Phenanthroline-Catalyzed Stereoselective Formation of α-1,2-*Cis* 2-Deoxy-2-Fluoro Glycosides:

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Total energies, retative energies and selected bond lengths

		Phenantholine						Pyridine				
		L0	L1	L2	L3	L4	L5	L6	L7	L8	L9	L10
	R	-H	-C6H5	-NMe2	-NC5H10	-NC4H8	-NC4H8O	-NC5H10	-NC4H8O	-NMe2	-C6H5	-H
Glycosyl-Br	E(Tz)	-3327.835423	-3327.835423	-3327.835423	-3327.835423	-3327.835423	-3327.835423	-3327.835423	-3327.835423	-3327.835423	-3327.835423	-3327.835423
	thermal(SV)	0.206786	0.206786	0.206786	0.206786	0.206786	0.206786	0.206786	0.206786	0.206786	0.206786	0.206786
	G	-3327.628637	-3327.628637	-3327.628637	-3327.628637	-3327.628637	-3327.628637	-3327.628637	-3327.628637	-3327.628637	-3327.628637	-3327.628637
Glycosyl-OMe	E(Tz)	-868.826317	-868.826317	-868.826317	-868.826317	-868.826317	-868.826317	-868.826317	-868.826317	-868.826317	-868.826317	-868.826317
	thermal(SV)	0.248643	0.248643	0.248643	0.248643	0.248643	0.248643	0.248643	0.248643	0.248643	0.248643	0.248643
	G	-868.577674	-868.577674	-868.577674	-868.577674	-868.577674	-868.577674	-868.577674	-868.577674	-868.577674	-868.577674	-868.577674
Glycosyl-OMe-HBr	E(Tz)	-3443.628961	-3443.628961	-3443.628961	-3443.628961	-3443.628961	-3443.628961	-3443.628961	-3443.628961	-3443.628961	-3443.628961	-3443.628961
	thermal(SV)	0.250647	0.250647	0.250647	0.250647	0.250647	0.250647	0.250647	0.250647	0.250647	0.250647	0.250647
	G	-3443.378314	-3443.378314	-3443.378314	-3443.378314	-3443.378314	-3443.378314	-3443.378314	-3443.378314	-3443.378314	-3443.378314	-3443.378314
Methanol	E(Tz)	-115.785128	-115.785128	-115.785128	-115.785128	-115.785128	-115.785128	-115.785128	-115.785128	-115.785128	-115.785128	-115.785128
	thermal(SV)	0.027819	0.027819	0.027819	0.027819	0.027819	0.027819	0.027819	0.027819	0.027819	0.027819	0.027819
	G	-115.757309	-115.757309	-115.757309	-115.757309	-115.757309	-115.757309	-115.757309	-115.757309	-115.757309	-115.757309	-115.757309
HBr	E(Tz)	-2574.794460	-2574.794460	-2574.794460	-2574.794460	-2574.794460	-2574.794460	-2574.794460	-2574.794460	-2574.794460	-2574.794460	-2574.794460
	thermal(SV)	-0.013269	-0.013269	-0.013269	-0.013269	-0.013269	-0.013269	-0.013269	-0.013269	-0.013269	-0.013269	-0.013269
	G	-2574.807729	-2574.807729	-2574.807729	-2574.807729	-2574.807729	-2574.807729	-2574.807729	-2574.807729	-2574.807729	-2574.807729	-2574.807729
IBO	E(Tz)	-232.547655	-232.547655	-232.547655	-232.547655	-232.547655	-232.547655	-232.547655	-232.547655	-232.547655	-232.547655	-232.547655
	thermal(SV)	0.084323	0.084323	0.084323	0.084323	0.084323	0.084323	0.084323	0.084323	0.084323	0.084323	0.084323
	G	-232.463332	-232.463332	-232.463332	-232.463332	-232.463332	-232.463332	-232.463332	-232.463332	-232.463332	-232.463332	-232.463332
IBO-HBr	E(Tz)	-2807.389785	-2807.389785	-2807.389785	-2807.389785	-2807.389785	-2807.389785	-2807.389785	-2807.389785	-2807.389785	-2807.389785	-2807.389785
	thermal(SV)	0.093021	0.093021	0.093021	0.093021	0.093021	0.093021	0.093021	0.093021	0.093021	0.093021	0.093021
	G	-2807.296764	-2807.296764	-2807.296764	-2807.296764	-2807.296764	-2807.296764	-2807.296764	-2807.296764	-2807.296764	-2807.296764	-2807.296764

