

**The Origin of Diastereofacial Control in Allylboration Reactions Using Tartrate Ester
Derived Allylboronates: Attractive Interactions Between The Boron-Coordinated
Aldehyde Carbonyl Group and An Ester Carbonyl Oxygen**

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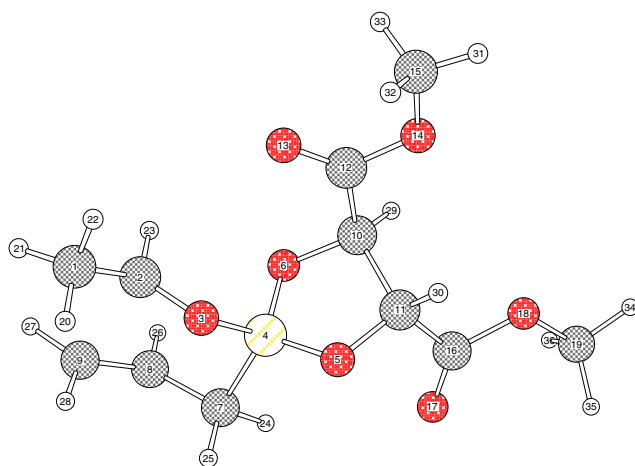
Supporting Information

Table Relative Energies (kcal/mol) for Transition States, Total Energies in atomic units in Parenthesis
Basis Set

Structure	HF/6-31G*	B3LYP/6-31G*	B3LYP/6-31G** ^a
11a	0.0 (-975.2384692)	0.0 (-980.8893318)	0.0 (-980.9133938)
11b	1.84 (-975.2355431)	1.64 (-980.8867259)	1.48 (-980.9110326)
11c	2.79 (-975.2340304)	2.37 (-980.8855591)	2.20 (-980.9098845)
12a	2.0 (-975.2352894)	1.75 (-980.8865351)	1.63 (-980.9107944)
12b	1.63 (-975.2358665)	1.84 (-980.886400)	1.86 (-980.9104351)
12c	2.75 (-975.2340902)	2.47 (-980.8853903)	2.37 (-980.9096095)
13	0.0 (-934.4041699)	0.0 (-939.9441363)	0.0 (-939.9724120)
14	2.23 (-934.4006209)	2.14 (-939.9407279)	2.18 (-939.9689309)

^a Single-point calculations using B3LYP/6-31G* structure.

Internal Coordinates from Optimized Structures (B3LYP/6-31G*)



11a

B(4)

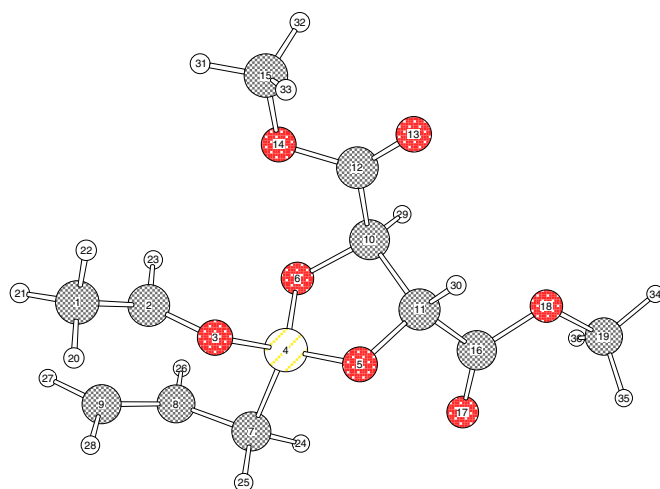
O(5) B(4) 1.435

O(6) B(4) 1.453 O(5) 108.064

C(10) O(6) 1.399 B(4) 107.584 O(5) -15.646 Dihedral

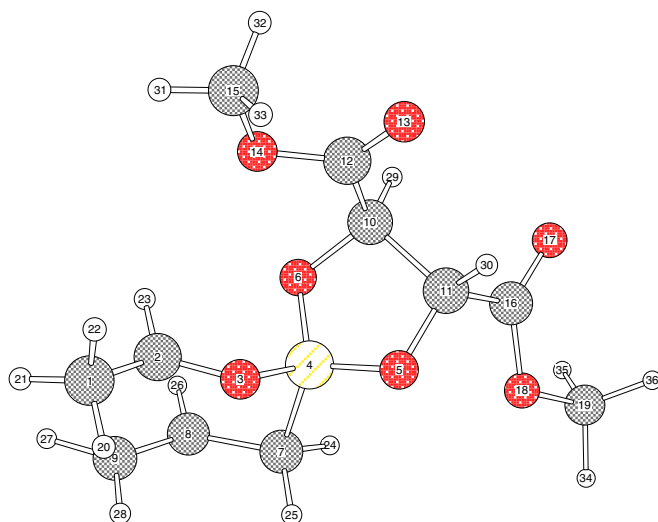
C(11) O(5) 1.398 B(4) 108.849 O(6) -2.417 Dihedral

