Supporting Information:

Enantioselectivity in the boron aldol reactions of methyl ketones.

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Computational Details:
Absolute energies and zero point energies (B3LYP/6-31G**), imaginary frequencies and Cartesian coordinates of all transition structures reported in the paper.

All calculations were performed with Jaguar version 4.2[1] and employed the 6-31G** basis-set[2] with the B3LYP density functional.[3] This level of theory has been shown to yield quantitative predictions in line with experimental diastereo- and enantioselectivities observed in boron aldol reactions.[4] Transition Structures were fully optimised in the gas phase and characterised by frequency calculations. The corresponding eigenvector was carefully inspected to check that it corresponded to the expected reaction coordinate.

The model transition structures in Fig. 1 were further optimised in solvent. These Solvent effects were evaluated by the Poisson-Boltzmann solver[5] as implemented in Jaguar, using a polarizable continuum dielectric model of the solvent used experimentally, diethyl ether. For the larger transition structures shown in Fig. 2 and Fig. 3 the effects of solvation were evaluated by single point calculations at the optimised gas-phase geometries.

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3. (a) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098-3100; (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785-789; (c) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652; (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623-11627.
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5. (a) Tannor, D. J.; Marten, B.; Murphy, R.; Friesner, R. A.; Sitkoff, D.; Nicholls, A.; Ringnalda, M. N.; Goddard III, W. A.; Honig, B. *J. Am. Chem. Soc.* **1994**, *116*, 11875; (b) B. Marten, B.; Kim, K.; Cortis, C.; Friesner, R. A.; Murphy, R. B.; Ringnalda, M. N.; Sitkoff, D.; Honig, J. *J. Phys. Chem.* **1996**, *100*, 11775.

B3LYP/6-31G** Energies:

Optimized Model Transition Structures (Fig. 1):
(Ether)

Structure	SCF energy (Hartrees)	ZPE (Hartrees)	Erel (kcal/mol)	Negative Freq (cm^{-1})
(Z)-boat A	-490.44395	0.23969	1.30	-59.7
(Z)-boat A'	-490.43733	0.23979	5.51	-111.1
(Z)-boat B	-490.44130	0.24033	3.37	-232.0
(Z)-boat B'	-490.43193	0.23997	9.01	-187.7
(Z)-Chair	-490.44683	0.24049	0.00	-189.4
(Z)-Chair'	-490.43867	0.23960	4.56	-144.0
(E)-boat A	-490.44752	0.24023	0.00	-157.0
(E)-boat A'	-490.44149	0.23962	3.40	-150.7 (-80.7)
(E)-boat B	-490.44638	0.24015	0.67	-103.4
(E)-boat B'	-490.43830	0.23910	5.08	-111.5 (-30.1)
(E)-Chair	-490.44657	0.24015	0.55	-167.0
(E)-Chair'	-490.43908	0.23950	4.84	-117.1
Unsub-boat A	-451.13144	0.21258	0.00	-213.9
Unsub-boat A'	-451.12670	0.21213	2.70	-188.8
Unsub-boat B	-451.12975	0.21237	0.93	-170.3
Unsub-boat B'	-451.12263	0.21166	4.95	-172.7
Unsub-boat C	-451.12854	0.21200	1.46	-190.8
Unsub-boat C'	-451.12134	0.21202	5.99	-150.2

Full list of optimized Transition Structures with (-)-Ipc ligands (Low energy structures shown in Fig. 2):
(Vacuum)

Structure	SCF energy (Hartrees)	ZPE (Hartrees)	Erel (kcal/mol)	Negative Freq (cm^{-1})
(Z)-Chair-*Re*	-1193.18592	0.66802	0.57	-131.4
(Z)-Chair-*Si*	-1193.18706	0.66825	0.00	-209.1
(E)-boat A-*Re*	-1193.19069	0.66776	0.00	-90.7
(E)-boat A-*Si*	-1193.18963	0.66773	0.65	-105.3
(E)-boat B-*Re*	-1193.18850	0.66777	1.38	-102.0
(E)-boat B-*Si*	-1193.18889	0.66757	1.02	-78.4
(E)-Chair-*Re*	-1193.18748	0.66706	1.57	-41.6
(E)-Chair-*Si*	-1193.18843	0.66717	1.05	-81.2
Unsub-boat A-*Re*	-1153.87435	0.64017	0.00	-188.9
Unsub-boat A-*Si*	-1153.87338	0.64010	0.56	-192.2
Unsub-boat B-*Re*	-1153.87128	0.63958	1.55	-32.6
Unsub-boat B-*Si*	-1153.87194	0.63951	1.10	-79.2
Unsub-Chair-*Re*	-1153.87006	0.63906	1.99	-68.1

Unsub-Chair-*Si*	-1153.87062	0.63932	1.81	-37.7

NB No boat transition structures were found for Z enolborinates

Full list of optimized Transition Structures with (-)-Ipc ligands (Low energy structures shown in Fig. 2):
(Single Point Calculations in Ether)

Structure	**Single Point energy** (Hartrees)	**Erel** (kcal/mol)
(Z)-Chair-Re	-1193.18958	1.23
(Z)-Chair-Si	-1193.19154	0.00
(E)-boat A-Re	-1193.19369	0.00
(E)-boat A-Si	-1193.19300	0.43
(E)-boat B-Re	-1193.19221	0.93
(E)-boat B-Si	-1193.19263	0.67
(E)-Chair-Re	-1193.19093	1.74
(E)-Chair-Si	-1193.19231	0.87
Unsub-boat A-Re	-1153.87788	0.00
Unsub-boat A-Si	-1153.87705	0.52
Unsub-boat B-Re	-1153.87529	1.62
Unsub-boat B-Si	-1153.87603	1.16
Unsub-Chair-Re	-1153.87403	2.42
Unsub-Chair-Si	-1153.87487	1.88

Full list of optimized Transition Structures with oxazolidinone auxiliaries (Low energy structures shown in Fig. 3):
(Vacuum)

Structure	**SCF energy** (Hartrees)	**ZPE** (Hartrees)	**Erel** (kcal/mol)	**Negative Freq** (cm-1)
(Z)-boat A-Si	-890.42253	0.36475	2.01	-48.4
(Z)-boat A-Re	-890.41329	0.36511	8.04	-58.6
(Z)-boat A-Re-II	-890.41550	0.36483	6.48	-61.6
(Z)-boat A-Re-III	-890.41442	0.36572	7.71	-206.9
(Z)-boat A-Re-IV	-890.41645	0.36593	6.57	-235.5
(Z)-boat B-Si	-890.41557	0.36560	6.92	-106.4
(Z)-boat B-Si-II	-890.41005	0.36547	10.30	-127.2
(Z)-boat B-Re	-890.42056	0.36562	3.80	-117.6
(Z)-boat B-Re-III	-890.42191	0.36562	2.95	-90.7
(Z)-boat B-Re-IV	-890.40818	0.36527	11.34	-68.7
(Z)-Chair-Si	-890.42671	0.36572	0.00	-91.7
(Z)-Chair-Si-II	-890.42510	0.36574	1.03	-99.7
(Z)-Chair-Si-III	-890.41212	0.36499	8.70	-81.0
(Z)-Chair-Re	-890.41578	0.36625	7.19	-260.4
(Z)-Chair-Re-II	-890.41258	0.36553	8.74	-45.3

