SUPPORTING INFORMATION FOR

"MODULAR AMINOALCOHOL LIGANDS CONTAINING BULKY ALKYL GROUPS AS CHIRAL CONTROLLERS FOR Et₂Zn ADDITION TO ALDEHYDES: ILLUSTRATION OF A DESIGN PRINCIPLE"

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Preparation Details

1-(Adamantyl)carbaldehyde. To a vigorously stirred mixture of 1-adamantylmethanol (4.5g, 27.1 mmol) and 2,2,5,5-tetramethylpiperidin-1-oxyl (TEMPO) (42 mg, 0.27 mmol) in CH₂Cl₂ (15 mL) and KBr (0.32 g, 2.71 mmol) in water (3 mL) cooled to -5°C were added 45 mL (29.8 mmol) of 0.67 M aqueous sodium hypochlorite. The mixture was stirred for 1h allowing to warm to room temperature. The organic phase was separated and the aqueous one extracted with CH₂Cl₂. The combined organic extracts were washed with 50 mL of 10% aqueous hydrochloric acid containing 0.8 g (0.005 mol) of potassium iodide, 50 mL of 10% aqueous sodium thiosulfate and 30 mL of water. The organic phase was dried over MgSO₄ and concentrated under reduced pressure affording 3.22 g (72% yield) of 1-(adamantyl)carbaldehyde as a white solid; mp: 137-139°C (lit.¹ mp: 139-141°C), ¹H-NMR (200 MHz, CDCl₃) δ 1.72 (m, 12H), 2.07 (m, 3H), 9.32 (s, 1H).

3-tert-Butyl ethyl acrylate, 7. Triethyl phosphonoacetate (39.2 mL, 0.197 mol) was added dropwise to a suspension of sodium hydride (9.2 g, ca.0.169 mol) in DME under N₂. The mixture was stirred for 15 min, and pivalaldehyde (15.5 mL, 0.141 mol) was added via syringe into the mixture. The reaction was left under stirring overnight. Water (200mL) was added and after 15 min of stirring the aqueous solution was extracted with ether (3x200 mL). The combined organic extracts were washed with water (200 mL), dried over MgSO₄, and concentrated carefully in vacuo (bath at 0 °C) until 1/4 of the original volume. The concentrated solution was rectified in vacuo affording 19.1 g (87% yield) of **7**,² bp 85°C/35 mmHg; ¹H-NMR (200 MHz, CDCl₃) δ 1.16 (s, 9H), 1.29

(1) Bott, K. *Angew. Chem. Int. Ed. Eng.* **1968**, 894.

(2) Marmor, R. S. *J. Org. Chem.* **1972**, 37, 2901.

(t, $J = 7$ Hz, 3H), 4.19 (q, $J = 7$ Hz, 2H), 5.73 (d, $J = 16$ Hz, 1H), 6.97 (d, $J = 16$ Hz, 1H).

3-(1-Adamantyl) ethyl acrilate, 8. The same procedure described above for the preparation of **7** was followed using the following amounts of reagents: NaH (1.0 g, ca. 23.4 mmol), triethyl phosphonoacetate (5.4 mL, 27.3 mmol) and 1-(adamantyl)carbaldehyde (3.2 g, 19.5 mmol) in DME (20mL). The workup was identical to the one described for **7** and after removal of the solvents in vacuo, 3.4 g (75% yield) of chemically pure **8**³ were obtained; ¹H-NMR (200 MHz, CDCl₃) δ 1.29 (t, $J = 7$ Hz, 3H), 1.63 (m, 12H), 2.01 (m, 3H), 4.18 (q, $J = 7$ Hz, 2H), 5.68 (d, $J = 16$ Hz, 1H), 6.82 (d, $J = 16$ Hz, 1H); ¹³C-NMR (50 MHz, CDCl₃) δ 14.3 (CH₃), 28.0 (CH), 35.6 (C), 36.6 (CH₂), 41.0 (CH₂), 60.1 (CH₂), 116.4 (CH), 158.6 (CH), 167.3 (C); IR (film) 2906, 2850, 1719, 1647, 1304, 1252, 1171, 1036 cm⁻¹; MS (CI, NH₃) m/z 252 (C₁₅H₂₂O₂+18, 77), 235 (C₁₅H₂₂O₂+1, 22).

(E)-3-tert-Butyl-2-propen-1-ol, 9. To a stirred solution of the stereochemically pure ester **7** (19.0 g, 0.122 mol) in anhydrous diethyl ether (20 mL) at -78 °C, under N₂, 1 M DIBALH in hexanes (268 mL, 0.268 mol) was added. After 3 hours of stirring at -78 °C methanol (200 mL) was carefully added and the mixture allowed to warm up. Precipitated aluminium oxide was separated by filtration and washed with ether (3x200 mL). This solution was washed with saturated brine (3x250 mL), dried over MgSO₄ and carefully concentrated in vacuo (bath at 0 °C) until 1/4 of its initial volume. The concentrated solution was rectified, obtaining 11.1 g (80% yield) of **9** bp 76-78 °C /

(3) Miryan, N.I.; Isaev, S.D.; Kovelava, S.A.; Petukh, N.V.; Dvornikova, E. V.; Kardakova, E.V.; Yurchenko, A.G. *Russ. J. Org. Chem.* **1999**, 35, 857-861.

25 mm Hg; ^1H -NMR (200 MHz, CDCl_3) δ 1.02 (s, 9H), 1.97 (b s, 1H), 4.10 (d, J = 6 Hz, 2H), 5.54 (dxt, J = 16 Hz, J' = 6 Hz, 1H), 5.73 (d, J = 16 Hz, 1H); ^{13}C -NMR (50 MHz, CDCl_3) δ 29.4 (CH_3), 32.7 (C), 63.9 (CH_2), 123.6 (CH), 143.9 (CH); IR (film) 3328, 2961, 1470, 1364, 1094, 1032, 974 cm^{-1} .

(E)-3-(1-Adamantyl)-2-propen-1-ol, 10. The same procedure described above for the preparation of **9** was followed, using the following amounts of reagents: ester **8** (2.0 g, 8.53 mmol) and DIBALH 1M in hexanes (19 mL, 18.78 mmol). The workup was identical to the one described for **9** and the crude was purified by flash chromatography using hexane:EtOAc (100:0-80:20) as eluent affording 1.4 g (88% yield) of **10**⁴ as an oil; ^1H -NMR (200 MHz, CDCl_3) δ 1.51-1.73 (m, 12H), 1.98 (m, 3H), 3.20 (b s, 1H), 4.10 (m, 2H), 5.52 (m, 2H). ^{13}C -NMR (50 MHz, CDCl_3) δ 28.3 (CH), 34.5 (C), 36.8 (CH_2), 42.1 (CH_2), 64.1 (CH_2), 123.7 (CH), 144.3 (CH); IR (film) 3330, 2904, 2848, 1451, 1017, 970 cm^{-1} ; MS (CI, NH_3) m/z 210 ($\text{C}_{13}\text{H}_{20}\text{O}+18$, 75), 192 ($\text{C}_{13}\text{H}_{20}\text{O}^+$, 100)

