90571100	1.22022000	C	-5.51908700	-1.48464700	-0.06290400
H	5.49482200	0.11455700	0.41950600	H	-4.07662300	0.05422700	0.40707500
H	5.98948200	-2.34075300	1.60399000	C	-5.72378900	-2.73650600	-0.64511200
N	3.87412300	-2.58091600	1.25796700	H	-4.79700800	-4.39124200	-1.66543400
C	3.64973600	-3.92198800	1.77855800	H	-6.35278200	-0.94555400	0.37536200
H	4.26499500	-4.64632400	1.24221900	H	-6.71533700	-3.17611400	-0.66250900
H	3.88710000	-3.96439300	2.84297000	6b			
H	2.60159800	-4.18401200	1.64192800	C	0.58838300	0.78783700	-0.22217600
N	-0.88782600	-1.46028500	-0.95419600	C	-0.48760800	1.20128100	0.18390400
N	0.23111200	-1.51417000	-1.17793700	Zn	2.43855800	1.02078700	-0.65165100
N	-1.93287100	-0.95924400	-0.53379300	C	3.73931200	2.28516900	-1.44397600
C	0.58838300	0.78783700	-0.22217600	H	4.46009700	1.72981900	-2.05885500
C	-0.48760800	1.20128100	0.18390400	H	4.33252100	2.71019800	-0.62166700
Zn	2.43855800	1.02078700	-0.65165100	C	3.12472100	3.42753900	-2.27080200
C	3.73931200	2.28516900	-1.44397600	H	2.42931000	4.03088600	-1.67848700
H	4.46009700	1.72981900	-2.05885500	H	3.88483500	4.11360400	-2.66847000
H	4.33252100	2.71019800	-0.62166700	H	2.55816200	3.04950800	-3.12814900
C	3.12472100	3.42753900	-2.27080200	C	-1.59302400	1.91109000	0.72158700
H	2.42931000	4.03088600	-1.67848700	C	-1.86559000	1.85501200	2.09804700
H	3.88483500	4.11360400	-2.66847000	C	-2.34568800	2.77700600	-0.08911000

C	-2.84312500	2.67127300	2.65344200	C	3.64996600	-3.92172900	1.77616900
H	-1.28402700	1.18631000	2.72305400	H	4.26700000	-4.64488300	1.24032300
C	-3.32248300	3.58998400	0.47271900	H	3.88663500	-3.96351200	2.84074900
H	-2.13510000	2.81985900	-1.15186600	H	2.60240700	-4.18558200	1.63876100
C	-3.56988400	3.54668800	1.84561300	H	-6.71024100	-3.17382100	-0.66238400
H	-3.03412200	2.63270900	3.72155700	7a			
H	-3.88693900	4.26843100	-0.15953100	N	-0.88432100	-1.46702500	-0.95624600
H	-4.32497700	4.19161500	2.28354200	N	0.24629800	-1.44912900	-1.15035200
N	3.47771900	-0.62203700	0.32162600	N	-1.92801700	-0.95306200	-0.53131400
C	2.94169200	-1.76589300	0.70689600	C	-3.16701100	-1.60209400	-0.60188000
C	4.81587500	-0.69580700	0.63663800	C	-3.36500700	-2.85638500	-1.18974900
H	1.90380500	-2.03373000	0.58837800	C	-4.24833800	-0.91263900	-0.03763300
C	5.07884900	-1.90359300	1.21970900	C	-4.63935000	-3.41337700	-1.20644200
H	5.49014300	0.11798200	0.42106400	H	-2.52710400	-3.38560400	-1.63263000
H	5.98822200	-2.33769700	1.60299900	C	-5.51554600	-1.48127000	-0.06194400
N	3.87314300	-2.58051700	1.25683100	H	-4.07641100	0.05930400	0.41012300
C	3.64994500	-3.92187700	1.77726500	C	-5.71917500	-2.73310900	-0.64437600
H	4.26615600	-4.64557000	1.24116900	H	-4.78892000	-4.38608900	-1.66463800
H	3.88691600	-3.96403500	2.84177200	H	-6.34998800	-0.94304600	0.37613500
H	2.60211600	-4.18489800	1.64020700	H	-6.71024100	-3.17382100	-0.66238400
7				7b			
N	-0.88432100	-1.46702500	-0.95624600	C	0.57292700	0.74877200	-0.23967400
N	0.24629800	-1.44912900	-1.15035200	C	-0.50293000	1.16754000	0.16971700
N	-1.92801700	-0.95306200	-0.53131400	Zn	2.42988800	1.01843700	-0.64950500
C	0.57292700	0.74877200	-0.23967400	C	3.72996200	2.28607500	-1.43880100
C	-0.50293000	1.16754000	0.16971700	H	4.45002100	1.72598900	-2.05031500
Zn	2.42988800	1.01843700	-0.64950500	H	4.32270300	2.71048900	-0.61598500
C	3.72996200	2.28607500	-1.43880100	C	3.12239100	3.42832400	-2.27053700
H	4.45002100	1.72598900	-2.05031500	H	2.42830700	4.03669200	-1.68184400
H	4.32270300	2.71048900	-0.61598500	H	3.88682800	4.10958400	-2.66801800
C	3.12239100	3.42832400	-2.27053700	H	2.55657900	3.05026000	-3.12829300
H	2.42830700	4.03669200	-1.68184400	C	-1.59176400	1.89988400	0.71496100
H	3.88682800	4.10958400	-2.66801800	C	-1.85891000	1.84931100	2.09287000
H	2.55657900	3.05026000	-3.12829300	C	-2.34020500	2.77187500	-0.09334500
C	-1.59176400	1.89988400	0.71496100	C	-2.83299800	2.66896200	2.64984500
C	-1.85891000	1.84931100	2.09287000	H	-1.28080500	1.17697200	2.71716700
C	-2.34020500	2.77187500	-0.09334500	C	-3.31335300	3.58836100	0.47005100
C	-2.83299800	2.66896200	2.64984500	H	-2.13418900	2.81169200	-1.15710000
H	-1.28080500	1.17697200	2.71716700	C	-3.56033400	3.54473900	1.84298100
C	-3.31335300	3.58836100	0.47005100	H	-3.02219600	2.63081800	3.71826600
H	-2.13418900	2.81169200	-1.15710000	H	-3.87688800	4.26795800	-0.16173200
C	-3.56033400	3.54473900	1.84298100	H	-4.31482600	4.18988100	2.28159900
H	-3.02219600	2.63081800	3.71826600	N	3.47438600	-0.62142800	0.32205600
H	-3.87688800	4.26795800	-0.16173200	C	2.93980000	-1.76657500	0.70621400
H	-4.31482600	4.18988100	2.28159900	C	4.81279500	-0.69382500	0.63713300
C	-3.16701100	-1.60209400	-0.60188000	H	1.90236700	-2.03558500	0.58626400
C	-3.36500700	-2.85638500	-1.18974900	C	5.07711200	-1.90175600	1.21925700
C	-4.24833800	-0.91263900	-0.03763300	H	5.48627300	0.12084400	0.42242700
C	-4.63935000	-3.41337700	-1.20644200	H	5.98699000	-2.33503000	1.60226600
H	-2.52710400	-3.38560400	-1.63263000	N	3.87218200	-2.58012000	1.25573800
C	-5.51554600	-1.48127000	-0.06194400	C	3.64996600	-3.92172900	1.77616900
H	-4.07641100	0.05930400	0.41012300	H	4.26700000	-4.64488300	1.24032300
C	-5.71917500	-2.73310900	-0.64437600	H	3.88663500	-3.96351200	2.84074900
H	-4.78892000	-4.38608900	-1.66463800	H	2.60240700	-4.18558200	1.63876100
H	-6.34998800	-0.94304600	0.37613500	8			
N	3.47438600	-0.62142800	0.32205600	N	-0.88105200	-1.47674200	-0.95948900
C	2.93980000	-1.76657500	0.70621400	N	0.25849300	-1.38420500	-1.12218100
C	4.81279500	-0.69382500	0.63713300	N	-1.92190100	-0.94506900	-0.52851200
H	1.90236700	-2.03558500	0.58626400	C	0.55603100	0.70598400	-0.25806100
C	5.07711200	-1.90175600	1.21925700	C	-0.51903300	1.13421900	0.15609600
H	5.48627300	0.12084400	0.42242700	Zn	2.42254700	1.01638800	-0.64753800
H	5.98699000	-2.33503000	1.60226600	C	3.72193800	2.28694200	-1.43472300
N	3.87218200	-2.58012000	1.25573800	H	4.44045900	1.72180700	-2.04340500

H	4.31474400	2.71027900	-0.61158200	H	3.88898300	4.10607700	-2.66773500
C	3.12068200	3.42914700	-2.27051800	H	2.55546200	3.05120800	-3.12862900
H	2.42796300	4.04195400	-1.68486800	C	-1.58978800	1.89070900	0.70930400
H	3.88898300	4.10607700	-2.66773500	C	-1.85270200	1.84500200	2.08858300
H	2.55546200	3.05120800	-3.12862900	C	-2.33497400	2.76803600	-0.09679300
C	-1.58978800	1.89070900	0.70930400	C	-2.82459200	2.66692600	2.64675300
C	-1.85270200	1.84500200	2.08858300	H	-1.27838600	1.16906000	2.71245600
C	-2.33497400	2.76803600	-0.09679300	C	-3.30571200	3.58688500	0.46779500
C	-2.82459200	2.66692600	2.64675300	H	-2.13373100	2.80481400	-1.16154500
H	-1.27838600	1.16906000	2.71245600	C	-3.55280800	3.54265800	1.84066700
C	-3.30571200	3.58688500	0.46779500	H	-3.01275700	2.62851700	3.71529900
H	-2.13373100	2.80481400	-1.16154500	H	-3.86892600	4.26683800	-0.16380600
C	-3.55280800	3.54265800	1.84066700	H	-4.30756200	4.18720200	2.27968000
H	-3.01275700	2.62851700	3.71529900	N	3.47146200	-0.62087700	0.32226200
H	-3.86892600	4.26683800	-0.16380600	C	2.93808200	-1.76729200	0.70538000
H	-4.30756200	4.18720200	2.27968000	C	4.81019600	-0.69211600	0.63751300
C	-3.16092100	-1.59416000	-0.59917100	H	1.90114500	-2.03752300	0.58310700
C	-3.35976200	-2.84927500	-1.18746600	C	5.07554700	-1.90015300	1.21886800
C	-4.24547500	-0.90811900	-0.03585500	H	5.48310700	0.12323400	0.42364900
C	-4.63310000	-3.40818400	-1.20518200	H	5.98582900	-2.33269600	1.60172600
H	-2.52089000	-3.37701900	-1.62984700	N	3.87126200	-2.57972300	1.25472700
C	-5.51230200	-1.47846400	-0.06120200	C	3.64988200	-3.92158200	1.77524100
H	-4.07710900	0.06397200	0.41308300	H	4.26765100	-4.64424300	1.23962200
C	-5.71495800	-2.73025300	-0.64380700	H	3.88632000	-3.96291400	2.83987600
H	-4.78048400	-4.38109100	-1.66392200	H	2.60256300	-4.18613100	1.63750700
H	-6.34744500	-0.94102600	0.37673800	9			
N	3.47146200	-0.62087700	0.32226200	N	-0.87525400	-1.49156900	-0.96451400
C	2.93808200	-1.76729200	0.70538000	N	0.27323700	-1.28862100	-1.08022900
C	4.81019600	-0.69211600	0.63751300	N	-1.91039300	-0.93066500	-0.52399000
H	1.90114500	-2.03752300	0.58310700	C	0.52759900	0.63442200	-0.28739500
C	5.07554700	-1.90015300	1.21886800	C	-0.54461600	1.08556100	0.13683800
H	5.48310700	0.12323400	0.42364900	Zn	2.41347100	1.01376800	-0.64496000
H	5.98582900	-2.33269600	1.60172600	C	3.71205500	2.28824700	-1.43009300
N	3.87126200	-2.57972300	1.25472700	H	4.42742800	1.71542000	-2.03517200
C	3.64988200	-3.92158200	1.77524100	H	4.30529300	2.70944200	-0.60648200
H	4.26765100	-4.64424300	1.23962200	C	3.11887800	3.43032300	-2.27072000
H	3.88632000	-3.96291400	2.83987600	H	2.42812600	4.04875400	-1.68874200
H	2.60256300	-4.18613100	1.63750700	H	3.89208100	4.10168700	-2.66751600
H	-6.70549800	-3.17220200	-0.66249400	H	2.55436500	3.05263500	-3.12924500
8a				C	-1.58576500	1.87982000	0.70214200
N	-0.88105200	-1.47674200	-0.95948900	C	-1.84443900	1.84024000	2.08345200
N	0.25849300	-1.38420500	-1.12218100	C	-2.32788700	2.76391700	-0.10095300
N	-1.92190100	-0.94506900	-0.52851200	C	-2.81449800	2.66427000	2.64289000
C	-3.16092100	-1.59416000	-0.59917100	H	-1.27604900	1.15914000	2.70706500
C	-3.35976200	-2.84927500	-1.18746600	C	-3.29647700	3.58492700	0.46497500
C	-4.24547500	-0.90811900	-0.03585500	H	-2.13378600	2.79640400	-1.16711700
C	-4.63310000	-3.40818400	-1.20518200	C	-3.54420200	3.53963200	1.83771300
H	-2.52089000	-3.37701900	-1.62984700	H	-3.00204500	2.62472700	3.71140600
C	-5.51230200	-1.47846400	-0.06120200	H	-3.85990900	4.26450900	-0.16666200
H	-4.07710900	0.06397200	0.41308300	H	-4.30014300	4.18255700	2.27699700
C	-5.71495800	-2.73025300	-0.64380700	C	-3.15104500	-1.58175300	-0.59512000
H	-4.78048400	-4.38109100	-1.66392200	C	-3.35194200	-2.83884300	-1.18416500
H	-6.34744500	-0.94102600	0.37673800	C	-4.24159800	-0.90218100	-0.03360300
H	-6.70549800	-3.17220200	-0.66249400	C	-4.62416000	-3.40075800	-1.20333600
8b				H	-2.51205600	-3.36467000	-1.62583500
C	0.55603100	0.70598400	-0.25806100	C	-5.50807300	-1.47506900	-0.06034700
C	-0.51903300	1.13421900	0.15609600	H	-4.07928200	0.07021000	0.41723200
Zn	2.42254700	1.01638800	-0.64753800	C	-5.70947100	-2.72672800	-0.64314800
C	3.72193800	2.28694200	-1.43472300	H	-4.76800200	-4.37399600	-1.66296600
H	4.44045900	1.72180700	-2.04340500	H	-6.34415000	-0.93860800	0.37744400
H	4.31474400	2.71027900	-0.61158200	N	3.46773400	-0.62014800	0.32235100
C	3.12068200	3.42914700	-2.27051800	C	2.93580100	-1.76841000	0.70401600
H	2.42796300	4.04195400	-1.68486800	C	4.80707100	-0.68996100	0.63798300

H	1.89968400	-2.04050600	0.57645600	C	0.52273800	0.58690200	-0.31998500
C	5.07352800	-1.89811300	1.21841800	C	-0.54623800	1.05948300	0.11299800
H	5.47944600	0.12612700	0.42531400	Zn	2.42478000	1.01742500	-0.65538400
H	5.98427400	-2.32973100	1.60118500	C	3.72306800	2.29423000	-1.43958100
N	3.86999300	-2.57913400	1.25340900	H	4.43614100	1.71648300	-2.04255500
C	3.64965000	-3.92137400	1.77410800	H	4.31654200	2.71387600	-0.61557100
H	4.26841000	-4.64334400	1.23878900	C	3.13428900	3.43607000	-2.28275600
H	3.88581100	-3.96197100	2.83881100	H	2.44468700	4.05756600	-1.70273400
H	2.60266200	-4.18677200	1.63585600	H	3.91012500	4.10437900	-2.67932100
H	-6.69922200	-3.17058200	-0.66290400	H	2.57017900	3.05845100	-3.14146400
9a				C	-1.56615800	1.87916700	0.68612000
N	-0.87525400	-1.49156900	-0.96451400	C	-1.82338500	1.84293900	2.06880800
N	0.27323700	-1.28862100	-1.08022900	C	-2.30742200	2.76703900	-0.11515500
N	-1.91039300	-0.93066500	-0.52399000	C	-2.79281900	2.66784000	2.62882200
C	-3.15104500	-1.58175300	-0.59512000	H	-1.25880200	1.15875600	2.69244000
C	-3.35194200	-2.83884300	-1.18416500	C	-3.27519000	3.58891000	0.45143500
C	-4.24159800	-0.90218100	-0.03360300	H	-2.11772500	2.79701500	-1.18214600
C	-4.62416000	-3.40075800	-1.20333600	C	-3.52346200	3.54293400	1.82410100
H	-2.51205600	-3.36467000	-1.62583500	H	-2.98034900	2.62734700	3.69723200
C	-5.50807300	-1.47506900	-0.06034700	H	-3.83898600	4.26794300	-0.18034200
H	-4.07928200	0.07021000	0.41723200	H	-4.28037500	4.18465200	2.26342700
C	-5.70947100	-2.72672800	-0.64314800	C	-3.12822500	-1.56827500	-0.60432800
H	-4.76800200	-4.37399600	-1.66296600	C	-3.33053800	-2.82706700	-1.19399400
H	-6.34415000	-0.93860800	0.37744400	C	-4.22289900	-0.89341700	-0.04418100
H	-6.69922200	-3.17058200	-0.66290400	C	-4.60228200	-3.39094800	-1.21406500
9b				H	-2.49014900	-3.35167400	-1.63516600
C	0.52759900	0.63442200	-0.28739500	C	-5.48928200	-1.46793800	-0.07176400
C	-0.54461600	1.08556100	0.13683800	H	-4.06469200	0.07920500	0.40785100
Zn	2.41347100	1.01376800	-0.64496000	C	-5.68990200	-2.71947700	-0.65466900
C	3.71205500	2.28824700	-1.43009300	H	-4.74378400	-4.36439200	-1.67429700
H	4.42742800	1.71542000	-2.03517200	H	-6.32594100	-0.93203900	0.36589500
H	4.30529300	2.70944200	-0.60648200	N	3.48195300	-0.61453100	0.31046200
C	3.11887800	3.43032300	-2.27072000	C	2.95078400	-1.76394800	0.69121100
H	2.42812600	4.04875400	-1.68874200	C	4.82173100	-0.68355900	0.62639800
H	3.89208100	4.10168700	-2.66751600	H	1.91528500	-2.03725100	0.55889000
H	2.55436500	3.05263500	-3.12924500	C	5.08870300	-1.89177900	1.20633300
C	-1.58576500	1.87982000	0.70214200	H	5.49389400	0.13289100	0.41450100
C	-1.84443900	1.84024000	2.08345200	H	5.99968200	-2.32288200	1.58911700
C	-2.32788700	2.76391700	-0.10095300	N	3.88554100	-2.57356600	1.24079400
C	-2.81449800	2.66427000	2.64289000	C	3.66574300	-3.91604500	1.76164500
H	-1.27604900	1.15914000	2.70706500	H	4.28513700	-4.63762300	1.22658900
C	-3.29647700	3.58492700	0.46497500	H	3.90163000	-3.95613800	2.82642000
H	-2.13378600	2.79640400	-1.16711700	H	2.61896400	-4.18189300	1.62293300
C	-3.54420200	3.53963200	1.83771300	H	-6.67918300	-3.16451800	-0.67514500
H	-3.00204500	2.62472700	3.71140600	10a			
H	-3.85990900	4.26450900	-0.16666200	N	-0.85432600	-1.49401700	-0.97888200
H	-4.30014300	4.18255700	2.27699700	N	0.29882200	-1.22150700	-1.06505800
N	3.46773400	-0.62014800	0.32235100	N	-1.88501600	-0.91513500	-0.53294300
C	2.93580100	-1.76841000	0.70401600	C	-3.12822500	-1.56827500	-0.60432800
C	4.80707100	-0.68996100	0.63798300	C	-3.33053800	-2.82706700	-1.19399400
H	1.89968400	-2.04050600	0.57645600	C	-4.22289900	-0.89341700	-0.04418100
C	5.07352800	-1.89811300	1.21841800	C	-4.60228200	-3.39094800	-1.21406500
H	5.47944600	0.12612700	0.42531400	H	-2.49014900	-3.35167400	-1.63516600
H	5.98427400	-2.32973100	1.60118500	C	-5.48928200	-1.46793800	-0.07176400
N	3.86999300	-2.57913400	1.25340900	H	-4.06469200	0.07920500	0.40785100
C	3.64965000	-3.92137400	1.77410800	C	-5.68990200	-2.71947700	-0.65466900
H	4.26841000	-4.64334400	1.23878900	H	-4.74378400	-4.36439200	-1.67429700
H	3.88581100	-3.96197100	2.83881100	H	-6.32594100	-0.93203900	0.36589500
H	2.60266200	-4.18677200	1.63585600	H	-6.67918300	-3.16451800	-0.67514500
10				10b			
N	-0.85432600	-1.49401700	-0.97888200	C	0.52273800	0.58690200	-0.31998500
N	0.29882200	-1.22150700	-1.06505800	C	-0.54623800	1.05948300	0.11299800
N	-1.88501600	-0.91513500	-0.53294300	Zn	2.42478000	1.01742500	-0.65538400