Unsub-boat A-Si	-851.10856	0.33754	0.00	-104.6
Unsub-boat A-Si-II	-851.10468	0.33669	1.90	-82.7
Unsub-boat A-Re	-851.10755	0.33741	0.55	-79.8
Unsub-boat A-Re-II	-851.10559	0.33773	1.98	-100.3
Unsub-boat A-Re-III	-851.10153	0.33774	4.54	-228.2
Unsub-boat B-Si	-851.10538	0.33582	0.92	-117.2
Unsub-boat B-Si-II	-851.09856	0.33721	6.07	-108.2
Unsub-boat B-Re	-851.10571	0.33716	1.55	-94.8
Unsub-boat B-Re-II	-851.10754	0.33685	0.21	-34.9
Unsub-boat B-Re-III	-851.09688	0.33692	6.94	-39.9
Unsub-Chair-Si	-851.10725	0.33791	1.05	-88.2
Unsub-Chair-Si-II	-851.09638	0.33738	7.54	-105.2
Unsub-Chair-Re	-851.10215	0.33754	4.03	-36.9
Unsub-Chair-Re-II	-851.09662	0.33745	7.44	-79.6

Full list of optimized Transition Structures with oxazolidinone auxiliaries (Low energy structures shown in Fig. 3):
(Single Point Calculations in Ether)

Structure	**Single Point energy** (Hartrees)	**Erel** (kcal/mol)
(Z)-boat A-Si	-890.43419	1.88
(Z)-boat A-Re	-890.42629	6.84
(Z)-boat A-Re-II	-890.42899	5.14
(Z)-boat A-Re-III	-890.42682	6.50
(Z)-boat A-Re-IV	-890.42831	5.57
(Z)-boat B-Si	-890.42592	7.07
(Z)-boat B-Si-II	-890.42327	8.73
(Z)-boat B-Re	-890.43007	4.46
(Z)-boat B-Re-III	-890.43221	3.12
(Z)-boat B-Re-IV	-890.42206	9.49
(Z)-Chair-Si	-890.43718	0.00
(Z)-Chair-Si-II	-890.43541	1.11
(Z)-Chair-Si-III	-890.42660	6.64
(Z)-Chair-Re	-890.42522	7.50
(Z)-Chair-Re-II	-890.42848	5.46
Unsub-boat A-Si	-851.12059	0.00
Unsub-boat A-Si-II	-851.11609	2.82
Unsub-boat A-Re	-851.12055	0.02
Unsub-boat A-Re-II	-851.11422	4.00
Unsub-boat A-Re-III	-851.11422	4.00
Unsub-boat B-Si	-851.11903	0.98
Unsub-boat B-Si-II	-851.11232	5.19
Unsub-boat B-Re	-851.11708	2.20

Unsub-boat B-Re-II	-851.11936	0.77
Unsub-boat B-Re-III	-851.11145	5.74

Unsub-Chair-Si	-851.11804	1.60
Unsub-Chair-Si-II	-851.11293	4.81
Unsub-Chair-Re	-851.11452	3.81
Unsub-Chair-Re-II	-851.11293	4.80

Cartesian Coordinates:

Optimized Model Transition Structures (Fig. 1):

(Z)-boat A

C1	-1.37481	2.25955	2.76605
C2	-0.83023	2.81958	1.65751
H3	-2.35526	2.63666	3.04527
C4	-1.52865	3.92751	0.90428
H5	-0.89210	4.82029	0.89032
H6	-1.69306	3.64825	-0.14454
H7	-2.48678	4.19187	1.35805
B8	1.03222	1.24119	0.78322
C9	2.19275	0.80039	1.80245
H10	3.02950	1.50672	1.72126
H11	1.89001	0.78215	2.85392
H12	2.59268	-0.19079	1.55346
C13	1.44868	1.21831	-0.77448
H14	2.19862	1.99575	-0.96701
H15	1.89416	0.26128	-1.07310
H16	0.60354	1.41971	-1.44699
C17	-1.29880	0.23572	0.53369
O18	-0.13053	0.05791	0.92385
H19	-1.54158	1.12157	-0.06102
C20	-2.35255	-0.78393	0.76123
H21	-3.21894	-0.31759	1.24395
H22	-2.70272	-1.15112	-0.21320
H23	-1.97768	-1.61434	1.36185
O24	0.36173	2.52011	1.10838
C25	-0.71788	1.30102	3.72334
H26	-0.44220	0.34656	3.26065
H27	0.20896	1.71883	4.13620
H28	-1.38216	1.08285	4.56448

(Z)-boat A'

C1	-1.43868	2.09997	2.64310
C2	-0.77514	2.81684	1.68728
H3	-2.41787	2.49941	2.89860
C4	-1.37323	4.08595	1.12503
H5	-0.70921	4.92725	1.35795
H6	-1.44679	4.03972	0.03209
H7	-2.35873	4.30041	1.54438
B8	1.07261	1.28235	0.71688
C9	2.22406	0.77667	1.72195
H10	3.09284	1.44337	1.64257

H11	1.93526	0.75697	2.77846
H12	2.57524	-0.22845	1.45512
C13	1.55885	1.37746	-0.81745
H14	2.37244	2.11010	-0.89613
H15	1.96299	0.42133	-1.17343
H16	0.78158	1.69067	-1.52392
C17	-1.33073	0.30441	0.58197
O18	-0.11197	0.15917	0.84112
H19	-2.01142	-0.36205	1.12410
O20	0.41479	2.55165	1.14146
C21	-1.90035	1.06161	-0.56783
H22	-2.92469	1.37088	-0.35038
H23	-1.28806	1.91235	-0.86095
H24	-1.93925	0.36085	-1.41678
C25	-0.92246	1.03831	3.57632
H26	-0.09933	0.46362	3.15623
H27	-0.56090	1.49419	4.50904
H28	-1.71878	0.34002	3.85862

(Z)-boat B

C1	-0.82153	-0.18401	0.31594
C2	-1.15968	1.15728	0.43673
H3	-0.72144	-0.72965	1.25243
C4	-1.27791	1.82590	1.77861
H5	-1.27631	1.11754	2.60956
H6	-0.44888	2.53598	1.89643
H7	-2.20267	2.41242	1.80565
B8	0.06788	2.43131	-1.37225
C9	0.12366	4.03261	-1.29365
H10	1.03872	4.43116	-1.75129
H11	-0.72126	4.47841	-1.83330
H12	0.08112	4.39976	-0.26080
C13	0.11823	1.81813	-2.86066
H14	-0.78008	2.11418	-3.41711
H15	0.97567	2.22344	-3.41416
H16	0.18201	0.72573	-2.92472
C17	1.23062	0.60471	-0.18939
O18	1.15058	1.87367	-0.43467
H19	1.15383	-0.07978	-1.03632
C20	2.08614	0.18819	0.96861
H21	3.13875	0.34529	0.69410
H22	1.87752	0.79895	1.85065
H23	1.95223	-0.86948	1.20465
O24	-1.24052	1.94847	-0.59925
C25	-1.11517	-1.02297	-0.90220
H26	-1.34408	-0.39958	-1.76748
H27	-0.28530	-1.69180	-1.16170
H28	-1.98404	-1.66349	-0.70520