O(3)	B(4)	1.527	O(5)	109.128	O(6)	112.324	Pro-R
C(7)	B(4)	1.710	O(3)	101.484	O(5)	114.971	Pro-S
C(12)	C(10)	1.534	O(6)	111.575	C(11)	111.833	Pro-R
C(16)	C(11)	1.532	O(5)	111.229	C(10)	109.755	Pro-R
H(29)	C(10)	1.097	O(6)	110.791	C(11)	111.627	Pro-S
H(30)	C(11)	1.095	O(5)	111.251	C(10)	111.710	Pro-S
C(2)	O(3)	1.282	B(4)	118.171	O(5)	162.762	Dihedral
C(1)	C(2)	1.500	O(3)	117.597	B(4)	174.901	Dihedral
H(23)	C(2)	1.090	C(1)	118.447	O(3)	117.431	Pro-R
C(8)	C(7)	1.444	B(4)	103.954	O(3)	61.253	Dihedral
H(24)	C(7)	1.092	B(4)	103.739	C(8)	115.053	Pro-S
H(25)	C(7)	1.093	B(4)	107.169	C(8)	114.539	Pro-R
C(9)	C(8)	1.373	C(7)	123.880	B(4)	-81.582	Dihedral
H(26)	C(8)	1.090	C(7)	116.776	C(9)	117.600	Pro-S
O(14)	C(12)	1.351	C(10)	110.152	O(6)	-175.048	Dihedral
O(13)	C(12)	1.210	C(10)	125.964	O(14)	123.883	Pro-S
C(15)	O(14)	1.437	C(12)	115.566	C(10)	-179.673	Dihedral
O(18)	C(16)	1.354	C(11)	110.049	O(5)	-161.796	Dihedral
O(17)	C(16)	1.209	C(11)	125.982	O(18)	123.942	Pro-R
C(19)	O(18)	1.437	C(16)	115.369	C(11)	-177.373	Dihedral
H(20)	C(1)	1.093	C(2)	111.130	O(3)	-38.328	Dihedral
H(21)	C(1)	1.093	C(2)	111.795	H(20)	110.214	Pro-R
H(22)	C(1)	1.099	C(2)	107.405	H(20)	108.133	Pro-S
H(27)	C(9)	1.087	C(8)	120.768	C(7)	175.010	Dihedral
H(28)	C(9)	1.087	C(8)	120.207	H(27)	116.103	Pro-S
H(31)	C(15)	1.090	O(14)	105.598	C(12)	179.789	Dihedral
H(32)	C(15)	1.093	O(14)	110.526	H(31)	110.608	Pro-R
H(33)	C(15)	1.093	O(14)	110.500	H(31)	110.597	Pro-S
H(34)	C(19)	1.090	O(18)	105.643	C(16)	179.170	Dihedral
H(35)	C(19)	1.093	O(18)	110.496	H(34)	110.570	Pro-S
H(36)	C(19)	1.093	O(18)	110.621	H(34)	110.620	Pro-R



