

Supporting Information
to accompany

**Vinylogous Mannich Reactions: Some Theoretical Studies on the
Origins of Diastereoselectivity**

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PDB files for the transitions states **A - D**:

HEADER

REMARK Transition State A

HETATM	1	H	UNK	0001	-2.466	-0.192	1.098
HETATM	2	O	UNK	0001	1.334	1.382	-0.026
HETATM	3	C	UNK	0001	1.192	1.330	-1.439
HETATM	4	C	UNK	0001	1.680	0.112	-1.844
HETATM	5	C	UNK	0001	2.010	-0.639	-0.700
HETATM	6	C	UNK	0001	1.772	0.170	0.375
HETATM	7	C	UNK	0001	2.300	0.950	2.619
HETATM	8	H	UNK	0001	1.131	2.268	-1.935
HETATM	9	H	UNK	0001	-1.001	0.593	-2.408
HETATM	10	H	UNK	0001	1.756	-0.218	-2.854
HETATM	11	H	UNK	0001	-2.417	2.195	1.261
HETATM	12	C	UNK	0001	-0.941	-1.511	-0.904
HETATM	13	H	UNK	0001	2.386	-1.632	-0.658
HETATM	14	H	UNK	0001	-0.774	-0.117	1.592
HETATM	15	O	UNK	0001	1.835	-0.078	1.664
HETATM	16	C	UNK	0001	-1.561	2.080	-0.753
HETATM	17	C	UNK	0001	-1.545	1.790	0.773
HETATM	18	C	UNK	0001	-1.502	0.243	0.887
HETATM	19	N	UNK	0001	-1.097	-0.173	-0.497
HETATM	20	H	UNK	0001	-1.327	-4.211	0.839
HETATM	21	H	UNK	0001	-2.580	2.173	-1.120
HETATM	22	H	UNK	0001	-1.022	2.971	-1.030
HETATM	23	H	UNK	0001	-0.658	2.217	1.209
HETATM	24	O	UNK	0001	-0.675	-1.803	-2.039
HETATM	25	O	UNK	0001	-1.153	-2.326	0.107
HETATM	26	H	UNK	0001	1.669	1.820	2.556
HETATM	27	H	UNK	0001	3.325	1.203	2.396
HETATM	28	H	UNK	0001	2.221	0.475	3.579
HETATM	29	C	UNK	0001	-1.065	-3.780	-0.109
HETATM	30	H	UNK	0001	-0.059	-4.037	-0.394
HETATM	31	H	UNK	0001	-1.758	-4.070	-0.882
HETATM	32	C	UNK	0001	-1.007	0.816	-1.365
CONNECT	1	18					
CONNECT	2	3	6				
CONNECT	3	2	8	4	32		
CONNECT	4	3	10	5			
CONNECT	5	4	13	6			
CONNECT	6	2	5	15			
CONNECT	7	15	26	27	28		
CONNECT	8	3					
CONNECT	9	32					
CONNECT	10	4					
CONNECT	11	17					

CONNECT 12 19 24 25
CONNECT 13 5
CONNECT 14 18
CONNECT 15 6 7
CONNECT 16 32 21 22 17
CONNECT 17 11 16 23 18
CONNECT 18 1 14 17 19
CONNECT 19 12 18 32
CONNECT 20 29
CONNECT 21 16
CONNECT 22 16
CONNECT 23 17
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CONNECT 25 12 29
CONNECT 26 7
CONNECT 27 7
CONNECT 28 7
CONNECT 29 20 25 30 31
CONNECT 30 29
CONNECT 31 29
CONNECT 32 3 9 16 19
END