(Z)-boat B'

C1	-0.08948	1.35212	0.59421
O2	0.22598	1.08250	1.84194
B3	1.32247	0.02002	2.17711

O4	1.03013	-1.08386	1.12430
C5	0.96748	-0.78734	-0.12657
C6	-0.91669	0.50610	-0.12557
C7	2.81040	0.62014	1.98796
C8	1.00581	-0.58671	3.62563
C9	0.54697	2.57010	-0.02259
H10	-1.11707	0.79093	-1.15654
H11	3.56541	-0.11516	2.29582
H12	3.06811	0.92964	0.96630
H13	2.94846	1.50112	2.62671
H14	1.70683	-1.39017	3.88594
H15	1.09968	0.18157	4.40328
H16	-0.00858	-0.99941	3.69497
H17	0.25941	2.70670	-1.06771
H18	0.23063	3.45310	0.54537
H19	1.63850	2.52295	0.05630
H20	1.63694	-0.01713	-0.51661
C21	0.56008	-1.86641	-1.08210
H22	0.26209	-1.45514	-2.04867
H23	1.43508	-2.51126	-1.24625
H24	-0.23858	-2.48437	-0.66749
C25	-1.87993	-0.45864	0.51351
H26	-2.16566	-1.25844	-0.17620
H27	-1.46008	-0.90436	1.41676
H28	-2.80235	0.06498	0.79684

(Z)-Chair

C1	-0.08948	1.35212	0.59421
O2	0.22598	1.08250	1.84194
B3	1.32247	0.02002	2.17711
O4	1.03013	-1.08386	1.12430
C5	0.96748	-0.78734	-0.12657
C6	-0.91669	0.50610	-0.12557
C7	2.81040	0.62014	1.98796
C8	1.00581	-0.58671	3.62563
C9	0.54697	2.57010	-0.02259
H10	-1.11707	0.79093	-1.15654
H11	3.56541	-0.11516	2.29582
H12	3.06811	0.92964	0.96630
H13	2.94846	1.50112	2.62671
H14	1.70683	-1.39017	3.88594
H15	1.09968	0.18157	4.40328
H16	-0.00858	-0.99941	3.69497
H17	0.25941	2.70670	-1.06771
H18	0.23063	3.45310	0.54537
H19	1.63850	2.52295	0.05630
H20	1.63694	-0.01713	-0.51661
C21	0.56008	-1.86641	-1.08210
H22	0.26209	-1.45514	-2.04867
H23	1.43508	-2.51126	-1.24625
H24	-0.23858	-2.48437	-0.66749
C25	-1.87993	-0.45864	0.51351
H26	-2.16566	-1.25844	-0.17620

H27	-1.46008	-0.90436	1.41676
H28	-2.80235	0.06498	0.79684

(Z)-Chair'

C1	-0.11438	-0.88476	-1.05036
O2	-1.35993	-0.49585	-1.27216
B3	-2.09184	0.49683	-0.36083
O4	-1.63030	-0.05640	1.05865
C5	-0.44066	-0.30251	1.44563
C6	0.15336	-1.93276	-0.19679
C7	-1.69360	2.04154	-0.60492
C8	-3.66740	0.20864	-0.45056
H9	-0.35368	-1.13266	2.15317
C10	0.97512	-0.13485	-1.77278
H11	1.20107	-2.19185	-0.05729
H12	-2.15375	2.68858	0.15341
H13	-0.62349	2.27440	-0.61800
H14	-2.09457	2.36671	-1.57389
H15	-4.23612	0.84203	0.24240
H16	-4.04257	0.42670	-1.45875
H17	-3.91744	-0.83571	-0.22683
H18	1.97235	-0.45891	-1.46621
H19	0.86715	-0.32113	-2.84868
H20	0.88073	0.94652	-1.63396
C21	0.67372	0.70056	1.50395
H22	1.63222	0.19411	1.63687
H23	0.71470	1.36333	0.64241
H24	0.49676	1.32074	2.39549
C25	-0.86433	-2.95340	0.23949
H26	-0.65983	-3.32843	1.24810
H27	-1.87349	-2.54006	0.21639
H28	-0.83783	-3.82048	-0.43390

(E)-boat A

C1	-1.17913	2.55953	2.42531
C2	-0.41498	3.24477	1.50109
H3	-0.75525	1.66496	2.86456
C4	-0.72487	4.64054	1.02184
H5	0.20894	5.20928	0.97389
H6	-1.12794	4.61070	0.00139
H7	-1.42740	5.17203	1.66382
B8	0.98153	1.26531	0.72744
C9	1.90395	0.76963	1.95339
H10	2.88762	1.25379	1.90684
H11	1.48127	0.99093	2.94104
H12	2.07684	-0.31287	1.90629
C13	1.58441	1.02201	-0.74500
H14	2.50105	1.60715	-0.89003
H15	1.84602	-0.03107	-0.90576
H16	0.88463	1.31549	-1.53866
C17	-1.49899	0.97784	0.67036
O18	-0.36334	0.43246	0.84845
H19	-1.59705	1.77831	-0.06666

C20	-2.73054	0.23311	1.06667
H21	-3.56666	0.91367	1.24217
H22	-3.01263	-0.42777	0.23395
H23	-2.54825	-0.38617	1.94788
O24	0.60427	2.72155	0.84117
C25	-2.37417	3.12993	3.14566
H26	-2.90449	3.88541	2.56004
H27	-3.09204	2.33614	3.38200
H28	-2.09481	3.59101	4.10352

(E)-boat A'

C1	-1.15997	2.56947	2.45834
C2	-0.38383	3.26894	1.56587
H3	-0.78882	1.61942	2.82047
C4	-0.63722	4.70168	1.17053
H5	0.30619	5.25476	1.22495
H6	-0.97637	4.75697	0.12863
H7	-1.36863	5.20114	1.80588
B8	1.02505	1.32567	0.73114
C9	1.84642	0.75171	1.99317
H10	2.83461	1.22787	2.03601
H11	1.36299	0.92336	2.96202
H12	2.01646	-0.32775	1.89542
C13	1.72199	1.10718	-0.69998
H14	2.66166	1.67178	-0.75347
H15	1.97342	0.05331	-0.87118
H16	1.09847	1.44003	-1.53908
C17	-1.52586	0.97159	0.57838
O18	-0.37629	0.48164	0.76683
H19	-2.34474	0.50199	1.13462
O20	0.63029	2.75511	0.87320
C21	-2.33716	3.13427	3.21288
H22	-2.84813	3.93418	2.67090
H23	-3.07648	2.34974	3.40943
H24	-2.04166	3.53620	4.19259
C25	-1.89710	1.80784	-0.60277
H26	-2.81502	2.36915	-0.41642
H27	-1.08620	2.46912	-0.91056
H28	-2.09328	1.11002	-1.43142