C	3.72306800	2.29423000	-1.43958100	H	-4.75819500	-4.36850400	-1.66228600
H	4.43614100	1.71648300	-2.04255500	H	-6.34188700	-0.93693600	0.37787200
H	4.31654200	2.71387600	-0.61557100	N	3.46514000	-0.61961000	0.32234700
C	3.13428900	3.43607000	-2.28275600	C	2.93414600	-1.76930800	0.70287000
H	2.44468700	4.05756600	-1.70273400	C	4.80502700	-0.68845200	0.63835700
H	3.91012500	4.10437900	-2.67932100	H	1.89880700	-2.04290900	0.56926400
H	2.57017900	3.05845100	-3.14146400	C	5.07211800	-1.89668800	1.21817200
C	-1.56615800	1.87916700	0.68612000	H	5.47714700	0.12807700	0.42663900
C	-1.82338500	1.84293900	2.06880800	H	5.98315500	-2.32767200	1.60094900
C	-2.30742200	2.76703900	-0.11515500	N	3.86904000	-2.57865200	1.25250800
C	-2.79281900	2.66784000	2.62882200	C	3.64937200	-3.92119300	1.77338000
H	-1.25880200	1.15875600	2.69244000	H	4.26889300	-4.64267400	1.23835400
C	-3.27519000	3.58891000	0.45143500	H	3.88523400	-3.96118300	2.83816300
H	-2.11772500	2.79701500	-1.18214600	H	2.60263700	-4.18713400	1.63458500
C	-3.52346200	3.54293400	1.82410100	H	-6.69465000	-3.16954400	-0.66335800
H	-2.98034900	2.62734700	3.69723200	11a			
H	-3.83898600	4.26794300	-0.18034200	N	-0.86948800	-1.50084100	-0.96751600
H	-4.28037500	4.18465200	2.26342700	N	0.28483700	-1.21132100	-1.04649900
N	3.48195300	-0.61453100	0.31046200	N	-1.89901700	-0.91768800	-0.52033900
C	2.95078400	-1.76394800	0.69121100	C	-3.14300200	-1.57138600	-0.59176900
C	4.82173100	-0.68355900	0.62639800	C	-3.34564100	-2.83063000	-1.18160700
H	1.91528500	-2.03725100	0.55889000	C	-4.23872300	-0.89775600	-0.03197700
C	5.08870300	-1.89177900	1.20633300	C	-4.61728500	-3.39501000	-1.20190000
H	5.49389400	0.13289100	0.41450100	H	-2.50513500	-3.35492800	-1.62265700
H	5.99968200	-2.32288200	1.58911700	C	-5.50508800	-1.47269200	-0.05976400
N	3.88554100	-2.57356600	1.24079400	H	-4.08156400	0.07492500	0.42036000
C	3.66574300	-3.91604500	1.76164500	C	-5.70549300	-2.72419400	-0.64270200
H	4.28513700	-4.63762300	1.22658900	H	-4.75819500	-4.36850400	-1.66228600
H	3.90163000	-3.95613800	2.82642000	H	-6.34188700	-0.93693600	0.37787200
H	2.61896400	-4.18189300	1.62293300	H	-6.69465000	-3.16954400	-0.66335800
11				11b			
N	-0.86948800	-1.50084100	-0.96751600	C	0.50088600	0.56814900	-0.31335500
N	0.28483700	-1.21132100	-1.04649900	C	-0.56715400	1.04662500	0.12198900
N	-1.89901700	-0.91768800	-0.52033900	Zn	2.40726900	1.01189800	-0.64315800
C	0.50088600	0.56814900	-0.31335500	C	3.70550500	2.28927400	-1.42717100
C	-0.56715400	1.04662500	0.12198900	H	4.41797600	1.71031900	-2.02966300
Zn	2.40726900	1.01189800	-0.64315800	H	4.29905500	2.70850800	-0.60306100
C	3.70550500	2.28927400	-1.42717100	C	3.11777300	3.43107800	-2.27091500
H	4.41797600	1.71031900	-2.02966300	H	2.42846900	4.05330200	-1.69133100
H	4.29905500	2.70850800	-0.60306100	H	3.89423500	4.09865800	-2.66742700
C	3.11777300	3.43107800	-2.27091500	H	2.55373700	3.05349800	-3.12966200
H	2.42846900	4.05330200	-1.69133100	C	-1.58162400	1.87270000	0.69704800
H	3.89423500	4.09865800	-2.66742700	C	-1.83858400	1.83725500	2.08008700
H	2.55373700	3.05349800	-3.12966200	C	-2.32277900	2.76146200	-0.10377600
C	-1.58162400	1.87270000	0.69704800	C	-2.80790300	2.66232400	2.64023800
C	-1.83858400	1.83725500	2.08008700	H	-1.27492200	1.15233200	2.70372700
C	-2.32277900	2.76146200	-0.10377600	C	-3.29038900	3.58349200	0.46297200
C	-2.80790300	2.66232400	2.64023800	H	-2.13415500	2.79085100	-1.17096500
H	-1.27492200	1.15233200	2.70372700	C	-3.53879000	3.53734100	1.83562400
C	-3.29038900	3.58349200	0.46297200	H	-2.99544600	2.62158100	3.70861900
H	-2.13415500	2.79085100	-1.17096500	H	-3.85430600	4.26236900	-0.16883400
C	-3.53879000	3.53734100	1.83562400	H	-4.29595800	4.17874500	2.27496200
H	-2.99544600	2.62158100	3.70861900	N	3.46514000	-0.61961000	0.32234700
H	-3.85430600	4.26236900	-0.16883400	C	2.93414600	-1.76930800	0.70287000
H	-4.29595800	4.17874500	2.27496200	C	4.80502700	-0.68845200	0.63835700
C	-3.14300200	-1.57138600	-0.59176900	H	1.89880700	-2.04290900	0.56926400
C	-3.34564100	-2.83063000	-1.18160700	C	5.07211800	-1.89668800	1.21817200
C	-4.23872300	-0.89775600	-0.03197700	H	5.47714700	0.12807700	0.42663900
C	-4.61728500	-3.39501000	-1.20190000	H	5.98315500	-2.32767200	1.60094900
H	-2.50513500	-3.35492800	-1.62265700	N	3.86904000	-2.57865200	1.25250800
C	-5.50508800	-1.47269200	-0.05976400	C	3.64937200	-3.92119300	1.77338000
H	-4.08156400	0.07492500	0.42036000	H	4.26889300	-4.64267400	1.23835400
C	-5.70549300	-2.72419400	-0.64270200	H	3.88523400	-3.96118300	2.83816300

H	2.60263700	-4.18713400	1.63458500
12			
C	0.50088600	0.56814900	-0.31335500
C	-0.56715400	1.04662500	0.12198900
Zn	2.40726900	1.01189800	-0.64315800
C	3.70550500	2.28927400	-1.42717100
H	4.41797600	1.71031900	-2.02966300
H	4.29905500	2.70850800	-0.60306100
C	3.11777300	3.43107800	-2.27091500
H	2.42846900	4.05330200	-1.69133100
H	3.89423500	4.09865800	-2.66742700
H	2.55373700	3.05349800	-3.12966200
C	-1.58162400	1.87270000	0.69704800
C	-1.83858400	1.83725500	2.08008700
C	-2.32277900	2.76146200	-0.10377600
C	-2.80790300	2.66232400	2.64023800
H	-1.27492200	1.15233200	2.70372700
C	-3.29038900	3.58349200	0.46297200
H	-2.13415500	2.79085100	-1.17096500
C	-3.53879000	3.53734100	1.83562400
H	-2.99544600	2.62158100	3.70861900
H	-3.85430600	4.26236900	-0.16883400
H	-4.29595800	4.17874500	2.27496200
N	3.46514000	-0.61961000	0.32234700
C	2.93414600	-1.76930800	0.70287000
C	4.80502700	-0.68845200	0.63835700
H	1.89880700	-2.04290900	0.56926400
C	5.07211800	-1.89668800	1.21817200
H	5.47714700	0.12807700	0.42663900
H	5.98315500	-2.32767200	1.60094900
N	3.86904000	-2.57865200	1.25250800
C	3.64937200	-3.92119300	1.77338000
H	4.26889300	-4.64267400	1.23835400
H	3.88523400	-3.96118300	2.83816300
H	2.60263700	-4.18713400	1.63458500
12a			
N	-0.86585700	-1.50476200	-0.96866500
N	0.29227500	-1.16594500	-1.02698700
N	-1.89170400	-0.90979100	-0.51828500
C	-3.13858800	-1.56527500	-0.58974100
C	-3.34203100	-2.82595600	-1.18015900
C	-4.23745700	-0.89547300	-0.03105200
C	-4.61342800	-3.39188100	-1.20110700
H	-2.50117600	-3.34928700	-1.62083700
C	-5.50377300	-1.47171200	-0.05944300
H	-4.08352100	0.07737800	0.42221200
C	-5.70343600	-2.72308400	-0.64250100
H	-4.75252300	-4.36551800	-1.66195900
H	-6.34096900	-0.93640100	0.37815900
H	-6.69219000	-3.16941500	-0.66369700
12b			
N	-0.86585700	-1.50476200	-0.96866500
N	0.29227500	-1.16594500	-1.02698700
N	-1.89170400	-0.90979100	-0.51828500
C	-3.13858800	-1.56527500	-0.58974100
C	-3.34203100	-2.82595600	-1.18015900
C	-4.23745700	-0.89547300	-0.03105200
C	-4.61342800	-3.39188100	-1.20110700
H	-2.50117600	-3.34928700	-1.62083700
C	-5.50377300	-1.47171200	-0.05944300
H	-4.08352100	0.07737800	0.42221200
C	-5.70343600	-2.72308400	-0.64250100
H	-4.75252300	-4.36551800	-1.66195900

H	-6.34096900	-0.93640100	0.37815900
H	-6.69219000	-3.16941500	-0.66369700
13			
N	-0.86064500	-1.50807700	-0.96944000
N	0.30331900	-1.10719300	-1.00211600
N	-1.88108100	-0.89901100	-0.51569400
C	0.45910100	0.46849200	-0.35085000
C	-0.60183000	0.99347000	0.10267100
Zn	2.39978300	1.00944500	-0.64114500
C	3.69799500	2.29077000	-1.42425500
H	4.40631000	1.70393100	-2.02375300
H	4.29198500	2.70709300	-0.59933200
C	3.11688200	3.43240400	-2.27136300
H	2.42963500	4.05924800	-1.69438600
H	3.89727100	4.09536600	-2.66762400
H	2.55315300	3.05516700	-3.13028700
C	-1.57522000	1.86497800	0.69088400
C	-1.83135100	1.83442100	2.07641300
C	-2.31662600	2.75936900	-0.10680000
C	-2.80015100	2.66025200	2.63749500
H	-1.27350200	1.14479700	2.70002200
C	-3.28356400	3.58208800	0.46086200
H	-2.13471300	2.78518600	-1.17519500
C	-3.53271200	3.53468900	1.83346500
H	-2.98795700	2.61783600	3.70565900
H	-3.84850900	4.25985500	-0.17103300
H	-4.29166600	4.17391300	2.27290000
C	-3.13295600	-1.55689900	-0.58690200
C	-3.33700800	-2.81956100	-1.17817500
C	-4.23565000	-0.89217800	-0.02974800
C	-4.60816700	-3.38762400	-1.20005800
H	-2.49560200	-3.34150400	-1.61830100
C	-5.50192900	-1.47024900	-0.05899500
H	-4.08595700	0.08090000	0.42464300
C	-5.70048700	-2.72142500	-0.64222200
H	-4.74480500	-4.36141400	-1.66153500
H	-6.33967900	-0.93555700	0.37847800
N	3.46228400	-0.61917600	0.32230500
C	2.93235700	-1.77069200	0.70120700
C	4.80286200	-0.68677100	0.63885000
H	1.89827500	-2.04623700	0.55736600
C	5.07073300	-1.89510700	1.21788800
H	5.47473200	0.13025500	0.42829400
H	5.98215100	-2.32536000	1.60057600
N	3.86814500	-2.57818100	1.25139600
C	3.64930700	-3.92111000	1.77229500
H	4.26949700	-4.64200500	1.23731400
H	3.88516900	-3.96058800	2.83709400
H	2.60281500	-4.18754200	1.63304000
H	-6.68872200	-3.16903400	-0.66417700
13a			
N	-0.86064500	-1.50807700	-0.96944000
N	0.30331900	-1.10719300	-1.00211600
N	-1.88108100	-0.89901100	-0.51569400
C	-3.13295600	-1.55689900	-0.58690200
C	-3.33700800	-2.81956100	-1.17817500
C	-4.23565000	-0.89217800	-0.02974800
C	-4.60816700	-3.38762400	-1.20005800
H	-2.49560200	-3.34150400	-1.61830100
C	-5.50192900	-1.47024900	-0.05899500
H	-4.08595700	0.08090000	0.42464300
C	-5.70048700	-2.72142500	-0.64222200
H	-4.74480500	-4.36141400	-1.66153500

H	-6.33967900	-0.93555700	0.37847800
H	-6.68872200	-3.16903400	-0.66417700
13b			
C	0.45910100	0.46849200	-0.35085000
C	-0.60183000	0.99347000	0.10267100
Zn	2.39978300	1.00944500	-0.64114500
C	3.69799500	2.29077000	-1.42425500
H	4.40631000	1.70393100	-2.02375300
H	4.29198500	2.70709300	-0.59933200
C	3.11688200	3.43240400	-2.27136300
H	2.42963500	4.05924800	-1.69438600
H	3.89727100	4.09536600	-2.66762400
H	2.55315300	3.05516700	-3.13028700
C	-1.57522000	1.86497800	0.69088400
C	-1.83135100	1.83442100	2.07641300
C	-2.31662600	2.75936900	-0.10680000
C	-2.80015100	2.66025200	2.63749500
H	-1.27350200	1.14479700	2.70002200
C	-3.28356400	3.58208800	0.46086200
H	-2.13471300	2.78518600	-1.17519500
C	-3.53271200	3.53468900	1.83346500
H	-2.98795700	2.61783600	3.70565900
H	-3.84850900	4.25985500	-0.17103300
H	-4.29166600	4.17391300	2.27290000
N	3.46228400	-0.61917600	0.32230500
C	2.93235700	-1.77069200	0.70120700
C	4.80286200	-0.68677100	0.63885000
H	1.89827500	-2.04623700	0.55736600
C	5.07073300	-1.89510700	1.21788800
H	5.47473200	0.13025500	0.42829400
H	5.98215100	-2.32536000	1.60057600
N	3.86814500	-2.57818100	1.25139600
C	3.64930700	-3.92111000	1.77229500
H	4.26949700	-4.64200500	1.23731400
H	3.88516900	-3.96058800	2.83709400
H	2.60281500	-4.18754200	1.63304000
14			
N	-0.85442700	-1.50989800	-0.96963900
N	0.31591200	-1.05220600	-0.97935000
N	-1.86845300	-0.88712400	-0.51311000
C	0.43299500	0.41199400	-0.37109200
C	-0.62704000	0.96001300	0.09122500
Zn	2.39505000	1.00778400	-0.63997500
C	3.69366000	2.29147700	-1.42262000
H	4.39993500	1.70058200	-2.02043300
H	4.28762900	2.70620500	-0.59703400
C	3.11632600	3.43308400	-2.27158300
H	2.43017800	4.06245200	-1.69607600
H	3.89890100	4.09349400	-2.66773300
H	2.55274100	3.05604000	-3.13061300
C	-1.57199900	1.86047500	0.68726400
C	-1.82733200	1.83278100	2.07410000
C	-2.31314900	2.75817600	-0.10846900
C	-2.79567300	2.65909700	2.63595900
H	-1.27250800	1.14042300	2.69737500
C	-3.27970600	3.58141800	0.45957100
H	-2.13457700	2.78195600	-1.17747300
C	-3.52917600	3.53308700	1.83212700
H	-2.98369700	2.61587900	3.70401800
H	-3.84527600	4.25869800	-0.17222300
H	-4.28920500	4.17102000	2.27163800
C	-3.12699300	-1.54732700	-0.58357900
C	-3.33103300	-2.81198800	-1.17580300

C	-4.23350300	-0.88809400	-0.02812400
C	-4.60191800	-3.38267300	-1.19888600
H	-2.48893400	-3.33242100	-1.61534600
C	-5.49971600	-1.46847500	-0.05844800
H	-4.08860200	0.08520900	0.42745700
C	-5.69677400	-2.71941100	-0.64192200
H	-4.73564100	-4.35658600	-1.66107700
H	-6.33809400	-0.93455500	0.37883600
N	3.46067300	-0.61897600	0.32228300
C	2.93136600	-1.77145600	0.70005700
C	4.80152700	-0.68576100	0.63925000
H	1.89815600	-2.04794900	0.54976400
C	5.06991800	-1.89417100	1.21783200
H	5.47318400	0.13163400	0.42943300
H	5.98153700	-2.32399900	1.60052800
N	3.86761200	-2.57792200	1.25075900
C	3.64923600	-3.92100000	1.77166000
H	4.26985500	-4.64164900	1.23684900
H	3.88493300	-3.96022700	2.83652000
H	2.60289100	-4.18773500	1.63204600
H	-6.68436300	-3.16854500	-0.66478600
14a			
N	-0.85442700	-1.50989800	-0.96963900
N	0.31591200	-1.05220600	-0.97935000
N	-1.86845300	-0.88712400	-0.51311000
C	-3.12699300	-1.54732700	-0.58357900
C	-3.33103300	-2.81198800	-1.17580300
C	-4.23350300	-0.88809400	-0.02812400
C	-4.60191800	-3.38267300	-1.19888600
H	-2.48893400	-3.33242100	-1.61534600
C	-5.49971600	-1.46847500	-0.05844800
H	-4.08860200	0.08520900	0.42745700
C	-5.69677400	-2.71941100	-0.64192200
H	-4.73564100	-4.35658600	-1.66107700
H	-6.33809400	-0.93455500	0.37883600
H	-6.68436300	-3.16854500	-0.66478600
14b			
C	0.43299500	0.41199400	-0.37109200
C	-0.62704000	0.96001300	0.09122500
Zn	2.39505000	1.00778400	-0.63997500
C	3.69366000	2.29147700	-1.42262000
H	4.39993500	1.70058200	-2.02043300
H	4.28762900	2.70620500	-0.59703400
C	3.11632600	3.43308400	-2.27158300
H	2.43017800	4.06245200	-1.69607600
H	3.89890100	4.09349400	-2.66773300
H	2.55274100	3.05604000	-3.13061300
C	-1.57199900	1.86047500	0.68726400
C	-1.82733200	1.83278100	2.07410000
C	-2.31314900	2.75817600	-0.10846900
C	-2.79567300	2.65909700	2.63595900
H	-1.27250800	1.14042300	2.69737500
C	-3.27970600	3.58141800	0.45957100
H	-2.13457700	2.78195600	-1.17747300
C	-3.52917600	3.53308700	1.83212700
H	-2.98369700	2.61587900	3.70401800
H	-3.84527600	4.25869800	-0.17222300
H	-4.28920500	4.17102000	2.27163800
N	3.46067300	-0.61897600	0.32228300
C	2.93136600	-1.77145600	0.70005700
C	4.80152700	-0.68576100	0.63925000
H	1.89815600	-2.04794900	0.54976400
C	5.06991800	-1.89417100	1.21783200