11b

B(4)						
O(5)	B(4)	1.431				
O(6)	B(4)	1.451	O(5)	108.316		
C(10)	O(6)	1.404	B(4)	107.565	O(5)	-12.217 Dihedral
C(11)	O(5)	1.402	B(4)	108.648	O(6)	-6.152 Dihedral
O(3)	B(4)	1.546	O(5)	108.884	O(6)	111.415 Pro-R
C(7)	B(4)	1.701	O(3)	101.262	O(5)	115.033 Pro-S
C(12)	C(10)	1.534	O(6)	115.082	C(11)	110.406 Pro-R
C(16)	C(11)	1.532	O(5)	111.178	C(10)	110.237 Pro-R
H(29)	C(10)	1.098	O(6)	110.215	C(11)	111.690 Pro-S
H(30)	C(11)	1.094	O(5)	111.442	C(10)	111.044 Pro-S
C(2)	O(3)	1.276	B(4)	118.461	O(5)	163.622 Dihedral
C(1)	C(2)	1.500	O(3)	118.077	B(4)	173.065 Dihedral
H(23)	C(2)	1.090	C(1)	118.864	O(3)	117.750 Pro-R
C(8)	C(7)	1.447	B(4)	105.106	O(3)	61.154 Dihedral
H(24)	C(7)	1.092	B(4)	103.466	C(8)	114.792 Pro-S
H(25)	C(7)	1.093	B(4)	107.466	C(8)	114.181 Pro-R
C(9)	C(8)	1.369	C(7)	124.098	B(4)	-83.583 Dihedral
H(26)	C(8)	1.091	C(7)	116.723	C(9)	117.656 Pro-S
O(14)	C(12)	1.348	C(10)	113.500	O(6)	-10.354 Dihedral
O(13)	C(12)	1.213	C(10)	122.761	O(14)	123.714 Pro-R
C(15)	O(14)	1.438	C(12)	114.596	C(10)	-178.241 Dihedral
O(18)	C(16)	1.352	C(11)	110.046	O(5)	-162.146 Dihedral
O(17)	C(16)	1.210	C(11)	126.017	O(18)	123.912 Pro-R
C(19)	O(18)	1.437	C(16)	115.459	C(11)	-177.579 Dihedral
H(20)	C(1)	1.093	C(2)	111.048	O(3)	-37.715 Dihedral
H(21)	C(1)	1.092	C(2)	111.780	H(20)	110.224 Pro-R
H(22)	C(1)	1.100	C(2)	107.860	H(20)	107.883 Pro-S
H(27)	C(9)	1.087	C(8)	121.036	C(7)	174.799 Dihedral
H(28)	C(9)	1.087	C(8)	120.433	H(27)	116.277 Pro-S
H(31)	C(15)	1.091	O(14)	105.598	C(12)	178.770 Dihedral
H(32)	C(15)	1.093	O(14)	110.567	H(31)	110.565 Pro-R
H(33)	C(15)	1.093	O(14)	110.544	H(31)	110.690 Pro-S
H(34)	C(19)	1.090	O(18)	105.617	C(16)	179.816 Dihedral
H(35)	C(19)	1.093	O(18)	110.483	H(34)	110.602 Pro-S
H(36)	C(19)	1.094	O(18)	110.614	H(34)	110.623 Pro-R

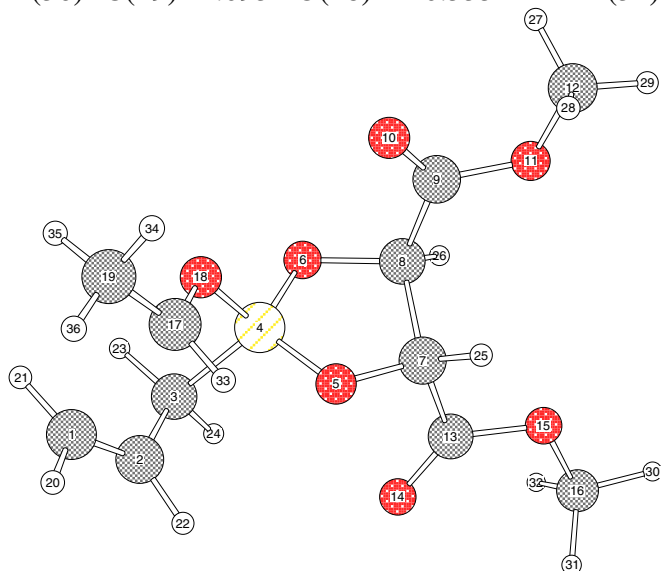


11c

B(4)