(2S,3S)-3-tert-Butyl-2,3-epoxypropan-1-ol, 5a. To a suspension of powdered, freshly activated 4 Å molecular sieves (3.8 g) in dry CH_2Cl_2 (500 mL), cooled at -20°C , under N_2 , were sequentially added via cannula L-(+)-diisopropyl tartrate (1.1 mL, 5.35 mmol), titanium tetrakisopropoxide (1.1 mL, 3.59 mmol) and a solution of tert-butyl hydroperoxide (TBHP) in isooctane (27 mL, 5.4 M, 145.8 mmol). The resulting mixture was stirred for 1 hour at -20°C , and a solution of (E)-3-tert-butyl-2-propen-1-ol (**9**) (8.2 g, 71.8 mmol) in anhydrous CH_2Cl_2 (20 mL) was added via cannula. The reaction mixture was stirred for 5 hours at -20°C and quenched adding an aqueous 10% NaOH

(4) Carlier, P.R.; Mungall, W.S.; Schröder, G.; Sharpless, K.B. *J. Am. Chem. Soc.* **1988**, *110*, 2978-2979.

solution in saturated brine (6 mL) and ether (75 mL). The mixture was allowed to warm to 10 °C, MgSO₄ (5.8 g) and Celite[®] (0.73 g) were added. After 15 min of stirring, it was filtered through a pad of Celite[®] and washed with ether (200 mL). The mother liquor was stirred with a solution of FeSO₄·7H₂O (24.6 g, 74.5 mmol) and tartaric acid (7.45 g, 74.5 mmol) in water (75 mL) for 15 min. Water (300 mL) was added, the layers were separated, and the aqueous one extracted with CH₂Cl₂ (3 x 200 mL). The combined organic extracts were then stirred for 1 hour with an aqueous 10% NaOH solution in saturated brine (200 mL). After this time, the organic phase was separated, and the aqueous layer extracted with CH₂Cl₂ (2 x 80 mL). The combined organic phases were dried (Na₂SO₄) and evaporated to an oil, which was purified by distillation at reduced pressure (water pump, 90-94 °C) to afford 8.4 g (90% yield) of epoxy alcohol **5a**. The enantiomeric purity of the product was determined to be of 96% by differential scanning calorimetry of the trityl derivative; [α]_D = -23.2 (c=1.30, CHCl₃), (lit.⁵: [α]_D=-20, c=1.7, CHCl₃); ¹H-NMR (200 MHz, CDCl₃) δ 0.92 (s, 9H), 1.81 (b s, 1H), 2.12 (d, J = 3 Hz, 1H), 2.40 (m, 1H), 2.94 (b d, J = 14 Hz, 1H), 3.28 (b d, J = 14 Hz, 1H); ¹³C-NMR (50 MHz, CDCl₃) δ 25.7 (CH₃), 30.4 (C), 55.5 (CH), 62.1 (CH₂), 63.6 (CH); IR (film) 3423, 2960, 1654, 1559, 1484, 1366, 1210 cm⁻¹.

(5) Roush, W. R.; Ando, K.; Powers, D. B.; Palkowitz, A. D.; Halterman, R.L.; *J. Amer. Chem. Soc.* **1990**, *112*, 6339.

General Procedure for the Enantioselective Amino Alcohol-Catalyzed Addition of Diethylzinc to Aldehydes. To a solution of chiral catalyst (0.05 mmol, 5mol%) in toluene (1.5 mL) was added diethylzinc (2 mL of a 1M hexanes solution, 2 mmol) via syringe. The mixture was cooled to 0°C and stirred for 15 min. Aldehyde (1 mmol) was added and the mixture stirred for 5h at 0°C. The reaction was quenched by the addition of a saturated NH₄Cl solution (10mL). The mixture was then extracted with CH₂Cl₂ (3x10mL). The combined organic extracts were dried and concentrated *in vacuo*. The enantiomeric excesses were determined from the crude mixture by GC analyses. Conditions of GC analyses have been reported elsewhere⁶.

Calculation Details

Calculations were performed at the PM3 level using PC Spartan Pro. All the transition states found had only one negative frequency (one negative eigenvalue). The Cartesian coordinates and energies for every TS that appear on the article are listed below:

Anti S TS for ligand 11b (14);

Heat of Formation: -25.757 kcal/mol

		Cartesian Coordinates (Angstroms)		
Atom		X	Y	Z
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1	Zn Zn1	0.0787212	-0.1703322	0.6821204
2	C C1	1.5119074	-1.6059194	0.7448557
3	H H6	1.0700173	-2.5694504	0.4472234
4	H H7	1.8679605	-1.7091334	1.7825881
5	N N1	0.6339265	1.6214944	1.7568619
6	O O1	-1.7089578	-0.2184833	1.8633735
7	C C2	-1.7112805	1.0657948	2.4632091
8	H H3	-1.9589953	1.8522820	1.6786771

⁶ Puigjaner, C.; Vidal-Ferran, A.; Moyano, A.; Pericàs,

M.A., Riera, A. *J. Org. Chem.* **1999**, *64*, 7902-7911

9	C	C3	-0.2681972	1.4492959	2.9924031
10	H	H11	-0.3819905	2.4388440	3.5275949
11	O	O2	-0.8644613	0.0025904	-1.2485047
12	Zn	Zn2	-2.9378263	-0.0174852	0.1361060
13	C	C4	-3.9293638	1.6370895	-0.5098479
14	H	H10	-3.2492257	2.1207535	-1.2301843
15	H	H14	-4.0854152	2.3262021	0.3392083
16	C	C5	-3.3584225	-1.7410067	-1.1976822
17	H	H19	-3.0929417	-2.5799324	-1.8564377
18	C	C6	-1.2565470	-1.2162298	-1.5167709
19	H	H18	-0.9733194	-2.0279555	-0.8034028
20	C	C7	2.5859234	-1.1438784	-0.1935459
21	H	H12	3.4579090	-1.8141064	-0.2089354
22	H	H17	2.9568786	-0.1398186	0.0871919
23	H	H21	2.2163811	-1.0715532	-1.2266201
24	C	C9	-5.2119144	1.1834111	-1.1322998
25	H	H16	-5.9163790	0.8093209	-0.3754922
26	H	H24	-5.0364627	0.3569665	-1.8458596
27	H	H25	-5.7246722	1.9859738	-1.6821134
28	C	C10	2.1170930	1.5555520	1.9994100
29	H	H4	2.5882830	1.3060957	1.0145024
30	H	H26	2.3312001	0.6786552	2.6550978
31	C	C11	0.2980723	2.8543698	0.9591354
32	H	H9	0.6925150	2.6867904	-0.0666114
33	H	H29	-0.8115699	2.9219685	0.8636185
34	C	C12	2.7090686	2.8306518	2.5904390
35	H	H5	3.8074504	2.7153016	2.6666688
36	H	H30	2.3494265	2.9769336	3.6299200
37	C	C13	0.8632200	4.1465294	1.5427024
38	H	H32	0.3659108	4.3914143	2.5040283
39	H	H33	0.6230333	4.9854818	0.8612653
40	C	C14	2.3662197	4.0446166	1.7430972
41	H	H28	2.8775724	3.9824260	0.7614670
42	H	H34	2.7495006	4.9650231	2.2237469
43	C	C15	-1.2614906	-1.5978842	-2.9713108
44	C	C16	-1.1757897	-2.3815119	-5.6530151
45	C	C17	-1.4885457	-0.6659461	-3.9866952
46	C	C18	-0.9931599	-2.9292462	-3.3138027
47	C	C19	-0.9485563	-3.3159899	-4.6467303
48	C	C20	-1.4458726	-1.0593843	-5.3208525
49	H	H27	-1.6995387	0.3802175	-3.7336368
50	H	H31	-0.8152411	-3.6729424	-2.5271365
51	H	H35	-0.7345110	-4.3580628	-4.9058134
52	H	H36	-1.6257996	-0.3223436	-6.1104661
53	H	H37	-1.1415912	-2.6884180	-6.7034246
54	H	H2	-4.0543514	-1.1069956	-1.7934892
55	C	C8	-3.9964874	-2.3165639	0.0510639
56	H	H20	-3.2774239	-2.9108748	0.6337044
57	H	H22	-4.8396937	-2.9814751	-0.1929631
58	H	H23	-4.4338138	-1.5540228	0.7502070
59	C	C21	-2.8608715	1.1992500	3.5344645