(E)-boat B

C1	-0.94040	-0.08650	0.29124
C2	-1.22356	1.22391	0.59448
H3	-0.90862	-0.34008	-0.76125
C4	-1.62479	1.71655	1.96105
H5	-1.91478	0.91552	2.64184
H6	-0.80248	2.28814	2.40905
H7	-2.46712	2.40755	1.85287
B8	-0.01576	2.32508	-1.34872
C9	0.22950	3.88683	-1.62232
H10	1.06874	4.05763	-2.30835
H11	-0.65516	4.34394	-2.08384
H12	0.43432	4.43748	-0.69645

C13	-0.25033	1.45119	-2.68668
H14	-1.19469	1.76184	-3.15249
H15	0.53867	1.65616	-3.42207
H16	-0.30688	0.36128	-2.57803
C17	1.38349	0.58875	-0.22029
O18	1.22065	1.81903	-0.48965
H19	1.21279	-0.15400	-1.00087
C20	2.21513	0.20181	0.95706
H21	3.26506	0.14668	0.63298
H22	2.14007	0.94706	1.75191
H23	1.93818	-0.78690	1.33019
O24	-1.08628	2.21293	-0.27374
C25	-1.03842	-1.24945	1.24315
H26	-0.86807	-0.96164	2.28377
H27	-2.02075	-1.73908	1.18961
H28	-0.29737	-2.01762	0.99132

(E)-boat B'

C1	0.03316	-0.81002	-1.11247
O2	-1.26190	-0.51335	-1.26679
B3	-2.43026	-1.41636	-1.30699
O4	-1.77919	-2.54736	-2.37969
C5	-0.90063	-3.41990	-2.19085
C6	0.48994	-1.92551	-0.47454
C7	-2.91561	-2.07758	0.07866
C8	-3.60124	-0.73114	-2.15821
H9	-0.10338	-3.48299	-2.94355
C10	0.90665	0.21732	-1.78681
H11	-3.68718	-2.83901	-0.09124
H12	-2.14857	-2.51978	0.72219
H13	-3.39268	-1.28579	0.67273
H14	-4.43929	-1.41670	-2.33464
H15	-4.00780	0.13383	-1.61831
H16	-3.24694	-0.37125	-3.13106
H17	1.97098	0.06301	-1.60667
H18	0.72333	0.21848	-2.86768
H19	0.63500	1.21297	-1.41922
H20	-0.22613	-2.48607	0.11254
C21	-1.02292	-4.58195	-1.25718
H22	-0.04240	-4.90571	-0.89915
H23	-1.69861	-4.38871	-0.42590
H24	-1.43643	-5.41184	-1.85186
C25	1.93199	-2.32096	-0.29401
H26	2.04550	-3.41022	-0.35666
H27	2.59245	-1.88379	-1.04693
H28	2.31637	-2.02826	0.69344

(E)-Chair

C1	0.02755	0.05457	-0.01048
O2	-0.19207	0.02291	1.29028
B3	0.95103	0.01204	2.33522
O4	1.95539	-0.99821	1.70742
C5	2.40834	-0.81812	0.52293

C6	0.45282	-1.08662	-0.66606
C7	1.62907	1.46995	2.49383
C8	0.39299	-0.64475	3.68556
C9	-0.16058	1.39680	-0.66738
H10	2.42241	1.45241	3.25250
H11	2.07472	1.88163	1.57807
H12	0.88302	2.19913	2.83277
H13	1.18093	-0.74121	4.44349
H14	-0.39968	-0.02778	4.12710
H15	-0.02606	-1.64392	3.51426
H16	-0.01381	1.37964	-1.74804
H17	-1.17854	1.74486	-0.45872
H18	0.51790	2.13274	-0.22134
H19	0.34281	-2.01109	-0.10619
H20	2.58176	0.20222	0.17272
C21	3.24655	-1.89874	-0.08459
H22	3.33144	-1.78106	-1.16621
H23	4.25800	-1.81063	0.33754
H24	2.85952	-2.88943	0.16391
C25	0.64732	-1.21911	-2.15458
H26	1.33552	-2.03847	-2.38470
H27	-0.29876	-1.45396	-2.66088
H28	1.04761	-0.31033	-2.61326

(E)-Chair'

C1	-0.03450	-0.82663	-1.10668
O2	-1.31335	-0.49832	-1.28815
B3	-2.08582	0.45178	-0.39645
O4	-1.65711	-0.13809	1.04443
C5	-0.49002	-0.35604	1.48619
C6	0.26715	-1.86850	-0.26654
C7	-1.72012	2.01551	-0.55993
C8	-3.65118	0.12581	-0.52672
H9	-0.39921	-1.22042	2.15336
C10	0.97163	-0.00710	-1.87124
H11	-2.21665	2.61640	0.21294
H12	-0.65724	2.27862	-0.53563
H13	-2.10564	2.37235	-1.52393
H14	-4.25104	0.72029	0.17414
H15	-4.01462	0.36262	-1.53487
H16	-3.87029	-0.93238	-0.34028
H17	2.00585	-0.26886	-1.64435
H18	0.80810	-0.16599	-2.94397
H19	0.82308	1.06121	-1.68759
H20	-0.58312	-2.46088	0.06206
C21	0.60636	0.65979	1.60014
H22	1.57446	0.16632	1.70886
H23	0.63281	1.36913	0.77611
H24	0.41931	1.22382	2.52607
C25	1.62886	-2.43854	0.01931
H26	1.72156	-2.72086	1.07469
H27	1.80440	-3.35258	-0.56365
H28	2.43965	-1.74303	-0.20991

Unsub-boat A

C1	-1.37026	2.03135	2.48654
C2	-0.78312	2.84459	1.53919
H3	-2.27809	2.37868	2.96799
H4	-0.82043	1.25049	2.99096
C5	-1.42518	4.13806	1.10568
H6	-0.70813	4.95554	1.23528
H7	-1.66978	4.09924	0.03817
H8	-2.32595	4.36288	1.67925
B9	0.98945	1.21331	0.74745
C10	2.03527	0.99779	1.94981
H11	2.87267	1.69904	1.85104
H12	1.60379	1.15150	2.94646
H13	2.45729	-0.01412	1.92907
C14	1.55185	1.04748	-0.74795
H15	2.29403	1.82436	-0.96760
H16	2.04521	0.07883	-0.89016
H17	0.76495	1.13304	-1.50957
C18	-1.36945	0.36562	0.81133
O19	-0.14090	0.10258	0.96784
H20	-1.66650	1.10290	0.06096
C21	-2.38933	-0.63510	1.25463
H22	-3.36086	-0.16543	1.41783
H23	-2.50333	-1.38468	0.45881
H24	-2.05756	-1.14873	2.15866
O25	0.28150	2.55039	0.83340

Unsub-boat A'