O(5)	B(4)	1.431			
O(6)	B(4)	1.448	O(5)	108.546	
C(10)	O(6)	1.410	B(4)	107.065	O(5) -14.548 Dihedral
C(11)	O(5)	1.406	B(4)	108.218	O(6) -4.266 Dihedral
O(3)	B(4)	1.542	O(5)	109.032	O(6) 111.873 Pro-R
C(7)	B(4)	1.709	O(3)	101.089	O(5) 114.833 Pro-S
C(12)	C(10)	1.534	O(6)	114.614	C(11) 110.960 Pro-R
C(16)	C(11)	1.534	O(5)	114.293	C(10) 110.163 Pro-R
H(29)	C(10)	1.096	O(6)	110.419	C(11) 111.020 Pro-S
H(30)	C(11)	1.096	O(5)	110.813	C(10) 110.719 Pro-S
C(2)	O(3)	1.279	B(4)	118.455	O(5) 164.139 Dihedral
C(1)	C(2)	1.500	O(3)	117.860	B(4) 173.650 Dihedral
H(23)	C(2)	1.090	C(1)	118.730	O(3) 117.628 Pro-R
C(8)	C(7)	1.446	B(4)	104.859	O(3) 60.877 Dihedral
H(24)	C(7)	1.092	B(4)	104.089	C(8) 114.334 Pro-S
H(25)	C(7)	1.093	B(4)	107.322	C(8) 114.450 Pro-R
C(9)	C(8)	1.371	C(7)	123.959	B(4) -82.910 Dihedral
H(26)	C(8)	1.090	C(7)	116.752	C(9) 117.685 Pro-S
O(14)	C(12)	1.349	C(10)	113.219	O(6) -16.670 Dihedral
O(13)	C(12)	1.212	C(10)	123.161	O(14) 123.576 Pro-R
C(15)	O(14)	1.438	C(12)	114.611	C(10) -176.989 Dihedral
O(18)	C(16)	1.344	C(11)	113.387	O(5) -8.662 Dihedral
O(17)	C(16)	1.214	C(11)	122.609	O(18) 123.997 Pro-R
C(19)	O(18)	1.437	C(16)	114.925	C(11) -178.154 Dihedral
H(20)	C(1)	1.093	C(2)	111.077	O(3) -38.251 Dihedral
H(21)	C(1)	1.092	C(2)	111.794	H(20) 110.226 Pro-R
H(22)	C(1)	1.099	C(2)	107.813	H(20) 107.873 Pro-S
H(27)	C(9)	1.087	C(8)	120.910	C(7) 174.828 Dihedral
H(28)	C(9)	1.087	C(8)	120.366	H(27) 116.232 Pro-S
H(31)	C(15)	1.091	O(14)	105.594	C(12) 178.768 Dihedral

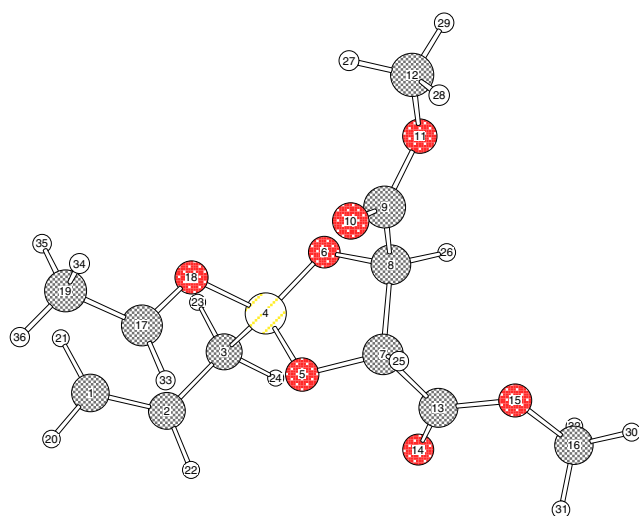
H(32)	C(15)	1.093	O(14)	110.562	H(31)	110.533	Pro-R
H(33)	C(15)	1.093	O(14)	110.593	H(31)	110.720	Pro-S
H(34)	C(19)	1.090	O(18)	105.498	C(16)	179.418	Dihedral
H(35)	C(19)	1.093	O(18)	110.609	H(34)	110.700	Pro-S
H(36)	C(19)	1.093	O(18)	110.535	H(34)	110.647	Pro-R



12a

B(4)						
O(5)	B(4)	1.452				
O(6)	B(4)	1.432	O(5)	108.158		
C(7)	O(5)	1.397	B(4)	108.633	O(6)	-6.930
C(8)	O(6)	1.399	B(4)	108.922	O(5)	-9.513
C(3)	B(4)	1.711	O(5)	112.891	O(6)	112.543
C(9)	C(8)	1.531	O(6)	111.970	C(7)	109.766
C(13)	C(7)	1.532	O(5)	111.097	C(8)	110.511
O(18)	B(4)	1.529	C(3)	101.263	O(5)	110.322
H(25)	C(7)	1.097	O(5)	111.225	C(8)	111.671
H(26)	C(8)	1.095	O(6)	110.801	C(7)	111.804
C(2)	C(3)	1.446	B(4)	104.626	O(5)	56.981
H(23)	C(3)	1.093	C(2)	114.534	B(4)	107.817
H(24)	C(3)	1.092	C(2)	113.650	B(4)	103.440
C(1)	C(2)	1.370	C(3)	124.169	B(4)	82.950
H(22)	C(2)	1.090	C(1)	117.892	C(3)	116.317
O(11)	C(9)	1.355	C(8)	109.910	O(6)	-157.591
O(10)	C(9)	1.209	C(8)	126.079	O(11)	123.977
C(12)	O(11)	1.436	C(9)	115.323	C(8)	-177.301
O(15)	C(13)	1.352	C(7)	110.074	O(5)	-165.279
O(14)	C(13)	1.210	C(7)	125.904	O(15)	124.010
C(16)	O(15)	1.437	C(13)	115.464	C(7)	-177.652
C(17)	O(18)	1.277	B(4)	119.086	C(3)	74.870
C(19)	C(17)	1.500	O(18)	117.943	B(4)	-173.682
H(33)	C(17)	1.091	O(18)	117.859	C(19)	118.597