60	C	C22	-2.8176928	0.1834014	4.6731376
61	H	H13	-1.9048686	0.2809419	5.2812239
62	H	H40	-2.8567127	-0.8481762	4.2981042
63	H	H41	-3.6732303	0.3174854	5.3500729
64	C	C23	-2.8202803	2.6103327	4.1275985
65	H	H8	-1.8205749	2.8442487	4.5293898
66	H	H42	-3.5449446	2.7220705	4.9444178
67	H	H43	-3.0557851	3.3747900	3.3744992
68	C	C24	-4.1910645	1.0107169	2.7923720
69	H	H39	-4.2705573	0.0054127	2.3356929
70	H	H44	-4.3203919	1.7513733	1.9808963
71	H	H45	-5.0444189	1.1197766	3.4762347
72	C	C25	0.3116672	0.4185944	3.9813959
73	H	H46	1.0632893	-0.2544841	3.5049576
74	H	H47	-0.4897818	-0.2290738	4.3958279
75	O	O3	0.9391106	1.1520560	5.0372078
76	C	C26	1.2313050	0.3715468	6.1656130
77	H	H38	0.3221992	-0.0262503	6.6339714
78	H	H48	1.7206743	1.0798342	6.8385360
79	H	H49	1.9109741	-0.4557258	5.9298460

Point Group = C1 Order = 1 Nsymop = 1

Anti S TS for ligand 11c, rotamer 1 (15a);

Heat of Formation: 1.967 kcal/mol

Cartesian Coordinates (Angstroms)

	Atom	X	Y	Z

1	Zn Zn1	-0.0235199	0.5070656	0.2115333
2	C C1	1.3811101	0.4780376	1.6752673
3	H H6	0.9228114	0.0958130	2.6004932
4	H H7	1.7173192	1.5100872	1.8695795
5	N N1	0.5729070	1.8065727	-1.4273405
6	O O1	-1.8144282	1.6569092	0.3114764
7	C C2	-1.8024263	2.4012450	-0.8928414
8	H H3	-2.0064658	1.7093647	-1.7748386
9	C C3	-0.3676187	3.0013152	-1.1811723
10	H H11	-0.4727984	3.6139666	-2.1262972
11	O O2	-0.9792676	-1.4143812	-0.0579842
12	Zn Zn2	-3.0292104	-0.0288942	-0.1678440
13	C C4	-3.8781949	-0.5413508	-1.9439892
14	H H10	-3.1230361	-1.1514379	-2.4656604
15	H H14	-4.0551557	0.3769138	-2.5325114
16	C C5	-3.6068206	-1.4036014	1.4659475
17	H H19	-3.4312081	-2.0964343	2.3008114
18	C C6	-1.4671484	-1.6909689	1.1268954
19	H H18	-1.2533766	-0.9793223	1.9614268
20	C C7	2.4801897	-0.4031172	1.1627681
21	H H12	3.3294366	-0.4763163	1.8579498

22	H	H17	2.8815078	-0.0235505	0.2040675
23	H	H21	2.1243866	-1.4271350	0.9787629
24	C	C9	-5.1372742	-1.2941035	-1.6497014
25	H	H16	-5.9330049	-0.6256153	-1.2910487
26	H	H24	-4.9737626	-2.0507953	-0.8597717
27	H	H25	-5.5321637	-1.8214753	-2.5301594
28	C	C10	2.0463507	2.0773333	-1.2892819
29	H	H4	2.5333184	1.0856489	-1.1069169
30	H	H26	2.2254699	2.6674780	-0.3528145
31	C	C11	0.3006099	1.1103575	-2.7356614
32	H	H9	0.7182493	0.0840516	-2.6408469
33	H	H29	-0.8032446	0.9924521	-2.8500707
34	C	C12	2.6649320	2.7870425	-2.4891553
35	H	H5	3.7566185	2.8780043	-2.3286315
36	H	H30	2.2845719	3.8272213	-2.5590741
37	C	C13	0.8917735	1.8151524	-3.9534195
38	H	H32	0.3784886	2.7825234	-4.1324182
39	H	H33	0.6965134	1.2031693	-4.8552084
40	C	C14	2.3849034	2.0397348	-3.7820716
41	H	H28	2.9188437	1.0682240	-3.7858169
42	H	H34	2.7862594	2.6064853	-4.6439244
43	C	C15	-1.4837045	-3.1469637	1.5036861
44	C	C16	-1.4293087	-5.8300829	2.2861354
45	C	C17	-1.6090595	-4.1624615	0.5527839
46	C	C18	-1.3324791	-3.4903621	2.8531727
47	C	C19	-1.3034262	-4.8238271	3.2395574
48	C	C20	-1.5823195	-5.4972110	0.9455970
49	H	H27	-1.7261464	-3.9093095	-0.5079143
50	H	H31	-1.2344914	-2.7038606	3.6116767
51	H	H35	-1.1812499	-5.0833416	4.2962307
52	H	H36	-1.6817177	-6.2867797	0.1934140
53	H	H37	-1.4073606	-6.8809417	2.5925816
54	H	H2	-4.2406038	-1.9694474	0.7436532
55	C	C8	-4.2873430	-0.1662116	2.0225844
56	H	H20	-3.6584650	0.3300559	2.7754066
57	H	H22	-5.2417878	-0.4150312	2.5109267
58	H	H23	-4.5547938	0.6252484	1.2613290
59	C	C21	-2.9930617	3.4340288	-0.9232900
60	C	C22	-3.0105493	4.4523214	0.2138199
61	H	H13	-2.1317319	5.1151483	0.1894385
62	H	H40	-3.0295642	3.9631424	1.1969693
63	H	H41	-3.9006081	5.0943021	0.1508444
64	C	C23	-2.9539739	4.1825613	-2.2584358
65	H	H8	-1.9550529	4.6126759	-2.4406902
66	H	H42	-3.6831951	5.0025221	-2.2810556
67	H	H43	-3.1816582	3.5191881	-3.1040717
68	C	C24	-4.2943154	2.6200449	-0.8397637
69	H	H39	-4.3802746	2.0475046	0.1117517
70	H	H44	-4.3812466	1.8945438	-1.6720254
71	H	H45	-5.1729766	3.2786396	-0.8889548
72	C	C25	0.1546633	3.9206770	-0.0600946

73	H	H46	0.9042357	3.4136812	0.5975304
74	H	H47	-0.6728383	4.2661595	0.5947334
75	O	O3	0.7705744	5.0450040	-0.6958742
76	C	C26	1.0699187	6.1229846	0.1622267
77	C	C39	2.3957639	6.0485482	0.8690295
78	C	C40	4.8378399	6.0519910	2.2264780
79	C	C41	3.0464869	4.8490201	1.1510056
80	C	C42	2.9801267	7.2530357	1.2722134
81	C	C43	4.1932108	7.2535433	1.9483219
82	C	C44	4.2628940	4.8518823	1.8260597
83	H	H48	2.5967990	3.8882507	0.8400307
84	H	H58	2.4781659	8.2024364	1.0531282
85	H	H59	4.6429484	8.2013260	2.2617549
86	H	H60	4.7650098	3.9033902	2.0439724
87	H	H61	5.7942305	6.0527530	2.7591500
88	H	H66	1.0605198	6.9687539	-0.5503660
89	H	H69	0.2633926	6.2893381	0.9054902