C1	-1.34217	2.03867	2.51637
C2	-0.74098	2.87379	1.60379
H3	-2.24081	2.38648	3.01402
H4	-0.82220	1.20846	2.97000
C5	-1.34483	4.20660	1.24119
H6	-0.61849	4.99946	1.44987
H7	-1.55933	4.24907	0.16754
H8	-2.25807	4.41004	1.80320
B9	1.02276	1.27243	0.74619
C10	2.00060	0.94862	1.98014
H11	2.86212	1.62763	1.95851
H12	1.53205	1.05568	2.96534
H13	2.39330	-0.07283	1.91355
C14	1.66069	1.16611	-0.72150
H15	2.46309	1.90476	-0.84042
H16	2.10582	0.17969	-0.89688
H17	0.93831	1.34944	-1.52725
C18	-1.40073	0.38070	0.76146
O19	-0.16627	0.15472	0.89082
H20	-2.07046	-0.25119	1.35588
O21	0.32253	2.59457	0.88090
C22	-2.00429	1.06919	-0.42541
H23	-3.01691	1.41496	-0.20994
H24	-1.37928	1.88905	-0.78049

H25	-2.05903	0.32239	-1.23043

Unsub-boat B

C1	-0.92664	-0.09971	0.27122
C2	-1.22517	1.20411	0.56826
H3	-0.86244	-0.43657	-0.75238
H4	-1.05265	-0.85955	1.03429
C5	-1.66995	1.62909	1.94427
H6	-1.82671	0.77738	2.60909
H7	-0.92853	2.30611	2.38325
H8	-2.60489	2.19325	1.86255
B9	-0.02632	2.34966	-1.34630
C10	0.23571	3.90734	-1.59528
H11	1.06570	4.07973	-2.29144
H12	-0.65132	4.38200	-2.03294
H13	0.46284	4.44034	-0.66460
C14	-0.25789	1.47077	-2.67765
H15	-1.17533	1.81833	-3.16871
H16	0.55548	1.63286	-3.39635
H17	-0.37204	0.38579	-2.56461
C18	1.42168	0.59263	-0.27136
O19	1.23224	1.82069	-0.47904
H20	1.22983	-0.12056	-1.07494
C21	2.26815	0.15997	0.88273
H22	3.32135	0.19097	0.56912
H23	2.14542	0.84118	1.72657
H24	2.03663	-0.86389	1.18125
O25	-1.07140	2.21956	-0.25378

Unsub-boat B'

C1	0.00583	-0.84032	-1.06764
O2	-1.26424	-0.51474	-1.25689
B3	-2.44987	-1.39460	-1.30293
O4	-1.76277	-2.54395	-2.39775
C5	-0.87808	-3.39946	-2.19131
C6	0.45094	-1.98113	-0.46874
C7	-2.92683	-2.08654	0.06613
C8	-3.59944	-0.71256	-2.17295
H9	-0.04593	-3.44061	-2.90853
C10	0.94522	0.16362	-1.68378
H11	1.51693	-2.16269	-0.39588
H12	-3.68172	-2.86072	-0.11822
H13	-2.15554	-2.51712	0.71258
H14	-3.42567	-1.31499	0.66782
H15	-4.43761	-1.39502	-2.35770
H16	-4.00816	0.15768	-1.64358
H17	-3.23021	-0.35985	-3.14213
H18	1.99139	-0.09922	-1.51555
H19	0.75718	0.24247	-2.76007
H20	0.75470	1.15275	-1.25409
H21	-0.19772	-2.59222	0.13883
C22	-1.03755	-4.59199	-1.29364
H23	-0.07124	-4.94653	-0.92922

H24	-1.71715	-4.39649	-0.46573
H25	-1.47299	-5.39246	-1.91018

Unsub-Chair

C1	0.00000	0.00000	0.00000
O2	0.00000	0.00000	1.31834
B3	1.27914	0.00000	2.16552
O4	2.13904	-1.12598	1.42765
C5	2.45741	-1.00932	0.20933
C6	0.26569	-1.14497	-0.70870
C7	2.06834	1.40696	2.10414
C8	0.93874	-0.56510	3.61937
C9	-0.24735	1.32804	-0.66863
H10	0.24427	-1.13687	-1.79336
H11	2.98207	1.37413	2.71073
H12	2.36650	1.74821	1.10242
H13	1.44007	2.20167	2.52415
H14	1.83932	-0.66808	4.23728
H15	0.26199	0.11402	4.15200
H16	0.44984	-1.54554	3.57737
H17	-0.24871	1.25234	-1.75829
H18	-1.21847	1.71275	-0.33897
H19	0.50291	2.05969	-0.35119
H20	0.24048	-2.10540	-0.20985
H21	2.60869	-0.01299	-0.21306
C22	3.09706	-2.16767	-0.49120
H23	2.97128	-2.09976	-1.57313
H24	4.17373	-2.13938	-0.27268
H25	2.69974	-3.11358	-0.11946

Unsub-Chair'

C1	-0.06651	-0.88100	-1.09755
O2	-1.31493	-0.50136	-1.28551
B3	-2.09238	0.46131	-0.40363
O4	-1.66394	-0.12925	1.05550
C5	-0.51020	-0.33039	1.51861
C6	0.23476	-1.87511	-0.20468
C7	-1.68408	2.01129	-0.57777
C8	-3.65375	0.14753	-0.52781
H9	-0.42613	-1.16410	2.22554
C10	0.98818	-0.15096	-1.89018
H11	1.25943	-2.20412	-0.06961
H12	-2.11797	2.62985	0.21809
H13	-0.61209	2.23913	-0.61281
H14	-2.10501	2.38251	-1.52078
H15	-4.24973	0.75872	0.16122
H16	-4.01053	0.37080	-1.54091
H17	-3.88224	-0.90486	-0.32464
H18	1.99501	-0.51722	-1.67763
H19	0.78242	-0.28548	-2.95775
H20	0.94172	0.92601	-1.69815
H21	-0.55606	-2.50123	0.18933
C22	0.59666	0.68286	1.58777

H23	1.55279	0.18986	1.77411
H24	0.66084	1.31059	0.70204
H25	0.37948	1.33648	2.44515

Optimized Transition Structures with (-)Ipc ligands (Fig.2):