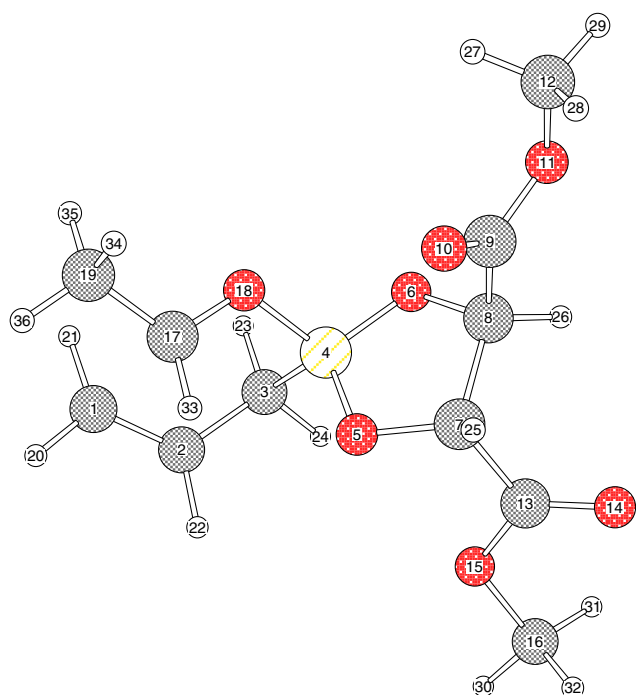
H(20)	C(1)	1.087	C(2)	120.961	C(3)	-174.853	Dihedral
H(21)	C(1)	1.087	C(2)	120.441	H(20)	116.182	Pro-R
H(27)	C(12)	1.093	O(11)	110.500	C(9)	-60.409	Dihedral
H(28)	C(12)	1.094	O(11)	110.647	H(27)	108.855	Pro-S
H(29)	C(12)	1.090	O(11)	105.659	H(27)	110.593	Pro-R
H(30)	C(16)	1.090	O(15)	105.615	C(13)	179.474	Dihedral
H(31)	C(16)	1.093	O(15)	110.482	H(30)	110.600	Pro-S
H(32)	C(16)	1.093	O(15)	110.580	H(30)	110.611	Pro-R
H(34)	C(19)	1.099	C(17)	107.813	O(18)	-79.587	Dihedral
H(35)	C(19)	1.093	C(17)	110.955	H(34)	107.858	Pro-S
H(36)	C(19)	1.093	C(17)	111.745	H(34)	108.064	Pro-R



12b

B(4)							
O(5)	B(4)	1.443					
O(6)	B(4)	1.433	O(5)	108.747			
C(7)	O(5)	1.401	B(4)	108.873	O(6)	-2.177	Dihedral
C(8)	O(6)	1.416	B(4)	108.158	O(5)	-11.789	Dihedral
C(3)	B(4)	1.708	O(5)	112.627	O(6)	112.782	Pro-S
C(9)	C(8)	1.534	O(6)	108.909	C(7)	111.645	Pro-R
C(13)	C(7)	1.530	O(5)	110.645	C(8)	110.251	Pro-R
O(18)	B(4)	1.539	C(3)	101.474	O(5)	110.431	Pro-R
H(25)	C(7)	1.095	O(5)	110.893	C(8)	110.867	Pro-S
H(26)	C(8)	1.095	O(6)	109.534	C(7)	113.163	Pro-S
C(2)	C(3)	1.447	B(4)	104.453	O(5)	57.255	Dihedral
H(23)	C(3)	1.093	C(2)	114.521	B(4)	108.128	Pro-R
H(24)	C(3)	1.092	C(2)	113.656	B(4)	103.407	Pro-S
C(1)	C(2)	1.370	C(3)	124.159	B(4)	83.041	Dihedral
H(22)	C(2)	1.090	C(1)	117.876	C(3)	116.360	Pro-S
O(11)	C(9)	1.347	C(8)	110.616	O(6)	-87.640	Dihedral
O(10)	C(9)	1.213	C(8)	125.491	O(11)	123.852	Pro-S
C(12)	O(11)	1.437	C(9)	115.377	C(8)	175.442	Dihedral

