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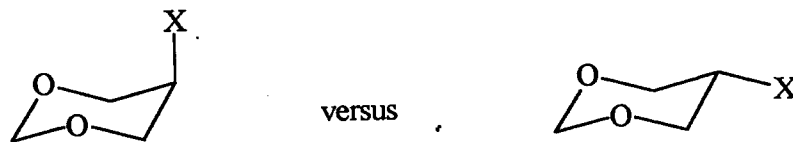
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Legend of Illustrations

- Figure 1.** Calculated structures (MOPAC/AM1) of minimum energy for axial and equatorial 5-carboxy-1,3-dioxane, in absence and presence of H^+ , Li^+ , Na^+ , and K^+ .
- Figure 2.** Calculated structures (MOPAC/AM1) of minimum energy for axial and equatorial 5-carbomethoxy-1,3-dioxane, in absence and presence of H^+ , Li^+ , Na^+ , and K^+ .
- Figure 3.** Calculated structures (MOPAC/AM1) of minimum energy for axial and equatorial 5-hydroxymethyl-1,3-dioxane, in absence and presence of H^+ , Li^+ , Na^+ , and K^+ .
- Figure 4.** Calculated structures (MOPAC/AM1) of minimum energy for axial and equatorial 5-*N*-methylcarboxamide-1,3-dioxane, in absence and presence of H^+ , Li^+ , Na^+ , and K^+ .
- Figure 5.** Calculated structures (MOPAC/AM1) of minimum energy for axial and equatorial 5-acetamide-1,3-dioxane, in absence and presence of H^+ , Li^+ , Na^+ , and K^+ .
- Figure 6.** Calculated structures (MOPAC/AM1) of minimum energy for axial and equatorial 5-hydroxy-1,3-dioxane, in absence and presence of H^+ , Li^+ , Na^+ , and K^+ .
- Figure 7.** Calculated structures (MOPAC/AM1) of minimum energy for axial and equatorial 5-nitro-1,3-dioxane, in absence and presence of H^+ , Li^+ , Na^+ , and K^+ .
- Figure 8.** Calculated structures (MOPAC/AM1) of minimum energy for axial and equatorial 5-*O*-acetyl-1,3-dioxane, in absence and presence of H^+ , Li^+ , Na^+ , and K^+ .

Table VIII. Differences in Heat of Formation (ΔH_f°) Calculated by the AM1 SemiempiricalMethod, in kcal/mol.^a

X substituent	Free system	In the presence of			
		H ⁺	Li ⁺	Na ⁺	K ⁺
-CO ₂ H	-1.81	+10.73	+4.36	+3.74	+4.10
-CO ₂ CH ₃	-2.05	+10.45	+1.66	+3.68	+1.93
-CH ₂ OH	-0.34	+18.59	+4.09	+5.44	+4.45
-CONHCH ₃	+2.50	+9.36	+7.26	+4.54	+4.02
-NHCOCH ₃	+2.21	+9.15	+2.48	+0.78	+0.55
-OH	+1.68	+11.70	+4.33	+4.67	+3.17
-NO ₂	-0.12	+6.31	+2.89	+3.14	+2.74
-OCOCH ₃	-0.84	+9.25	-0.36	-0.13	-2.44

^a Positive values correspond to axial preference.