(Z)-Chair-*Re*

C1	0.98771	0.65590	-0.81787
O2	-0.22157	0.44051	-1.30216
B3	-1.46891	0.13742	-0.43765
O4	-0.81744	-0.76999	0.68899
C5	0.16540	-0.34569	1.37281
C6	1.81052	-0.36833	-0.39879
C7	1.44184	2.09284	-0.71767
H8	2.77897	-0.06412	-0.00675
H9	2.46375	2.17368	-0.34018
H10	1.40103	2.54375	-1.71502
H11	0.77204	2.68283	-0.08506
H12	0.26424	0.72657	1.55459
C13	0.83169	-1.27604	2.33501
H14	1.83009	-0.92653	2.60474
H15	0.22160	-1.30106	3.24878
H16	0.87670	-2.28966	1.93329
C17	1.66210	-1.81988	-0.75955
H18	2.24948	-2.45535	-0.08924
H19	0.62111	-2.14622	-0.73172
H20	2.03002	-1.99817	-1.77804
H21	-1.16473	2.07903	0.58566
H22	-3.18304	-0.07337	-1.76799
C23	-2.81198	2.47166	-0.70176
C24	-2.04579	1.50326	0.27423
C25	-2.83658	1.21875	1.60514
H26	-2.14417	1.29408	2.45607
C27	-1.89190	-1.61799	-2.45029
C28	-2.51828	-0.78860	-1.27117
C29	-3.45124	-1.64263	-0.33623
H30	-4.37825	-1.08806	-0.14299
C31	-3.98892	3.19225	-0.00534
H32	-4.42479	3.94590	-0.67452
C33	-4.03771	2.15073	1.83766
H34	-4.50454	1.95510	2.81197
C35	-4.93195	2.10085	0.57125
C36	-3.71991	3.64378	1.48067
H37	-4.96681	1.15057	0.02868
H38	-5.95471	2.44236	0.74195
H39	-3.28660	1.87168	-1.49020
H40	-3.21666	0.19218	1.62450
C41	-4.82442	4.59910	1.97187
H42	-4.68330	5.59783	1.54109
H43	-5.83179	4.26834	1.70842
H44	-4.78469	4.70207	3.06319
C45	-2.38144	4.25605	1.91303
H46	-1.51682	3.63711	1.67531

H47	-2.23184	5.23359	1.43888
H48	-2.38001	4.42190	2.99805
C49	-1.87189	3.44589	-1.42738
H50	-2.43473	4.08221	-2.12075
H51	-1.34456	4.10573	-0.72943
H52	-1.12342	2.89904	-2.00717
C53	-2.56301	-2.99789	-2.61661
H54	-2.17939	-3.50749	-3.51082
C55	-3.78786	-3.03754	-0.89008
H56	-4.48915	-3.56304	-0.22838
C57	-2.45421	-3.73917	-1.25479
C58	-4.12734	-3.01211	-2.41914
H59	-2.53272	-4.82567	-1.33172
H60	-1.58813	-3.49160	-0.63076
H61	-0.84449	-1.83660	-2.20864
H62	-2.98221	-1.79913	0.64277
C63	-4.72816	-4.34783	-2.89630
H64	-5.75414	-4.46092	-2.52514
H65	-4.76938	-4.37675	-3.99200
H66	-4.15984	-5.22112	-2.56661
C67	-5.02596	-1.89717	-2.96853
H68	-5.02841	-1.90554	-4.06526
H69	-6.06169	-2.06076	-2.64394
H70	-4.73621	-0.89830	-2.64497
C71	-1.86197	-0.80904	-3.75677
H72	-1.31037	0.12469	-3.61418
H73	-1.36739	-1.37410	-4.55666
H74	-2.86923	-0.55638	-4.10373

(Z)-Chair-*Si*

C1	-0.36713	-0.72406	1.19966
O2	-1.33774	-0.34171	0.40805
B3	-1.15774	0.84526	-0.60611
O4	0.27587	0.51812	-1.13447
C5	1.26613	0.35601	-0.33483
C6	0.63853	-1.56802	0.75215
C7	-0.33863	-0.15061	2.59511
H8	1.41513	-1.80827	1.47643
H9	0.47802	-0.56048	3.19360
H10	-1.28917	-0.38649	3.08512
H11	-0.26252	0.94093	2.57306
H12	1.31771	0.96664	0.56930
C13	2.57420	-0.07584	-0.92534
H14	3.25128	-0.46726	-0.16333
H15	3.04407	0.80929	-1.37539
H16	2.42387	-0.81320	-1.71556
C17	0.50394	-2.50161	-0.41807
H18	1.47302	-2.72063	-0.87755
H19	-0.16597	-2.09822	-1.17716
H20	0.08830	-3.45970	-0.08017
H21	-0.27287	2.28396	0.84746
H22	-2.35063	1.65485	-2.25580
C23	-0.85391	3.51040	-0.79933

C24	-1.13427	2.29279	0.16416
C25	-2.39003	2.50020	1.08806
H26	-2.11768	2.27015	2.12625
C27	-1.74517	-0.23982	-3.01168
C28	-2.23400	0.65770	-1.81633
C29	-3.66359	0.26505	-1.28775
H30	-4.26878	1.17368	-1.17477
C31	-1.72475	4.73915	-0.45845
H32	-1.44565	5.59296	-1.09033
C33	-2.99411	3.91190	1.02123
H34	-3.84519	4.00739	1.70806
C35	-3.20963	4.28238	-0.46937
C36	-1.89736	5.02995	1.08011
H37	-3.46581	3.46466	-1.15037
H38	-3.92064	5.09701	-0.62039
H39	-1.15956	3.22854	-1.81643
H40	-3.18185	1.78970	0.83174
C41	-2.50643	6.42527	1.31111
H42	-1.75183	7.20368	1.14422
H43	-3.35133	6.64160	0.65287
H44	-2.85890	6.52361	2.34509
C45	-0.73023	4.88040	2.06337
H46	-0.24813	3.90354	2.02467
H47	0.03810	5.63970	1.87313
H48	-1.08505	5.03263	3.09073
C49	0.64042	3.86182	-0.89555
H50	0.79580	4.71050	-1.57229
H51	1.06605	4.13207	0.07644
H52	1.21605	3.02066	-1.29494
C53	-2.87727	-1.11162	-3.59420
H54	-2.52928	-1.64791	-4.48766
C55	-4.40842	-0.74112	-2.18049
H56	-5.41704	-0.93652	-1.79303
C57	-3.46760	-1.94904	-2.42526
C58	-4.28037	-0.40217	-3.70452
H59	-3.98539	-2.85567	-2.74551
H60	-2.78125	-2.20089	-1.60967
H61	-1.00469	-0.95732	-2.63432
H62	-3.59348	-0.18384	-0.29085
C63	-5.25017	-1.23588	-4.56277
H64	-6.28043	-0.88467	-4.42712
H65	-5.00404	-1.13166	-5.62672
H66	-5.23107	-2.30233	-4.32461
C67	-4.41792	1.05547	-4.16131
H68	-4.13594	1.16070	-5.21614
H69	-5.46451	1.37508	-4.07558
H70	-3.81466	1.75576	-3.58478
C71	-1.01865	0.58804	-4.08363
H72	-0.17436	1.13052	-3.64635
H73	-0.62612	-0.05735	-4.87933
H74	-1.68175	1.32336	-4.55038