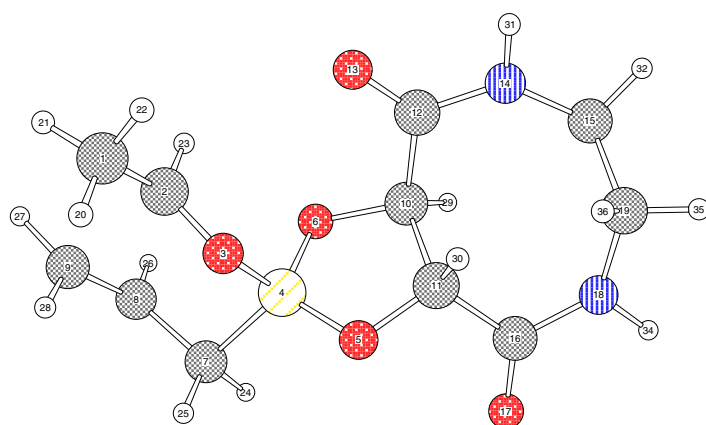
O(15)	C(13)	1.354	C(7)	109.906	O(5)	-166.533	Dihedral
O(14)	C(13)	1.209	C(7)	126.118	O(15)	123.959	Pro-R
C(16)	O(15)	1.437	C(13)	115.429	C(7)	-177.434	Dihedral
C(17)	O(18)	1.278	B(4)	118.461	C(3)	74.858	Dihedral
C(19)	C(17)	1.500	O(18)	118.030	B(4)	-173.780	Dihedral
H(33)	C(17)	1.091	O(18)	117.750	C(19)	118.602	Pro-R
H(20)	C(1)	1.087	C(2)	120.925	C(3)	-175.061	Dihedral
H(21)	C(1)	1.087	C(2)	120.455	H(20)	116.205	Pro-R
H(27)	C(12)	1.093	O(11)	110.414	C(9)	-60.882	Dihedral
H(28)	C(12)	1.093	O(11)	110.552	H(27)	108.969	Pro-S
H(29)	C(12)	1.090	O(11)	105.603	H(27)	110.602	Pro-R
H(30)	C(16)	1.090	O(15)	105.648	C(13)	179.572	Dihedral
H(31)	C(16)	1.093	O(15)	110.508	H(30)	110.570	Pro-S
H(32)	C(16)	1.093	O(15)	110.601	H(30)	110.592	Pro-R
H(34)	C(19)	1.099	C(17)	107.777	O(18)	-79.724	Dihedral
H(35)	C(19)	1.093	C(17)	111.028	H(34)	107.969	Pro-S
H(36)	C(19)	1.092	C(17)	111.736	H(34)	107.963	Pro-R



12c

B(4)						
O(5)	B(4)	1.442				
O(6)	B(4)	1.430	O(5)	108.864		
C(7)	O(5)	1.405	B(4)	108.853	O(6)	2.560
C(8)	O(6)	1.419	B(4)	107.820	O(5)	-15.444
C(3)	B(4)	1.715	O(5)	112.369	O(6)	112.614
C(9)	C(8)	1.533	O(6)	108.679	C(7)	111.667
C(13)	C(7)	1.529	O(5)	114.031	C(8)	110.117
						Pro-R