Point Group = C1 Order = 1 Nsymop = 1

Anti S TS for ligand 11c, rotamer 2 (15b);

Heat of Formation: 2.189 kcal/mol

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
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1	Zn	Zn1	0.0271811	0.4880938	0.1458792
2	C	C1	1.4455966	0.4661311	1.5952573
3	H	H6	0.9929966	0.0955167	2.5281628
4	H	H7	1.7852250	1.4988928	1.7758565
5	N	N1	0.5858486	1.7474078	-1.5354087
6	O	O1	-1.7582880	1.6359883	0.2528501
7	C	C2	-1.7709136	2.3664605	-0.9598454
8	H	H3	-1.9981435	1.6656933	-1.8296025
9	C	C3	-0.3419326	2.9542883	-1.2976342
10	H	H11	-0.4711136	3.5416796	-2.2556365
11	O	O2	-0.9359045	-1.4401866	-0.0841631
12	Zn	Zn2	-2.9840651	-0.0546334	-0.1869121
13	C	C4	-3.8584565	-0.5874366	-1.9447382
14	H	H10	-3.1105584	-1.2034762	-2.4698919
15	H	H14	-4.0439413	0.3238508	-2.5414409
16	C	C5	-3.5417749	-1.4081561	1.4722784
17	H	H19	-3.3569664	-2.0903358	2.3138955
18	C	C6	-1.4072363	-1.6989525	1.1110490
19	H	H18	-1.1831542	-0.9744885	1.9316982
20	C	C7	2.5378125	-0.4246434	1.0850833
21	H	H12	3.3953467	-0.4862084	1.7711557
22	H	H17	2.9276911	-0.0625332	0.1150683
23	H	H21	2.1792952	-1.4514436	0.9234605
24	C	C9	-5.1130720	-1.3368474	-1.6241253

25	H	H16	-5.9039784	-0.6643002	-1.2624132
26	H	H24	-4.9383903	-2.0840790	-0.8276137
27	H	H25	-5.5199868	-1.8746997	-2.4926975
28	C	C10	2.0630711	2.0009737	-1.4143934
29	H	H4	2.5397053	1.0066816	-1.2164758
30	H	H26	2.2435154	2.6010774	-0.4914777
31	C	C11	0.2891696	1.0335703	-2.8283227
32	H	H9	0.6897297	0.0018613	-2.7202055
33	H	H29	-0.8178086	0.9336465	-2.9295843
34	C	C12	2.6847425	2.6764072	-2.6324724
35	H	H5	3.7792402	2.7492998	-2.4827321
36	H	H30	2.3237014	3.7217325	-2.7217763
37	C	C13	0.8814696	1.7077145	-4.0627795
38	H	H32	0.3834830	2.6807571	-4.2535680
39	H	H33	0.6677435	1.0843008	-4.9524628
40	C	C14	2.3798390	1.9091092	-3.9082223
41	H	H28	2.8964717	0.9283282	-3.8974977
42	H	H34	2.7835040	2.4516670	-4.7844545
43	C	C15	-1.4171302	-3.1491099	1.5107309
44	C	C16	-1.3498635	-5.8197307	2.3339510
45	C	C17	-1.5535582	-4.1793576	0.5774121
46	C	C18	-1.2481702	-3.4714024	2.8632766
47	C	C19	-1.2127913	-4.7986892	3.2699275
48	C	C20	-1.5203784	-5.5078297	0.9904839
49	H	H27	-1.6844346	-3.9427176	-0.4854768
50	H	H31	-1.1412469	-2.6730878	3.6081010
51	H	H35	-1.0767947	-5.0416477	4.3288350
52	H	H36	-1.6285653	-6.3090608	0.2519873
53	H	H37	-1.3229047	-6.8656737	2.6563517
54	H	H2	-4.1845552	-1.9826293	0.7649341
55	C	C8	-4.2142787	-0.1627759	2.0206794
56	H	H20	-3.5749088	0.3439084	2.7575706
57	H	H22	-5.1619567	-0.4041169	2.5256752
58	H	H23	-4.4921297	0.6177646	1.2518666
59	C	C21	-2.9589536	3.4021341	-0.9682740
60	C	C22	-2.9623109	4.4063319	0.1811423
61	H	H13	-2.1142309	5.1090519	0.1193626
62	H	H40	-2.9133337	3.9084834	1.1584915
63	H	H41	-3.8796884	5.0120586	0.1684807
64	C	C23	-2.9330169	4.1685450	-2.2930423
65	H	H8	-1.9411133	4.6190497	-2.4680442
66	H	H42	-3.6756787	4.9766455	-2.3027008
67	H	H43	-3.1498033	3.5132878	-3.1475858
68	C	C24	-4.2596356	2.5876570	-0.8795088
69	H	H39	-4.3395408	2.0161890	0.0733075
70	H	H44	-4.3506100	1.8614066	-1.7104819
71	H	H45	-5.1392263	3.2453405	-0.9243530
72	C	C25	0.2155230	3.9068419	-0.2223014
73	H	H46	0.9342440	3.3955068	0.4609390
74	H	H47	-0.5966396	4.3301300	0.4041863
75	O	O3	0.8799817	4.9686775	-0.9137033

76	C	C26	1.3293423	6.0161193	-0.0830235
77	C	C27	0.2495449	6.9382464	0.4105064
78	C	C28	-1.6754931	8.7361286	1.3292487
79	C	C29	0.3639657	7.5017013	1.6824498
80	C	C30	-0.8364800	7.2772147	-0.3970592
81	C	C31	-1.7956952	8.1727378	0.0634856
82	C	C32	-0.5951472	8.3989094	2.1379368
83	H	H15	1.2121701	7.2379508	2.3248514
84	H	H50	-0.9357742	6.8302278	-1.3945140
85	H	H51	-2.6469693	8.4336668	-0.5738402
86	H	H52	-0.4996595	8.8392241	3.1358700
87	H	H53	-2.4303841	9.4426481	1.6892231
88	H	H62	1.9289268	5.6168775	0.7592734
89	H	H73	2.0088503	6.5576724	-0.7658839

Point Group = C1 Order = 1 Nsymop = 1

Anti S TS for ligand 11c, rotamer 3 (15c) ;

Heat of Formation: 2.500 kcal/mol

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
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1	Zn	Zn1	-0.0106719	0.5847693	0.0813666
2	C	C1	1.4583066	0.6176615	1.4803993
3	H	H6	1.0399569	0.2732787	2.4390840
4	H	H7	1.7998369	1.6560705	1.6196004
5	N	N1	0.4791287	1.8016002	-1.6574534
6	O	O1	-1.8037143	1.7195223	0.2229382
7	C	C2	-1.8650960	2.4045606	-1.0146812
8	H	H3	-2.1065793	1.6688269	-1.8511666
9	C	C3	-0.4554967	3.0017470	-1.4102921
10	H	H11	-0.6232659	3.5694444	-2.3748096
11	O	O2	-0.9592690	-1.3561277	-0.0578665
12	Zn	Zn2	-3.0273039	0.0031936	-0.1124734
13	C	C4	-3.9665457	-0.5997668	-1.8133058
14	H	H10	-3.2358448	-1.2309089	-2.3446114
15	H	H14	-4.1817457	0.2878949	-2.4350609
16	C	C5	-3.4983723	-1.3027344	1.6102179
17	H	H19	-3.2689429	-1.9563775	2.4634467
18	C	C6	-1.3792608	-1.5890933	1.1618250
19	H	H18	-1.1261517	-0.8435714	1.9546457
20	C	C7	2.5364043	-0.2842244	0.9596018
21	H	H12	3.4172487	-0.3223901	1.6172121
22	H	H17	2.8910210	0.0501005	-0.0336433
23	H	H21	2.1769834	-1.3165887	0.8409263
24	C	C9	-5.2023136	-1.3433977	-1.4154050
25	H	H16	-5.9816506	-0.6623154	-1.0446388
26	H	H24	-4.9903819	-2.0618303	-0.6016439
27	H	H25	-5.6413929	-1.9128540	-2.2473929