HEADER

REMARK Transition State B

HETATM	1	H	UNK	0001	2.522	1.645	-1.727
HETATM	2	O	UNK	0001	-2.365	-0.025	0.395
HETATM	3	C	UNK	0001	-1.433	-0.835	-0.314
HETATM	4	C	UNK	0001	-1.016	-1.807	0.554
HETATM	5	C	UNK	0001	-1.592	-1.564	1.822
HETATM	6	C	UNK	0001	-2.416	-0.486	1.667
HETATM	7	C	UNK	0001	-4.187	1.115	2.122
HETATM	8	H	UNK	0001	-1.487	-0.781	-1.374
HETATM	9	H	UNK	0001	0.195	0.333	1.071
HETATM	10	H	UNK	0001	-0.337	-2.594	0.323
HETATM	11	H	UNK	0001	0.514	2.775	-2.450
HETATM	12	C	UNK	0001	2.257	-0.785	-0.137
HETATM	13	H	UNK	0001	-1.451	-2.116	2.719
HETATM	14	H	UNK	0001	1.863	0.311	-2.672
HETATM	15	O	UNK	0001	-3.169	0.140	2.535
HETATM	16	C	UNK	0001	-0.232	1.859	-0.597
HETATM	17	C	UNK	0001	0.344	1.793	-2.036
HETATM	18	C	UNK	0001	1.667	1.005	-1.874
HETATM	19	N	UNK	0001	1.422	0.248	-0.600
HETATM	20	H	UNK	0001	5.072	-1.806	-1.370
HETATM	21	H	UNK	0001	0.173	2.714	-0.059
HETATM	22	H	UNK	0001	-1.305	1.892	-0.537
HETATM	23	H	UNK	0001	-0.335	1.255	-2.681

HETATM 24 O UNK 0001 1.988 -1.435 0.838
HETATM 25 O UNK 0001 3.305 -0.912 -0.923
HETATM 26 H UNK 0001 -4.865 0.661 1.418
HETATM 27 H UNK 0001 -3.709 1.977 1.684
HETATM 28 H UNK 0001 -4.690 1.374 3.035
HETATM 29 C UNK 0001 4.324 -1.930 -0.609
HETATM 30 H UNK 0001 3.875 -2.909 -0.651
HETATM 31 H UNK 0001 4.723 -1.743 0.374
HETATM 32 C UNK 0001 0.347 0.631 0.056
CONNECT 1 18
CONNECT 2 3 6
CONNECT 3 2 8 4 32
CONNECT 4 3 10 5
CONNECT 5 4 13 6
CONNECT 6 2 5 15
CONNECT 7 15 26 27 28
CONNECT 8 3
CONNECT 9 32
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CONNECT 11 17
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CONNECT 28 7
CONNECT 29 20 25 30 31
CONNECT 30 29
CONNECT 31 29
CONNECT 32 3 9 16 19
END