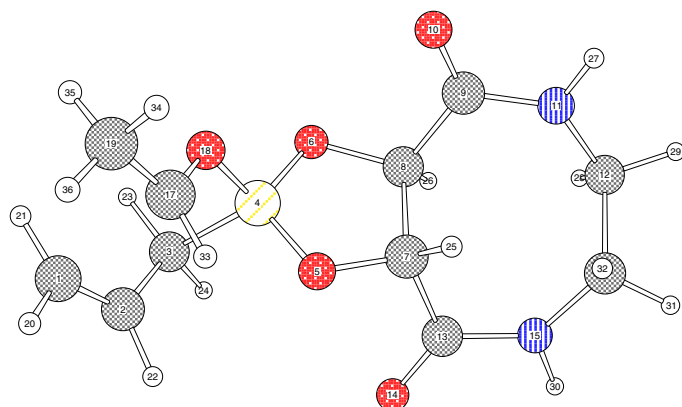
O(18)	B(4)	1.537	C(3)	101.193	O(5)	110.840	Pro-R
H(25)	C(7)	1.096	O(5)	110.525	C(8)	110.264	Pro-S
H(26)	C(8)	1.094	O(6)	109.776	C(7)	112.827	Pro-S
C(2)	C(3)	1.444	B(4)	104.105	O(5)	57.370	Dihedral
H(23)	C(3)	1.093	C(2)	114.712	B(4)	107.739	Pro-R
H(24)	C(3)	1.092	C(2)	113.975	B(4)	103.756	Pro-S
C(1)	C(2)	1.372	C(3)	123.977	B(4)	82.170	Dihedral
H(22)	C(2)	1.090	C(1)	117.754	C(3)	116.536	Pro-S
O(11)	C(9)	1.346	C(8)	110.624	O(6)	-86.511	Dihedral
O(10)	C(9)	1.213	C(8)	125.435	O(11)	123.897	Pro-S
C(12)	O(11)	1.437	C(9)	115.434	C(8)	175.704	Dihedral
O(15)	C(13)	1.345	C(7)	113.774	O(5)	3.158	Dihedral
O(14)	C(13)	1.214	C(7)	122.206	O(15)	124.018	Pro-S
C(16)	O(15)	1.437	C(13)	114.831	C(7)	179.946	Dihedral
C(17)	O(18)	1.280	B(4)	118.418	C(3)	74.822	Dihedral
C(19)	C(17)	1.501	O(18)	117.763	B(4)	-174.520	Dihedral
H(33)	C(17)	1.091	O(18)	117.535	C(19)	118.419	Pro-R
H(20)	C(1)	1.087	C(2)	120.753	C(3)	-175.099	Dihedral
H(21)	C(1)	1.087	C(2)	120.319	H(20)	116.109	Pro-R
H(27)	C(12)	1.093	O(11)	110.415	C(9)	-61.190	Dihedral
H(28)	C(12)	1.093	O(11)	110.534	H(27)	109.002	Pro-S
H(29)	C(12)	1.090	O(11)	105.585	H(27)	110.604	Pro-R
H(30)	C(16)	1.090	O(15)	105.543	C(13)	179.455	Dihedral
H(31)	C(16)	1.093	O(15)	110.589	H(30)	110.648	Pro-S
H(32)	C(16)	1.093	O(15)	110.549	H(30)	110.642	Pro-R
H(34)	C(19)	1.099	C(17)	107.692	O(18)	-78.889	Dihedral
H(35)	C(19)	1.093	C(17)	111.056	H(34)	107.938	Pro-S
H(36)	C(19)	1.093	C(17)	111.814	H(34)	107.984	Pro-R



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C(10)						
C(11)	C(10)	1.589				
O(5)	C(11)	1.395	C(10)	105.648		
C(16)	C(11)	1.531	C(10)	110.091	O(5)	111.806
						Pro-S

O(6)	C(10)	1.395	C(11)	105.149	O(5)	-1.940	Dihedral
C(12)	C(10)	1.533	C(11)	110.098	O(6)	112.115	Pro-S
B(4)	O(5)	1.427	C(11)	108.793	C(10)	-10.067	Dihedral
N(14)	C(12)	1.374	C(10)	115.581	C(11)	73.285	Dihedral
C(15)	N(14)	1.460	C(12)	129.506	C(10)	6.728	Dihedral
N(18)	C(16)	1.380	C(11)	114.995	C(10)	74.732	Dihedral
C(19)	C(15)	1.554	N(14)	116.236	C(12)	-73.911	Dihedral
O(3)	B(4)	1.529	O(5)	110.244	O(6)	111.604	Pro-R
C(7)	B(4)	1.714	O(3)	101.724	O(5)	113.877	Pro-S
H(29)	C(10)	1.099	O(6)	109.305	C(11)	110.859	Pro-S
H(30)	C(11)	1.101	O(5)	110.021	C(10)	109.923	Pro-S
O(13)	C(12)	1.224	C(10)	123.274	N(14)	121.085	Pro-R
O(17)	C(16)	1.219	C(11)	123.640	N(18)	121.283	Pro-R
H(31)	N(14)	1.012	C(12)	112.763	C(15)	117.633	Pro-S
H(32)	C(15)	1.094	N(14)	105.633	C(19)	108.095	Pro-R
H(33)	C(15)	1.097	N(14)	110.979	C(19)	108.729	Pro-S
H(34)	N(18)	1.012	C(16)	112.638	C(19)	117.722	Pro-S
H(35)	C(19)	1.094	C(15)	107.893	N(18)	105.819	Pro-S
H(36)	C(19)	1.097	C(15)	108.763	N(18)	111.154	Pro-R
C(2)	O(3)	1.287	B(4)	117.629	O(5)	163.836	Dihedral
C(1)	C(2)	1.502	O(3)	117.144	B(4)	175.821	Dihedral
H(23)	C(2)	1.090	C(1)	117.974	O(3)	117.057	Pro-R
C(8)	C(7)	1.442	B(4)	103.281	O(3)	60.775	Dihedral
H(24)	C(7)	1.092	B(4)	104.262	C(8)	114.780	Pro-S
H(25)	C(7)	1.093	B(4)	106.982	C(8)	114.909	Pro-R
C(9)	C(8)	1.377	C(7)	123.710	B(4)	-79.921	Dihedral
H(26)	C(8)	1.090	C(7)	116.797	C(9)	117.592	Pro-S
H(20)	C(1)	1.093	C(2)	111.213	O(3)	-39.154	Dihedral
H(21)	C(1)	1.093	C(2)	111.830	H(20)	110.175	Pro-R
H(22)	C(1)	1.099	C(2)	107.292	H(20)	108.213	Pro-S
H(27)	C(9)	1.087	C(8)	120.418	C(7)	175.510	Dihedral
H(28)	C(9)	1.087	C(8)	119.957	H(27)	115.950	Pro-S