28	C	C10	1.9576652	2.0675251	-1.5807472
29	H	H4	2.4441940	1.0785416	-1.3794195
30	H	H26	2.1608428	2.6831694	-0.6723390
31	C	C11	0.1525938	1.0746704	-2.9349936
32	H	H9	0.5694375	0.0490960	-2.8345895
33	H	H29	-0.9555021	0.9607481	-3.0015738
34	C	C12	2.5515170	2.7272229	-2.8209562
35	H	H5	3.6517108	2.7802843	-2.7032541
36	H	H30	2.2149631	3.7878496	-2.9007326
37	C	C13	0.6983898	1.7524568	-4.1886932
38	H	H32	0.1883978	2.7225351	-4.3627323
39	H	H33	0.4586597	1.1277015	-5.0708100
40	C	C14	2.1998350	1.9619058	-4.0853731
41	H	H28	2.7204321	0.9830926	-4.0949327
42	H	H34	2.5698517	2.5074826	-4.9745694
43	C	C15	-1.3615283	-3.0291835	1.5956343
44	C	C16	-1.2390511	-5.6788232	2.4781280
45	C	C17	-1.5308926	-4.0823400	0.6937958
46	C	C18	-1.1316311	-3.3178926	2.9468004
47	C	C19	-1.0688875	-4.6347978	3.3828115
48	C	C20	-1.4701006	-5.4002945	1.1363762
49	H	H27	-1.7097025	-3.8720780	-0.3676676
50	H	H31	-0.9982790	-2.5013342	3.6671879
51	H	H35	-0.8852306	-4.8514599	4.4402380
52	H	H36	-1.6045124	-6.2196631	0.4224845
53	H	H37	-1.1904915	-6.7165568	2.8237267
54	H	H2	-4.1662328	-1.9047921	0.9507236
55	C	C8	-4.1587346	-0.0468420	2.1494334
56	H	H20	-3.4935154	0.4871154	2.8428896
57	H	H22	-5.0816967	-0.2807410	2.7015168
58	H	H23	-4.4764212	0.7079428	1.3704290
59	C	C21	-3.0673008	3.4237414	-1.0296319
60	C	C22	-3.0307675	4.4978853	0.0540975
61	H	H13	-2.1689326	5.1724411	-0.0630402
62	H	H40	-2.9761745	4.0595260	1.0595048
63	H	H41	-3.9353630	5.1213825	0.0179077
64	C	C23	-3.1116851	4.1048499	-2.4002831
65	H	H8	-2.1302238	4.5362779	-2.6585952
66	H	H42	-3.8517285	4.9150780	-2.4221377
67	H	H43	-3.3769369	3.3979153	-3.1983205
68	C	C24	-4.3525978	2.6040771	-0.8325203
69	H	H39	-4.3788459	2.0783613	0.1490909
70	H	H44	-4.4786983	1.8384545	-1.6227898
71	H	H45	-5.2397762	3.2523589	-0.8633817
72	C	C25	0.1272383	3.9768492	-0.3687211
73	H	H46	0.8784403	3.4813540	0.2927189
74	H	H47	-0.6636443	4.3939990	0.2880394
75	O	O3	0.7063391	5.0530139	-1.1043236
76	C	C26	1.5021607	5.9179760	-0.3076694
77	C	C33	2.1790814	6.8954188	-1.2244792
78	C	C34	3.4836872	8.7276802	-2.8724128

79	C	C35	2.1907057	8.2513002	-0.8946990
80	C	C36	2.8200409	6.4621086	-2.3859753
81	C	C37	3.4679732	7.3777620	-3.2070840
82	C	C38	2.8447898	9.1626413	-1.7161050
83	H	H38	1.6834733	8.6005231	0.0120580
84	H	H54	2.8015654	5.3934369	-2.6556598
85	H	H55	3.9672617	7.0341367	-4.1188219
86	H	H56	2.8539290	10.2252507	-1.4523434
87	H	H57	3.9966507	9.4470053	-3.5189170
88	H	H62	2.2658950	5.3413373	0.2539364
89	H	H69	0.8573632	6.4294424	0.4343069

Point Group = C1 Order = 1 Nsymop = 1

Anti S TS for ligand 11d (16) ;

Heat of Formation: 69.819 kcal/mol

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
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1	Zn	Zn1	0.0359696	0.5089058	0.1403812
2	C	C1	1.4830012	0.4823266	1.5630262
3	H	H6	1.0402317	0.1362048	2.5099080
4	H	H7	1.8422791	1.5133138	1.7187853
5	N	N1	0.5872100	1.7949941	-1.5300589
6	O	O1	-1.7168307	1.6935095	0.2981546
7	C	C2	-1.7489655	2.4316413	-0.9094925
8	H	H3	-1.9978588	1.7357573	-1.7774254
9	C	C3	-0.3239960	3.0133348	-1.2815766
10	H	H11	-0.4752217	3.5876597	-2.2445563
11	O	O2	-0.9446719	-1.4063621	-0.0777594
12	Zn	Zn2	-2.9736226	0.0158460	-0.1248873
13	C	C4	-3.8820946	-0.5086818	-1.8687998
14	H	H10	-3.1533972	-1.1411337	-2.4012519
15	H	H14	-4.0587991	0.4034603	-2.4667483
16	C	C5	-3.5160147	-1.3421045	1.5368845
17	H	H19	-3.3217895	-2.0330433	2.3692330
18	C	C6	-1.3945393	-1.6653021	1.1257510
19	H	H18	-1.1407554	-0.9504564	1.9463256
20	C	C7	2.5529083	-0.4340449	1.0517233
21	H	H12	3.4186668	-0.5001486	1.7270506
22	H	H17	2.9354692	-0.0922356	0.0716596
23	H	H21	2.1753635	-1.4568596	0.9099497
24	C	C9	-5.1460722	-1.2325328	-1.5271750
25	H	H16	-5.9165582	-0.5441025	-1.1514597
26	H	H24	-4.9730744	-1.9840883	-0.7344396
27	H	H25	-5.5787843	-1.7609569	-2.3890471
28	C	C10	2.0706843	2.0177486	-1.4297756
29	H	H4	2.5249983	1.0160984	-1.2156964
30	H	H26	2.2803768	2.6360069	-0.5197735