HEADER

REMARK Transition State C

HETATM 1 H UNK 0001 2.980 1.061 -0.478
HETATM 2 O UNK 0001 -1.607 -1.166 -0.123
HETATM 3 C UNK 0001 -0.873 -1.703 -1.220

HETATM	4	C	UNK	0001	0.102	-2.503	-0.678
HETATM	5	C	UNK	0001	0.076	-2.370	0.719
HETATM	6	C	UNK	0001	-0.992	-1.551	1.005
HETATM	7	C	UNK	0001	-2.726	-0.398	2.257
HETATM	8	H	UNK	0001	-1.397	-1.741	-2.145
HETATM	9	H	UNK	0001	-0.740	0.669	-1.607
HETATM	10	H	UNK	0001	0.772	-3.115	-1.238
HETATM	11	H	UNK	0001	3.350	-0.107	-2.530
HETATM	12	C	UNK	0001	0.417	1.133	0.695
HETATM	13	H	UNK	0001	0.708	-2.834	1.437
HETATM	14	H	UNK	0001	2.675	-0.531	0.212
HETATM	15	O	UNK	0001	-1.423	-1.096	2.149
HETATM	16	C	UNK	0001	1.164	-0.035	-2.689
HETATM	17	C	UNK	0001	2.485	-0.465	-1.993
HETATM	18	C	UNK	0001	2.407	0.154	-0.573
HETATM	19	N	UNK	0001	0.953	0.505	-0.447
HETATM	20	H	UNK	0001	1.874	1.764	3.514
HETATM	21	H	UNK	0001	1.302	0.898	-3.230
HETATM	22	H	UNK	0001	0.769	-0.767	-3.373
HETATM	23	H	UNK	0001	2.542	-1.541	-1.931
HETATM	24	O	UNK	0001	-0.713	1.540	0.743
HETATM	25	O	UNK	0001	1.333	1.210	1.636
HETATM	26	H	UNK	0001	-3.500	-1.021	1.840
HETATM	27	H	UNK	0001	-2.654	0.540	1.738
HETATM	28	H	UNK	0001	-2.862	-0.264	3.314
HETATM	29	C	UNK	0001	0.956	1.743	2.958
HETATM	30	H	UNK	0001	0.238	1.073	3.402
HETATM	31	H	UNK	0001	0.537	2.729	2.842
HETATM	32	C	UNK	0001	0.247	0.267	-1.534
CONNECT	1	18					
CONNECT	2	3	6				
CONNECT	3	2	8	4	32		
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CONNECT	7	15	26	27	28		
CONNECT	8	3					
CONNECT	9	32					
CONNECT	10	4					
CONNECT	11	17					
CONNECT	12	19	24	25			
CONNECT	13	5					
CONNECT	14	18					
CONNECT	15	6	7				
CONNECT	16	32	21	22	17		
CONNECT	17	11	16	23	18		
CONNECT	18	1	14	17	19		
CONNECT	19	12	18	32			

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CONNECT 29 20 25 30 31
CONNECT 30 29
CONNECT 31 29
CONNECT 32 3 9 16 19
END

HEADER

REMARK Transition State **D**

HETATM	1	H	UNK	0001	-1.974	-1.796	-1.994
HETATM	2	O	UNK	0001	0.551	1.533	1.005
HETATM	3	C	UNK	0001	0.354	2.041	-0.312
HETATM	4	C	UNK	0001	1.576	2.473	-0.752
HETATM	5	C	UNK	0001	2.551	2.147	0.211
HETATM	6	C	UNK	0001	1.872	1.601	1.273
HETATM	7	C	UNK	0001	1.437	0.670	3.479
HETATM	8	H	UNK	0001	-0.644	2.315	-0.554
HETATM	9	H	UNK	0001	1.352	-0.147	-0.801
HETATM	10	H	UNK	0001	1.756	2.963	-1.682
HETATM	11	H	UNK	0001	-1.738	-0.213	-3.796
HETATM	12	C	UNK	0001	-0.599	-1.347	0.488
HETATM	13	H	UNK	0001	3.598	2.323	0.172
HETATM	14	H	UNK	0001	-2.699	-0.431	-1.147
HETATM	15	O	UNK	0001	2.324	1.167	2.414
HETATM	16	C	UNK	0001	0.152	0.181	-2.746
HETATM	17	C	UNK	0001	-1.398	0.156	-2.841
HETATM	18	C	UNK	0001	-1.831	-0.774	-1.682
HETATM	19	N	UNK	0001	-0.634	-0.723	-0.775
HETATM	20	H	UNK	0001	-2.958	-3.035	1.929
HETATM	21	H	UNK	0001	0.581	-0.655	-3.295
HETATM	22	H	UNK	0001	0.604	1.091	-3.097
HETATM	23	H	UNK	0001	-1.793	1.150	-2.691
HETATM	24	O	UNK	0001	0.390	-1.388	1.168
HETATM	25	O	UNK	0001	-1.775	-1.876	0.755
HETATM	26	H	UNK	0001	0.935	-0.213	3.129
HETATM	27	H	UNK	0001	0.732	1.440	3.750
HETATM	28	H	UNK	0001	2.104	0.453	4.293
HETATM	29	C	UNK	0001	-1.968	-2.625	2.008
HETATM	30	H	UNK	0001	-1.890	-1.947	2.842
HETATM	31	H	UNK	0001	-1.222	-3.400	2.082

HETATM 32 C UNK 0001 0.400 -0.092 -1.286

CONNECT 1 18
CONNECT 2 3 6
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