		Phenantholine						Pyridine				
		L0	L1	L2	L3	L4	L5	L6	L7	L8	L9	L10
	R	-H	-C6H5	-NMe2	-NC5H10	-NC4H8	-NC4H8O	-NC5H10	-NC4H8O	-NMe2	-C6H5	-H
Catalyst	E(Tz)	-571.883945	-1034.220522	-839.954262	-1073.558177	-994.874196	-1145.366953	-499.247830	-535.153205	-382.449604	-479.571245	-248.406079
	thermal(SV)	0.136194	0.285570	0.272353	0.400767	0.341975	0.353141	0.193202	0.168567	0.128741	0.135910	0.061489
	G	-571.747751	-1033.934952	-839.681909	-1073.157410	-994.532221	-1145.013812	-499.054628	-534.984638	-382.320863	-479.435335	-248.344590
TS1	E(Tz)	-3899.690467	-4362.028170	-4167.766148	-4401.369964	-4322.685917	-4473.177473	-3827.060235	-3862.964251	-3710.261598	-3807.385850	-3576.213701
	thermal(SV)	0.365308	0.514994	0.499217	0.627400	0.570984	0.580268	0.418808	0.394954	0.354941	0.362241	0.287608
	G	-3899.325159	-4361.513176	-4167.266931	-4400.742564	-4322.114933	-4472.597205	-3826.641427	-3862.569297	-3709.906657	-3807.023609	-3575.926093
Int1	E(Tz)	-3899.721067	-4362.058883	-4167.802489	-4401.405423	-4322.722218	-4473.211992	-3827.116260	-3863.015673	-3710.313688	-3807.430929	-3576.256986
	thermal(SV)	0.368077	0.517299	0.505430	0.632265	0.574904	0.584709	0.422920	0.398376	0.357950	0.365132	0.291128
	G	-3899.352990	-4361.541584	-4167.297059	-4400.773158	-4322.147314	-4472.627283	-3826.693340	-3862.617297	-3709.955738	-3807.065797	-3575.965858
TS2	E(Tz)	-4015.489392	-4477.827789	-4283.564780	-4517.168533	-4438.484572	-4588.976146	-3942.855550	-3978.759631	-3826.056806	-3923.180685	-3692.009613
	thermal(SV)	0.412961	0.561914	0.545904	0.676461	0.616751	0.630034	0.464854	0.440944	0.400599	0.410278	0.333701
	G	-4015.076431	-4477.265875	-4283.018876	-4516.492072	-4437.867821	-4588.346112	-3942.390696	-3978.318687	-3825.656207	-3922.770407	-3691.675912
Int2	E(Tz)	-4015.521273	-4477.858896	-4283.592609	-4517.196643	-4438.508267	-4589.005313	-3942.881405	-3978.788400	-3826.086681	-3923.215029	-3692.039784
	thermal(SV)	0.406797	0.556451	0.542621	0.671100	0.612172	0.622266	0.463930	0.436950	0.399783	0.407147	0.328051
	G	-4015.114476	-4477.302445	-4283.049988	-4516.525543	-4437.896095	-4588.383047	-3942.417475	-3978.351450	-3825.686898	-3922.807882	-3691.711733
Reactant	G(hartree)	-4015.133697	-4477.320898	-4283.067855	-4516.543356	-4437.918167	-4588.399758	-3942.440574	-3978.370584	-3825.706809	-3922.821281	-3691.730535
TS1	G(hartree)	-4015.082468	-4477.270485	-4283.024240	-4516.499873	-4437.872241	-4588.354514	-3942.398736	-3978.326605	-3825.663966	-3922.780918	-3691.683402
Int1	G(hartree)	-4015.110299	-4477.298893	-4283.054368	-4516.530467	-4437.904623	-4588.384592	-3942.450649	-3978.374605	-3825.713047	-3922.823106	-3691.723167
TS2	G(hartree)	-4015.076431	-4477.265875	-4283.018876	-4516.492072	-4437.867821	-4588.346112	-3942.390696	-3978.318687	-3825.656207	-3922.770407	-3691.675912
Int2	G(hartree)	-4015.114476	-4477.302445	-4283.049988	-4516.525543	-4437.896095	-4588.383047	-3942.417475	-3978.351450	-3825.686898	-3922.807882	-3691.711733
Product	G(hartree)	-4015.126065	-4477.313267	-4283.060224	-4516.535724	-4437.910536	-4588.392127	-3942.432942	-3978.362953	-3825.699177	-3922.813649	-3691.722904
Product w/IBO-HBr	G(hartree)	-4015.158857	-4477.346058	-4283.093015	-4516.568516	-4437.943327	-4588.424918	-3942.465734	-3978.395744	-3825.731969	-3922.846441	-3691.755696

		Phenantholine						Pyridine				
		L0	L1	L2	L3	L4	L5	L6	L7	L8	L9	L10
	R	-H	-C6H5	-NMe2	-NC5H10	-NC4H8	-NC4H8O	-NC5H10	-NC4H8O	-NMe2	-C6H5	-H
Reactant	G(kcal/mol)	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TS1	G(kcal/mol)	32.1	31.6	27.4	27.3	28.8	28.4	26.3	27.6	26.9	25.3	29.6
Int1	G(kcal/mol)	14.7	13.8	8.5	8.1	8.5	9.5	-6.3	-2.5	-3.9	-1.1	4.6
TS2	G(kcal/mol)	35.9	34.5	30.7	32.2	31.6	33.7	31.3	32.6	31.8	31.9	34.3
Int2	G(kcal/mol)	12.1	11.6	11.2	11.2	13.9	10.5	14.5	12.0	12.5	8.4	11.8
Product	G(kcal/mol)	4.8	4.8	4.8	4.8	4.8	4.8	4.8	4.8	4.8	4.8	4.8
Product w/IBO-HBr	G(kcal/mol)	-15.8	-15.8	-15.8	-15.8	-15.8	-15.8	-15.8	-15.8	-15.8	-15.8	-15.8
	TS1 R(C-N)	2.007	2.005	2.050	2.038	2.047	2.030	2.141	2.129	2.139	2.086	2.075
	TS1 R(C-Br)	3.061	3.054	3.023	3.031	3.027	3.033	2.827	2.840	2.829	2.880	2.900
	TS2 R(C-N)	2.199	2.162	2.207	2.195	2.199	2.179	2.306	2.296	2.304	2.229	2.242
	TS2 R(C-O)	2.484	2.583	2.476	2.486	2.484	2.506	2.250	2.266	2.252	2.332	2.335
	Yield %		33	0	68	56	43	66	37	38	20	
	α:β ratio		10	0	10	10	10	10	10	10	10	
	unreacted %		34	12	39	25	29	9	4	3	4	