31	C	C11	0.2594964	1.0793152	-2.8152221
32	H	H9	0.6396272	0.0396765	-2.7048811
33	H	H29	-0.8503243	1.0013899	-2.9034955
34	C	C12	2.7046135	2.6504499	-2.6643904
35	H	H5	3.8028398	2.6799210	-2.5255182
36	H	H30	2.3903499	3.7153667	-2.7639275
37	C	C13	0.8510540	1.7317439	-4.0611977
38	H	H32	0.3813307	2.7197785	-4.2464242
39	H	H33	0.6037291	1.1134639	-4.9457321
40	C	C14	2.3569745	1.8845841	-3.9293009
41	H	H28	2.8410874	0.8873304	-3.9182173
42	H	H34	2.7664016	2.4072331	-4.8149726
43	C	C15	-1.4198966	-3.1179625	1.5151872
44	C	C16	-1.3785731	-5.7953780	2.3175776
45	C	C17	-1.5966575	-4.1386866	0.5781623
46	C	C18	-1.2238546	-3.4531459	2.8609289
47	C	C19	-1.2013618	-4.7838622	3.2571552
48	C	C20	-1.5763048	-5.4705795	0.9809097
49	H	H27	-1.7493305	-3.8918788	-0.4795054
50	H	H31	-1.0853262	-2.6623659	3.6085778
51	H	H35	-1.0439037	-5.0370333	4.3106853
52	H	H36	-1.7161844	-6.2643029	0.2396280
53	H	H37	-1.3617208	-6.8440194	2.6318056
54	H	H2	-4.1828553	-1.9020614	0.8404236
55	C	C8	-4.1583262	-0.0921536	2.1099792
56	H	H20	-3.4926184	0.4037724	2.8307432
57	H	H22	-5.0938555	-0.3254660	2.6408343
58	H	H23	-4.4491790	0.6942918	1.3527574
59	C	C21	-2.9356089	3.4677865	-0.8898855
60	C	C22	-2.9138482	4.4634200	0.2655887
61	H	H13	-2.0785473	5.1794248	0.1826698
62	H	H40	-2.8260427	3.9596357	1.2371634
63	H	H41	-3.8387163	5.0577102	0.2878201
64	C	C23	-2.9378048	4.2384302	-2.2124605
65	H	H8	-1.9427421	4.6651358	-2.4228112
66	H	H42	-3.6604735	5.0642848	-2.1931681
67	H	H43	-3.2009540	3.5915532	-3.0604525
68	C	C24	-4.2368872	2.6562314	-0.7782008
69	H	H39	-4.3026616	2.0855594	0.1762661
70	H	H44	-4.3460555	1.9317958	-1.6086807
71	H	H45	-5.1150058	3.3170032	-0.8069611
72	C	C25	0.2675495	3.9876307	-0.2395084
73	H	H46	0.9792008	3.4759384	0.4540950
74	H	H47	-0.5287007	4.4557931	0.3752449
75	O	O3	0.9853488	4.9754685	-0.9767347
76	C	C26	1.3276119	6.2028433	-0.3104343
77	C	C27	0.0461001	6.8733804	0.1894698
78	C	C28	-2.3185104	8.1041124	1.0419142
79	C	C29	-0.2945448	6.8929930	1.5431968
80	C	C30	-0.8272022	7.4532202	-0.7359366
81	C	C31	-1.9991482	8.0681266	-0.3114494

82	C	C32	-1.4669840	7.5103848	1.9664716
83	H	H15	0.3699084	6.4249846	2.2812372
84	H	H50	-0.5778528	7.4252754	-1.8040385
85	H	H51	-2.6712590	8.5239576	-1.0459078
86	H	H52	-1.7183098	7.5248809	3.0321948
87	H	H53	-3.2389974	8.5932242	1.3767252
88	C	C33	1.9950861	7.0578239	-1.3979500
89	C	C34	3.2226394	8.6844463	-3.3198740
90	C	C35	2.0993768	8.4398865	-1.2048709
91	C	C36	2.5371614	6.4993074	-2.5562483
92	C	C37	3.1420720	7.3111473	-3.5116391
93	C	C38	2.7040229	9.2475823	-2.1581526
94	H	H38	1.7156423	8.8769246	-0.2693257
95	H	H54	2.5016388	5.4126932	-2.7332339
96	H	H55	3.5590784	6.8609194	-4.4185040
97	H	H56	2.7743244	10.3274587	-1.9923656
98	H	H57	3.6967045	9.3197651	-4.0747705
99	C	C39	2.3703489	6.0448983	0.7999475
100	C	C40	4.3373063	5.8900857	2.7939841
101	C	C41	3.0019112	4.8351108	1.0842551
102	C	C42	2.7462134	7.1804166	1.5290146
103	C	C43	3.7176701	7.1049480	2.5170894
104	C	C44	3.9771258	4.7583200	2.0744588
105	H	H48	2.7254776	3.9167770	0.5374311
106	H	H58	2.2695679	8.1461820	1.2926256
107	H	H59	3.9975670	8.0039615	3.0757922
108	H	H60	4.4583138	3.7973382	2.2857609
109	H	H61	5.1039581	5.8280038	3.5729194

Point Group = C1 Order = 1 Nsymop = 1

Anti R TS for ligand 11c, rotamer 1 (17a);

Heat of Formation: 12.266 kcal/mol

Cartesian Coordinates (Angstroms)

Atom	X	Y	Z

1 Zn Zn1	-0.3803108	0.1332348	1.2231514
2 C C1	1.2016371	-1.1022821	1.5870884
3 H H6	0.9538485	-2.0614683	1.0911976
4 H H7	1.2835598	-1.2802643	2.6688773
5 N N1	-0.0268198	2.2204250	2.0242634
6 O O1	-2.2327150	0.5400930	2.2481271
7 C C2	-2.5292009	1.9176444	2.2336479
8 H H3	-2.7600040	2.2293507	1.1685817
9 C C3	-1.2944287	2.8299178	2.6161094
10 H H11	-1.5007227	3.7943462	2.0697133
11 O O2	-0.8191601	0.1352398	-0.8472867
12 Zn Zn2	-3.2456298	-0.2428874	0.5756626
13 C C4	-4.6008515	0.2509307	-0.8696067

14	H	H10	-5.5919061	-0.0964256	-0.5408756
15	H	H14	-4.2957963	-0.3495532	-1.7475850
16	H	H1	-1.5224320	-1.8838732	1.4736387
17	C	C5	-2.0266128	-2.1105598	0.4977602
18	H	H19	-1.3602294	-2.8508633	0.0289823
19	C	C6	-1.4661688	-0.9175884	-1.2291711
20	C	C7	2.4334269	-0.4958096	0.9872113
21	H	H12	3.2699323	-1.2087396	0.9302009
22	H	H17	2.7976244	0.3677702	1.5694925
23	H	H21	2.2466721	-0.1352844	-0.0368584
24	C	C8	-3.3908538	-2.7505877	0.6944736
25	H	H8	-3.8632215	-2.9844059	-0.2710458
26	H	H22	-4.1265040	-2.1214002	1.2705886
27	H	H23	-3.3283278	-3.6910017	1.2627635
28	C	C9	-4.5443726	1.7214906	-1.1367636
29	H	H16	-3.5199848	2.0501033	-1.3660625
30	H	H24	-4.8834401	2.3016253	-0.2601560
31	H	H25	-5.1788665	2.0197347	-1.9842490
32	C	C10	1.1586194	2.1756545	2.9421351
33	H	H4	1.8439388	1.3883429	2.5453027
34	H	H26	0.8165565	1.8206521	3.9572910
35	C	C11	0.3588217	2.8402983	0.7016535
36	H	H9	1.0339139	2.1097331	0.1889848
37	H	H29	-0.5465445	2.9252517	0.0628671
38	C	C12	1.8958693	3.5077363	3.0785154
39	H	H5	2.7972533	3.3561242	3.7028253
40	H	H30	1.2611114	4.2351321	3.6364395
41	C	C13	1.0595896	4.1914624	0.8268992
42	H	H32	0.3626843	4.9603652	1.2193141
43	H	H33	1.3552447	4.5443211	-0.1799473
44	C	C14	2.2801097	4.0839993	1.7267911
45	H	H28	3.0500929	3.4462356	1.2474570
46	H	H34	2.7493831	5.0782094	1.8546971
47	H	H38	-2.5071925	-0.7383836	-1.6245578
48	C	C15	-0.7336341	-1.9640840	-2.0341439
49	C	C16	0.5868738	-3.8207226	-3.6518787
50	C	C17	-1.3188448	-2.4092490	-3.2239661
51	C	C18	0.5134672	-2.4678727	-1.6575596
52	C	C19	1.1697164	-3.3905133	-2.4649396
53	C	C20	-0.6593223	-3.3305346	-4.0286564
54	H	H20	-2.3006646	-2.0284782	-3.5312873
55	H	H27	0.9627050	-2.1359934	-0.7009492
56	H	H31	2.1480481	-3.7782257	-2.1623252
57	H	H35	-1.1221301	-3.6702863	-4.9608985
58	H	H36	1.1059185	-4.5452440	-4.2876990
59	C	C21	-3.8687822	2.1611269	3.0398627
60	C	C22	-3.8179087	1.7694898	4.5161035
61	H	H13	-3.3172813	2.5394197	5.1248988
62	H	H40	-3.2831764	0.8240194	4.6712490
63	H	H41	-4.8294426	1.6513916	4.9299486
64	C	C23	-4.2735190	3.6335414	2.9309281