H	5.47318400	0.13163400	0.42943300	C	3.11487100	3.43418200	-2.27179100
H	5.98153700	-2.32399900	1.60052800	H	2.43072600	4.06842600	-1.69926800
N	3.86761200	-2.57792200	1.25075900	H	3.90203400	4.08951800	-2.66738800
C	3.64923600	-3.92100000	1.77166600	H	2.55150200	3.05820400	-3.13141100
H	4.26985500	-4.64164900	1.23684900	C	-1.57435600	1.84833700	0.67997700
H	3.88493300	-3.96022700	2.83652000	C	-1.82093200	1.82841100	2.06851100
H	2.60289100	-4.18773500	1.63204600	C	-2.30796500	2.75484400	-0.11186600
15				C	-2.78573000	2.65786600	2.63307200
C	0.43299500	0.41199400	-0.37109200	H	-1.27104700	1.13022800	2.68982900
C	-0.62704000	0.96001300	0.09122500	C	-3.27153000	3.58148600	0.45732900
Zn	2.39505000	1.00778400	-0.63997500	H	-2.13484100	2.77427400	-1.18194700
C	3.69366000	2.29147700	-1.42262000	C	-3.52132700	3.53037900	1.82954500
H	4.39993500	1.70058200	-2.02043300	H	-2.97264400	2.61466500	3.70132400
H	4.28762900	2.70620500	-0.59703400	H	-3.83710700	4.25961700	-0.17353400
C	3.11632600	3.43308400	-2.27158300	H	-4.28317800	4.16589300	2.26951900
H	2.43017800	4.06245200	-1.69607600	N	3.45745500	-0.61879800	0.32200600
H	3.89890100	4.09349400	-2.66773300	C	2.92977800	-1.77284000	0.69731300
H	2.55274100	3.05604000	-3.13061300	C	4.79829700	-0.68354500	0.64035500
C	-1.57199900	1.86047500	0.68726400	H	1.89829300	-2.05136700	0.53862000
C	-1.82733200	1.83278100	2.07410000	C	5.06807200	-1.89211700	1.21804600
C	-2.31314900	2.75817600	-0.10846900	H	5.46896400	0.13510200	0.43222800
C	-2.79567300	2.65909700	2.63595900	H	5.98000300	-2.32084400	1.60123800
H	-1.27250800	1.14042300	2.69737500	N	3.86663100	-2.57766200	1.24928700
C	-3.27970600	3.58141800	0.45957100	C	3.64919500	-3.92080900	1.77018200
H	-2.13457700	2.78195600	-1.17747300	H	4.27077900	-4.64112500	1.23599900
C	-3.52917600	3.53308700	1.83212700	H	3.88419600	-3.95961900	2.83523500
H	-2.98369700	2.61587900	3.70401800	H	2.60316000	-4.18836800	1.62984100
H	-3.84527600	4.25869800	-0.17222300	16			
H	-4.28920500	4.17102000	2.27163800	N	-0.82481700	-1.51635000	-0.97304300
N	3.46067300	-0.61897600	0.32228300	N	0.34856100	-0.99286300	-0.95727800
C	2.93136600	-1.77145600	0.70005700	N	-1.81140100	-0.83982300	-0.50242300
C	4.80152700	-0.68576100	0.63925000	C	0.38221300	0.34020700	-0.39171800
H	1.89815600	-2.04794900	0.54976400	C	-0.75796500	0.81619200	0.04631300
C	5.06991800	-1.89417100	1.21783200	Zn	2.37151900	1.00205300	-0.63477000
H	5.47318400	0.13163400	0.42943300	C	3.67584200	2.28960300	-1.41606400
H	5.98153700	-2.32399900	1.60052800	H	4.38283200	1.69416600	-2.00877400
N	3.86761200	-2.57792200	1.25075900	H	4.26773000	2.70227900	-0.58777800
C	3.64923600	-3.92100000	1.77166600	C	3.11316400	3.43418800	-2.27133500
H	4.26985500	-4.64164900	1.23684900	H	2.43020200	4.07178600	-1.70106000
H	3.88493300	-3.96022700	2.83652000	H	3.90385900	4.08602100	-2.66587500
H	2.60289100	-4.18773500	1.63204600	H	2.55017900	3.05973900	-3.13195800
15a				C	-1.58784600	1.82851800	0.67152500
N	-0.83973400	-1.51264900	-0.97036900	C	-1.81936600	1.82097100	2.06191800
N	0.33675500	-1.00057000	-0.95916400	C	-2.30766800	2.74836300	-0.11542900
N	-1.83963100	-0.86341400	-0.50835000	C	-2.77611300	2.65839800	2.63046700
C	-3.11370700	-1.52435900	-0.57547600	H	-1.27366200	1.11834300	2.68218300
C	-3.31555300	-2.79210200	-1.16950700	C	-3.26370800	3.58328500	0.45628900
C	-4.22718400	-0.87596500	-0.02334700	H	-2.13985200	2.76524500	-1.18654700
C	-4.58501400	-3.36970700	-1.19600000	C	-3.51355400	3.53009000	1.82807900
H	-2.47172200	-3.30953900	-1.60794500	H	-2.95845800	2.61809300	3.69969200
C	-5.49257200	-1.46302200	-0.05692500	H	-3.82612100	4.26546500	-0.17313200
H	-4.09346100	0.09772400	0.43492700	H	-4.27483200	4.16561400	2.26918600
C	-5.68543500	-2.71354300	-0.64118500	C	-3.10095200	-1.49899800	-0.56635300
H	-4.71090400	-4.34377200	-1.65995000	C	-3.29834700	-2.76948900	-1.16242100
H	-6.33263300	-0.93139900	0.37982200	C	-4.22000900	-0.86066600	-0.01726700
H	-6.67118200	-3.16662300	-0.66629700	C	-4.56564000	-3.35466100	-1.19266000
15b				H	-2.45315300	-3.28451700	-1.59987800
C	0.39644000	0.35439800	-0.38909000	C	-5.48346500	-1.45564500	-0.05493000
C	-0.69163700	0.88884100	0.06882500	H	-4.09748800	0.11310400	0.44370100
Zn	2.38344700	1.00425100	-0.63732700	C	-5.67137300	-2.70588600	-0.64012200
C	3.68417400	2.29149400	-1.41925800	H	-4.68338300	-4.32893000	-1.65828100
H	4.38935700	1.69621500	-2.01399300	H	-6.32576600	-0.92715700	0.38111700
H	4.27704500	2.70421700	-0.59192200	N	3.45475800	-0.61891300	0.32155000

C	2.92890700	-1.77399300	0.69520000	N	0.35788200	-0.98923300	-0.95736900
C	4.79520400	-0.68162000	0.64142200	N	-1.78304000	-0.81158800	-0.49412100
H	1.89854800	-2.05476900	0.53491600	C	0.37188900	0.33048900	-0.39314900
C	5.06651500	-1.89024100	1.21854800	C	-0.82191100	0.74124100	0.02290800
H	5.46468100	0.13832600	0.43454200	Zn	2.36123600	1.00118700	-0.63263200
H	5.97871000	-2.31779500	1.60245400	C	3.66971700	2.28724700	-1.41339700
N	3.86616300	-2.57776800	1.24799000	H	4.37838000	1.69233900	-2.00485700
C	3.64938800	-3.92083700	1.76884700	H	4.26105100	2.70030900	-0.58468600
H	4.27181600	-4.64100800	1.23540300	C	3.11167000	3.43345100	-2.27050800
H	3.88351500	-3.95940000	2.83413100	H	2.42922000	4.07309300	-1.70180200
H	2.60362200	-4.18916800	1.62781200	H	3.90465400	4.08322300	-2.66407100
H	-6.65514000	-3.16316300	-0.66741100	H	2.54911800	3.06024100	-3.13205700
16a				C	-1.60448100	1.80419200	0.66203900
N	-0.82481700	-1.51635000	-0.97304300	C	-1.82078100	1.81125200	2.05446700
N	0.34856100	-0.99286300	-0.95727800	C	-2.31000500	2.73900700	-0.11890400
N	-1.81140100	-0.83982300	-0.50242300	C	-2.76755600	2.65900800	2.62759200
C	-3.10095200	-1.49899800	-0.56635300	H	-1.27959800	1.10494000	2.67488800
C	-3.29834700	-2.76948900	-1.16242100	C	-3.25650700	3.58475300	0.45581500
C	-4.22000900	-0.86066600	-0.01726700	H	-2.14816800	2.75464800	-1.19117400
C	-4.56564000	-3.35466100	-1.19266000	C	-3.50602300	3.53135900	1.82730500
H	-2.45315300	-3.28451700	-1.59987800	H	-2.94338600	2.62244600	3.69812000
C	-5.48346500	-1.45564500	-0.05493000	H	-3.81386700	4.27214200	-0.17255400
H	-4.09748800	0.11310400	0.44370100	H	-4.26450800	4.16921400	2.26995200
C	-5.67137300	-2.70588600	-0.64012200	C	-3.08964800	-1.47305700	-0.55680500
H	-4.68338300	-4.32893000	-1.65828100	C	-3.28171400	-2.74672900	-1.15524300
H	-6.32576600	-0.92715700	0.38111700	C	-4.21399800	-0.84526000	-0.01097000
H	-6.65514000	-3.16316300	-0.66741100	C	-4.54707800	-3.33961600	-1.18919200
16b				H	-2.43524300	-3.25937300	-1.59170800
C	0.38221300	0.34020700	-0.39171800	C	-5.47529500	-1.44818700	-0.05278300
C	-0.75796500	0.81619200	0.04631300	H	-4.10256400	0.12851600	0.45256700
Zn	2.37151900	1.00205300	-0.63477000	C	-5.65794700	-2.69811700	-0.63889200
C	3.67584200	2.28960300	-1.41606400	H	-4.65654100	-4.31400600	-1.65641800
H	4.38283200	1.69416600	-2.00877400	H	-6.31982900	-0.92288500	0.38254200
H	4.26773000	2.70227900	-0.58777800	N	3.45278000	-0.61917300	0.32125000
C	3.11316400	3.43418800	-2.27133500	C	2.92851600	-1.77492100	0.69391500
H	2.43020200	4.07178600	-1.70106000	C	4.79285500	-0.68024800	0.64222500
H	3.90385900	4.08602100	-2.66587500	H	1.89902900	-2.05772200	0.53348400
H	2.55017900	3.05973900	-3.13195800	C	5.06554700	-1.88884300	1.21904500
C	-1.58784600	1.82851800	0.67152500	H	5.46125700	0.14078400	0.43614400
C	-1.81936600	1.82097100	2.06191800	H	5.97800200	-2.31537700	1.60349100
C	-2.30766800	2.74836300	-0.11542900	N	3.86611900	-2.57801100	1.24717500
C	-2.77611300	2.65839800	2.63046700	C	3.64975500	-3.92099900	1.76788700
H	-1.27366200	1.11834300	2.68218300	H	4.27282000	-4.64109300	1.23502900
C	-3.26370800	3.58328500	0.45628900	H	3.88307700	-3.95952600	2.83337400
H	-2.13985200	2.76524500	-1.18654700	H	2.60419400	-4.18988100	1.62617600
C	-3.51355400	3.53009000	1.82807900	H	-6.63968200	-3.15958600	-0.66830400
H	-2.95845800	2.61809300	3.69969200	17a			
H	-3.82612100	4.26546500	-0.17313200	N	-0.81147800	-1.52015100	-0.97636100
H	-4.27483200	4.16561400	2.26918600	N	0.35788200	-0.98923300	-0.95736900
N	3.45475800	-0.61891300	0.32155000	N	-1.78304000	-0.81158800	-0.49412100
C	2.92890700	-1.77399300	0.69520000	C	-3.08964800	-1.47305700	-0.55680500
C	4.79520400	-0.68162000	0.64142200	C	-3.28171400	-2.74672900	-1.15524300
H	1.89854800	-2.05476900	0.53491600	C	-4.21399800	-0.84526000	-0.01097000
C	5.06651500	-1.89024100	1.21854800	C	-4.54707800	-3.33961600	-1.18919200
H	5.46468100	0.13832600	0.43454200	H	-2.43524300	-3.25937300	-1.59170800
H	5.97871000	-2.31779500	1.60245400	C	-5.47529500	-1.44818700	-0.05278300
N	3.86616300	-2.57776800	1.24799000	H	-4.10256400	0.12851600	0.45256700
C	3.64938800	-3.92083700	1.76884700	C	-5.65794700	-2.69811700	-0.63889200
H	4.27181600	-4.64100800	1.23540300	H	-4.65654100	-4.31400600	-1.65641800
H	3.88351500	-3.95940000	2.83413100	H	-6.31982900	-0.92288500	0.38254200
H	2.60362200	-4.18916800	1.62781200	H	-6.63968200	-3.15958600	-0.66830400
17				17b			
N	-0.81147800	-1.52015100	-0.97636100	C	0.37188900	0.33048900	-0.39314900

C	-0.82191100	0.74124100	0.02290800	H	-4.12399800	0.17883600	0.48124400
Zn	2.36123600	1.00118700	-0.63263200	C	-5.61609700	-2.67317600	-0.63480100
C	3.66971700	2.28724700	-1.41339700	H	-4.56979700	-4.26389300	-1.64974200
H	4.37838000	1.69233900	-2.00485700	H	-6.30644600	-0.91080600	0.38737900
H	4.26105100	2.70030900	-0.58468600	N	3.44849400	-0.62026600	0.32099300
C	3.11167000	3.43345100	-2.27050800	C	2.92839200	-1.77733700	0.69218500
H	2.42922000	4.07309300	-1.70180200	C	4.78793700	-0.67757500	0.64384300
H	3.90465400	4.08322300	-2.66407100	H	1.90054600	-2.06463200	0.53417400
H	2.54911800	3.06024100	-3.13205700	C	5.06430500	-1.88596100	1.22025900
C	-1.60448100	1.80419200	0.66203900	H	5.45376500	0.14589600	0.43903700
C	-1.82078100	1.81125200	2.05446700	H	5.97760800	-2.30995800	1.60558700
C	-2.31000500	2.73900700	-0.11890400	N	3.86707400	-2.57893300	1.24610900
C	-2.76755600	2.65900800	2.62759200	C	3.65141700	-3.92177900	1.76614900
H	-1.27959800	1.10494000	2.67488800	H	4.27581400	-4.64174200	1.23452400
C	-3.25650700	3.58475300	0.45581500	H	3.88270400	-3.96070100	2.83213900
H	-2.14816800	2.75464800	-1.19117400	H	2.60629300	-4.19166300	1.62260600
C	-3.50602300	3.53135900	1.82730500	H	-6.59025600	-3.14990400	-0.67212100
H	-2.94338600	2.62244600	3.69812000	18a			
H	-3.81386700	4.27214200	-0.17255400	N	-0.77618000	-1.53252200	-0.98733400
H	-4.26450800	4.16921400	2.26995200	N	0.38238600	-0.97545000	-0.95691000
N	3.45278000	-0.61917300	0.32125000	N	-1.70944400	-0.72249400	-0.46620400
C	2.92851600	-1.77492100	0.69391500	C	-3.05855300	-1.39046700	-0.52553600
C	4.79285500	-0.68024800	0.64222500	C	-3.23055800	-2.67075600	-1.13067300
H	1.89902900	-2.05772200	0.53348400	C	-4.20030000	-0.79452500	0.01055600
C	5.06554700	-1.88884300	1.21904500	C	-4.48749200	-3.28957800	-1.17730900
H	5.46125700	0.14078400	0.43614400	H	-2.37800300	-3.17309900	-1.56354200
H	5.97800200	-2.31537700	1.60349100	C	-5.45339700	-1.42418500	-0.04494100
N	3.86611900	-2.57801100	1.24717500	H	-4.12399800	0.17883600	0.48124400
C	3.64975500	-3.92099900	1.76788700	C	-5.61609700	-2.67317600	-0.63480100
H	4.27282000	-4.64109300	1.23502900	H	-4.56979700	-4.26389300	-1.64974200
H	3.88307700	-3.95952600	2.83337400	H	-6.30644600	-0.91080600	0.38737900
H	2.60419400	-4.18988100	1.62617600	H	-6.59025600	-3.14990400	-0.67212100
18				18b			
N	-0.77618000	-1.53252200	-0.98733400	C	0.33544800	0.30272100	-0.39662900
N	0.38238600	-0.97545000	-0.95691000	C	-0.99484700	0.53094300	-0.04251800
N	-1.70944400	-0.72249400	-0.46620400	Zn	2.33359500	1.00181800	-0.62686300
C	0.33544800	0.30272100	-0.39662900	C	3.65681500	2.28018300	-1.40713800
C	-0.99484700	0.53094300	-0.04251800	H	4.36738800	1.68476400	-1.99612800
Zn	2.33359500	1.00181800	-0.62686300	H	4.24731300	2.69322000	-0.57742100
C	3.65681500	2.28018300	-1.40713800	C	3.10820400	3.42981500	-2.26744400
H	4.36738800	1.68476400	-1.99612800	H	2.42603300	4.07261000	-1.70173300
H	4.24731300	2.69322000	-0.57742100	H	3.90533200	4.07640200	-2.65845600
C	3.10820400	3.42981500	-2.26744400	H	2.54702300	3.05915900	-3.13120900
H	2.42603300	4.07261000	-1.70173300	C	-1.66876500	1.70881600	0.62763100
H	3.90533200	4.07640200	-2.65845600	C	-1.83360900	1.76848300	2.02680300
H	2.54702300	3.05915900	-3.13120900	C	-2.32459000	2.69599000	-0.13235100
C	-1.66876500	1.70881600	0.62763100	C	-2.74062700	2.65605200	2.61475300
C	-1.83360900	1.76848300	2.02680300	H	-1.30715500	1.05373200	2.65135700
C	-2.32459000	2.69599000	-0.13235100	C	-3.23215900	3.58321300	0.45305800
C	-2.74062700	2.65605200	2.61475300	H	-2.18260100	2.71158600	-1.20809100
H	-1.30715500	1.05373200	2.65135700	C	-3.47895300	3.53668800	1.82453200
C	-3.23215900	3.58321300	0.45305800	H	-2.88957000	2.63353700	3.68997800
H	-2.18260100	2.71158600	-1.20809100	H	-3.76722000	4.28999700	-0.17356800
C	-3.47895300	3.53668800	1.82453200	H	-4.22070400	4.18990000	2.27326800
H	-2.88957000	2.63353700	3.68997800	N	3.44849400	-0.62026600	0.32099300
H	-3.76722000	4.28999700	-0.17356800	C	2.92839200	-1.77733700	0.69218500
H	-4.22070400	4.18990000	2.27326800	C	4.78793700	-0.67757500	0.64384300
C	-3.05855300	-1.39046700	-0.52553600	H	1.90054600	-2.06463200	0.53417400
C	-3.23055800	-2.67075600	-1.13067300	C	5.06430500	-1.88596100	1.22025900
C	-4.20030000	-0.79452500	0.01055600	H	5.45376500	0.14589600	0.43903700
C	-4.48749200	-3.28957800	-1.17730900	H	5.97760800	-2.30995800	1.60558700
H	-2.37800300	-3.17309900	-1.56354200	N	3.86707400	-2.57893300	1.24610900
C	-5.45339700	-1.42418500	-0.04494100	C	3.65141700	-3.92177900	1.76614900

H	4.27581400	-4.64174200	1.23452400
H	3.88270400	-3.96070100	2.83213900

H	2.60629300	-4.19166300	1.62260600
---	------------	-------------	------------

9.2 B3LYP-D3BJ geometries for 20-ts

1			
N	0.05709000	-1.79382300	-1.03840000
N	1.02877200	-2.04389200	-1.55706100
N	-0.92571500	-1.44243800	-0.37772300
C	1.42793200	0.26265300	0.89571000
C	2.57797400	0.07458300	0.52644100
Zn	-0.40332800	0.40947400	1.55334100
C	3.94346700	-0.12690600	0.15932600
C	4.97031900	0.43505100	0.94105100
C	4.30364700	-0.88868500	-0.96819200
C	6.30583500	0.24292300	0.60571000
H	4.70323100	1.01949000	1.81466800
C	5.64242100	-1.07752800	-1.29785500
H	3.52477100	-1.33416800	-1.57522400
C	6.64964600	-0.51357500	-0.51506300
H	7.08269600	0.68352300	1.22319500
H	5.90055500	-1.67140300	-2.16948900
H	7.69292000	-0.66397800	-0.77409800
C	-2.20551000	-1.87004200	-0.82792100
C	-2.40477500	-2.58706800	-2.01212300
C	-3.29193000	-1.53454600	-0.01640300
C	-3.69379900	-2.96740800	-2.37479100
H	-1.56489700	-2.85191900	-2.64648300
C	-4.57355100	-1.92180700	-0.39019300
H	-3.11713900	-0.98488400	0.89995500
C	-4.78223100	-2.63854900	-1.56870200
H	-3.84451100	-3.52677900	-3.29247200
H	-5.41390700	-1.66543900	0.24666300
C	-1.68236200	0.14560400	3.05385000
H	-1.48573100	0.96261100	3.76266600
H	-2.71392600	0.31744800	2.71547700
C	-1.60251000	-1.19482100	3.80390100
H	-2.29696000	-1.24478000	4.65349000
H	-1.83571500	-2.04464200	3.15330800
H	-0.59928100	-1.37483800	4.20287900
N	-1.19512500	2.02319400	0.25626300
C	-0.58079800	2.46326400	-0.82588500
C	-2.31003300	2.81469100	0.41432100
H	0.34681900	2.06958100	-1.21391100
C	-2.35925200	3.73959900	-0.59184400
H	-2.99212800	2.66863700	1.23701200
H	-3.06193400	4.52564900	-0.81741500
C	-0.87166600	4.23380200	-2.58336600
H	-0.70840800	5.28827100	-2.35437600
H	0.05308500	3.81434700	-2.97702800
H	-1.64935800	4.14578400	-3.34402600
N	-1.24911500	3.50353700	-1.38165400
H	-5.78382800	-2.94116700	-1.85479600
1a			
N	0.05709000	-1.79382300	-1.03840000
N	1.02877200	-2.04389200	-1.55706100
N	-0.92571500	-1.44243800	-0.37772300

C	-2.20551000	-1.87004200	-0.82792100
C	-2.40477500	-2.58706800	-2.01212300
C	-3.29193000	-1.53454600	-0.01640300
C	-3.69379900	-2.96740800	-2.37479100
H	-1.56489700	-2.85191900	-2.64648300
C	-4.57355100	-1.92180700	-0.39019300
H	-3.11713900	-0.98488400	0.89995500
C	-4.78223100	-2.63854900	-1.56870200
H	-3.84451100	-3.52677900	-3.29247200
H	-5.41390700	-1.66543900	0.24666300
H	-5.78382800	-2.94116700	-1.85479600
1b			
C	1.42793200	0.26265300	0.89571000
C	2.57797400	0.07458300	0.52644100
Zn	-0.40332800	0.40947400	1.55334100
C	3.94346700	-0.12690600	0.15932600
C	4.97031900	0.43505100	0.94105100
C	4.30364700	-0.88868500	-0.96819200
C	6.30583500	0.24292300	0.60571000
H	4.70323100	1.01949000	1.81466800
C	5.64242100	-1.07752800	-1.29785500
H	3.52477100	-1.33416800	-1.57522400
C	6.64964600	-0.51357500	-0.51506300
H	7.08269600	0.68352300	1.22319500
H	5.90055500	-1.67140300	-2.16948900
H	7.69292000	-0.66397800	-0.77409800
C	-1.68236200	0.14560400	3.05385000
H	-1.48573100	0.96261100	3.76266600
H	-2.71392600	0.31744800	2.71547700
C	-1.60251000	-1.19482100	3.80390100
H	-2.29696000	-1.24478000	4.65349000
H	-1.83571500	-2.04464200	3.15330800
H	-0.59928100	-1.37483800	4.20287900
N	-1.19512500	2.02319400	0.25626300
C	-0.58079800	2.46326400	-0.82588500
C	-2.31003300	2.81469100	0.41432100
H	0.34681900	2.06958100	-1.21391100
C	-2.35925200	3.73959900	-0.59184400
H	-2.99212800	2.66863700	1.23701200
H	-3.06193400	4.52564900	-0.81741500
C	-0.87166600	4.23380200	-2.58336600
H	-0.70840800	5.28827100	-2.35437600
H	0.05308500	3.81434700	-2.97702800
H	-1.64935800	4.14578400	-3.34402600
N	-1.24911500	3.50353700	-1.38165400
2			
N	0.09466300	-1.75866300	-1.02151400
N	1.07150500	-2.00457100	-1.53313200
N	-0.89011100	-1.40586800	-0.36475300
C	1.40494400	0.23928500	0.88354000
C	2.54242400	0.02690800	0.49134900
Zn	-0.42875400	0.39124600	1.53656400