Unsub-boat A-*Re*

B1	9.14586	0.79772	-0.18358
H2	9.89696	-0.97316	-1.26035
H3	9.85848	2.80436	-0.72354
C4	10.63529	0.65140	-2.43350
C5	10.31094	0.01602	-1.03031
C6	11.58369	-0.26470	-0.14756
H7	11.53762	-1.29630	0.22464
C8	8.01899	3.21301	0.27787
C9	9.35263	2.38764	0.15486
C10	10.32977	2.60748	1.36686
H11	11.34324	2.78646	0.98737
C12	12.15037	0.65287	-2.73341
H13	12.33895	1.02727	-3.74848
C14	12.91443	-0.03542	-0.88097
H15	13.76705	-0.27124	-0.23073
C16	12.86823	1.36238	-1.55260
C17	12.91467	-0.66152	-2.31667
H18	12.30186	2.14280	-1.03425
H19	13.85307	1.75870	-1.80798
H20	10.35433	1.71470	-2.41253
H21	11.59100	0.36863	0.74437
C22	14.32560	-0.69422	-2.93240
H23	14.27105	-0.94477	-3.99889
H24	14.85665	0.25699	-2.84591
H25	14.93907	-1.46134	-2.44425
C26	12.30155	-2.05230	-2.51862
H27	11.31245	-2.16288	-2.07471
H28	12.21882	-2.29047	-3.58603
H29	12.95130	-2.81400	-2.06880
C30	9.81592	0.02050	-3.57220
H31	10.03772	0.51144	-4.52767
H32	10.03278	-1.04582	-3.69058
H33	8.74455	0.12629	-3.38134
C34	8.07792	4.26861	1.40248
H35	7.17231	4.89038	1.39356
C36	9.91913	3.75204	2.30811
H37	10.66384	3.89146	3.10245
C38	8.44073	3.52609	2.71811
C39	9.45186	5.02938	1.53164
H40	8.14580	4.05866	3.62456
H41	8.11285	2.48348	2.79519
H42	7.20695	2.53900	0.59247
H43	10.38685	1.70116	1.97977
C44	9.31440	6.25077	2.45957
H45	10.30380	6.62067	2.75454
H46	8.79848	7.06776	1.94046
H47	8.75528	6.03858	3.37429
C48	10.24480	5.48611	0.30101
H49	9.70982	6.27995	-0.23446
H50	11.20901	5.90531	0.61563
H51	10.45321	4.68675	-0.40919
C52	7.58969	3.81478	-1.07020

H53	7.50822	3.04010	-1.83919
H54	6.61657	4.31461	-0.98639
H55	8.31140	4.55542	-1.42743
C56	7.58737	-1.78559	0.25906
C57	8.09361	-0.99727	1.26929
H58	6.94719	-2.61800	0.53058
H59	8.02428	-1.80995	-0.72802
C60	7.70490	-1.21530	2.70858
H61	8.61200	-1.29984	3.31597
H62	7.15099	-0.34841	3.08710
H63	7.10324	-2.11632	2.83934
C64	6.72334	0.23080	-0.63069
O65	7.84073	0.62150	-1.08553
H66	6.42042	0.52931	0.37413
C67	5.65632	-0.18395	-1.59302
H68	4.90348	-0.80633	-1.10596
H69	5.16016	0.72425	-1.96341
H70	6.08704	-0.70649	-2.44919
O71	8.83169	0.07805	1.10545

Unsub-boat A-*Si*

H1	8.41573	-1.75415	-1.61328
H2	9.19086	1.78081	-2.53202
C3	9.49225	-0.97795	-3.26648
C4	9.28715	-1.09842	-1.71508
C5	10.45443	-1.85890	-0.99796
H6	10.02593	-2.51792	-0.22980
C7	8.74688	2.98528	-0.81824
C8	9.42874	1.72028	-1.46208
C9	10.99626	1.73215	-1.35196
H10	11.43027	1.50484	-2.33322
C11	10.53507	-1.99383	-3.78984
H12	10.54705	-2.00053	-4.88794
C13	11.34461	-2.67432	-1.95363
H14	12.07480	-3.27545	-1.39590
C15	11.87174	-1.71089	-3.04917
C16	10.52609	-3.40166	-3.07798
H17	12.05291	-0.67551	-2.74613
H18	12.75537	-2.08104	-3.57246
H19	9.92446	0.00558	-3.49644
H20	11.10668	-1.16664	-0.45273
C21	11.39566	-4.40939	-3.85592
H22	10.86524	-4.75626	-4.75104
H23	12.35345	-3.99778	-4.18219
H24	11.60721	-5.28978	-3.23689
C25	9.22403	-4.13439	-2.72643
H26	8.53876	-3.55564	-2.10918
H27	8.68708	-4.42339	-3.63814
H28	9.45410	-5.06012	-2.18346
C29	8.15629	-1.05212	-4.02163
H30	8.30552	-0.90833	-5.09836
H31	7.66651	-2.02173	-3.87974
H32	7.46597	-0.27855	-3.67043

C33	9.77221	4.07373	-0.43417
H34	9.25834	4.97238	-0.06687
C35	11.58385	3.04986	-0.82192
H36	12.68070	3.01057	-0.80231
C37	10.83826	3.41819	0.48673
C38	10.92263	4.30363	-1.48707
H39	11.37749	4.12887	1.11647
H40	10.50155	2.58104	1.10861
H41	8.28896	2.69490	0.14046
H42	11.34444	0.93920	-0.68017
C43	11.69770	5.59814	-1.17975
H44	12.63955	5.62287	-1.74110
H45	11.11116	6.47446	-1.48148
H46	11.94175	5.71553	-0.12088
C47	10.65358	4.28447	-2.99628
H48	10.04370	5.14570	-3.29467
H49	11.60234	4.35810	-3.54297
H50	10.14757	3.38270	-3.33954
C51	7.60279	3.53667	-1.68474
H52	6.86689	2.75516	-1.88958
H53	7.09318	4.36604	-1.17831
H54	7.96769	3.91137	-2.64564
C55	6.68020	-1.24969	0.51903
C56	6.39760	-0.25334	-0.39231
H57	5.85529	-1.67793	1.07833
H58	7.59106	-1.82859	0.48196
C59	5.00314	0.29482	-0.54984
H60	4.70792	0.22676	-1.60227
H61	4.98052	1.35738	-0.28255
H62	4.27783	-0.24928	0.05756
B63	8.78977	0.29794	-0.99524
C64	8.21662	0.27586	1.46427
O65	9.08215	0.09695	0.55452
H66	7.47725	1.07011	1.35321
C67	8.50666	-0.23171	2.84083
H68	7.59017	-0.34890	3.42187
H69	9.14104	0.50708	3.35074
H70	9.05497	-1.17461	2.79678
O71	7.28333	0.40535	-1.10635

Optimized Transition Structures with oxazolidinone auxiliaries (Fig. 3):

(Z)-Chair-Si

N1	10.09158	1.16986	-0.43593
C2	10.18488	2.18063	-1.50295
C3	11.05857	3.23083	-0.78776
O4	11.71116	2.52999	0.28775
H5	9.19217	2.58524	-1.70627
H6	11.83017	3.66232	-1.42717
H7	10.45548	4.03716	-0.35752
C8	11.05697	1.36383	0.54154
O9	11.30728	0.66072	1.49533
C10	10.76072	1.61001	-2.82102

