

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1997 American Chemical Society

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^+ .

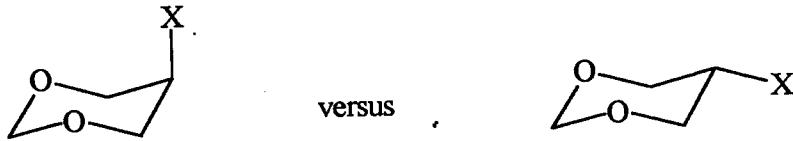
Figure 5. Calculated structures (MOPAC/AM1) of minimum energy for axial and equatorial 5-acetamide-1,3-dioxane, in absence and presence of H^+ , Li^+ , Na^+ , and K^+ .

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 Semiempirical Method, in kcal/mol.*



X substituent	Free system	In the presence of			
		H^+	Li^+	Na^+	K^+
$-CO_2H$	-1.81	+10.73	+4.36	+3.74	+4.10
$-CO_2CH_3$	-2.05	+10.45	+1.66	+3.68	+1.93
$-CH_2OH$	-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

* Positive values correspond to axial preference.