C	3.91026800	-0.16940700	0.13115800	C	6.25880300	0.24302200	0.61140600
C	4.91615600	0.40835300	0.92822200	H	4.62474200	0.98626600	1.79833800
C	4.29863600	-0.92394900	-0.99169300	C	5.64578100	-1.08649100	-1.30283600
C	6.25880300	0.24302200	0.61140600	H	3.53779300	-1.38219900	-1.61136000
H	4.62474200	0.98626600	1.79833800	C	6.63147500	-0.50399900	-0.50648600
C	5.64578100	-1.08649100	-1.30283600	H	7.01859900	0.69733200	1.24012600
H	3.53779300	-1.38219900	-1.61136000	H	5.92740800	-1.67365500	-2.17179400
C	6.63147500	-0.50399900	-0.50648600	H	7.68072200	-0.63315400	-0.75260800
H	7.01859900	0.69733200	1.24012600	C	-1.68492600	0.14797000	3.06146600
H	5.92740800	-1.67365500	-2.17179400	H	-1.46037700	0.96558400	3.76136500
H	7.68072200	-0.63315400	-0.75260800	H	-2.72225100	0.33165100	2.74775900
C	-2.16681100	-1.84159800	-0.81263500	C	-1.60413200	-1.18947200	3.81687900
C	-2.36093300	-2.56069600	-1.99590300	H	-2.27469300	-1.22411700	4.68629300
C	-3.25382600	-1.51189800	-0.00008500	H	-1.86915000	-2.03920100	3.17819200
C	-3.64733900	-2.95043200	-2.35662000	H	-0.59267300	-1.38298100	4.18801200
H	-1.51938200	-2.81989000	-2.63032500	N	-1.20835600	2.01694100	0.24856900
C	-4.53279500	-1.90838600	-0.37210400	C	-0.60179900	2.44780700	-0.84162700
H	-3.08160800	-0.96001100	0.91533300	C	-2.30330400	2.83151400	0.42686200
C	-4.73693800	-2.62839700	-1.54934500	H	0.31154900	2.03686300	-1.24521300
H	-3.79539300	-3.51191500	-3.27341300	C	-2.34864800	3.76086700	-0.57539600
H	-5.37443600	-1.65721900	0.26509700	H	-2.97481300	2.69753100	1.26024400
C	-1.68492600	0.14797000	3.06146600	H	-3.03748900	4.56291400	-0.78687400
H	-1.46037700	0.96558400	3.76136500	C	-0.88493500	4.22815500	-2.59074300
H	-2.72225100	0.33165100	2.74775900	H	-0.70670800	5.28088500	-2.36514600
C	-1.60413200	-1.18947200	3.81687900	H	0.03023100	3.79760100	-2.99467800
H	-2.27469300	-1.22411700	4.68629300	H	-1.67261700	4.14830900	-3.34202500
H	-1.86915000	-2.03920100	3.17819200	N	-1.25642300	3.50410200	-1.38340900
H	-0.59267300	-1.38298100	4.18801200	3			
N	-1.20835600	2.01694100	0.24856900	N	0.13344300	-1.72222000	-1.00234500
C	-0.60179900	2.44780700	-0.84162700	N	1.12712700	-1.94918500	-1.48919200
C	-2.30330400	2.83151400	0.42686200	N	-0.85739900	-1.37067300	-0.35335500
H	0.31154900	2.03686300	-1.24521300	C	1.38420900	0.21886900	0.87841100
C	-2.34864800	3.76086700	-0.57539600	C	2.50029700	-0.03298900	0.44503200
H	-2.97481300	2.69753100	1.26024400	Zn	-0.45267900	0.37338800	1.51957300
H	-3.03748900	4.56291400	-0.78687400	C	3.86980300	-0.22280800	0.09248800
C	-0.88493500	4.22815500	-2.59074300	C	4.84581500	0.37630600	0.91036000
H	-0.70670800	5.28088500	-2.36514600	C	4.29639300	-0.96658000	-1.02314500
H	0.03023100	3.79760100	-2.99467800	C	6.19689800	0.24792800	0.61951500
H	-1.67261700	4.14830900	-3.34202500	H	4.52115800	0.94451400	1.77478100
N	-1.25642300	3.50410200	-1.38340900	C	5.65379200	-1.09281600	-1.30807400
H	-5.73655900	-2.93879600	-1.83392500	H	3.56117700	-1.44182200	-1.65977000
2a				C	6.60892400	-0.48567100	-0.49346300
N	0.09466300	-1.75866300	-1.02151400	H	6.93245000	0.72055500	1.26330500
N	1.07150500	-2.00457100	-1.53313200	H	5.96742200	-1.67021200	-2.17258400
N	-0.89011100	-1.40586800	-0.36475300	H	7.66538200	-0.58598900	-0.72138300
C	-2.16681100	-1.84159800	-0.81263500	C	-2.12997100	-1.81452500	-0.79846200
C	-2.36093300	-2.56069600	-1.99590300	C	-2.31988800	-2.53589800	-1.98049200
C	-3.25382600	-1.51189800	-0.00008500	C	-3.21703800	-1.48956900	0.01550000
C	-3.64733900	-2.95043200	-2.35662000	C	-3.60410600	-2.93426500	-2.33827600
H	-1.51938200	-2.81989000	-2.63032500	H	-1.47679100	-2.79003800	-2.61490800
C	-4.53279500	-1.90838600	-0.37210400	C	-4.49369500	-1.89435400	-0.35383100
H	-3.08160800	-0.96001100	0.91533300	H	-3.04673000	-0.93610500	0.93024500
C	-4.73693800	-2.62839700	-1.54934500	C	-4.69430900	-2.61763000	-1.52956800
H	-3.79539300	-3.51191500	-3.27341300	H	-3.75053300	-3.49816100	-3.25383800
H	-5.37443600	-1.65721900	0.26509700	H	-5.33615000	-1.64769800	0.28402400
H	-5.73655900	-2.93879600	-1.83392500	C	-1.68324800	0.15102600	3.06984500
2b				H	-1.42601200	0.96670200	3.76082700
C	1.40494400	0.23928500	0.88354000	H	-2.72589100	0.35053900	2.78476200
C	2.54242400	0.02690800	0.49134900	C	-1.60311700	-1.18508000	3.82773800
Zn	-0.42875400	0.39124600	1.53656400	H	-2.24563600	-1.20413800	4.71856300
C	3.91026800	-0.16940700	0.13115800	H	-1.90504700	-2.03178300	3.20139100
C	4.91615600	0.40835300	0.92822200	H	-0.58398600	-1.39678300	4.16659900
C	4.29863600	-0.92394900	-0.99169300	N	-1.21309500	2.01373000	0.24339800

C	-0.61324900	2.43906700	-0.85266800	N	1.18783300	-1.88414600	-1.43041900
C	-2.29481200	2.84224500	0.43620900	N	-0.83272500	-1.34471200	-0.34719700
H	0.29023800	2.01764000	-1.26741800	C	1.36971400	0.19998800	0.87439900
C	-2.33964200	3.77420300	-0.56360200	C	2.46070700	-0.08712900	0.40239100
H	-2.95808800	2.71518100	1.27721600	Zn	-0.47026300	0.35894500	1.50525700
H	-3.02030000	4.58564800	-0.76544400	C	3.83222200	-0.27202300	0.05445200
C	-0.89664700	4.22430100	-2.59727600	C	4.77855300	0.34680200	0.89175300
H	-0.70950700	5.27627600	-2.37552800	C	4.29522200	-1.00503700	-1.05353200
H	0.01168400	3.78732900	-3.00966200	C	6.13622100	0.25352600	0.62695800
H	-1.69250000	4.14805200	-3.34030500	H	4.42205000	0.90512500	1.74984600
N	-1.26032000	3.50501400	-1.38470900	C	5.66131700	-1.09681300	-1.31198900
H	-5.69227600	-2.93498900	-1.81225000	H	3.58616400	-1.49621000	-1.70645400
3a				C	6.58589900	-0.46700400	-0.47987100
N	0.13344300	-1.72222000	-1.00234500	H	6.84746900	0.74322200	1.28513700
N	1.12712700	-1.94918500	-1.48919200	H	6.00574800	-1.66454200	-2.17121500
N	-0.85739900	-1.37067300	-0.35335500	H	7.64841300	-0.54006600	-0.68929600
C	-2.12997100	-1.81452500	-0.79846200	C	-2.10137300	-1.79471300	-0.78848600
C	-2.31988800	-2.53589800	-1.98049200	C	-2.28954200	-2.51800100	-1.96920800
C	-3.21703800	-1.48956900	0.01550000	C	-3.18769300	-1.47244400	0.02733800
C	-3.60410600	-2.93426500	-2.33827600	C	-3.57263700	-2.92178900	-2.32363500
H	-1.47679100	-2.79003800	-2.61490800	H	-1.44541800	-2.76873100	-2.60368700
C	-4.49369500	-1.89435400	-0.35383100	C	-4.46317500	-1.88218100	-0.33890300
H	-3.04673000	-0.93610500	0.93024500	H	-3.01794900	-0.91799600	0.94158300
C	-4.69430900	-2.61763000	-1.52956800	C	-4.66253100	-2.60783200	-1.51326500
H	-3.75053300	-3.49816100	-3.25383800	H	-3.71905100	-3.48766700	-3.23796800
H	-5.33615000	-1.64769800	0.28402400	H	-5.30549300	-1.63802500	0.30007400
H	-5.69227600	-2.93498900	-1.81225000	C	-1.67806300	0.15474000	3.07651000
3b				H	-1.39190200	0.96676600	3.76046700
C	1.38420900	0.21886900	0.87841100	H	-2.72384200	0.37013400	2.81551000
C	2.50029700	-0.03298900	0.44503200	C	-1.60111200	-1.18162300	3.83419100
Zn	-0.45267900	0.37338800	1.51957300	H	-2.22195400	-1.18943200	4.74043200
C	3.86980300	-0.22280800	0.09248800	H	-1.93202500	-2.02403300	3.21669000
C	4.84581500	0.37630600	0.91036000	H	-0.57759200	-1.40955000	4.14846600
C	4.29639300	-0.96658000	-1.02314500	N	-1.21163100	2.01293300	0.24116300
C	6.19689800	0.24792800	0.61951500	C	-0.61716700	2.43544400	-0.85890000
H	4.52115800	0.94451400	1.77478100	C	-2.28680100	2.84756800	0.44266200
C	5.65379200	-1.09281600	-1.30807400	H	0.28058500	2.00895000	-1.28082800
H	3.56117700	-1.44182200	-1.65977000	C	-2.33383100	3.78016200	-0.55638900
C	6.60892400	-0.48567100	-0.49346300	H	-2.94433700	2.72363100	1.28860700
H	6.93245000	0.72055500	1.26330500	H	-3.01129400	4.59560700	-0.75274800
H	5.96742200	-1.67021200	-2.17258400	C	-0.90537300	4.22194500	-2.60177000
H	7.66538200	-0.58598900	-0.72138300	H	-0.71325200	5.27358900	-2.38278800
C	-1.68324800	0.15102600	3.06984500	H	-0.00158700	3.78161000	-3.02050800
H	-1.42601200	0.96670200	3.76082700	H	-1.70712500	4.14730600	-3.33861300
H	-2.72589100	0.35053900	2.78476200	N	-1.26218600	3.50534000	-1.38558500
C	-1.60311700	-1.18508000	3.82773800	H	-5.65969300	-2.92948400	-1.79385600
H	-2.24563600	-1.20413800	4.71856300	4a			
H	-1.90504700	-2.03178300	3.20139100	N	0.16576600	-1.69324000	-0.98682100
H	-0.58398600	-1.39678300	4.16659900	N	1.18783300	-1.88414600	-1.43041900
N	-1.21309500	2.01373000	0.24339800	N	-0.83272500	-1.34471200	-0.34719700
C	-0.61324900	2.43906700	-0.85266800	C	-2.10137300	-1.79471300	-0.78848600
C	-2.29481200	2.84224500	0.43620900	C	-2.28954200	-2.51800100	-1.96920800
H	0.29023800	2.01764000	-1.26741800	C	-3.18769300	-1.47244400	0.02733800
C	-2.33964200	3.77420300	-0.56360200	C	-3.57263700	-2.92178900	-2.32363500
H	-2.95808800	2.71518100	1.27721600	H	-1.44541800	-2.76873100	-2.60368700
H	-3.02030000	4.58564800	-0.76544400	C	-4.46317500	-1.88218100	-0.33890300
C	-0.89664700	4.22430100	-2.59727600	H	-3.01794900	-0.91799600	0.94158300
H	-0.70950700	5.27627600	-2.37552800	C	-4.66253100	-2.60783200	-1.51326500
H	0.01168400	3.78732900	-3.00966200	H	-3.71905100	-3.48766700	-3.23796800
H	-1.69250000	4.14805200	-3.34030500	H	-5.30549300	-1.63802500	0.30007400
N	-1.26032000	3.50501400	-1.38470900	H	-5.65969300	-2.92948400	-1.79385600
4				4b			
N	0.16576600	-1.69324000	-0.98682100	C	1.36971400	0.19998800	0.87439900

C	2.46070700	-0.08712900	0.40239100
Zn	-0.47026300	0.35894500	1.50525700
C	3.83222200	-0.27202300	0.05445200
C	4.77855300	0.34680200	0.89175300
C	4.29522200	-1.00503700	-1.05353200
C	6.13622100	0.25352600	0.62695800
H	4.42205000	0.90512500	1.74984600
C	5.66131700	-1.09681300	-1.31198900
H	3.58616400	-1.49621000	-1.70645400
C	6.58589900	-0.46700400	-0.47987100
H	6.84746900	0.74322200	1.28513700
H	6.00574800	-1.66454200	-2.17121500
H	7.64841300	-0.54006600	-0.68929600
C	-1.67806300	0.15474000	3.07651000
H	-1.39190200	0.96676600	3.76046700
H	-2.72384200	0.37013400	2.81551000
C	-1.60111200	-1.18162300	3.83419100
H	-2.22195400	-1.18943200	4.74043200
H	-1.93202500	-2.02403300	3.21669000
H	-0.57759200	-1.40955000	4.14846600
N	-1.21163100	2.01293300	0.24116300
C	-0.61716700	2.43544400	-0.85890000
C	-2.28680100	2.84756800	0.44266200
H	0.28058500	2.00895000	-1.28082800
C	-2.33383100	3.78016200	-0.55638900
H	-2.94433700	2.72363100	1.28860700
H	-3.01129400	4.59560700	-0.75274800
C	-0.90537300	4.22194500	-2.60177000
H	-0.71325200	5.27358900	-2.38278800
H	-0.00158700	3.78161000	-3.02050800
H	-1.70712500	4.14730600	-3.33861300
N	-1.26218600	3.50534000	-1.38558500

5

N	0.19519100	-1.67300500	-0.97864800
N	1.25304000	-1.80598000	-1.35465400
N	-0.81088000	-1.32378700	-0.34487200
C	1.35818400	0.18159200	0.87123600
C	2.42217600	-0.14188800	0.35866200
Zn	-0.48495900	0.34615300	1.49207300
C	3.79611900	-0.31932200	0.01592900
C	4.71205000	0.31883600	0.87165900
C	4.29422700	-1.04098600	-1.08377300
C	6.07491500	0.25857300	0.63328900
H	4.32494300	0.86734000	1.72254000
C	5.66736600	-1.10001200	-1.31527900
H	3.61160700	-1.54701100	-1.75223400
C	6.56110400	-0.44973500	-0.46586100
H	6.76171700	0.76414400	1.30529900
H	6.04154700	-1.65814200	-2.16832200
H	7.62870700	-0.49753800	-0.65588200
C	-2.07620100	-1.77818800	-0.77975100
C	-2.26392400	-2.50312300	-1.95929200
C	-3.16155100	-1.45764500	0.03792700
C	-3.54591900	-2.91081100	-2.31077200
H	-1.41866700	-2.75089300	-2.59343300
C	-4.43628000	-1.87078600	-0.32569500
H	-2.99236700	-0.90259300	0.95189600
C	-4.63525800	-2.59823200	-1.49884500
H	-3.69281200	-3.47835600	-3.22404600
H	-5.27833800	-1.62831100	0.31428500
C	-1.67030100	0.15952000	3.08300300
H	-1.35798800	0.96645200	3.76148200
H	-2.71757500	0.39081600	2.84246700

C	-1.59878900	-1.17852400	3.83805100
H	-2.20642900	-1.17997500	4.75323900
H	-1.94893100	-2.01618800	3.22467700
H	-0.57363400	-1.41921900	4.13717300
N	-1.20758900	2.01348100	0.24070700
C	-0.61813900	2.43389800	-0.86280900
C	-2.27934200	2.85084100	0.44802900
H	0.27542900	2.00435800	-1.29042100
C	-2.32995100	3.78276900	-0.55141000
H	-2.93233900	2.72858700	1.29770500
H	-3.00666700	4.59960700	-0.74449900
C	-0.91215400	4.22023300	-2.60496800
H	-0.71670800	5.27161000	-2.38765200
H	-0.01162500	3.77784400	-3.02853500
H	-1.71817900	4.14679400	-3.33724500
N	-1.26361400	3.50502100	-1.38641500
H	-5.63204800	-2.92275500	-1.77752900

5a

N	0.19519100	-1.67300500	-0.97864800
N	1.25304000	-1.80598000	-1.35465400
N	-0.81088000	-1.32378700	-0.34487200
C	-2.07620100	-1.77818800	-0.77975100
C	-2.26392400	-2.50312300	-1.95929200
C	-3.16155100	-1.45764500	0.03792700
C	-3.54591900	-2.91081100	-2.31077200
H	-1.41866700	-2.75089300	-2.59343300
C	-4.43628000	-1.87078600	-0.32569500
H	-2.99236700	-0.90259300	0.95189600
C	-4.63525800	-2.59823200	-1.49884500
H	-3.69281200	-3.47835600	-3.22404600
H	-5.27833800	-1.62831100	0.31428500
H	-5.63204800	-2.92275500	-1.77752900

5b

C	1.35818400	0.18159200	0.87123600
C	2.42217600	-0.14188800	0.35866200
Zn	-0.48495900	0.34615300	1.49207300
C	3.79611900	-0.31932200	0.01592900
C	4.71205000	0.31883600	0.87165900
C	4.29422700	-1.04098600	-1.08377300
C	6.07491500	0.25857300	0.63328900
H	4.32494300	0.86734000	1.72254000
C	5.66736600	-1.10001200	-1.31527900
H	3.61160700	-1.54701100	-1.75223400
C	6.56110400	-0.44973500	-0.46586100
H	6.76171700	0.76414400	1.30529900
H	6.04154700	-1.65814200	-2.16832200
H	7.62870700	-0.49753800	-0.65588200
C	-1.67030100	0.15952000	3.08300300
H	-1.35798800	0.96645200	3.76148200
H	-2.71757500	0.39081600	2.84246700
C	-1.59878900	-1.17852400	3.83805100
H	-2.20642900	-1.17997500	4.75323900
H	-1.94893100	-2.01618800	3.22467700
H	-0.57363400	-1.41921900	4.13717300
N	-1.20758900	2.01348100	0.24070700
C	-0.61813900	2.43389800	-0.86280900
C	-2.27934200	2.85084100	0.44802900
H	0.27542900	2.00435800	-1.29042100
C	-2.32995100	3.78276900	-0.55141000
H	-2.93233900	2.72858700	1.29770500
H	-3.00666700	4.59960700	-0.74449900
C	-0.91215400	4.22023300	-2.60496800
H	-0.71670800	5.27161000	-2.38765200

H	-0.01162500	3.77784400	-3.02853500
H	-1.71817900	4.14679400	-3.33724500
N	-1.26361400	3.50502100	-1.38641500
6			
N	0.21653400	-1.66632100	-0.98187300
N	1.31112800	-1.72779200	-1.27540200
N	-0.79046300	-1.30703800	-0.34422800
C	1.34896300	0.16319900	0.86525100
C	2.38712200	-0.19414900	0.31604600
Zn	-0.49653000	0.33651500	1.48198300
C	3.76597600	-0.35836900	-0.01725000
C	4.65467200	0.29651300	0.85372700
C	4.29269200	-1.06973900	-1.10932200
C	6.02121500	0.26213400	0.63806700
H	4.24249600	0.83664100	1.69795700
C	5.67044000	-1.10225200	-1.31787900
H	3.63189800	-1.58807200	-1.78951300
C	6.53758300	-0.43652700	-0.45343700
H	6.68729700	0.77982400	1.32146500
H	6.06922800	-1.65224200	-2.16500100
H	7.60880300	-0.46459900	-0.62594000
C	-2.05385000	-1.76414200	-0.77105000
C	-2.24223200	-2.49055300	-1.94983800
C	-3.13959800	-1.44565100	0.04699400
C	-3.52272400	-2.90135400	-2.30001000
H	-1.39572400	-2.73571600	-2.58323100
C	-4.41372300	-1.86144500	-0.31552600
H	-2.97257800	-0.89034500	0.96126000
C	-4.61242800	-2.59001900	-1.48779200
H	-3.66904900	-3.47007600	-3.21269100
H	-5.25572700	-1.62025100	0.32507100
C	-1.66221900	0.16456600	3.08929100
H	-1.33208700	0.96641600	3.76520500
H	-2.70960300	0.40788600	2.86167400
C	-1.59681400	-1.17619200	3.83995400
H	-2.20012000	-1.17602900	4.75800900
H	-1.95575500	-2.00953200	3.22585300
H	-0.57196100	-1.42494200	4.13359300
N	-1.20311200	2.01468300	0.24123600
C	-0.61802100	2.43344300	-0.86518900
C	-2.27348400	2.85284000	0.45209300
H	0.27196000	2.00156900	-1.29779000
C	-2.32778200	3.78352800	-0.54826600
H	-2.92328400	2.73136800	1.30429700
H	-3.00510100	4.60024000	-0.73968500
C	-0.91671700	4.21915100	-2.60697400
H	-0.71923600	5.27030200	-2.39040200
H	-0.01823600	3.77556900	-3.03362500
H	-1.72532800	4.14662200	-3.33647200
N	-1.26484400	3.50447600	-1.38714800
H	-5.60881400	-2.91653100	-1.76551600
6a			
N	0.21653400	-1.66632100	-0.98187300
N	1.31112800	-1.72779200	-1.27540200
N	-0.79046300	-1.30703800	-0.34422800
C	-2.05385000	-1.76414200	-0.77105000
C	-2.24223200	-2.49055300	-1.94983800
C	-3.13959800	-1.44565100	0.04699400
C	-3.52272400	-2.90135400	-2.30001000
H	-1.39572400	-2.73571600	-2.58323100
C	-4.41372300	-1.86144500	-0.31552600
H	-2.97257800	-0.89034500	0.96126000
C	-4.61242800	-2.59001900	-1.48779200