H11	10.06461	0.81730	-3.12313
C12	10.74068	2.68483	-3.91760
H13	9.73986	3.11212	-4.04280
H14	11.43275	3.50611	-3.69618
H15	11.04375	2.25752	-4.87816
C16	12.15427	0.98750	-2.65867
H17	12.89885	1.72538	-2.33914
H18	12.15062	0.17436	-1.92691
H19	12.49516	0.57089	-3.61167
C20	9.53176	-1.16726	0.03421
C21	9.25083	0.03106	-0.56516
H22	10.46213	-1.24743	0.58263
B23	6.87176	0.76851	-0.57931
C24	5.61542	0.34658	-1.47100
H25	5.64345	0.85225	-2.44415
H26	5.58601	-0.73175	-1.66786
H27	4.66629	0.62299	-0.99572
C28	6.94558	2.32080	-0.14427
H29	6.96386	2.96266	-1.03415
H30	6.04686	2.60483	0.41740
H31	7.80905	2.60711	0.47033
C32	7.79462	-0.11678	1.55853
O33	6.83820	-0.14079	0.73104
H34	8.41776	0.77546	1.64363
C35	7.83309	-1.10385	2.67569
H36	8.85344	-1.23637	3.03961
H37	7.22845	-0.70282	3.50153
H38	7.39956	-2.05779	2.37053
O39	8.15199	0.23602	-1.26688
C40	8.75353	-2.41896	-0.25330
H41	7.72802	-2.19917	-0.55492
H42	9.22541	-2.98086	-1.07040
H43	8.73554	-3.08528	0.61587

(Z)-Chair-Re:

C1	-0.20042	-9.77309	-0.90523
O2	-1.16226	-9.83273	-0.03314
B3	-0.93343	-10.62670	1.34853
O4	-0.14694	-11.85324	0.85159
C5	0.94442	-11.70522	0.18659
C6	0.09281	-10.83659	-1.74272
C7	-0.05907	-9.75089	2.38067
C8	-2.36893	-11.11012	1.85431
H9	0.92256	-10.71460	-2.42784
H10	0.16982	-10.34243	3.27658
H11	0.89586	-9.37594	1.99138
H12	-0.62381	-8.87654	2.72624
H13	-2.28866	-11.71119	2.76866
H14	-3.01219	-10.25421	2.09202
H15	-2.89615	-11.71655	1.10802
H16	1.58559	-10.85013	0.40034
C17	1.62221	-12.93126	-0.33901
H18	2.35560	-12.67085	-1.10366

H19	2.15354	-13.40409	0.49842
H20	0.89824	-13.65146	-0.72450
C21	-0.92512	-11.90390	-2.04848
H22	-0.44529	-12.79546	-2.46287
H23	-1.49620	-12.18728	-1.16309
H24	-1.63638	-11.54174	-2.80165
N25	0.61492	-8.60338	-0.86288
C26	0.10748	-7.19747	-0.85894
C27	1.43150	-6.49224	-0.54883
O28	2.43820	-7.32888	-1.14284
H29	1.50893	-5.49723	-0.98635
H30	1.61683	-6.44027	0.53053
C31	1.96697	-8.60171	-1.20700
O32	2.66865	-9.54516	-1.49554
C33	-1.06816	-6.82260	0.07236
H34	-0.97108	-7.41112	0.98886
H35	-0.18651	-6.95290	-1.89247
C36	-1.00779	-5.32583	0.43664
H37	-0.11157	-5.05974	1.00501
H38	-1.04455	-4.69408	-0.45929
H39	-1.87206	-5.06356	1.05358
C40	-2.42895	-7.12065	-0.57836
H41	-2.55835	-6.51878	-1.48686
H42	-2.54043	-8.17405	-0.83348
H43	-3.23886	-6.85712	0.10929

Unsub-boat A-Si:

N1	10.73642	0.88432	-0.57250
C2	10.77751	2.15782	-1.31303
C3	12.09996	2.72974	-0.76962
O4	12.83683	1.59604	-0.28123
H5	9.93120	2.77773	-1.01058
H6	12.70446	3.22451	-1.53119
H7	11.93539	3.42261	0.06311
C8	11.99021	0.54841	-0.06862
O9	12.33779	-0.46969	0.47988
C10	10.71857	1.96745	-2.84865
H11	9.77306	1.44785	-3.04080
C12	10.64909	3.33239	-3.54876
H13	9.81701	3.93604	-3.16998
H14	11.57251	3.90860	-3.41465
H15	10.50359	3.20271	-4.62538
C16	11.86061	1.10261	-3.40031
H17	12.84203	1.56175	-3.23625
H18	11.87303	0.10894	-2.94304
H19	11.74022	0.96591	-4.47956
C20	9.55537	-1.18116	-0.00541
C21	9.57086	0.08532	-0.51596
H22	10.48034	-1.64287	0.30377
H23	8.67236	-1.78862	-0.12286
B24	7.06661	0.44825	-0.77574
C25	6.56224	-0.66052	-1.82300
H26	6.56705	-0.23916	-2.83598

H27	7.17574	-1.56789	-1.85242
H28	5.53156	-0.96755	-1.61020
C29	6.23849	1.82163	-0.71298
H30	6.33064	2.36540	-1.66125
H31	5.16952	1.64842	-0.54417
H32	6.59516	2.49487	0.07842
C33	7.78499	-0.12311	1.57397
O34	6.91521	-0.25437	0.67997
H35	8.45480	0.73952	1.55391
C36	7.72860	-0.95760	2.80764
H37	8.73547	-1.18107	3.16651
H38	7.21527	-0.38458	3.59278
H39	7.17153	-1.87767	2.62538
O40	8.52409	0.79344	-0.91312

Unsub-boat A-Re:

N1	10.88344	0.60885	-0.18367
C2	12.21440	0.01563	-0.36354
C3	13.07329	1.30240	-0.32601
O4	12.17030	2.39298	-0.57349
H5	13.53589	1.45265	0.65511
H6	13.84961	1.32158	-1.09270
C7	10.88246	1.98409	-0.38827
O8	9.93714	2.73247	-0.36140
C9	9.40238	-0.91254	0.95635
C10	9.68424	-0.15006	-0.16597
H11	10.12612	-0.91814	1.76355
H12	8.71335	-1.74323	0.89691
B13	7.36731	-0.17329	-1.21936
C14	7.04861	-1.63345	-1.81041
H15	7.36993	-1.70782	-2.85602
H16	7.53946	-2.44722	-1.26079
H17	5.97062	-1.83389	-1.78893
C18	6.73201	1.09076	-1.97287
H19	7.07456	1.13343	-3.01365
H20	5.63721	1.03220	-1.99424
H21	7.01206	2.04210	-1.50454
C22	7.56738	0.38088	1.19535
O23	6.89357	-0.18978	0.27144
H24	8.10669	1.30325	0.96435
C25	7.14298	0.15220	2.61364
H26	7.93898	0.40910	3.31465
H27	6.28430	0.80613	2.81939
H28	6.82359	-0.88120	2.76160
O29	8.90149	0.05636	-1.17150
C30	12.33055	-0.83145	-1.65358
H31	11.58374	-1.63139	-1.55053
C32	13.71181	-1.49724	-1.73221
H33	14.51097	-0.75911	-1.86832
H34	13.93647	-2.07286	-0.82708
H35	13.75737	-2.18273	-2.58348
C36	11.99683	-0.04220	-2.92728
H37	12.68658	0.79534	-3.08162

H38	12.07371	-0.69415	-3.80294
H39	10.97845	0.35286	-2.89545
H40	12.45936	-0.62407	0.49255