65	H	H18	-3.5504945	4.2838819	3.4506067
66	H	H42	-5.2561792	3.8074231	3.3892528
67	H	H43	-4.3334064	3.9663541	1.8858650
68	C	C24	-4.9613176	1.3099598	2.3722712
69	H	H39	-4.7497911	0.2223362	2.4292518
70	H	H44	-5.1034433	1.5910923	1.3116310
71	H	H45	-5.9325543	1.4543455	2.8698157
72	C	C25	-1.1693725	3.3272118	4.0714359
73	H	H37	-0.4484131	4.1798479	4.1038861
74	H	H47	-2.1629697	3.7092025	4.4103840
75	O	O3	-0.7157554	2.3146544	4.9584946
76	C	C26	-0.5977232	2.7746246	6.3012219
77	C	C39	0.2174778	1.7831606	7.0787045
78	C	C40	1.7479410	0.0096903	8.5911085
79	C	C41	1.3403282	1.1722166	6.5193789
80	C	C42	-0.1389649	1.4967741	8.3975743
81	C	C43	0.6274759	0.6149553	9.1506605
82	C	C44	2.1008521	0.2868217	7.2747461
83	H	H49	1.6094871	1.3809082	5.4709101
84	H	H58	-1.0251735	1.9647258	8.8411162
85	H	H59	0.3452175	0.3940694	10.1851569
86	H	H60	2.9773510	-0.1950198	6.8292486
87	H	H61	2.3484059	-0.6870360	9.1848137
88	H	H62	-1.6144845	2.8907538	6.7277905
89	H	H70	-0.1028094	3.7672929	6.3430174

Point Group = C1 Order = 1 Nsymop = 1

Anti R TS for ligand 11c, rotamer 2 (17b);

Heat of Formation: 11.242 kcal/mol

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
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1	Zn	Zn1	-0.4637702	0.0376599	1.2180125
2	C	C1	1.1386965	-1.1629510	1.6103215
3	H	H6	0.9624058	-2.0946232	1.0373191
4	H	H7	1.1574913	-1.4110826	2.6810526
5	N	N1	-0.2678116	2.0824518	2.1495187
6	O	O1	-2.3988430	0.2896406	2.1291875
7	C	C2	-2.7573933	1.6520774	2.1830240
8	H	H3	-2.9300965	2.0249031	1.1263476
9	C	C3	-1.5957911	2.5881038	2.7077938
10	H	H11	-1.8185937	3.5801991	2.2205796
11	O	O2	-0.7562959	0.1549841	-0.8762113
12	Zn	Zn2	-3.2575165	-0.4139961	0.3384118
13	C	C4	-4.5296501	0.1236604	-1.1654811
14	H	H10	-5.5254867	-0.2816401	-0.9311463
15	H	H14	-4.1396666	-0.4053761	-2.0557214

16	H	H1	-1.5312365	-2.0434801	1.2473308
17	C	C5	-1.9570003	-2.2236745	0.2258393
18	H	H19	-1.2284218	-2.9036907	-0.2416439
19	C	C6	-1.3290161	-0.8928862	-1.3722605
20	C	C7	2.3818753	-0.4742748	1.1353249
21	H	H12	3.2444111	-1.1551208	1.0742369
22	H	H17	2.6815922	0.3506897	1.8038556
23	H	H21	2.2427220	-0.0392123	0.1327836
24	C	C8	-3.3021867	-2.9282526	0.2819946
25	H	H8	-3.6964786	-3.1132787	-0.7281204
26	H	H22	-4.1023558	-2.3693117	0.8441781
27	H	H23	-3.2378697	-3.9024411	0.7900141
28	C	C9	-4.5168796	1.6097592	-1.3341002
29	H	H16	-3.4935798	1.9913786	-1.4652666
30	H	H24	-4.9424908	2.1173630	-0.4503333
31	H	H25	-5.1009491	1.9391939	-2.2059506
32	C	C10	0.8587975	2.0156314	3.1363738
33	H	H4	1.6038035	1.2878135	2.7335181
34	H	H26	0.4507082	1.5737408	4.0831921
35	C	C11	0.1657763	2.8189960	0.9049589
36	H	H9	0.9025096	2.1591712	0.3823688
37	H	H29	-0.7028753	2.9162622	0.2190019
38	C	C12	1.5264886	3.3610553	3.4202045
39	H	H5	2.3975464	3.1977316	4.0830442
40	H	H30	0.8292315	4.0153340	3.9944105
41	C	C13	0.7933091	4.1843535	1.1776668
42	H	H32	0.0383265	4.8893742	1.5824550
43	H	H33	1.1321255	4.6280758	0.2216550
44	C	C14	1.9612221	4.0583619	2.1426076
45	H	H28	2.7880448	3.4943214	1.6655559
46	H	H34	2.3739836	5.0586786	2.3751593
47	H	H38	-2.3466042	-0.7271607	-1.8297586
48	C	C15	-0.4972928	-1.8527220	-2.1890852
49	C	C16	1.0120374	-3.5420468	-3.8249728
50	C	C17	-0.9780249	-2.2372952	-3.4449752
51	C	C18	0.7409933	-2.3329344	-1.7567646
52	C	C19	1.4913095	-3.1721972	-2.5731297
53	C	C20	-0.2247060	-3.0752773	-4.2583526
54	H	H20	-1.9514461	-1.8742436	-3.7971745
55	H	H27	1.1075533	-2.0502846	-0.7503997
56	H	H31	2.4619049	-3.5419034	-2.2263168
57	H	H35	-0.6060655	-3.3677623	-5.2420701
58	H	H36	1.6050523	-4.2008337	-4.4675623
59	C	C21	-4.1572758	1.7842584	2.9066899
60	C	C22	-4.1910232	1.2806494	4.3481523
61	H	H13	-3.7343269	2.0015274	5.0470079
62	H	H40	-3.6586541	0.3279791	4.4632025
63	H	H41	-5.2250455	1.1256492	4.6878980
64	C	C23	-4.6134877	3.2451993	2.8823163
65	H	H18	-3.9598154	3.8750710	3.5083229
66	H	H42	-5.6346143	3.3461371	3.2734883