H	-3.66904900	-3.47007600	-3.21269100
H	-5.25572700	-1.62025100	0.32507100
H	-5.60881400	-2.91653100	-1.76551600
6b			
C	1.34896300	0.16319900	0.86525100
C	2.38712200	-0.19414900	0.31604600
Zn	-0.49653000	0.33651500	1.48198300
C	3.76597600	-0.35836900	-0.01725000
C	4.65467200	0.29651300	0.85372700
C	4.29269200	-1.06973900	-1.10932200
C	6.02121500	0.26213400	0.63806700
H	4.24249600	0.83664100	1.69795700
C	5.67044000	-1.10225200	-1.31787900
H	3.63189800	-1.58807200	-1.78951300
C	6.53758300	-0.43652700	-0.45343700
H	6.68729700	0.77982400	1.32146500
H	6.06922800	-1.65224200	-2.16500100
H	7.60880300	-0.46459900	-0.62594000
C	-1.66221900	0.16456600	3.08929100
H	-1.33208700	0.96641600	3.76520500
H	-2.70960300	0.40788600	2.86167400
C	-1.59681400	-1.17619200	3.83995400
H	-2.20012000	-1.17602900	4.75800900
H	-1.95575500	-2.00953200	3.22585300
H	-0.57196100	-1.42494200	4.13359300
N	-1.20311200	2.01468300	0.24123600
C	-0.61802100	2.43344300	-0.86518900
C	-2.27348400	2.85284000	0.45209300
H	0.27196000	2.00156900	-1.29779000
C	-2.32778200	3.78352800	-0.54826600
H	-2.92328400	2.73136800	1.30429700
H	-3.00510100	4.60024000	-0.73968500
C	-0.91671700	4.21915100	-2.60697400
H	-0.71923600	5.27030200	-2.39040200
H	-0.01823600	3.77556900	-3.03362500
H	-1.72532800	4.14662200	-3.33647200
N	-1.26484400	3.50447600	-1.38714800
7			
N	0.22520000	-1.66647000	-0.98621400
N	1.33575700	-1.69208400	-1.23845200
N	-0.78017300	-1.29921300	-0.34330500
C	1.34525700	0.15458700	0.86160000
C	2.37056900	-0.21968400	0.29472200
Zn	-0.50126900	0.33284800	1.47815200
C	3.75315800	-0.37447600	-0.03123500
C	4.62986200	0.28757100	0.84609700
C	4.29152300	-1.08117800	-1.11992300
C	5.99789500	0.26335900	0.63994900
H	4.20749200	0.82411600	1.68751100
C	5.67080600	-1.10303000	-1.31893500
H	3.63949200	-1.60456600	-1.80452400
C	6.52674000	-0.43146100	-0.44805300
H	6.65525800	0.78573400	1.32809800
H	6.07963100	-1.64957900	-2.16344200
H	7.59930500	-0.45174700	-0.61284800
C	-2.04329500	-1.75779600	-0.76674500
C	-2.23260800	-2.48500400	-1.94534000
C	-3.13000100	-1.44072100	0.05075200
C	-3.51241200	-2.89715900	-2.29533600
H	-1.38561400	-2.72913400	-2.57835200
C	-4.40396700	-1.85762700	-0.31157400
H	-2.96471100	-0.88538000	0.96533800
C	-4.60270800	-2.58655300	-1.48347000

H	-3.65797300	-3.46631400	-3.20791200	C	-2.32713100	3.78358900	-0.54717000
H	-5.24588100	-1.61688700	0.32936500	H	-2.91982000	2.73222000	1.30676800
C	-1.65857000	0.16688500	3.09216000	H	-3.00499300	4.59995000	-0.73812400
H	-1.32297600	0.96658100	3.76782200	C	-0.91832400	4.21878400	-2.60766600
H	-2.70572800	0.41433600	2.86812200	H	-0.72016700	5.26984600	-2.39128000
C	-1.59602100	-1.17531900	3.84047700	H	-0.02052800	3.77478500	-3.03532400
H	-2.19919300	-1.17533200	4.75861300	H	-1.72774800	4.14657600	-3.33627600
H	-1.95685600	-2.00677600	3.22500500	N	-1.26538300	3.50424300	-1.38744900
H	-0.57166600	-1.42679100	4.13361000	8			
N	-1.20105300	2.01534200	0.24163200	N	0.23921600	-1.66921500	-0.99527500
C	-0.61787200	2.43343100	-0.86604100	N	1.37061200	-1.63840100	-1.18206100
C	-2.27118800	2.85352400	0.45367000	N	-0.76280500	-1.28705700	-0.34104000
H	0.27036300	2.00049000	-1.30107700	C	1.34032700	0.14179800	0.85554900
C	-2.32713100	3.78358900	-0.54717000	C	2.34342500	-0.26152300	0.25904100
H	-2.91982000	2.73222000	1.30676800	Zn	-0.50777400	0.32815100	1.47328200
H	-3.00499300	4.59995000	-0.73812400	C	3.73425900	-0.39694800	-0.05094200
C	-0.91832400	4.21878400	-2.60766600	C	4.59356000	0.27539800	0.83530600
H	-0.72016700	5.26984600	-2.39128000	C	4.28909400	-1.09649500	-1.13450800
H	-0.02052800	3.77478500	-3.03532400	C	5.96388700	0.26476200	0.64246100
H	-1.72774800	4.14657600	-3.33627600	H	4.15792400	0.80702900	1.67309500
N	-1.26538300	3.50424300	-1.38744900	C	5.67020200	-1.10392400	-1.32029700
H	-5.59888600	-2.91383800	-1.76102600	H	3.64844700	-1.62645700	-1.82474400
7a				C	6.51039100	-0.42477800	-0.44027800
N	0.22520000	-1.66647000	-0.98621400	H	6.60923900	0.79320300	1.33722000
N	1.33575700	-1.69208400	-1.23845200	H	6.09261400	-1.64567200	-2.16110200
N	-0.78017300	-1.29921300	-0.34330500	H	7.58472400	-0.43471000	-0.59396000
C	-2.04329500	-1.75779600	-0.76674500	C	-2.02653700	-1.74822300	-0.76000700
C	-2.23260800	-2.48500400	-1.94534000	C	-2.21842800	-2.47690000	-1.93848500
C	-3.13000100	-1.44072100	0.05075200	C	-3.11591600	-1.43396400	0.05580100
C	-3.51241200	-2.89715900	-2.29533600	C	-3.49741500	-2.89097700	-2.28849300
H	-1.38561400	-2.72913400	-2.57835200	H	-1.37114800	-2.71997600	-2.57114300
C	-4.40396700	-1.85762700	-0.31157400	C	-4.38992000	-1.85241300	-0.30637000
H	-2.96471100	-0.88538000	0.96533800	H	-2.95422000	-0.87864400	0.97107500
C	-4.60270800	-2.58655300	-1.48347000	C	-4.58909800	-2.58171800	-1.47769500
H	-3.65797300	-3.46631400	-3.20791200	H	-3.64146500	-3.46066200	-3.20110200
H	-5.24588100	-1.61688700	0.32936500	H	-5.23159900	-1.61216800	0.33520900
H	-5.59888600	-2.91383800	-1.76102600	C	-1.65323500	0.17029300	3.09639800
7b				H	-1.31244100	0.96709200	3.77264900
C	1.34525700	0.15458700	0.86160000	H	-2.69985500	0.42232800	2.87517400
C	2.37056900	-0.21968400	0.29472200	C	-1.59495800	-1.17420700	3.84100500
Zn	-0.50126900	0.33284800	1.47815200	H	-2.19916300	-1.17501400	4.75844200
C	3.75315800	-0.37447600	-0.03123500	H	-1.95719600	-2.00292900	3.22282400
C	4.62986200	0.28757100	0.84609700	H	-0.57158500	-1.42908900	4.13475100
C	4.29152300	-1.08117800	-1.11992300	N	-1.19804900	2.01639800	0.24233200
C	5.99789500	0.26335900	0.63994900	C	-0.61765500	2.43356200	-0.86714400
H	4.20749200	0.82411600	1.68751100	C	-2.26815000	2.85437900	0.45575800
C	5.67080600	-1.10303000	-1.31893500	H	0.26779600	1.99902500	-1.30607600
H	3.63949200	-1.60456600	-1.80452400	C	-2.32642600	3.78351000	-0.54581100
C	6.52674000	-0.43146100	-0.44805300	H	-2.91538300	2.73316700	1.30990300
H	6.65525800	0.78573400	1.32809800	H	-3.00528600	4.59912600	-0.73633000
H	6.07963100	-1.64957900	-2.16344200	C	-0.92029600	4.21834000	-2.60852100
H	7.59930500	-0.45174700	-0.61284800	H	-0.72130400	5.26928500	-2.39231000
C	-1.65857000	0.16688500	3.09216000	H	-0.02332100	3.77379600	-3.03734000
H	-1.32297600	0.96658100	3.76782200	H	-1.73062500	4.14653100	-3.33612600
H	-2.70572800	0.41433600	2.86812200	N	-1.26615700	3.50395600	-1.38785500
C	-1.59602100	-1.17531900	3.84047700	H	-5.58498500	-2.91001600	-1.75525400
H	-2.19919300	-1.17533200	4.75861300	8a			
H	-1.95685600	-2.00677600	3.22500500	N	0.23921600	-1.66921500	-0.99527500
H	-0.57166600	-1.42679100	4.13361000	N	1.37061200	-1.63840100	-1.18206100
N	-1.20105300	2.01534200	0.24163200	N	-0.76280500	-1.28705700	-0.34104000
C	-0.61787200	2.43343100	-0.86604100	C	-2.02653700	-1.74822300	-0.76000700
C	-2.27118800	2.85352400	0.45367000	C	-2.21842800	-2.47690000	-1.93848500
H	0.27036300	2.00049000	-1.30107700	C	-3.11591600	-1.43396400	0.05580100

C	-3.49741500	-2.89097700	-2.28849300
H	-1.37114800	-2.71997600	-2.57114300
C	-4.38992000	-1.85241300	-0.30637000
H	-2.95422000	-0.87864400	0.97107500
C	-4.58909800	-2.58171800	-1.47769500
H	-3.64146500	-3.46066200	-3.20110200
H	-5.23159900	-1.61216800	0.33520900
H	-5.58498500	-2.91001600	-1.75525400

8b

C	1.34032700	0.14179800	0.85554900
C	2.34342500	-0.26152300	0.25904100
Zn	-0.50777400	0.32815100	1.47328200
C	3.73425900	-0.39694800	-0.05094200
C	4.59356000	0.27539800	0.83530600
C	4.28909400	-1.09649500	-1.13450800
C	5.96388700	0.26476200	0.64246100
H	4.15792400	0.80702900	1.67309500
C	5.67020200	-1.10392400	-1.32029700
H	3.64844700	-1.62645700	-1.82474400
C	6.51039100	-0.42477800	-0.44027800
H	6.60923900	0.79320300	1.33722000
H	6.09261400	-1.64567200	-2.16110200
H	7.58472400	-0.43471000	-0.59396000
C	-1.65323500	0.17029300	3.09639800
H	-1.31244100	0.96709200	3.77264900
H	-2.69985500	0.42232800	2.87517400
C	-1.59495800	-1.17420700	3.84100500
H	-2.19916300	-1.17501400	4.75844200
H	-1.95719600	-2.00292900	3.22282400
H	-0.57158500	-1.42908900	4.13475100
N	-1.19804900	2.01639800	0.24233200
C	-0.61765500	2.43356200	-0.86714400
C	-2.26815000	2.85437900	0.45575800
H	0.26779600	1.99902500	-1.30607600
C	-2.32642600	3.78351000	-0.54581100
H	-2.91538300	2.73316700	1.30990300
H	-3.00528600	4.59912600	-0.73633000
C	-0.92029600	4.21834000	-2.60852100
H	-0.72130400	5.26928500	-2.39231000
H	-0.02332100	3.77379600	-3.03734000
H	-1.73062500	4.14653100	-3.33612600
N	-1.26615700	3.50395600	-1.38785500

9

N	0.25480400	-1.67281800	-1.00508300
N	1.40433400	-1.58555500	-1.12582100
N	-0.74314300	-1.27456000	-0.33767100
C	1.33658500	0.12968600	0.84903200
C	2.31178100	-0.30902700	0.21720500
Zn	-0.51335700	0.32445300	1.46950200
C	3.71544100	-0.41693000	-0.06858000
C	4.55891600	0.26483100	0.82555700
C	4.28600800	-1.10925900	-1.14688100
C	5.93187200	0.26558700	0.64452100
H	4.11272000	0.79222400	1.66064500
C	5.66849300	-1.10445300	-1.32122600
H	3.65458800	-1.64479000	-1.84154100
C	6.49475700	-0.41911900	-0.43312300
H	6.56635100	0.79900900	1.34537600
H	6.10233700	-1.64204600	-2.15875100
H	7.57054600	-0.42019400	-0.57643600
C	-2.00933500	-1.73884500	-0.75321600
C	-2.20507800	-2.46938000	-1.93177400
C	-3.10272900	-1.42813200	0.06001500

C	-3.48366000	-2.88512000	-2.28205400
H	-1.35800800	-2.71189800	-2.56430600
C	-4.37719000	-1.84795400	-0.30207200
H	-2.94553000	-0.87273500	0.97609100
C	-4.57720800	-2.57747800	-1.47281500
H	-3.62579400	-3.45512200	-3.19492700
H	-5.21845100	-1.60789700	0.34032100
C	-1.64831600	0.17343900	3.10035400
H	-1.30554900	0.96779800	3.77822900
H	-2.69425200	0.42831100	2.87935100
C	-1.59407600	-1.17334800	3.84130000
H	-2.20008400	-1.17522900	4.75751200
H	-1.95664600	-1.99953000	3.22010600
H	-0.57179600	-1.43100900	4.13658900
N	-1.19530500	2.01746200	0.24309700
C	-0.61749900	2.43379700	-0.86804900
C	-2.26567200	2.85506200	0.45747400
H	0.26506400	1.99773300	-1.31104800
C	-2.32597000	3.78333000	-0.54478200
H	-2.91186200	2.73385900	1.31237900
H	-3.00592200	4.59806200	-0.73511700
C	-0.92178100	4.21800800	-2.60919200
H	-0.72213900	5.26885000	-2.39306700
H	-0.02544600	3.77297900	-3.03884800
H	-1.73273500	4.14649700	-3.33608200
N	-1.26683400	3.50375600	-1.38818500
H	-5.57282400	-2.90661000	-1.75059600

9a

N	0.25480400	-1.67281800	-1.00508300
N	1.40433400	-1.58555500	-1.12582100
N	-0.74314300	-1.27456000	-0.33767100
C	-2.00933500	-1.73884500	-0.75321600
C	-2.20507800	-2.46938000	-1.93177400
C	-3.10272900	-1.42813200	0.06001500
C	-3.48366000	-2.88512000	-2.28205400
H	-1.35800800	-2.71189800	-2.56430600
C	-4.37719000	-1.84795400	-0.30207200
H	-2.94553000	-0.87273500	0.97609100
C	-4.57720800	-2.57747800	-1.47281500
H	-3.62579400	-3.45512200	-3.19492700
H	-5.21845100	-1.60789700	0.34032100
H	-5.57282400	-2.90661000	-1.75059600

9b

C	1.33658500	0.12968600	0.84903200
C	2.31178100	-0.30902700	0.21720500
Zn	-0.51335700	0.32445300	1.46950200
C	3.71544100	-0.41693000	-0.06858000
C	4.55891600	0.26483100	0.82555700
C	4.28600800	-1.10925900	-1.14688100
C	5.93187200	0.26558700	0.64452100
H	4.11272000	0.79222400	1.66064500
C	5.66849300	-1.10445300	-1.32122600
H	3.65458800	-1.64479000	-1.84154100
C	6.49475700	-0.41911900	-0.43312300
H	6.56635100	0.79900900	1.34537600
H	6.10233700	-1.64204600	-2.15875100
H	7.57054600	-0.42019400	-0.57643600
C	-1.64831600	0.17343900	3.10035400
H	-1.30554900	0.96779800	3.77822900
H	-2.69425200	0.42831100	2.87935100
C	-1.59407600	-1.17334800	3.84130000
H	-2.20008400	-1.17522900	4.75751200
H	-1.95664600	-1.99953000	3.22010600

H	-0.57179600	-1.43100900	4.13658900
N	-1.19530500	2.01746200	0.24309700
C	-0.61749900	2.43379700	-0.86804900
C	-2.26567200	2.85506200	0.45747400
H	0.26506400	1.99773300	-1.31104800
C	-2.32597000	3.78333000	-0.54478200
H	-2.91186200	2.73385900	1.31237900
H	-3.00592200	4.59806200	-0.73511700
C	-0.92178100	4.21800800	-2.60919200
H	-0.72213900	5.26885000	-2.39306700
H	-0.02544600	3.77297900	-3.03884800
H	-1.73273500	4.14649700	-3.33608200
N	-1.26683400	3.50375600	-1.38818500

10

N	0.26593400	-1.67489000	-1.01128600
N	1.42679000	-1.55106600	-1.08873600
N	-0.72908700	-1.26638100	-0.33499800
C	1.33484600	0.12208600	0.84435400
C	2.28752800	-0.34418700	0.18535600
Zn	-0.51650700	0.32252500	1.46757300
C	3.70292900	-0.42851900	-0.07880400
C	4.53732800	0.25877100	0.81983400
C	4.28371000	-1.11617400	-1.15351400
C	5.91232000	0.26585300	0.64561600
H	4.08598600	0.78381100	1.65386600
C	5.66689600	-1.10451300	-1.32157300
H	3.65736000	-1.65515600	-1.85041700
C	6.48518600	-0.41591900	-0.42883400
H	6.54033600	0.80196400	1.35018800
H	6.10693000	-1.63982000	-2.15724700
H	7.56178000	-0.41198700	-0.56588800
C	-1.99819600	-1.73291200	-0.74880600
C	-2.19693600	-2.46480400	-1.92759000
C	-3.09471300	-1.42473900	0.06236500
C	-3.47547100	-2.88152900	-2.27811700
H	-1.35014200	-2.70724900	-2.55994900
C	-4.36967800	-1.84543400	-0.29966300
H	-2.94082300	-0.86929400	0.97902800
C	-4.57038400	-2.57500500	-1.47004100
H	-3.61623200	-3.45171500	-3.19120400
H	-5.21057600	-1.60539800	0.34334500
C	-1.64542900	0.17531100	3.10275400
H	-1.30257800	0.96829600	3.78201200
H	-2.69087100	0.43135000	2.88090700
C	-1.59357700	-1.17290800	3.84140500
H	-2.20086200	-1.17551100	4.75673700
H	-1.95608400	-1.99757000	3.21828700
H	-0.57199100	-1.43211400	4.13785400
N	-1.19370600	2.01813600	0.24359700
C	-0.61742400	2.43398500	-0.86853700
C	-2.26433400	2.85544300	0.45841500
H	0.26323500	1.99692900	-1.31418900
C	-2.32576600	3.78318900	-0.54426000
H	-2.91000600	2.73420600	1.31368500
H	-3.00640300	4.59734300	-0.73456400
C	-0.92253900	4.21783900	-2.60955000
H	-0.72256300	5.26862200	-2.39344700
H	-0.02655000	3.77253000	-3.03963500
H	-1.73380200	4.14646700	-3.33607300
N	-1.26720900	3.50366600	-1.38835600
H	-5.56584900	-2.90457700	-1.74804200

10a

N	0.26593400	-1.67489000	-1.01128600
---	------------	-------------	-------------

N	1.42679000	-1.55106600	-1.08873600
N	-0.72908700	-1.26638100	-0.33499800
C	-1.99819600	-1.73291200	-0.74880600
C	-2.19693600	-2.46480400	-1.92759000
C	-3.09471300	-1.42473900	0.06236500
C	-3.47547100	-2.88152900	-2.27811700
H	-1.35014200	-2.70724900	-2.55994900
C	-4.36967800	-1.84543400	-0.29966300
H	-2.94082300	-0.86929400	0.97902800
C	-4.57038400	-2.57500500	-1.47004100
H	-3.61623200	-3.45171500	-3.19120400
H	-5.21057600	-1.60539800	0.34334500
H	-5.56584900	-2.90457700	-1.74804200