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C(7)

C(8)	C(7)	1.585				
O(5)	C(7)	1.395	C(8)	105.453		
C(13)	C(7)	1.532	C(8)	109.537	O(5)	111.744 Pro-S
O(6)	C(8)	1.394	C(7)	105.738	O(5)	-3.285 Dihedral
C(9)	C(8)	1.532	C(7)	109.447	O(6)	112.808 Pro-S
B(4)	O(5)	1.444	C(7)	109.717	C(8)	2.967 Dihedral
N(11)	C(9)	1.380	C(8)	114.847	C(7)	75.403 Dihedral
C(12)	N(11)	1.458	C(9)	129.584	C(8)	4.911 Dihedral
N(15)	C(13)	1.377	C(7)	115.233	C(8)	75.121 Dihedral
C(16)	C(12)	1.555	N(11)	116.236	C(9)	-73.088 Dihedral
C(3)	B(4)	1.708	O(5)	111.859	O(6)	113.495 Pro-S
O(18)	B(4)	1.540	C(3)	101.286	O(5)	110.743 Pro-R
H(25)	C(7)	1.100	O(5)	109.932	C(8)	110.661 Pro-S
H(26)	C(8)	1.100	O(6)	109.337	C(7)	110.428 Pro-S
O(10)	C(9)	1.219	C(8)	123.745	N(11)	121.320 Pro-R
O(14)	C(13)	1.221	C(7)	123.222	N(15)	121.455 Pro-R
H(27)	N(11)	1.012	C(9)	112.699	C(12)	117.708 Pro-S
H(28)	C(12)	1.097	N(11)	111.059	C(16)	108.754 Pro-S
H(29)	C(12)	1.094	N(11)	105.761	C(16)	107.919 Pro-R
H(30)	N(15)	1.012	C(13)	112.803	C(16)	117.705 Pro-S
H(31)	C(16)	1.094	C(12)	108.026	N(15)	105.693 Pro-S
H(32)	C(16)	1.097	C(12)	108.704	N(15)	110.935 Pro-R
C(2)	C(3)	1.448	B(4)	105.125	O(5)	57.355 Dihedral
H(23)	C(3)	1.093	C(2)	114.493	B(4)	108.135 Pro-R
H(24)	C(3)	1.093	C(2)	113.360	B(4)	103.367 Pro-S
C(1)	C(2)	1.368	C(3)	124.239	B(4)	83.831 Dihedral
H(22)	C(2)	1.090	C(1)	117.945	C(3)	116.298 Pro-S
C(17)	O(18)	1.275	B(4)	119.096	C(3)	74.503 Dihedral
C(19)	C(17)	1.499	O(18)	118.192	B(4)	-173.118 Dihedral
H(33)	C(17)	1.091	O(18)	117.951	C(19)	118.769 Pro-R
H(20)	C(1)	1.087	C(2)	121.056	C(3)	-174.889 Dihedral
H(21)	C(1)	1.087	C(2)	120.549	H(20)	116.268 Pro-R
H(34)	C(19)	1.100	C(17)	107.853	O(18)	-80.189 Dihedral
H(35)	C(19)	1.093	C(17)	110.974	H(34)	107.832 Pro-S
H(36)	C(19)	1.092	C(17)	111.760	H(34)	107.964 Pro-R