67	H	H43	-4.6070215	3.6602456	1.8654276
68	C	C24	-5.1648761	0.9484340	2.1004025
69	H	H39	-4.9131144	-0.1321747	2.0923166
70	H	H44	-5.2440110	1.3039109	1.0557365
71	H	H45	-6.1734166	1.0193379	2.5355926
72	C	C25	-1.5786459	2.9825997	4.2002697
73	H	H37	-0.9067164	3.8647357	4.3320861
74	H	H47	-2.6067620	3.2877982	4.5104127
75	O	O3	-1.1468650	1.9262181	5.0529280
76	C	C26	-0.7923351	2.3432531	6.3583360
77	C	C33	-1.9294423	2.8873992	7.1760860
78	C	C34	-4.0038105	3.8796860	8.7522245
79	C	C35	-2.9767407	2.0510790	7.5642108
80	C	C36	-1.9257180	4.2223001	7.5809682
81	C	C37	-2.9607109	4.7154873	8.3677844
82	C	C38	-4.0111936	2.5483002	8.3491122
83	H	H46	-2.9811570	1.0022646	7.2423530
84	H	H54	-1.1040002	4.8834770	7.2821624
85	H	H55	-2.9527847	5.7632160	8.6855709
86	H	H56	-4.8317288	1.8889439	8.6507981
87	H	H57	-4.8177313	4.2690668	9.3724692
88	H	H62	-0.4136147	1.3970970	6.7846668
89	H	H69	0.0489542	3.0654089	6.3128204

Point Group = C1 Order = 1 Nsymop = 1

Anti R TS for ligand 11c, rotamer 3 (17c);

Heat of Formation: 9.422 kcal/mol

Cartesian Coordinates (Angstroms)

Atom			X	Y	Z
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1	Zn	Zn1	-0.3763925	0.2030783	1.2853539
2	C	C1	1.1962464	-1.0235365	1.7150839
3	H	H6	0.9421533	-2.0050029	1.2683829
4	H	H7	1.2780154	-1.1473527	2.8042836
5	N	N1	-0.0368519	2.3279805	1.9520952
6	O	O1	-2.2381899	0.6484905	2.2851575
7	C	C2	-2.5362319	2.0229355	2.1960261
8	H	H3	-2.7673279	2.2771060	1.1155952
9	C	C3	-1.3031252	2.9566262	2.5272441
10	H	H11	-1.5193452	3.8942899	1.9393948
11	O	O2	-0.8116196	0.0944037	-0.7833620
12	Zn	Zn2	-3.2394674	-0.2163325	0.6439982
13	C	C4	-4.5914800	0.2044286	-0.8270607
14	H	H10	-5.5842936	-0.1213397	-0.4820311
15	H	H14	-4.2865323	-0.4438591	-1.6704523

16	H	H1	-1.5224175	-1.8094153	1.6260370
17	C	C5	-2.0231156	-2.0857877	0.6615515
18	H	H19	-1.3545548	-2.8477664	0.2322938
19	C	C6	-1.4548954	-0.9769783	-1.1170472
20	C	C7	2.4316694	-0.4566075	1.0842090
21	H	H12	3.2555407	-1.1850219	1.0409365
22	H	H17	2.8164272	0.4180011	1.6357864
23	H	H21	2.2401009	-0.1246653	0.0512541
24	C	C8	-3.3877189	-2.7161731	0.8841963
25	H	H8	-3.8567094	-2.9963674	-0.0705598
26	H	H22	-4.1253654	-2.0602343	1.4266555
27	H	H23	-3.3268708	-3.6281503	1.4972491
28	C	C9	-4.5295061	1.6579771	-1.1741548
29	H	H16	-3.5027519	1.9712164	-1.4142647
30	H	H24	-4.8730156	2.2864001	-0.3333680
31	H	H25	-5.1575808	1.9104753	-2.0410777
32	C	C10	1.1549404	2.3204239	2.8636179
33	H	H4	1.8397492	1.5183141	2.4955983
34	H	H26	0.8119000	2.0057749	3.8832124
35	C	C11	0.3389726	2.9003698	0.6064620
36	H	H9	1.0192640	2.1576047	0.1203877
37	H	H29	-0.5682358	2.9524917	-0.0329862
38	C	C12	1.8961805	3.6543427	2.9489124
39	H	H5	2.8131743	3.5152975	3.5534942
40	H	H30	1.2781562	4.3957720	3.5165776
41	C	C13	1.0241687	4.2630222	0.6837039
42	H	H32	0.3205845	5.0357083	1.0563632
43	H	H33	1.3085967	4.5871361	-0.3359788
44	C	C14	2.2523778	4.1996808	1.5769173
45	H	H28	3.0283284	3.5619372	1.1071545
46	H	H34	2.7065125	5.2045601	1.6726141
47	H	H38	-2.4940128	-0.8184500	-1.5263840
48	C	C15	-0.7173092	-2.0599011	-1.8674070
49	C	C16	0.6123068	-3.9905449	-3.3882711
50	C	C17	-1.2958640	-2.5610949	-3.0380801
51	C	C18	0.5277292	-2.5448736	-1.4606184
52	C	C19	1.1885178	-3.5044492	-2.2198249
53	C	C20	-0.6318401	-3.5191554	-3.7946641
54	H	H20	-2.2759879	-2.1956411	-3.3685390
55	H	H27	0.9718730	-2.1678838	-0.5184726
56	H	H31	2.1652542	-3.8769555	-1.8938284
57	H	H35	-1.0894437	-3.9027282	-4.7123612
58	H	H36	1.1349487	-4.7441033	-3.9862705
59	C	C21	-3.8784140	2.3080089	2.9854303
60	C	C22	-3.8432250	1.9745028	4.4759236
61	H	H13	-3.2916291	2.7328860	5.0615923
62	H	H40	-3.3685563	1.0035575	4.6658006
63	H	H41	-4.8588675	1.9352616	4.8947613
64	C	C23	-4.2765416	3.7759922	2.8145033
65	H	H18	-3.5597358	4.4448123	3.3187766
66	H	H42	-5.2654280	3.9703246	3.2508733

67	H	H43	-4.3199970	4.0678508	1.7564744
68	C	C24	-4.9711527	1.4341045	2.3473462
69	H	H39	-4.7644914	0.3490701	2.4515789
70	H	H44	-5.1045522	1.6696204	1.2746565
71	H	H45	-5.9449889	1.6035751	2.8315992
72	C	C25	-1.1718072	3.5202487	3.9564682
73	H	H37	-0.4549519	4.3794555	3.9565683
74	H	H47	-2.1688498	3.9065819	4.2785599
75	O	O3	-0.6517172	2.5786997	4.8906339
76	C	C26	-0.9844758	2.8322205	6.2383254
77	C	C27	-0.2880786	3.9847207	6.9066482
78	C	C28	0.9548153	6.0662094	8.2950787
79	C	C29	-0.5620843	4.1951336	8.2617706
80	C	C30	0.6105841	4.8271641	6.2551724
81	C	C31	1.2293281	5.8627451	6.9482982
82	C	C32	0.0559932	5.2299436	8.9509405
83	H	H15	-1.2671271	3.5361039	8.7812462
84	H	H50	0.8311777	4.6786283	5.1812763
85	H	H51	1.9360132	6.5176785	6.4281699
86	H	H52	-0.1632186	5.3867585	10.0121739
87	H	H53	1.4436243	6.8807222	8.8391852
88	H	H62	-0.6798138	1.8793452	6.7086846
89	H	H69	-2.0891013	2.9362803	6.3428299

Point Group = C1 Order = 1 Nsymop = 1