10b

C	1.33484600	0.12208600	0.84435400
C	2.28752800	-0.34418700	0.18535600
Zn	-0.51650700	0.32252500	1.46757300
C	3.70292900	-0.42851900	-0.07880400
C	4.53732800	0.25877100	0.81983400
C	4.28371000	-1.11617400	-1.15351400
C	5.91232000	0.26585300	0.64561600
H	4.08598600	0.78381100	1.65386600
C	5.66689600	-1.10451300	-1.32157300
H	3.65736000	-1.65515600	-1.85041700
C	6.48518600	-0.41591900	-0.42883400
H	6.54033600	0.80196400	1.35018800
H	6.10693000	-1.63982000	-2.15724700
H	7.56178000	-0.41198700	-0.56588800
C	-1.64542900	0.17531100	3.10275400
H	-1.30257800	0.96829600	3.78201200
H	-2.69087100	0.43135000	2.88090700
C	-1.59357700	-1.17290800	3.84140500
H	-2.20086200	-1.17551100	4.75673700
H	-1.95608400	-1.99757000	3.21828700
H	-0.57199100	-1.43211400	4.13785400
N	-1.19370600	2.01813600	0.24359700
C	-0.61742400	2.43398500	-0.86853700
C	-2.26433400	2.85544300	0.45841500
H	0.26323500	1.99692900	-1.31418900
C	-2.32576600	3.78318900	-0.54426000
H	-2.91000600	2.73420600	1.31368500
H	-3.00640300	4.59734300	-0.73456400
C	-0.92253900	4.21783900	-2.60955000
H	-0.72256300	5.26862200	-2.39344700
H	-0.02655000	3.77253000	-3.03963500
H	-1.73380200	4.14646700	-3.33607300
N	-1.26720900	3.50366600	-1.38835600

11

N	0.28034400	-1.67698400	-1.01823500
N	1.45514000	-1.50924000	-1.04362900
N	-0.71078000	-1.25653300	-0.33165700
C	1.33312800	0.11253200	0.83785600
C	2.25394700	-0.39134800	0.14174500
Zn	-0.51992000	0.32061900	1.46571700
C	3.68728000	-0.44110400	-0.08983700
C	4.51200500	0.25211000	0.81360800
C	4.28052800	-1.12316900	-1.16015500
C	5.88980200	0.26604000	0.64685100
H	4.05616400	0.77473000	1.64712200
C	5.66445800	-1.10430100	-1.32162200
H	3.65948000	-1.66612500	-1.85932100
C	6.47410400	-0.41231100	-0.42387800
H	6.51055100	0.80495100	1.35568400

H	6.11092100	-1.63724100	-2.15530900	H	-1.29994700	0.96884900	3.78655100
H	7.55155000	-0.40293800	-0.55386500	H	-2.68714400	0.43448100	2.88223100
C	-1.98492900	-1.72582900	-0.74350000	C	-1.59302400	-1.17249500	3.84144600
C	-2.18736700	-2.45946100	-1.92272400	H	-2.20173300	-1.17596600	4.75578300
C	-3.08536700	-1.42082800	0.06505800	H	-1.95538200	-1.99545700	3.21615100
C	-3.46601400	-2.87728400	-2.27356500	H	-0.57220700	-1.43336700	4.13919400
H	-1.34091900	-2.70184200	-2.55472500	N	-1.19200900	2.01891400	0.24418200
C	-4.36107800	-1.84257600	-0.29692000	C	-0.61737200	2.43423700	-0.86903300
H	-2.93560100	-0.86526900	0.98241200	C	-2.26298600	2.85585600	0.45941000
C	-4.56259000	-2.57215200	-1.46687000	H	0.26108500	1.99604700	-1.31773500
H	-3.60510400	-3.44764400	-3.18693600	C	-2.32560500	3.78302600	-0.54372700
H	-5.20152900	-1.60252700	0.34682200	H	-2.90813500	2.73457800	1.31504200
C	-1.64229300	0.17739400	3.10547600	H	-3.00700400	4.59652300	-0.73405200
H	-1.29994700	0.96884900	3.78655100	C	-0.92332700	4.21768400	-2.60989700
H	-2.68714400	0.43448100	2.88223100	H	-0.72302100	5.26839900	-2.39378800
C	-1.59302400	-1.17249500	3.84144600	H	-0.02769700	3.77208000	-3.04041600
H	-2.20173300	-1.17596600	4.75578300	H	-1.73489500	4.14643600	-3.33604400
H	-1.95538200	-1.99545700	3.21615100	N	-1.26762600	3.50359400	-1.38850700
H	-0.57220700	-1.43336700	4.13919400	12			
N	-1.19200900	2.01891400	0.24418200	N	0.30577300	-1.68911600	-1.01347600
C	-0.61737200	2.43423700	-0.86903300	N	1.49081900	-1.48914700	-1.00050900
C	-2.26298600	2.85585600	0.45941000	N	-0.68154100	-1.25944400	-0.31915500
H	0.26108500	1.99604700	-1.31773500	C	1.34442700	0.09288300	0.84166800
C	-2.32560500	3.78302600	-0.54372700	C	2.23899700	-0.44089000	0.11568400
H	-2.90813500	2.73457800	1.31504200	Zn	-0.50928300	0.30871300	1.47461200
H	-3.00700400	4.59652300	-0.73405200	C	3.68744400	-0.46102700	-0.08765100
C	-0.92332700	4.21768400	-2.60989700	C	4.50471100	0.23639400	0.81933100
H	-0.72302100	5.26839900	-2.39378800	C	4.29069600	-1.13867600	-1.15457300
H	-0.02769700	3.77208000	-3.04041600	C	5.88475400	0.25578200	0.65842800
H	-1.73489500	4.14643600	-3.33604400	H	4.04570700	0.75713500	1.65268200
N	-1.26762600	3.50359400	-1.38850700	C	5.67518500	-1.11432400	-1.31102000
H	-5.55789100	-2.90220300	-1.74516400	H	3.67355100	-1.68456300	-1.85547900
11a				C	6.47803600	-0.41969200	-0.40934800
N	0.28034400	-1.67698400	-1.01823500	H	6.49976300	0.79682800	1.37062900
N	1.45514000	-1.50924000	-1.04362900	H	6.12669100	-1.64533100	-2.14317300
N	-0.71078000	-1.25653300	-0.33165700	H	7.55610600	-0.40592900	-0.53375800
C	-1.98492900	-1.72582900	-0.74350000	C	-1.96054400	-1.73044200	-0.72895100
C	-2.18736700	-2.45946100	-1.92272400	C	-2.16554800	-2.46540500	-1.90857500
C	-3.08536700	-1.42082800	0.06505800	C	-3.06378200	-1.42783800	0.07768800
C	-3.46601400	-2.87728400	-2.27356500	C	-3.44425000	-2.88415800	-2.25964600
H	-1.34091900	-2.70184200	-2.55472500	H	-1.31927900	-2.70760800	-2.54016600
C	-4.36107800	-1.84257600	-0.29692000	C	-4.34004600	-1.85057900	-0.28429100
H	-2.93560100	-0.86526900	0.98241200	H	-2.91724200	-0.87214300	0.99553600
C	-4.56259000	-2.57215200	-1.46687000	C	-4.54205000	-2.58017500	-1.45390800
H	-3.60510400	-3.44764400	-3.18693600	H	-3.58200800	-3.45464300	-3.17323700
H	-5.20152900	-1.60252700	0.34682200	H	-5.18019400	-1.61064100	0.35997200
H	-5.55789100	-2.90220300	-1.74516400	C	-1.62670700	0.16828100	3.11766500
11b				H	-1.28442300	0.95844100	3.80011000
C	1.33312800	0.11253200	0.83785600	H	-2.67117900	0.42628900	2.89381100
C	2.25394700	-0.39134800	0.14174500	C	-1.57915000	-1.18299800	3.85130600
Zn	-0.51992000	0.32061900	1.46571700	H	-2.18900800	-1.18750400	4.76483400
C	3.68728000	-0.44110400	-0.08983700	H	-1.94115400	-2.00464000	3.22416200
C	4.51200500	0.25211000	0.81360800	H	-0.55888000	-1.44497800	4.15001200
C	4.28052800	-1.12316900	-1.16015500	N	-1.17753700	2.00872700	0.25477600
C	5.88980200	0.26604000	0.64685100	C	-0.60401500	2.42374300	-0.85916600
H	4.05616400	0.77473000	1.64712200	C	-2.24877100	2.84536300	0.47032800
C	5.66445800	-1.10430100	-1.32162200	H	0.27293500	1.98481800	-1.30996500
H	3.65948000	-1.66612500	-1.85932100	C	-2.31221300	3.77217300	-0.53308700
C	6.47410400	-0.41231100	-0.42387800	H	-2.89356400	2.72398200	1.32619700
H	6.51055100	0.80495100	1.35568400	H	-2.99418900	4.58518500	-0.72340400
H	6.11092100	-1.63724100	-2.15530900	C	-0.91060300	4.20699900	-2.59984400
H	7.55155000	-0.40293800	-0.55386500	H	-0.71021400	5.25768300	-2.38367300
C	-1.64229300	0.17739400	3.10547600	H	-0.01514700	3.76130700	-3.03061900

H	-1.72235600	4.13576500	-3.32575200
N	-1.25460700	3.49288800	-1.37833300
H	-5.53719800	-2.91069400	-1.73242300
12a			
N	0.30577300	-1.68911600	-1.01347600
N	1.49081900	-1.48914700	-1.00050900
N	-0.68154100	-1.25944400	-0.31915500
C	-1.96054400	-1.73044200	-0.72895100
C	-2.16554800	-2.46540500	-1.90857500
C	-3.06378200	-1.42783800	0.07768800
C	-3.44425000	-2.88415800	-2.25964600
H	-1.31927900	-2.70760800	-2.54016600
C	-4.34004600	-1.85057900	-0.28429100
H	-2.91724200	-0.87214300	0.99553600
C	-4.54205000	-2.58017500	-1.45390800
H	-3.58200800	-3.45464300	-3.17323700
H	-5.18019400	-1.61064100	0.35997200
H	-5.53719800	-2.91069400	-1.73242300
12b			
C	1.34442700	0.09288300	0.84166800
C	2.23899700	-0.44089000	0.11568400
Zn	-0.50928300	0.30871300	1.47461200
C	3.68744400	-0.46102700	-0.08765100
C	4.50471100	0.23639400	0.81933100
C	4.29069600	-1.13867600	-1.15457300
C	5.88475400	0.25578200	0.65842800
H	4.04570700	0.75713500	1.65268200
C	5.67518500	-1.11432400	-1.31102000
H	3.67355100	-1.68456300	-1.85547900
C	6.47803600	-0.41969200	-0.40934800
H	6.49976300	0.79682800	1.37062900
H	6.12669100	-1.64533100	-2.14317300
H	7.55610600	-0.40592900	-0.53375800
C	-1.62670700	0.16828100	3.11766500
H	-1.28442300	0.95844100	3.80011000
H	-2.67117900	0.42628900	2.89381100
C	-1.57915000	-1.18299800	3.85130600
H	-2.18900800	-1.18750400	4.76483400
H	-1.94115400	-2.00464000	3.22416200
H	-0.55888000	-1.44497800	4.15001200
N	-1.17753700	2.00872700	0.25477600
C	-0.60401500	2.42374300	-0.85916600
C	-2.24877100	2.84536300	0.47032800
H	0.27293500	1.98481800	-1.30996500
C	-2.31221300	3.77217300	-0.53308700
H	-2.89356400	2.72398200	1.32619700
H	-2.99418900	4.58518500	-0.72340400
C	-0.91060300	4.20699900	-2.59984400
H	-0.71021400	5.25768300	-2.38367300
H	-0.01514700	3.76130700	-3.03061900
H	-1.72235600	4.13576500	-3.32575200
N	-1.25460700	3.49288800	-1.37833300
13			
N	0.30163000	-1.68069100	-1.02909800
N	1.49297200	-1.46086900	-0.99176600
N	-0.68140900	-1.24320200	-0.32870200
C	1.32793200	0.09450700	0.82529900
C	2.20483300	-0.45885000	0.07922600
Zn	-0.52459300	0.31859800	1.46403900
C	3.66290200	-0.45829500	-0.10450800
C	4.47325900	0.24259800	0.80540600
C	4.27405800	-1.13275900	-1.16866600
C	5.85471000	0.26699000	0.64975300

H	4.01062300	0.76161600	1.63810300
C	5.65901500	-1.10349900	-1.32047100
H	3.66044800	-1.68121800	-1.87107100
C	6.45558900	-0.40611100	-0.41538500
H	6.46470400	0.81008400	1.36469200
H	6.11534900	-1.63292400	-2.15099400
H	7.53416900	-0.38836500	-0.53492100
C	-1.96438400	-1.71459100	-0.73553700
C	-2.17144500	-2.45055100	-1.91522300
C	-3.06896000	-1.41346500	0.07034000
C	-3.45019500	-2.86999700	-2.26588700
H	-1.32548800	-2.69265400	-2.54674400
C	-4.34573200	-1.83697800	-0.29114100
H	-2.92435800	-0.85762500	0.98846100
C	-4.54848400	-2.56669600	-1.46036900
H	-3.58738900	-3.44069200	-3.17946900
H	-5.18538200	-1.59701700	0.35381100
C	-1.63797700	0.18082700	3.10989200
H	-1.29407500	0.96980200	3.79281400
H	-2.68212200	0.44069600	2.88676000
C	-1.59223000	-1.17136800	3.84206800
H	-2.20197100	-1.17577500	4.75563900
H	-1.95545000	-1.99184900	3.21417300
H	-0.57230400	-1.43505000	4.14045900
N	-1.18974900	2.02046200	0.24515400
C	-0.61731500	2.43472100	-0.86968400
C	-2.26090500	2.85720000	0.46099100
H	0.25842700	1.99499100	-1.32197200
C	-2.32517700	3.78332400	-0.54298600
H	-2.90508200	2.73632700	1.31738400
H	-3.00740000	4.59611200	-0.73333400
C	-0.92465300	4.21727100	-2.61075900
H	-0.72343900	5.26784900	-2.39486500
H	-0.02984400	3.77090500	-3.04217500
H	-1.73698900	4.14639100	-3.33602600
N	-1.26821600	3.50356900	-1.38885300
H	-5.54364300	-2.89753700	-1.73854300
13a			
N	0.30163000	-1.68069100	-1.02909800
N	1.49297200	-1.46086900	-0.99176600
N	-0.68140900	-1.24320200	-0.32870200
C	-1.96438400	-1.71459100	-0.73553700
C	-2.17144500	-2.45055100	-1.91522300
C	-3.06896000	-1.41346500	0.07034000
C	-3.45019500	-2.86999700	-2.26588700
H	-1.32548800	-2.69265400	-2.54674400
C	-4.34573200	-1.83697800	-0.29114100
H	-2.92435800	-0.85762500	0.98846100
C	-4.54848400	-2.56669600	-1.46036900
H	-3.58738900	-3.44069200	-3.17946900
H	-5.18538200	-1.59701700	0.35381100
H	-5.54364300	-2.89753700	-1.73854300
13b			
C	1.32793200	0.09450700	0.82529900
C	2.20483300	-0.45885000	0.07922600
Zn	-0.52459300	0.31859800	1.46403900
C	3.66290200	-0.45829500	-0.10450800
C	4.47325900	0.24259800	0.80540600
C	4.27405800	-1.13275900	-1.16866600
C	5.85471000	0.26699000	0.64975300
H	4.01062300	0.76161600	1.63810300
C	5.65901500	-1.10349900	-1.32047100
H	3.66044800	-1.68121800	-1.87107100

C	6.45558900	-0.40611100	-0.41538500	H	-2.90186800	2.73988800	1.32034100
H	6.46470400	0.81008400	1.36469200	H	-3.00616700	4.59759900	-0.73202100
H	6.11534900	-1.63292400	-2.15099400	C	-0.92624400	4.21612500	-2.61198800
H	7.53416900	-0.38836500	-0.53492100	H	-0.72346300	5.26656100	-2.39690500
C	-1.63797700	0.18082700	3.10989200	H	-0.03273000	3.76846700	-3.04472900
H	-1.29407500	0.96980200	3.79281400	H	-1.73993400	4.14578800	-3.33576700
H	-2.68212200	0.44069600	2.88676000	N	-1.26858500	3.50342000	-1.38908100
C	-1.59223000	-1.17136800	3.84206800	H	-5.53142900	-2.89034100	-1.72553100
H	-2.20197100	-1.17577500	4.75563900	14a			
H	-1.95545000	-1.99184900	3.21417300	N	0.31200200	-1.69020300	-1.04335700
H	-0.57230400	-1.43505000	4.14045900	N	1.50777500	-1.46118900	-0.99225500
N	-1.18974900	2.02046200	0.24515400	N	-0.66054200	-1.24006900	-0.33373700
C	-0.61731500	2.43472100	-0.86968400	C	-1.94897000	-1.70664900	-0.73226800
C	-2.26090500	2.85720000	0.46099100	C	-2.16006500	-2.44307100	-1.91143700
H	0.25842700	1.99499100	-1.32197200	C	-3.05151200	-1.40506900	0.07591000
C	-2.32517700	3.78332400	-0.54298600	C	-3.43919600	-2.86275100	-2.25857700
H	-2.90508200	2.73632700	1.31738400	H	-1.31563600	-2.68544400	-2.54432600
H	-3.00740000	4.59611200	-0.73333400	C	-4.32946600	-1.82891900	-0.28228700
C	-0.92465300	4.21727100	-2.61075900	H	-2.90613000	-0.84925100	0.99393900
H	-0.72343900	5.26784900	-2.39486500	C	-4.53551200	-2.55927700	-1.45032800
H	-0.02984400	3.77090500	-3.04217500	H	-3.57839900	-3.43387600	-3.17159800
H	-1.73698900	4.14639100	-3.33602600	H	-5.16731300	-1.58862400	0.36489400
N	-1.26821600	3.50356900	-1.38885300	H	-5.53142900	-2.89034100	-1.72553100
14				14b			
N	0.31200200	-1.69020300	-1.04335700	C	1.31784000	0.07689600	0.81261300
N	1.50777500	-1.46118900	-0.99225500	C	2.18301700	-0.48910000	0.05209200
N	-0.66054200	-1.24006900	-0.33373700	Zn	-0.52734000	0.31914900	1.46495700
C	1.31784000	0.07689600	0.81261300	C	3.64676000	-0.46928800	-0.11319800
C	2.18301700	-0.48910000	0.05209200	C	4.44431800	0.23705100	0.80216200
Zn	-0.52734000	0.31914900	1.46495700	C	4.26940900	-1.13928900	-1.17338000
C	3.64676000	-0.46928800	-0.11319800	C	5.82677700	0.27100000	0.65587200
C	4.44431800	0.23705100	0.80216200	H	3.97280400	0.75240400	1.63235300
C	4.26940900	-1.13928900	-1.17338000	C	5.65491400	-1.10064200	-1.31613200
C	5.82677700	0.27100000	0.65587200	H	3.66312100	-1.69178700	-1.87910800
H	3.97280400	0.75240400	1.63235300	C	6.43982900	-0.39773700	-0.40508800
C	5.65491400	-1.10064200	-1.31613200	H	6.42819600	0.81798600	1.37508900
H	3.66312100	-1.69178700	-1.87910800	H	6.12077700	-1.62673500	-2.14348500
C	6.43982900	-0.39773700	-0.40508800	H	7.51912200	-0.37231000	-0.51664400
H	6.42819600	0.81798600	1.37508900	C	-1.63461500	0.18424600	3.11452300
H	6.12077700	-1.62673500	-2.14348500	H	-1.28502000	0.97073400	3.79738000
H	7.51912200	-0.37231000	-0.51664400	H	-2.67836300	0.44875000	2.89524200
C	-1.94897000	-1.70664900	-0.73226800	C	-1.59161100	-1.16945300	3.84408000
C	-2.16006500	-2.44307100	-1.91143700	H	-2.19932600	-1.17330000	4.75894900
C	-3.05151200	-1.40506900	0.07591000	H	-1.95892000	-1.98761700	3.21559400
C	-3.43919600	-2.86275100	-2.25857700	H	-0.57189300	-1.43694600	4.13971600
H	-1.31563600	-2.68544400	-2.54432600	N	-1.18855700	2.02185000	0.24621000
C	-4.32946600	-1.82891900	-0.28228700	C	-0.61761800	2.43463900	-0.87005700
H	-2.90613000	-0.84925100	0.99393900	C	-2.25885200	2.85954500	0.46291200
C	-4.53551200	-2.55927700	-1.45032800	H	0.25646400	1.99333300	-1.32395600
H	-3.57839900	-3.43387600	-3.17159800	C	-2.32408500	3.78464700	-0.54188700
H	-5.16731300	-1.58862400	0.36489400	H	-2.90186800	2.73988800	1.32034100
C	-1.63461500	0.18424600	3.11452300	H	-3.00616700	4.59759900	-0.73202100
H	-1.28502000	0.97073400	3.79738000	C	-0.92624400	4.21612500	-2.61198800
H	-2.67836300	0.44875000	2.89524200	H	-0.72346300	5.26656100	-2.39690500
C	-1.59161100	-1.16945300	3.84408000	H	-0.03273000	3.76846700	-3.04472900
H	-2.19932600	-1.17330000	4.75894900	H	-1.73993400	4.14578800	-3.33576700
H	-1.95892000	-1.98761700	3.21559400	N	-1.26858500	3.50342000	-1.38908100
H	-0.57189300	-1.43694600	4.13971600	15			
N	-1.18855700	2.02185000	0.24621000	C	1.31784000	0.07689600	0.81261300
C	-0.61761800	2.43463900	-0.87005700	C	2.18301700	-0.48910000	0.05209200
C	-2.25885200	2.85954500	0.46291200	Zn	-0.52734000	0.31914900	1.46495700
H	0.25646400	1.99333300	-1.32395600	C	3.64676000	-0.46928800	-0.11319800
C	-2.32408500	3.78464700	-0.54188700	C	4.44431800	0.23705100	0.80216200

C	4.26940900	-1.13928900	-1.17338000	H	-1.96311700	-1.98131200	3.21862500
C	5.82677700	0.27100000	0.65587200	H	-0.57091700	-1.43909300	4.13993300
H	3.97280400	0.75240400	1.63235300	N	-1.18834900	2.02272800	0.24848200
C	5.65491400	-1.10064200	-1.31613200	C	-0.61911100	2.43263300	-0.86990800
H	3.66312100	-1.69178700	-1.87910800	C	-2.25632900	2.86315100	0.46659800
C	6.43982900	-0.39773700	-0.40508800	H	0.25237400	1.98802800	-1.32551800
H	6.42819600	0.81798600	1.37508900	C	-2.32183500	3.78687600	-0.53934300
H	6.12077700	-1.62673500	-2.14348500	H	-2.89766000	2.74616100	1.32564600
H	7.51912200	-0.37231000	-0.51664400	H	-3.00260300	4.60102600	-0.72902800
C	-1.63461500	0.18424600	3.11452300	C	-0.92813700	4.21263200	-2.61333600
H	-1.28502000	0.97073400	3.79738000	H	-0.72300800	5.26294200	-2.39994300
H	-2.67836300	0.44875000	2.89524200	H	-0.03646900	3.76280300	-3.04759600
C	-1.59161100	-1.16945300	3.84408000	H	-1.74369600	4.14280800	-3.33503500
H	-2.19932600	-1.17330000	4.75894900	N	-1.26895300	3.50209600	-1.38863300
H	-1.95892000	-1.98761700	3.21559400	16			
H	-0.57189300	-1.43694600	4.13971600	N	0.34793000	-1.78644900	-1.13992800
N	-1.18855700	2.02185000	0.24621000	N	1.55473300	-1.55532000	-1.07301300
C	-0.61761800	2.43463900	-0.87005700	N	-0.58220800	-1.28330100	-0.40840600
C	-2.25885200	2.85954500	0.46291200	C	1.24266900	-0.01586900	0.71387100
H	0.25646400	1.99333300	-1.32395600	C	2.11774800	-0.59132400	-0.04812500
C	-2.32408500	3.78464700	-0.54188700	Zn	-0.51716900	0.35286900	1.49555200
H	-2.90186800	2.73988800	1.32034100	C	3.59397800	-0.50101400	-0.14076600
H	-3.00616700	4.59759900	-0.73202100	C	4.33405000	0.22730700	0.80374400
C	-0.92624400	4.21612500	-2.61198800	C	4.27773500	-1.14551600	-1.17982400
H	-0.72346300	5.26656100	-2.39690500	C	5.71989800	0.30736900	0.70659300
H	-0.03273000	3.76846700	-3.04472900	H	3.81889000	0.72304000	1.62008700
H	-1.73993400	4.14578800	-3.33576700	C	5.66502300	-1.06164900	-1.27333900
N	-1.26858500	3.50342000	-1.38908100	H	3.71458300	-1.71516800	-1.90697100
15a				C	6.39301400	-0.33670300	-0.33281600
N	0.32209900	-1.71244500	-1.06833400	H	6.27706600	0.87068700	1.44854500
N	1.52124600	-1.48265500	-1.01196600	H	6.17687700	-1.56950500	-2.08480700
N	-0.63813200	-1.24752800	-0.35101600	H	7.47428300	-0.27539600	-0.40468500
C	-1.93421100	-1.70352000	-0.73668300	C	-1.90023900	-1.70722800	-0.75899200
C	-2.15800700	-2.43893300	-1.91438200	C	-2.16495100	-2.43743100	-1.93251500
C	-3.02905000	-1.39687300	0.07968100	C	-2.97226800	-1.38426600	0.08102200
C	-3.44101300	-2.85400200	-2.25095800	C	-3.46118500	-2.83276400	-2.23932000
H	-1.31939900	-2.68486200	-2.55325400	H	-1.34506000	-2.69670100	-2.58958000
C	-4.31151900	-1.81591400	-0.26823300	C	-4.26942700	-1.78261500	-0.23765900
H	-2.87541400	-0.84199700	0.99695300	H	-2.79215200	-0.83467800	0.99680200
C	-4.52963900	-2.54634800	-1.43387500	C	-4.52620800	-2.50943700	-1.39742700
H	-3.58961600	-3.42496200	-3.16260800	H	-3.63885800	-3.40098300	-3.14753300
H	-5.14318500	-1.57213500	0.38559100	H	-5.08154800	-1.52634000	0.43569800
H	-5.52895500	-2.87407500	-1.70061000	C	-1.61381700	0.20473400	3.14582400
15b				H	-1.25401400	0.97960000	3.83645700
C	1.30095100	0.05255100	0.78929600	H	-2.65452200	0.48300400	2.93048200
C	2.16402500	-0.51863600	0.02410300	C	-1.58257500	-1.15839700	3.85794400
Zn	-0.52681100	0.32489400	1.47025200	H	-2.18756200	-1.16499900	4.77429600
C	3.63154500	-0.47960700	-0.12142900	H	-1.96131300	-1.96452800	3.22113600
C	4.41268700	0.23357400	0.80186500	H	-0.56511300	-1.44057300	4.14689600
C	4.27053500	-1.14322800	-1.17590400	N	-1.18857600	2.02586900	0.25888300
C	5.79618200	0.28068300	0.66886500	C	-0.62315100	2.42554300	-0.86570400
H	3.92861500	0.74372700	1.62813600	C	-2.25117200	2.87325900	0.47775800
C	5.65674700	-1.09167000	-1.30536000	H	0.24209700	1.97122900	-1.32348000
H	3.67570600	-1.70092000	-1.88721300	C	-2.31696000	3.79084500	-0.53342800
C	6.42580900	-0.38169400	-0.38632600	H	-2.88873300	2.76497400	1.34072300
H	6.38554000	0.83282000	1.39410800	H	-2.99449100	4.60734300	-0.72451000
H	6.13567000	-1.61296900	-2.12827900	C	-0.93173200	4.19812300	-2.61662800
H	7.50587100	-0.34589700	-0.48711400	H	-0.72019100	5.24824100	-2.40878800
C	-1.62939800	0.18926800	3.12174000	H	-0.04466200	3.74160400	-3.05321400
H	-1.27447000	0.97273100	3.80530600	H	-1.75141000	4.12914300	-3.33364500
H	-2.67234300	0.45892800	2.90533200	N	-1.27017100	3.49511100	-1.38664100
C	-1.59021700	-1.16634300	3.84786300	H	-5.53630400	-2.82210000	-1.64066300
H	-2.19535600	-1.16915100	4.76436100	16a			

N	0.34793000	-1.78644900	-1.13992800	H	6.17241700	0.89771600	1.49543400
N	1.55473300	-1.55532000	-1.07301300	H	6.19920400	-1.52966100	-2.04739800
N	-0.58220800	-1.28330100	-0.40840600	H	7.43567900	-0.21714700	-0.33221500
C	-1.90023900	-1.70722800	-0.75899200	C	-1.85749800	-1.70679200	-0.77726600
C	-2.16495100	-2.43743100	-1.93251500	C	-2.15976500	-2.43153300	-1.94726300
C	-2.97226800	-1.38426600	0.08102200	C	-2.91063700	-1.37239500	0.08213000
C	-3.46118500	-2.83276400	-2.23932000	C	-3.46621300	-2.81101700	-2.22890900
H	-1.34506000	-2.69670100	-2.58958000	H	-1.35739700	-2.70177400	-2.62044600
C	-4.26942700	-1.78261500	-0.23765900	C	-4.22033800	-1.75337000	-0.21250900
H	-2.79215200	-0.83467800	0.99680200	H	-2.71092200	-0.82969700	0.99820000
C	-4.52620800	-2.50943700	-1.39742700	C	-4.51097100	-2.47597500	-1.36653900
H	-3.63885800	-3.40098300	-3.14753300	H	-3.66705500	-3.37617900	-3.13421900
H	-5.08154800	-1.52634000	0.43569800	H	-5.01479600	-1.48731500	0.47793600
H	-5.53630400	-2.82210000	-1.64066300	C	-1.60199300	0.22173800	3.17419200
16b				H	-1.24237200	0.98666800	3.87564100
C	1.24266900	-0.01586900	0.71387100	H	-2.64083900	0.50557000	2.95792800
C	2.11774800	-0.59132400	-0.04812500	C	-1.57569800	-1.15144900	3.86713100
Zn	-0.51716900	0.35286900	1.49555200	H	-2.18290600	-1.16732900	4.78166200
C	3.59397800	-0.50101400	-0.14076600	H	-1.95574200	-1.94770300	3.21903000
C	4.33405000	0.22730700	0.80374400	H	-0.55988200	-1.44047300	4.15449900
C	4.27773500	-1.14551600	-1.17982400	N	-1.18933700	2.03206800	0.27125900
C	5.71989800	0.30736900	0.70659300	C	-0.62545700	2.42169500	-0.85835100
H	3.81889000	0.72304000	1.62008700	C	-2.24975300	2.88343600	0.48638600
C	5.66502300	-1.06164900	-1.27333900	H	0.23600100	1.95929200	-1.31510700
H	3.71458300	-1.71516800	-1.90697100	C	-2.31549000	3.79334400	-0.53131500
C	6.39301400	-0.33670300	-0.33281600	H	-2.88581600	2.78303000	1.35139000
H	6.27706600	0.87068700	1.44854500	H	-2.99162600	4.60990800	-0.72690800
H	6.17687700	-1.56950500	-2.08480700	C	-0.93330000	4.18464100	-2.61925000
H	7.47428300	-0.27539600	-0.40468500	H	-0.71750500	5.23486300	-2.41651500
C	-1.61381700	0.20473400	3.14582400	H	-0.04911800	3.72276800	-3.05594800
H	-1.25401400	0.97960000	3.83645700	H	-1.75526000	4.11523900	-3.33351900
H	-2.65452200	0.48300400	2.93048200	N	-1.27132000	3.48875500	-1.38476700
C	-1.58257500	-1.15839700	3.85794400	H	-5.52963300	-2.77592900	-1.58922900
H	-2.18756200	-1.16499900	4.77429600	17a			
H	-1.96131300	-1.96452800	3.22113600	N	0.37878600	-1.86569400	-1.21659600
H	-0.56511300	-1.44057300	4.14689600	N	1.59336700	-1.62987000	-1.13764800
N	-1.18857600	2.02586900	0.25888300	N	-0.51281200	-1.31866400	-0.46549100
C	-0.62315100	2.42554300	-0.86570400	C	-1.85749800	-1.70679200	-0.77726600
C	-2.25117200	2.87325900	0.47775800	C	-2.15976500	-2.43153300	-1.94726300
H	0.24209700	1.97122900	-1.32348000	C	-2.91063700	-1.37239500	0.08213000
C	-2.31696000	3.79084500	-0.53342800	C	-3.46621300	-2.81101700	-2.22890900
H	-2.88873300	2.76497400	1.34072300	H	-1.35739700	-2.70177400	-2.62044600
H	-2.99449100	4.60734300	-0.72451000	C	-4.22033800	-1.75337000	-0.21250900
C	-0.93173200	4.19812300	-2.61662800	H	-2.71092200	-0.82969700	0.99820000
H	-0.72019100	5.24824100	-2.40878800	C	-4.51097100	-2.47597500	-1.36653900
H	-0.04466200	3.74160400	-3.05321400	H	-3.66705500	-3.37617900	-3.13421900
H	-1.75141000	4.12914300	-3.33364500	H	-5.01479600	-1.48731500	0.47793600
N	-1.27017100	3.49511100	-1.38664100	H	-5.52963300	-2.77592900	-1.58922900
17				17b			
N	0.37878600	-1.86569400	-1.21659600	C	1.15103800	-0.10321700	0.62467700
N	1.59336700	-1.62987000	-1.13764800	C	2.06599900	-0.66554400	-0.11965200
N	-0.51281200	-1.31866400	-0.46549100	Zn	-0.50854400	0.38703400	1.52803400
C	1.15103800	-0.10321700	0.62467700	C	3.54919500	-0.51874300	-0.15647600
C	2.06599900	-0.66554400	-0.11965200	C	4.25570200	0.21985900	0.80543800
Zn	-0.50854400	0.38703400	1.52803400	C	4.27448600	-1.14380000	-1.18210900
C	3.54919500	-0.51874300	-0.15647600	C	5.64361800	0.32677500	0.73859700
C	4.25570200	0.21985900	0.80543800	H	3.71691100	0.70274200	1.61443600
C	4.27448600	-1.14380000	-1.18210900	C	5.66114100	-1.03403700	-1.24528000
C	5.64361800	0.32677500	0.73859700	H	3.74029100	-1.72243300	-1.92317900
H	3.71691100	0.70274200	1.61443600	C	6.35434700	-0.29949300	-0.28616800
C	5.66114100	-1.03403700	-1.24528000	H	6.17241700	0.89771600	1.49543400
H	3.74029100	-1.72243300	-1.92317900	H	6.19920400	-1.52966100	-2.04739800
C	6.35434700	-0.29949300	-0.28616800	H	7.43567900	-0.21714700	-0.33221500

C	-1.60199300	0.22173800	3.17419200	H	-0.05041400	3.71403500	-3.05666500
H	-1.24237200	0.98666800	3.87564100	H	-1.75615300	4.10871600	-3.33376000
H	-2.64083900	0.50557000	2.95792800	N	-1.27192700	3.48600900	-1.38390500
C	-1.57569800	-1.15144900	3.86713100	H	-5.51671000	-2.75253600	-1.56097700
H	-2.18290600	-1.16732900	4.78166200	18a			
H	-1.95574200	-1.94770300	3.21903000	N	0.40046700	-1.91439800	-1.26545900
H	-0.55988200	-1.44047300	4.15449900	N	1.62049500	-1.67403900	-1.17843900
N	-1.18933700	2.03206800	0.27125900	N	-0.45791200	-1.33297500	-0.49489000
C	-0.62545700	2.42169500	-0.85835100	C	-1.82550600	-1.69855900	-0.78042100
C	-2.24975300	2.88343600	0.48638600	C	-2.14755200	-2.42138300	-1.94911200
H	0.23600100	1.95929200	-1.31510700	C	-2.87168300	-1.36255100	0.08684600
C	-2.31549000	3.79334400	-0.53131500	C	-3.45830900	-2.79588600	-2.21942100
H	-2.88581600	2.78303000	1.35139000	H	-1.35497600	-2.69629400	-2.63098700
H	-2.99162600	4.60990800	-0.72690800	C	-4.18753600	-1.73714900	-0.19756400
C	-0.93330000	4.18464100	-2.61925000	H	-2.66704000	-0.82452800	1.00474200
H	-0.71750500	5.23486300	-2.41651500	C	-4.49447100	-2.45750700	-1.34830100
H	-0.04911800	3.72276800	-3.05594800	H	-3.66771100	-3.35953900	-3.12372000
H	-1.75526000	4.11523900	-3.33351900	H	-4.97300600	-1.46743600	0.50168600
N	-1.27132000	3.48875500	-1.38476700	H	-5.51671000	-2.75253600	-1.56097700
18				18b			
N	0.40046700	-1.91439800	-1.26545900	C	1.06499900	-0.17472700	0.55579100
N	1.62049500	-1.67403900	-1.17843900	C	2.03050000	-0.71227500	-0.16382400
N	-0.45791200	-1.33297500	-0.49489000	Zn	-0.50480200	0.40692100	1.54802300
C	1.06499900	-0.17472700	0.55579100	C	3.51757500	-0.52721300	-0.16334200
C	2.03050000	-0.71227500	-0.16382400	C	4.20919500	0.21551300	0.80647300
Zn	-0.50480200	0.40692100	1.54802300	C	4.26748500	-1.14109900	-1.18176400
C	3.51757500	-0.52721300	-0.16334200	C	5.59885300	0.33524700	0.75474600
C	4.20919500	0.21551300	0.80647300	H	3.66046900	0.69250500	1.61251800
C	4.26748500	-1.14109900	-1.18176400	C	5.65324700	-1.01938100	-1.22999100
C	5.59885300	0.33524700	0.75474600	H	3.74963400	-1.72399400	-1.93032900
H	3.66046900	0.69250500	1.61251800	C	6.32938700	-0.28117100	-0.26158200
C	5.65324700	-1.01938100	-1.22999100	H	6.11247700	0.90959300	1.51953200
H	3.74963400	-1.72399400	-1.93032900	H	6.20340800	-1.50891600	-2.02770400
C	6.32938700	-0.28117100	-0.26158200	H	7.41041800	-0.18837500	-0.29378100
H	6.11247700	0.90959300	1.51953200	C	-1.59701000	0.23231400	3.19126500
H	6.20340800	-1.50891600	-2.02770400	H	-1.23881500	0.99090700	3.90009800
H	7.41041800	-0.18837500	-0.29378100	H	-2.63491800	0.51885500	2.97429000
C	-1.82550600	-1.69855900	-0.78042100	C	-1.57284900	-1.14736300	3.87171500
C	-2.14755200	-2.42138300	-1.94911200	H	-2.18188300	-1.17007300	4.78474700
C	-2.87168300	-1.36255100	0.08684600	H	-1.95245200	-1.93773200	3.21629700
C	-3.45830900	-2.79588600	-2.21942100	H	-0.55791200	-1.43967800	4.15852200
H	-1.35497600	-2.69629400	-2.63098700	N	-1.19042000	2.03655000	0.27815900
C	-4.18753600	-1.73714900	-0.19756400	C	-0.62652200	2.42074700	-0.85380100
H	-2.66704000	-0.82452800	1.00474200	C	-2.25023800	2.88948200	0.49009100
C	-4.49447100	-2.45750700	-1.34830100	H	0.23340000	1.95411400	-1.30920300
H	-3.66771100	-3.35953900	-3.12372000	C	-2.31557600	3.79496200	-0.53130700
H	-4.97300600	-1.46743600	0.50168600	H	-2.88607300	2.79327400	1.35575000
C	-1.59701000	0.23231400	3.19126500	H	-2.99120000	4.61117900	-0.73008200
H	-1.23881500	0.99090700	3.90009800	C	-0.93346200	4.17842800	-2.62041300
H	-2.63491800	0.51885500	2.97429000	H	-0.71584700	5.22870400	-2.42002200
C	-1.57284900	-1.14736300	3.87171500	H	-0.05041400	3.71403500	-3.05666500
H	-2.18188300	-1.17007300	4.78474700	H	-1.75615300	4.10871600	-3.33376000
H	-1.95245200	-1.93773200	3.21629700	N	-1.27192700	3.48600900	-1.38390500
H	-0.55791200	-1.43967800	4.15852200	19			
N	-1.19042000	2.03655000	0.27815900	N	0.42429500	-1.95962700	-1.31241600
C	-0.62652200	2.42074700	-0.85380100	N	1.65024400	-1.71142600	-1.21453100
C	-2.25023800	2.88948200	0.49009100	N	-0.38756400	-1.33228800	-0.51075500
H	0.23340000	1.95411400	-1.30920300	C	0.94053100	-0.26913700	0.46732900
C	-2.31557600	3.79496200	-0.53130700	C	1.99154400	-0.75842400	-0.20732900
H	-2.88607300	2.79327400	1.35575000	Zn	-0.50224300	0.42314400	1.56549200
H	-2.99120000	4.61117900	-0.73008200	C	3.48403000	-0.53241100	-0.16675200
C	-0.93346200	4.17842800	-2.62041300	C	4.16872000	0.21227900	0.80752200
H	-0.71584700	5.22870400	-2.42002200	C	4.25782000	-1.13699100	-1.17936200

C	5.56106200	0.34073200	0.76659200	H	3.75437700	-1.72298800	-1.93434300
H	3.61580300	0.68642400	1.61268400	C	6.30736300	-0.26774100	-0.24230700
C	5.64268400	-1.00786400	-1.21726800	H	6.06287400	0.91738300	1.53758800
H	3.75437700	-1.72298800	-1.93434300	H	6.20032300	-1.49350000	-2.01231100
C	6.30736300	-0.26774100	-0.24230700	H	7.38805200	-0.16753600	-0.26381900
H	6.06287400	0.91738300	1.53758800	C	-1.59419900	0.24199200	3.20604100
H	6.20032300	-1.49350000	-2.01231100	H	-1.23886000	0.99472000	3.92234100
H	7.38805200	-0.16753600	-0.26381900	H	-2.63167000	0.53015700	2.98867600
C	-1.79023700	-1.68018600	-0.77253300	C	-1.57110000	-1.14378800	3.87500600
C	-2.12687600	-2.40444400	-1.94161800	H	-2.18181700	-1.17346400	4.78660600
C	-2.83663400	-1.34999200	0.09629500	H	-1.94954800	-1.92933500	3.21311400
C	-3.44067900	-2.77961200	-2.20674500	H	-0.55675900	-1.43837400	4.16135700
H	-1.34268400	-2.68230400	-2.63047200	N	-1.19222300	2.04122800	0.28383900
C	-4.15696800	-1.72351000	-0.18421000	C	-0.62756600	2.42067600	-0.84981300
H	-2.63649600	-0.81594900	1.01749700	C	-2.25158100	2.89514600	0.49239700
C	-4.47402500	-2.44216700	-1.33243400	H	0.23147600	1.95047100	-1.30338600
H	-3.65105300	-3.34251800	-3.11123800	C	-2.31615400	3.79686700	-0.53208900
H	-4.93636100	-1.45262100	0.52128700	H	-2.88746900	2.80243900	1.35842100
C	-1.59419900	0.24199200	3.20604100	H	-2.99125700	4.61276800	-0.73393300
H	-1.23886000	0.99472000	3.92234100	C	-0.93321700	4.17427100	-2.62127000
H	-2.63167000	0.53015700	2.98867600	H	-0.71437800	5.22457500	-2.42244000
C	-1.57110000	-1.14378800	3.87500600	H	-0.05082400	3.70812500	-3.05692000
H	-2.18181700	-1.17346400	4.78660600	H	-1.75621200	4.10439800	-3.33421500
H	-1.94954800	-1.92933500	3.21311400	N	-1.27245700	3.48437700	-1.38341900
H	-0.55675900	-1.43837400	4.16135700	20			
N	-1.19222300	2.04122800	0.28383900	N	0.44251000	-1.98844200	-1.34336200
C	-0.62756600	2.42067600	-0.84981300	N	1.67170200	-1.73271100	-1.23572200
C	-2.25158100	2.89514600	0.49239700	N	-0.32566200	-1.31804600	-0.50908400
H	0.23147600	1.95047100	-1.30338600	C	0.82055600	-0.35724800	0.38666300
C	-2.31615400	3.79686700	-0.53208900	C	1.96249600	-0.78819100	-0.23513500
H	-2.88746900	2.80243900	1.35842100	Zn	-0.50055100	0.43167000	1.57529500
H	-2.99125700	4.61276800	-0.73393300	C	3.45989000	-0.53387500	-0.16687000
C	-0.93321700	4.17427100	-2.62127000	C	4.14501900	0.21075900	0.80833500
H	-0.71437800	5.22457500	-2.42244000	C	4.25017500	-1.13321500	-1.17643100
H	-0.05082400	3.70812500	-3.05692000	C	5.53976800	0.34312400	0.77243200
H	-1.75621200	4.10439800	-3.33421500	H	3.59250000	0.68462400	1.61425400
N	-1.27245700	3.48437700	-1.38341900	C	5.63452300	-1.00157400	-1.20975800
H	-5.49789200	-2.73572700	-1.53938700	H	3.75623400	-1.72067000	-1.93579800
19a				C	6.29471500	-0.26091300	-0.23187200
N	0.42429500	-1.95962700	-1.31241600	H	6.03517700	0.92092100	1.54687100
N	1.65024400	-1.71142600	-1.21453100	H	6.19474800	-1.48578700	-2.00402500
N	-0.38756400	-1.33228800	-0.51075500	H	7.37522900	-0.15720500	-0.24793100
C	-1.79023700	-1.68018600	-0.77253300	C	-1.76408000	-1.66074400	-0.75962700
C	-2.12687600	-2.40444400	-1.94161800	C	-2.10702900	-2.38853600	-1.93027500
C	-2.83663400	-1.34999200	0.09629500	C	-2.81544300	-1.33972200	0.10593500
C	-3.44067900	-2.77961200	-2.20674500	C	-3.42287000	-2.76749700	-2.19605200
H	-1.34268400	-2.68230400	-2.63047200	H	-1.32788200	-2.66773400	-2.62304700
C	-4.15696800	-1.72351000	-0.18421000	C	-4.13792000	-1.71568300	-0.17600600
H	-2.63649600	-0.81594900	1.01749700	H	-2.62418600	-0.80774100	1.02995200
C	-4.47402500	-2.44216700	-1.33243400	C	-4.45810100	-2.43329200	-1.32319600
H	-3.65105300	-3.34251800	-3.11123800	H	-3.62913600	-3.33028000	-3.10149700
H	-4.93636100	-1.45262100	0.52128700	H	-4.91482400	-1.44529200	0.53232100
H	-5.49789200	-2.73572700	-1.53938700	C	-1.59289800	0.24863500	3.21521200
19b				H	-1.24161200	0.99721600	3.93768500
C	0.94053100	-0.26913700	0.46732900	H	-2.63042800	0.53705700	2.99722600
C	1.99154400	-0.75842400	-0.20732900	C	-1.57029500	-1.14147700	3.87648900
Zn	-0.50224300	0.42314400	1.56549200	H	-2.18210000	-1.17632000	4.78714500
C	3.48403000	-0.53241100	-0.16675200	H	-1.94762400	-1.92421200	3.21044400
C	4.16872000	0.21227900	0.80752200	H	-0.55625000	-1.43734400	4.16251300
C	4.25782000	-1.13699100	-1.17936200	N	-1.19377000	2.04487900	0.28727100
C	5.56106200	0.34073200	0.76659200	C	-0.62832800	2.42107400	-0.84731200
H	3.61580300	0.68642400	1.61268400	C	-2.25284600	2.89904400	0.49333900
C	5.64268400	-1.00786400	-1.21726800	H	0.23058300	1.94884500	-1.29930100

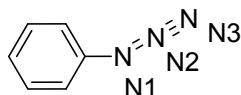
C	-2.31678600	3.79840800	-0.53306600	C	4.25017500	-1.13321500	-1.17643100
H	-2.88870800	2.80852200	1.35964700	C	5.53976800	0.34312400	0.77243200
H	-2.99150800	4.61411200	-0.73704200	H	3.59250000	0.68462400	1.61425400
C	-0.93290800	4.17237300	-2.62178600	C	5.63452300	-1.00157400	-1.20975800
H	-0.71344500	5.22267900	-2.42369300	H	3.75623400	-1.72067000	-1.93579800
H	-0.05074900	3.70536700	-3.05696300	C	6.29471500	-0.26091300	-0.23187200
H	-1.75591900	4.10251600	-3.33470500	H	6.03517700	0.92092100	1.54687100
N	-1.27282500	3.48381700	-1.38335000	H	6.19474800	-1.48578700	-2.00402500
H	-5.48197800	-2.72774300	-1.52911400	H	7.37522900	-0.15720500	-0.24793100
20a				C	-1.59289800	0.24863500	3.21521200
N	0.44251000	-1.98844200	-1.34336200	H	-1.24161200	0.99721600	3.93768500
N	1.67170200	-1.73271100	-1.23572200	H	-2.63042800	0.53705700	2.99722600
N	-0.32566200	-1.31804600	-0.50908400	C	-1.57029500	-1.14147700	3.87648900
C	-1.76408000	-1.66074400	-0.75962700	H	-2.18210000	-1.17632000	4.78714500
C	-2.10702900	-2.38853600	-1.93027500	H	-1.94762400	-1.92421200	3.21044400
C	-2.81544300	-1.33972200	0.10593500	H	-0.55625000	-1.43734400	4.16251300
C	-3.42287000	-2.76749700	-2.19605200	N	-1.19377000	2.04487900	0.28727100
H	-1.32788200	-2.66773400	-2.62304700	C	-0.62832800	2.42107400	-0.84731200
C	-4.13792000	-1.71568300	-0.17600600	C	-2.25284600	2.89904400	0.49333900
H	-2.62418600	-0.80774100	1.02995200	H	0.23058300	1.94884500	-1.29930100
C	-4.45810100	-2.43329200	-1.32319600	C	-2.31678600	3.79840800	-0.53306600
H	-3.62913600	-3.33028000	-3.10149700	H	-2.88870800	2.80852200	1.35964700
H	-4.91482400	-1.44529200	0.53232100	H	-2.99150800	4.61411200	-0.73704200
H	-5.48197800	-2.72774300	-1.52911400	C	-0.93290800	4.17237300	-2.62178600
20b				H	-0.71344500	5.22267900	-2.42369300
C	0.82055600	-0.35724800	0.38666300	H	-0.05074900	3.70536700	-3.05696300
C	1.96249600	-0.78819100	-0.23513500	H	-1.75591900	4.10251600	-3.33470500
Zn	-0.50055100	0.43167000	1.57529500	N	-1.27282500	3.48381700	-1.38335000
C	3.45989000	-0.53387500	-0.16687000				
C	4.14501900	0.21075900	0.80833500				

10. The orbital energies of the model complex

	LUMO		HOMO	
	Hartree	eV	Hartree	eV
2	-0.05226	-1.421472	-0.53388	-14.521536
7	0.08138	2.213536	-0.2346	-6.38112
15	0.05599	1.522928	-0.2096	-5.70112
22	0.06903	1.877616	-0.1885	-5.1272

11. The values of proportions which represent the weight of the atomic orbitals in the ground state molecular orbitals

11.1 The values for the proportions of 2 in the ground state molecular orbitals

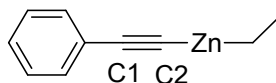


Eigenvalues	HOMO		LUMO	
	19	19 ²	32	33 ²
N1 1S	0.03466	0.001201	-0.01175	1.6E-09
2S	0.05572	0.003105	-0.01885	4.9E-09
2PX	-0.00183	3.35E-06	-0.00601	4E-10
2PY	0.09291	0.008632	-0.08453	2.25E-08
2PZ	-0.00024	5.76E-08	-0.00016	0.002718
3S	-0.16302	0.026576	0.04298	3.24E-08
3PX	-0.01065	0.000113	-0.00315	9E-10
3PY	0.13624	0.018561	-0.12256	4.84E-08
3PZ	-0.00038	1.44E-07	-0.00023	0.006371
4S	-0.19155	0.036691	0.12696	5.48E-07
4PX	0.0044	1.94E-05	-0.08361	1.6E-09
4PY	0.07484	0.005601	-0.17447	3.24E-08
4PZ	-0.00021	4.41E-08	-0.00031	0.011092
5S	1.31667	1.73362	1.67422	0.000247
5PX	0.20616	0.042502	0.40969	8.94E-06
5PY	0.21288	0.045318	0.23408	6.86E-06
5PZ	0.00027	7.29E-08	0.0001	0.004598
6D 0	-0.00369	1.36E-05	0.00757	1E-10
6D+1	-0.00004	1.6E-09	0.00003	0.000677
6D-1	-0.00003	9E-10	0.00002	2.96E-05
6D+2	-0.02469	0.00061	-0.02624	2.5E-09
6D-2	0.00404	1.63E-05	0.01019	9E-10
N2 1S	-0.02335	0.000545	-0.00053	4E-10
2S	-0.03785	0.001433	-0.00054	1.6E-09
2PX	-0.12307	0.015146	-0.12048	1E-08
2PY	0.14105	0.019895	0.17971	1.68E-07
2PZ	-0.00054	2.92E-07	0.00034	0.023688
3S	0.11352	0.012887	-0.00951	1.96E-08
3PX	-0.1835	0.033672	-0.18095	2.56E-08
3PY	0.21434	0.045942	0.28177	3.97E-07
3PZ	-0.00081	6.56E-07	0.00053	0.056084
4S	0.15862	0.02516	0.09102	2.25E-08
4PX	-0.1372	0.018824	-0.30775	1E-08
4PY	0.16313	0.026611	0.30228	7.92E-07
4PZ	-0.00057	3.25E-07	0.00063	0.09997

5S	-0.27848	0.077551	-0.42149	2.34E-05
5PX	0.70933	0.503149	0.65051	5.31E-05
5PY	0.46832	0.219324	0.79981	3.47E-05
5PZ	0.00065	4.23E-07	0.00125	0.045959
6D 0	-0.00109	1.19E-06	0.00517	1E-10
6D+1	0	0	-0.00003	0.000195
6D-1	0	0	-0.00004	8.76E-05
6D+2	-0.00341	1.16E-05	0.02145	1.6E-09
6D-2	0.00518	2.68E-05	-0.01796	1E-10
N3 1S	0.02169	0.00047	0.00392	1E-10
2S	0.03502	0.001226	0.00632	4E-10
2PX	-0.08013	0.006421	0.12233	1.21E-08
2PY	0.07967	0.006347	-0.17065	1.3E-07
2PZ	-0.00032	1.02E-07	-0.00033	0.020964
3S	-0.1038	0.010774	-0.02094	4.9E-09
3PX	-0.11615	0.013491	0.18338	2.56E-08
3PY	0.12524	0.015685	-0.25642	2.92E-07
3PZ	-0.00048	2.3E-07	-0.0005	0.046695
4S	-0.12216	0.014923	0.00343	1.69E-08
4PX	-0.05419	0.002937	0.22216	1.02E-07
4PY	0.06652	0.004425	-0.35514	4.76E-07
4PZ	-0.00025	6.25E-08	-0.00068	0.087515
5S	-1.05796	1.119279	-1.17766	0.000118
5PX	0.15065	0.022695	0.35955	3.42E-06
5PY	0.10727	0.011507	-0.14242	1.76E-07
5PZ	0.00001	1E-10	-0.00047	0.050968
6D 0	-0.00057	3.25E-07	0.00055	1E-10
6D+1	0.00007	4.9E-09	-0.00001	5.17E-05
6D-1	0.00003	9E-10	-0.00001	1.85E-05
6D+2	0.02523	0.000637	0.00994	4E-10
6D-2	-0.01018	0.000104	-0.00535	1E-10

* The data of 5 tracks is not used in the calculated for the proportion

11.2 The values for the proportions of 7 in the ground state molecular orbitals

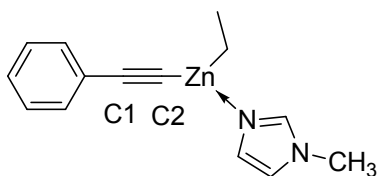


Eigenvalues	HOMO	LUMO
-------------	------	------

	45	45 ²	64	64 ²
C1 1S	0	0	0.00094	8.836E-07
2S	0	0	0.0019	0.00000361
2PX	0	0	-0.00796	6.3362E-05
2PY	0	0	-0.10714	0.01147898
2PZ	0.10652	0.011347	0	0
3S	0	0	-0.0101	0.00010201
3PX	0	0	-0.01953	0.00038142
3PY	0	0	-0.15742	0.02478106
3PZ	0.16061	0.025796	0.00001	1E-10
4S	-0.00002	4E-10	0.28245	0.079778
4PX	-0.00002	4E-10	0.26166	0.06846596
4PY	0	0	-0.40188	0.16150753
4PZ	0.13294	0.017673	0.00002	4E-10
5S	0	0	-2.89468	8.3791723
5PX	0	0	1.38596	1.92088512
5PY	0	0	-0.51203	0.26217472
5PZ	0.03565	0.001271	-0.00042	1.764E-07
6D 0	0	0	0.00352	1.239E-05
6D+1	0.03041	0.000925	0	0
6D-1	-0.00172	2.96E-06	0	0
6D+2	0	0	-0.00114	1.2996E-06
6D-2	0	0	0.03059	0.00093575
C2 1S	0	0	0.00391	1.5288E-05
2S	0	0	0.00674	4.5428E-05
2PX	0	0	0.00739	5.4612E-05
2PY	0	0	0.1282	0.01643524
2PZ	0.14701	0.021612	-0.00001	1E-10
3S	0	0	-0.03345	0.0011189
3PX	0	0	-0.00672	4.5158E-05
3PY	0	0	0.18942	0.03587994
3PZ	0.21689	0.047041	-0.00001	1E-10
4S	0.00003	9E-10	-0.04045	0.0016362
4PX	-0.00002	4E-10	0.45617	0.20809107
4PY	0	0	0.37946	0.14398989
4PZ	0.19898	0.039593	-0.00004	1.6E-09
5S	0	0	0.22022	0.04849685
5PX	-0.00001	1E-10	1.62321	2.6348107
5PY	0	0	-0.62989	0.39676141
5PZ	0.01908	0.000364	0.00049	2.401E-07
6D 0	0	0	0.00053	2.809E-07
6D+1	-0.00998	9.96E-05	0	0
6D-1	0.00058	3.36E-07	0	0
6D+2	0	0	0.00377	1.4213E-05
6D-2	0	0	0.01997	0.0003988

* The date of 5 tracks is not used in the calculated for the proportion

11.3 The values for the proportions of 15 in the ground state molecular orbitals

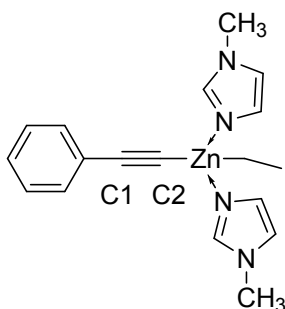


Eigenvalues	HOMO		LUMO	
	67	67 ²	84	84 ²
C1 1S	-0.00177	3.13E-06	0.00051	2.601E-07
2S	-0.00291	8.47E-06	0.00056	3.136E-07
2PX	-0.04062	0.00165	0.00681	4.6376E-05
2PY	-0.11066	0.012246	0.02344	0.00054943
2PZ	0.0242	0.000586	0.03453	0.00119232
3S	0.00782	6.12E-05	0.00497	2.4701E-05
3PX	-0.05985	0.003582	0.00706	4.9844E-05
3PY	-0.16563	0.027433	0.03472	0.00120548
3PZ	0.03641	0.001326	0.05129	0.00263066
4S	0.01539	0.000237	-0.08679	0.0075325
4PX	-0.04818	0.002321	0.00293	8.5849E-06
4PY	-0.15104	0.022813	0.08169	0.00667326
4PZ	0.03084	0.000951	0.0957	0.00915849
5S	-0.00197	3.88E-06	-1.24764	1.55660557
5PX	0.00787	6.19E-05	-0.97272	0.9461842
5PY	-0.1554	0.024149	-0.89662	0.80392742
5PZ	-0.02795	0.000781	-6.50635	42.3325903
6D 0	-0.0006	3.6E-07	0.00053	2.809E-07
6D+1	-0.00568	3.23E-05	0.01509	0.00022771
6D-1	0.00188	3.53E-06	-0.00502	2.52E-05
6D+2	0.01494	0.000223	0.00348	1.211E-05
6D-2	0.02065	0.000426	0.00324	1.0498E-05
C2 1S	0.00475	2.26E-05	-0.00217	4.7089E-06
2S	0.00765	5.85E-05	-0.00376	1.4138E-05
2PX	-0.03005	0.000903	-0.00831	6.9056E-05
2PY	-0.13596	0.018485	-0.02458	0.00060418
2PZ	0.03118	0.000972	-0.06645	0.0044156
3S	-0.02143	0.000459	0.01621	0.00026276
3PX	-0.04543	0.002064	-0.0143	0.00020449
3PY	-0.19898	0.039593	-0.03853	0.00148456
3PZ	0.04576	0.002094	-0.10688	0.01142333
4S	-0.04176	0.001744	-0.02313	0.000535
4PX	-0.03982	0.001586	-0.0157	0.00024649
4PY	-0.17778	0.031606	-0.0635	0.00403225
4PZ	0.04225	0.001785	-0.11317	0.01280745
5S	-0.08598	0.007393	-1.31479	1.72867274
5PX	0.15712	0.024687	1.29782	1.68433675
5PY	0.05506	0.003032	-0.01024	0.00010486
5PZ	0.02089	0.000436	3.15463	9.95169044
6D 0	0.00014	1.96E-08	0.00096	9.216E-07
6D+1	0.00252	6.35E-06	0.00833	6.9389E-05

6D-1	-0.00097	9.41E-07	-0.00252	6.3504E-06
6D+2	-0.0094	8.84E-05	0.00351	1.232E-05
6D-2	-0.01191	0.000142	0.00551	3.036E-05

* The date of 5 tracks is not used in the calculated for the proportion

11.4 The values for the proportions of 22 in the ground state molecular orbitals



Eigenvalues	HOMO		LUMO	
	89	89 ²	115	115 ²
C1 1S	0.00403	1.62E-05	-0.0037	1.37E-05
2S	0.00656	4.3E-05	-0.00602	3.62E-05
2PX	-0.02985	0.000891	0.00713	5.08E-05
2PY	-0.03658	0.001338	-0.05925	0.003511
2PZ	0.09068	0.008223	-0.03435	0.00118
3S	-0.0179	0.00032	0.0195	0.00038
3PX	-0.04214	0.001776	0.01606	0.000258
3PY	-0.05486	0.00301	-0.09057	0.008203
3PZ	0.13538	0.018328	-0.05602	0.003138
4S	-0.03482	0.001212	0.0305	0.00093
4PX	-0.01489	0.000222	-0.13084	0.017119
4PY	-0.0465	0.002162	-0.14987	0.022461
4PZ	0.1363	0.018578	-0.10119	0.010239
5S	-0.05373	0.002887	-0.3057	0.093452
5PX	0.07805	0.006092	0.71336	0.508882
5PY	-0.10299	0.010607	1.15193	1.326943
5PZ	0.04518	0.002041	-0.44515	0.198159
6D 0	0.00573	3.28E-05	0.00241	5.81E-06
6D+1	0.01385	0.000192	0.00992	9.84E-05
6D-1	-0.00114	1.3E-06	0.00447	2E-05
6D+2	-0.0035	1.23E-05	-0.00008	6.4E-09
6D-2	-0.00784	6.15E-05	0.01018	0.000104
C2 1S	-0.00929	8.63E-05	-0.00185	3.42E-06
2S	-0.01496	0.000224	-0.00295	8.7E-06

2PX	0.00513	2.63E-05	-0.01168	0.000136
2PY	-0.0428	0.001832	0.03855	0.001486
2PZ	0.09884	0.009769	0.04129	0.001705
3S	0.04269	0.001822	0.0103	0.000106
3PX	0.00543	2.95E-05	-0.01945	0.000378
3PY	-0.0625	0.003906	0.05773	0.003333
3PZ	0.14457	0.0209	0.06536	0.004272
4S	0.05059	0.002559	0.1307	0.017082
4PX	0.00232	5.38E-06	-0.07198	0.005181
4PY	-0.05807	0.003372	0.10723	0.011498
4PZ	0.12045	0.014508	0.08496	0.007218
5S	-0.0114	0.00013	0.76029	0.578041
5PX	-0.01674	0.00028	-0.92145	0.84907
5PY	0.06286	0.003951	0.06975	0.004865
5PZ	0.01861	0.000346	0.29263	0.085632
6D 0	-0.00596	3.55E-05	0.00315	9.92E-06
6D+1	-0.01353	0.000183	0.00875	7.66E-05
6D-1	0.0007	4.9E-07	0.0046	2.12E-05
6D+2	0.00259	6.71E-06	-0.00152	2.31E-06
6D-2	0.00474	2.25E-05	0.01156	0.000134

* The date of 5 tracks is not used in the calculated for the proportion